Numerical Investigation of the Influence of Particle–Particle and Particle–Wall Collisions in Turbulent Wall–Bounded Flows at High Mass Loadings

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Abstract

The present work deals with the simulation of turbulent particle–laden flows at high mass loadings. In order to achieve this goal, the fluid flow is described by means of the eddy–resolving concept known as Large–Eddy Simulation (LES) and the particles are described in a Lagrangian frame of reference. Special emphasis is placed on the inter–particle collisions and the impact of solid particles on rough walls. Both mechanisms are shown to be crucial for the correct description of the particle dynamics in wall–bounded flows.

In order to distinguish the present methodology from the variety of methods available in the literature to treat turbulent flows laden with solid particles, the thesis starts with an overview of different simulation techniques to calculate this class of flows. In this overview special care is taken to underline the parameter space, where the different simulation methods are valid. After that, the governing equations and the boundary conditions applied for the continuous phase of the Euler–Lagrange approach used in the present thesis are given. In the subsequent section the governing equations for the solid particles and their interaction with smooth and rough walls are discussed. Here a new wall roughness model for the particles which incorporates an amplitude parameter used in technical applications such as the mean roughness height or the root–mean–squared roughness is presented. After that, the coupling mechanisms between the phases and the algorithmic realization are discussed. Furthermore, a new agglomeration model capable to treat inter–particle collisions with friction is presented. However, the agglomeration model is not evaluated in such a detail as the inter–particle collisions and the particle–wall collisions. The reason is that it does not represent a central aspect of this thesis. The numerical methods for the continuous and the disperse phase are presented in the subsequent section. The efficient algorithm to detect the inter–particle collisions is described in detail. With this efficient algorithm it is possible to detect the inter–particle collisions with computational costs which scale linearly with the number of particles present in the computational domain. The resulting methodology is validated based on a variety of test cases. The validation process starts with two turbulent channel flows at different Reynolds numbers and one turbulent pipe flow. Using this simple test cases possible error sources can be detected easily. After that, a turbulent pipe flow is simulated, where the gravity points vertical to the mean streamwise direction. The appearance of an interesting secondary flow of second kind, for which the particles are only indirectly responsible, is analyzed in detail. In order to demonstrate the applicability of the present methodology in practically relevant turbulent flow configurations, the particle–laden cold flow in a combustion chamber model and the flow in a cyclone separator are tackled. The results are discussed in detail, compared with experimental reference data and interpreted from a physical point of view. Regarding the combustion chamber model, good agreement is found with the reference experiment. Furthermore, it is shown that the present methodology is capable to reproduce in the high mass loading case the disappearance of two stagnation points present on the axis of the low mass loading configuration. Regarding the cyclone separator flow, in the core region still some differences with the reference experiment remain.
Überblick


Nomenclature

Greek Symbols

$\alpha_R$ ................. random wall inclination

$\omega_p^+$ ................ particle angular velocity after a collision

$\omega_p^-$ ................ particle angular velocity before a collision

$\Delta$ ..................... filter width used in LES

$\delta^-$ .................... particle incident angle

$\delta_0$ .................... minimal contact distance

$\delta_{Ch}$ ................ channel half-width

$\eta_K$ ..................... Kolmogorov length scale

$\eta$ ....................... mass loading

$\mu_T$ ...................... turbulent viscosity

$\mu_{dy,p}$ ................ dynamic coefficients of friction for a particle–particle collision

$\mu_{dy,w}$ ................ dynamic coefficients of friction for a particle–wall collision

$\mu_{st,p}$ ................ static coefficients of friction for a particle–particle collision

$\mu_{st,w}$ ................ static coefficients of friction for a particle–wall collision

$\sigma$ ....................... yield pressure

$\Phi$ ....................... volume fraction

$\rho_p$ ...................... particle density

$\sigma_w$ ..................... standard deviation of the wall inclination

$\tau_\eta$ ..................... Kolmogorov time

$\tau_p$ ...................... particle relaxation time

$\tau_{ani}$ ................ anisotropic part of the subgrid–scale stress tensor

$\tau_{iso}$ ................ isotropic part of the subgrid–scale stress tensor

$\tau_{SGS}$ ................ subgrid–scale stress tensor

$\tau_{le}$ .................... large–eddy turn over time

$\tau_{vis}$ .................. viscous time

Roman Symbols

$n_c$ ...................... collision normal vector
$F_p$ ................. forces acting on a particle

$T_p$ ................. torque acting on a particle

$n_R$ .................. randomly inclined wall normal vector of the rough wall

$n_w$ ................. wall normal vector of the nominally smooth wall

$n_{Rnew}$ ............ wall normal vector in case of a shadow event

$u^+_p$ ............... particle velocity after a collision

$u^-_p$ ............... particle velocity before a collision

$d_{p,M}$ .............. mass–averaged diameter

$d_{p,N}$ .............. number–averaged diameter

$\overline{\mu}_i$ ........ filtered velocity field

$Re_r$ ................. Reynolds number of particle rotation

$Re_{bulk}$ ............ bulk Reynolds number

$C_s$ ................. Smagorinsky constant

$C_{surface}$ ........ surface texture factor

$d_{body}$ ............. diameter of the cyclone body

$e_{n,p}$ ............... normal restitution coefficients for a particle–particle collision

$e_{n,p}$ ............... tangential restitution coefficients for a particle–particle collision

$e_{n,w}$ ............... normal restitution coefficients for a particle–wall collision

$e_{n,w}$ ............... tangential restitution coefficients for a particle–wall collision

$H$ ..................... Hamaker constant

$I_p$ ................. particle moment of inertia

$k_s$ ................. sandgrain roughness

$m_p$ ................. particle mass

$N_p$ ................. total number of particles

$Q_0(d_p)$ ............ cumulative number distribution function

$q_0(d_p)$ ............ number distribution function

$Q_3(d_p)$ ............ cumulative distribution function

$q_3(d_p)$ ............ mass distribution function

$R_a$ ................. arithmetic average roughness
\( R_q \) ............... root–mean–squared roughness
\( R_z \) ............... mean roughness
\( R_{pipe} \) ............... pipe radius
\( U_B \) ............... bulk velocity
\( U_e \) ............... annular flow velocity
\( u_i \) ............... unfiltered velocity field
\( u'_i \) ............... subgrid–scale velocity field
\( U_{jet} \) ............... particle–laden air flow of the chamber
\( U_{in} \) ............... inlet velocity of the cyclone
\( Re_p \) ............... particle Reynolds number
\( St \) ............... Stokes number

**Subscripts and Superscrips**

* ............... Dimensional Quantities
[-] ............... Dimensionalless Quantities
1 Introduction

Because of its ability to treat problems in complex geometries and its lower cost compared to experiments, in the last decades computational fluid dynamics (CFD) has become a main pillar of engineering applications. It is therefore a must to develop reliable simulation tools to efficiently design industrial devices. In this spirit, the scope of this thesis was to take a step towards the development of a reliable and efficient two-phase simulation tool applicable within a wide parameter space by combining Large–Eddy Simulations (LES) with a Lagrangian approach for the particles including two–way coupling, particle–particle and particle–wall collisions. Special emphasis is taken respect the prediction of turbulent particle–laden flow at high mass loadings. Furthermore, the extended tool based on the in–house CFD code \textit{LESOCC} (Breuer, 1998, 2002; Breuer et al., 2006) is tested in complex wall–bounded turbulent flows to prove its applicability in engineering applications.

1.1 Motivation

To underline the importance of the present research field and to elucidate potential application fields, in the first part of this section a few examples are given in which LES was applied in complex flow configurations with a Lagrangian approach for the particles. The examples are restricted to this topic to show that until now very few four–way coupled investigations were carried out in this framework. The reason of the lag of four–way coupled LES are the rather high computational costs to solve the equations for the continuous flow due to the fine resolution needed for eddy–revolving techniques. Furthermore, introducing a high amount of solid particles into the computational domain implicates two additional critical issues concerning the performance of the CFD code. One regards the localization of the computational cell containing the particle after advancing the trajectory by a time step. This issue has already been solved in the previous version of the code (see Breuer et al., 2006). The second issue regards the deterministic treatment of the inter–particle collisions. If they are not tackled adequately, this would end to a completely intractable problem. However, in § 6.2.3 a newly developed algorithm is presented (see also Breuer and Alletto, 2012b) allowing a considerable acceleration of the collision detection compared to a brute force approach and hence, it is possible to circumvent the necessity to use a stochastic collision model (see, e.g., Sommerfeld, 2001). Later on in § 8.7 one of the first four–way coupled LES predictions in complex geometries is shown although since until now most investigations were restricted to one– or two–way coupled simulations because of the afore mentioned reason.

The second part of this section summarizes the wall roughness models for the particulate phase available in the literature to show that none of them incorporates a commonly used roughness parameter. Hence, the model presented in § 4.3.2 is the first wall roughness model for the particles known to the author which incorporates a commonly used roughness parameter such the mean roughness $R_{z}^*$ or the root–mean squared roughness $R_q^*$ to characterize technically rough surfaces. For this reason the model developed in this thesis has a great potential to be applied in designing industrial devices.

A possible application area of the method developed in this work is the flow in pneumatic conveying systems. Because of its versatility they are used to transport solids in

\footnote{Note that in this thesis the superscript * is adopted in order to mark the dimensional quantities. Quantities without the superscript * are dimensionless.}
many industrial branches like chemical, pharmaceutical, food, mineral processing and electric power generation (see Fokeer et al., 2004). The influence of the particles on the continuous phase is a crucial point to correctly reproduce the pressure loss in pipe systems (Huber and Sommerfeld, 1998; Lain and Sommerfeld, 2012). It is therefore important to incorporate all relevant effects influencing the particle dynamics such as gravitational settling, inertial effects in pipe bends, turbulent transport of the particles, Magnus and Saffman lift forces, inter–particle collisions, modulation of the turbulence by the particle and the effect of the wall roughness on the particles to optimize such devices (Huber and Sommerfeld, 1998; Fokeer et al., 2004). Furthermore, the correct description of the particle dynamics is a must to identify those mechanical components predominantly effected by abrasion (see Fokeer et al., 2004, and references therein). Because of the multiplicity of physical effects governing the flow in a horizontal conveying system it still remains a challenging application for computational tools and very few studies are known which treat this problem by adopting a four–way coupled eddy-resolving technique with additionally taking the effect of the wall roughness on the particles into account. In case of a horizontal channel flow in this work (see § 8.3) one of the first results (see, also Konan et al., 2009; Breuer et al., 2012; Mallouppas and van Wachem, 2013) obtained by means of four–way coupled LES including the influence of rough walls on the particle motion is shown. Until now horizontal pipe flows were only investigated by mean of four–way coupled RANS (see, e.g., Huber and Sommerfeld, 1998; Kartushinsky et al., 2011; Lain and Sommerfeld, 2012). In § 8.6 one of the first results (some results were recently published in Alletto and Breuer, 2013) obtained by means of a four–way coupled LES including additionally the influence of the wall roughness will be presented to underline the wide application area of the method developed in this thesis.

In pulverized coal combustion primary air and coal particles are injected in the center of the combustion chamber and a secondary stream of air is introduced on the periphery. For this kind of configuration a cone–shaped body is located close to the exit of the primary air in order to generate a recirculation region to stabilizes the flame generated by the combustion of the coal particles (Xu et al., 1995; Shi et al., 1997). The same stabilizing recirculation region can, however, also be achieved by a swirling jet expanding in a surrounding fluid at rest (Apte et al., 2003b; Oefelein et al., 2007) or an annular flow entering in a cylindrical geometry generating a bluff–body like flow (Riber et al., 2009; Alletto and Breuer, 2012; Breuer and Alletto, 2012b). To rise the efficiency and reduce the emissions of such devices it is therefore important to precisely predict the particle dispersion and the local particle concentration in such complicated flow configurations. Foregoing researches investigated the cold flow in model combustion chambers prevalently by means of the two–way coupling assumption (see, e.g., Apte et al., 2003b; Oefelein et al., 2007; Riber et al., 2009). For higher mass loading, however, the particle–particle collisions became important and also this interaction mechanism has to be considered in order to reliably predict the two–phase flow. In this work results obtained with LES combined with a point–particle approach considering particle–fluid (two–way coupling) and particle–particle (four–way coupling) interaction in a complex geometry are shown for the first time in § 8.7 proving the applicability of the approach in technically relevant applications. Note that some results were already published in Alletto and Breuer (2012) and Breuer and Alletto (2012b) by the author of the present work.

In cyclone separators (see, e.g., Obermair et al., 2003, 2005) the particle–laden gas flow enters the cyclone barrel tangentially inducing a highly rotatory flow. Centrifugal forces
lead to a migration of the particles towards the cyclone walls where they are transported downwards and collected in the dust bin located at the bottom of the apparatus. The air leaves the cyclone through the vortex finder located at the top of the device. The complicated flow structures (curved streamlines, secondary flows and a precessing vortex core) and the experimentally proved particle agglomeration (see Obermair et al., 2005) turn the optimization of a cyclone separator regarding pressure loss and separation efficiency to a challenge for the simulation tool. Because of the huge number of particles present in a cyclone separator until now this flow configuration remained unexplored in the framework of four–way coupled LES. Numerical investigations were yet restricted to one–way coupled (see, e.g., Derksen, 2003; de Souza et al., 2012) or two–way coupled simulations (see, e.g., Derksen et al., 2006, 2008). Hence, four–way coupled simulation have a great potential in providing additional understanding of the phenomena influencing the flow in this interesting configuration. In § 8.8 fist results of one– and two–way coupled simulations including the effect of particles hitting a rough wall are compared with the experiments of Obermair et al. (2003) and Obermair et al. (2005). Unfortunately no four–way coupled simulations were possible because of the tremendous computational costs simulating the \( \mathcal{O}(10^9) \) particles present in the computational domain in the case if each single particle is tracked.

The accurate prediction of the flow structure and the related particle deposition in the respiratory system is crucial for understanding the \( \text{O}_2–\text{CO}_2 \) exchange, the deposition of toxic materials and the optimal aerosol–drug targeting (Kleinstreuer and Zhang, 2010). Due to the complex flow structure present in nasal cavities and oral airways (i.e., laminar–turbulent transition, large pressure drops, secondary flows and merging streams (Kleinstreuer and Zhang, 2010) and possible particle–particle collisions and agglomeration (Kleinstreuer and Zhang, 2010) LES combined with a Lagrangian particle approach seems the right way to follow in order to reach the ultimate goal in this research field, i.e., a patient–specific drug delivery optimum (Kleinstreuer and Zhang, 2010). Unfortunately, until now only one–way coupled LES were performed in this research field (see, e.g., Breuer et al., 2007; Lambert et al., 2011) and hence, the method presented in this work could also be used to advance the knowledge about the particulate flow in a respiratory system.

Summing up, it is evident that there is a lag of four–way coupled LES in wall–bounded turbulent flows in complex geometries. Therefore, one of the objectives of this thesis is to make a step towards filling this gap by proving the applicability of four–way coupled LES first of all for simple geometries such as turbulent channel (§ 8.1, § 8.2 and § 8.3) and turbulent pipe flows (§ 8.4 and § 8.6). In a second step the methodology is applied in geometrically more complex configurations. These are a model combustion chamber (see, § 8.7) and a cyclone separator (see, § 8.8). Furthermore, by a detailed physical analysis of the test cases supplementary information not deliverable by experiments were gathered to improve the knowledge about the physics governing such complicated flows.

As already mentioned, a further objective of this thesis was to develop a simple model which mimics the rebound behavior of solid particles at rough walls employable in engineering applications which will be described in § 4.3.2. Note that the model presented in this thesis was already published by the present author as coauthor in Breuer, Alletto, and Langfeldt (2012).

The background for the wall modeling issue was the experimental finding of the significant alteration of the fluid and particle statistics by the particles rebounding at rough
walls (Kussin and Sommerfeld, 2002; Sommerfeld, 2003; Sommerfeld and Kussin, 2003; Benson et al., 2005). In their channel flow experiments both groups reported diminishing mean particle velocities and rising particle fluctuations in streamwise and wall–normal directions with increasing wall roughness. Benson et al. (2005) found a smaller mean velocity for the particles than for the fluid, although the flow pointed in the gravitational direction. They directly attributed this effect to the momentum loss of the particles during the wall collision and the strong cross–stream mixing. Similar experimental findings (mean particle velocity lower than fluid velocity and high particle fluctuations) were made in vertical downward directed channel and pipe flows, see, e.g., Kulick et al. (1994); Paris (2001); Caraman et al. (2003); Borée and Caraman (2005). Hence, such wall roughness models should be at least capable to describe (I) the intensified momentum loss at the rough wall in comparison to a smooth wall and (II) the increased resuspension of particles due to the wall roughness which leads to an equalization of the particle mean velocity and concentration. In general, the momentum loss of the particle at the wall (I) can be achieved by introducing normal \((e_{n,w})\) and tangential \((e_{t,w})\) restitution coefficients and static \((\mu_{st,w})\) and dynamic \((\mu_{dy,w})\) friction coefficients (see § 4.3.1 for a detailed explanation). Precondition (II) can be taken into account by modeling the so–called shadow effect, i.e., a particle can not hit a roughness structure which has a negative inclination angle with respect to the particle trajectory identified by Sommerfeld and Huber (1999) as a basic mechanism influencing the particle dynamics. This effect leads to a redistribution of the streamwise momentum carried by the particle towards the wall–normal direction. Some models already exist which comply with this condition. Unfortunately, none of the models found in the literature and described in the following incorporated an amplitude parameter like the mean roughness \(R^*_z\) or the root–mean–squared roughness \(R^*_q\) which are commonly used in industrial applications to characterize rough surfaces.

Available wall roughness models in the literature applied in the context of dispersed multiphase flows and used in an Euler–Lagrange formalism assume a certain random distribution of the surface inclination hit by the particles. Squires and Simonin (2006) simulated the effect of the wall roughness on a one–way coupled turbulent channel flow using LES. To account for the wall roughness, they computed the normal vector of the surface according to \(\mathbf{n} = [n_x, n_y, n_z] = [\sin \alpha \cos \phi, \cos \alpha, \sin \alpha \sin \phi]\) sampling random Gaussian distributed angles \(\alpha_R\) and \(\phi\). Here the \(x\)–coordinate pointed in streamwise, the \(y\)–coordinate in wall–normal and the \(z\)–coordinate in spanwise direction (see Fig. 1). Consequently, the normal vector lays on a point of the unit sphere surface described by the polar angle \(\alpha_R\) and the azimuthal angle \(\phi\). \(\alpha = \phi = 0\) represents the smooth wall case. The collisions between the particles and the wall were assumed to take place at a specular wall, i.e., without friction and a wall–normal restitution coefficient of unity. In case the particle velocity after the wall collision was not directed inside the flow domain, they resampled the normal vector. This procedure modeled the shadow effect by turning the mean of the probability distribution of the normal vector towards the incoming particle trajectory. Squires and Simonin (2006) reported the following results: The mean particle velocity became more uniform for increasing roughness, the velocity fluctuations in streamwise and wall–normal direction increased and the concentration was found to be more uniform across the channel. No significant alteration of the spanwise velocity fluctuations were reported. The reason may be that the azimuthal angle \(\phi\) is Gaussian distributed and hence angles \(\phi\) which lay around the \(x\)–axis are predominant, i.e., deviations in \(z\)–direction are more seldom.

\[
\begin{align*}
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\]
Figure 1: Definition of the normal vector $\mathbf{n}$ in Squires and Simonin (2006) and of the angle $\delta^-$ in Lain and Sommerfeld (2008).

For two-dimensional RANS predictions Sommerfeld and Huber (1999) assumed in their pioneering work a random Gaussian distribution with a standard deviation $\sigma_w$ of the wall inclination. The standard deviation was obtained by experimentally measuring the incident and the reflection angle of different particle–wall material pairings. To account for the shadow effect, they recomputed the random wall inclination angle $\alpha_R$, if $\alpha_R$ was greater than the particle incident angle $\delta^-$ (see Fig. 1). For the normal restitution coefficient $e_{n,w}$ and the friction coefficients ($\mu_{st,w} = \mu_{dy,w}$) they used experimentally obtained correlations depending on the impact angle $\delta^-$. Unfortunately, they did not mention how to proceed in the general 3-D case. Sommerfeld (2003) and Sommerfeld and Kussin (2003) used this model to analyze the influence of the wall roughness on the particle behavior in a horizontal channel flow. The mean fluid velocity required to compute the fluid forces on the particles was assumed to obey the $1/7$-power law and the distributions of the fluid velocity fluctuations in streamwise and wall–normal directions needed for a random–walk model describing the effect of turbulence on the particles were taken from experiments. Sommerfeld (2003) found that by applying the wall roughness model the wall collision frequency was reduced for particles with a small relaxation time and increased for particles with a large relaxation time. Additionally, it led to a considerable equalization of the particle concentration across the channel preventing gravitational settling. Analyzing the integral properties of the particles, Sommerfeld and Kussin (2003) drew the following conclusions: The wall roughness leads to (i) a decrease of the mean particle velocity, where the effect is more pronounced for larger particles, (ii) the particle turbulent kinetic energy is considerably increased, (iii) the particle velocity fluctuations become more isotropic, (iv) a much better agreement with experiments is found compared to the case neglecting the effect of the wall roughness. Lain and Sommerfeld (2008) applied the model developed by Sommerfeld and Huber (1999) in two–dimensional RANS computations of the flow in a horizontal channel. They found an excellent agreement of the predicted results with the fluid and particle statistics of Kussin and Sommerfeld (2002), if they adjusted the standard deviation $\sigma_w$ of the wall inclination in such a way that the simulated pressure drop matches the measured one. The findings of the authors for increasing wall roughness were: (i) the particle mean velocities were diminishing, (ii) the velocity fluctuations in streamwise and wall–normal direction were increasing, (iii) the concentration became more uniform and (iv) no significant effects on the fluid statistics were visible.

Konan et al. (2009) pointed out that the model developed by Sommerfeld and Huber (1999) led to a non–zero probability of particles hitting the wall with a small incident angle to remain grazing, i.e., to leave the wall with a very small or zero rebound angle. Konan et al. (2009) argued that even if a particle after its first wall collision would still move
towards the wall or leave the wall with a very small deflection angle, it would hit anyway a second wall asperity. This mechanism deflects the particle towards the inner part of the domain. These multiple collisions at the wall lead to a zero probability of the particles to remain grazing and hence Konan et al. (2009) claimed that the model of Sommerfeld and Huber (1999) would not reproduce the proper particle deflection angle. Konan et al. (2009) accounted for this effect by recomputing the wall inclination if the actually computed wall inclination led to a non–zero probability of the particle to make a second rebound. Unfortunately, the model was evaluated only for a two–dimensional roughness and no hint was given how to proceed in the general three–dimensional case. Similar to the model of Sommerfeld and Huber (1999) also this model assumed a Gaussian distributed wall inclination seen by the particle with a standard deviation of $\sigma_w$. Hence, no relation to a parameter used to characterize the wall roughness in technical applications is established.

Konan et al. (2011) compared the particle statistics obtained adopting the model described in Konan et al. (2009) with the statistics obtained implementing the model described in Sommerfeld and Huber (1999). A Detached–Eddy Simulation (DES) of a particle–laden turbulent horizontal channel flow was carried out the perceive this scope. In spite of the three dimensional channel they assumed a two–dimensional roughness, i.e., they allowed the virtual wall only to incline around the axis parallel to the spanwise direction (the wall was only able to incline in the $x$–$y$ plane depicted in Fig. 1). They compared their statistics with the measurements performed by Kussin and Sommerfeld (2002) for 100 $\mu$m particles at a mass loading of $\eta = 20\%$ and a mean roughness height of $R_z = 6.8 \mu$m (denoted R2 in the experiment). For increasing standard deviation of the wall inclination $\sigma_w$ both models evaluated led to a diminishing of the mean streamwise particle velocity and an increase of the particle velocity fluctuations. It is worth to mention that applying the model described in Konan et al. (2011) led to the maximum particle concentration located near the middle of the channel, whereas applying the model of Sommerfeld and Huber (1999) predicted a concentration maximum at the bottom wall. Since in the experiment of Kussin and Sommerfeld (2002) the particle concentration showed a maximum at the bottom wall the refined model of Konan et al. (2009) yields qualitatively incorrect results for this quantity. Good agreement was found applying the model of Konan et al. (2009) for the particles streamwise and wall–normal velocity fluctuations, whereas the mean particle velocity was lower than the measured one. Using the model of Sommerfeld and Huber (1999) yields good agreement between the simulation and the experiment regarding the mean particle velocity, the particle concentration and the particle streamwise fluctuations. The particle wall–normal fluctuations were predicted too low. Summing up, the model of Sommerfeld and Huber (1999) led to a better accordance with the experiments of Kussin and Sommerfeld (2002) than the model described in Konan et al. (2009).

In his DNS predictions Vreman (2007) applied a very simple wall roughness model adding to each component of the wall–normal vector a uniformly distributed random number. The resulting maximum inclination of the virtual wall was $\alpha_{\text{max}} = 22^\circ$. The model parameters of the inelastic wall with friction were $\epsilon_{t,w} = 0.3$, $\mu_{st,w} = \mu_{dy,w} = 0.3$ and $\epsilon_{n,w} = 0.97$ (see § 4.3.1). Applying this model he observed a significant reduction of the particle axial velocity and an increase of the radial particle fluctuations and the particle shear stress for a mass loading of $\eta = 110\%$. For a mass loading of $\eta = 11\%$, however, no significant changes in the particle statistics could be observed. This rather simple formulation can describe the randomly distributed roughness structures, but not the shadow effect.
Another approach was provided by Frank et al. (1993), who carried out two-dimensional channel flow simulations postulating the 1/7-power law for the mean axial gas velocity. The influence of the fluid turbulence on the particle motion was neglected. They described the wall surface as a polygonal chain with randomly distributed base points \((x_n, y_n)\). \(y_n\) is the wall-normal coordinate of the base point and \(x_n\) denotes the coordinate pointing in streamwise direction. They computed the coordinates \((x_n, y_n)\) using uniformly distributed random numbers varying between \([-y_{\text{max}}, y_{\text{max}}]\) and \([1/2 \overline{x}, 3/2 \overline{x}]\). They mentioned that the two roughness parameters had to be predicted by microscopical examinations of the wall material specimens. Unfortunately, Frank et al. (1993) did not suggest how the two parameters \(\overline{x}\) and \(y_{\text{max}}\) are correlated to commonly employed roughness parameters used to describe the surface asperities. They obtained reasonable agreement between their numerical predictions and their mean particle velocities measured in a square duct. However, they did not refer which parameters they used for \(\overline{x}\) and \(y_{\text{max}}\).

As already mentioned, in spite of the reasonable agreement between simulation and experiment, one of the major disadvantages of the aforementioned roughness models that they are not based on an explicit correlation between some characteristic factors describing the roughness of the wall and the deviation of the normal vector. Instead, either fully empirical or experimentally determined correlations are required which are in general not available. Hence, in § 4.3.2.2, a model is presented for which the only parameters required to establish a relation between the inclination of the normal vector and the wall roughness are the particle diameter \(d_p^*\) and the mean roughness height \(R_z^*\) or the root-mean-squared roughness \(R_q^*\), which are commonly used parameters to describe the wall roughness of manufactured surfaces. The model proposed can be applied in general three-dimensional domains with no restrictions to the bounding surfaces. Hence, it is suitable for DNS, LES, RANS and hybrid LES–RANS.

1.2 Objectives of the Present Work

Recapitulating, this thesis is motivated by the lag of four-way coupled LES predictions in complex geometries which are indispensable for the validation of the method described in this work in view of its applicability to design industrial devices. By means of the newly developed collision detection algorithm it is possible to efficiently account for the momentum transfer between the particles and hence, to reliably predict disperse multiphase flows at regimes of high mass loadings. Furthermore, a new wall model mimicking the rebound of solid particles at rough walls is developed incorporating an amplitude parameter for the roughness. This model is shown to reliably reproduce the momentum change of particles hitting a rough domain boundary and in the view of the author represents the first model applicable in designing industrial devices. Hence, accounting for both effects (particle–particle and particle–wall interactions), together with an accurate description of the feedback of the disperse phase on the carrier phase, leads to an extended simulation tool ² able to take the most relevant physical mechanism governing disperse two-phase flows containing solid particles into account.

Furthermore, the objective of this work was to carefully choose and evaluate different test cases in order to elucidate the influence of the different modeling assumptions for the solid phase on the particle dynamics and via the particle–fluid coupling also on the continuous phase. The following measures were taken in order to reach the goal of the

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²The original CFD code LE$S$OCC is accurately described in Breuer (1998, 2002); Breuer et al. (2006).
present thesis:

- Different interpolation schemes to determine the fluid velocity at the particle position were tested in order to allow conclusions on their filtering effect.

- Since for tiny particles the subgrid–scale velocity became important, their effect is considered by a simple but still sufficient model.

- A fast collision detection algorithm was implemented in the underlying CFD code order to take the influence of the particle–particle interaction with affordable computational costs into account.

- A new wall model which mimics the rebound behavior of solid particles at rough walls was developed to correctly describe the experimentally proven effect of rough asperities on the particle motion.

Furthermore, the resulting method is scrupulously validated against experimental data and other numerical simulation data which are assumed to be more accurate than LES, i.e., DNS. As already mentioned, for this scope different test cases are considered. To compare two different schemes to interpolate the fluid velocity at particle position (the trilinear interpolations scheme and the one proposed by Marchioli et al. (2007a)), channel flow simulations at zero gravity at Re = 10,935 are performed. The statistics of tracers which perfectly follow the fluid are compared with the fluid statistics to assert the damping features of the two schemes. After implementing the the subgrid–scale model for the particles, it is check if the statistics obtained for tiny particles coincide with the DNS results of Kim et al. (1987). The collision detection algorithm was validated with the experiments of Benson et al. (2005) in a downward channel flow with smooth walls at the same Reynolds number mentioned above. The wall roughness model was carefully compared with the experiments of Kussin and Sommerfeld (2002) and Kussin (2004) for different wall roughness heights, particle diameters and mass–loadings. The resulting methodology is further tested and compared with experiments in a downward and a horizontal pipe flow to gain further confidence about its reliability. After successfully validating the resulting CFD code in simple geometries more challenging test cases like a cold flow in a combustion chamber and the flow in a cyclone separator were tackled. For both cases the quality of the results are supported by experimental works from the literature. After asserting the reliability of the numerical method, the simulations are evaluated in detail in order to provide additional information about the physical mechanism governing particle–laden turbulent wall–bounded flows which are not measurable by experimental studies.

Last but not least, a model for the occurrence of agglomeration of dry particles valid for frictional inter–particles collisions is presented. This model extends the works of Löffler and Muhr (1972), Hiller (1981), Ho (2004) and Jürgens (2012) which presented agglomeration models only valid for frictionless collisions. All this model assumed an increased van–der–Waals attraction after the collision due to the plastic deformation of the particles and hence a flattening of the particles surface. In contrast to the wall roughness model for the particles and the deterministic collision handling, the agglomeration model is not evaluated in detail but only a proof of its applicability is provided. The detailed evaluation is not the scope of this thesis and will be performed in an ongoing project.
1.3 Outline of the Thesis

The thesis is organized as follows: First, the classification of gas–solid flows and a literature review on simulation methods for gas-solid flows is given in § 2 to trace out the parameter space in which the present method can be applied and to underline its advantages and drawbacks compared to other simulation methods. Then the theoretical background of LES (§ 3) and the point-particle approach (§ 4) is discussed and the modeling of the coupling mechanisms between the phases (§ 5) is described. After that the numerical methods adopted to solve the equations of motion for the continuous and the disperse phase are discussed in § 6. The description of the numerical methods is followed by the description and the numerical setup of the different test cases (§ 7) and the results obtained in turbulent channel flows (§ 8.1, § 8.2 and § 8.3), turbulent pipe flows (§ 8.4 and § 8.6), a cold flow in a model combustion chamber (§ 8.7) and the flow in a cyclone separator (§ 8.8). Last but not least, conclusions are drawn and an outlook about future work is given in § 9.

In the following section the classification and simulation methods for gaseous flows carrying solid particles are briefly reviewed to trace out the parameter space in which the method employed in this thesis can be applied and to underline its advantages and drawbacks compared to other simulation methods.

2.1 Classification of Gas–Solid Flows

In principle the flow around each particle can be fully resolved and the inter–particle collisions and the particle collisions with bounding walls can be treated by continuum mechanical approaches to keep the modeling assumptions at a minimum. Unfortunately, this procedure will turn the problem to be completely intractable due to huge computational costs. Hence, some modeling assumptions have to be taken into account to treat the problem within a reasonable amount of time. Since modeling is always associated with simplifications and simplifications are only valid in a certain range of a parameter space, a description of gas–solid flows depending on some characteristic parameters is mandatory to choose the appropriate modeling and hence reliably predict the flow.

Considering a single phase flow, the classification is rather simple. Assuming that the flow configuration has only one characteristic length $L_f^*$, a characteristic velocity $U_f^*$, a constant density $\rho_f^*$ and a constant dynamic viscosity $\mu_f^*$, a dimensional analysis turns out that the flow regime (without considering the temperature difference) is fully defined by one dimensionless parameter, i.e., the Reynolds number $\text{Re} = U_f^* L_f^* \rho_f^* / \mu_f^*$. Here it is also assumed that the flow is isothermal and that the gravity does not influence the behavior of the continuous phase. Note that in the following if no other specification is given, quantities with the superscript $^*$ are dimensional quantities and all quantities without such a superscript have to be seen as dimensionless.

Adding to the same configuration a certain number $N_p$ of particles with a density of $\rho_p^*$ and a diameter of $d_p^*$ leads to three additional dimensionless parameters characterizing the system when adopting again a dimensional analysis. If the influence of the gravity on the particles cannot be neglected (e.g., in case of a horizontal conveying system) an additional fourth parameter is involved further complicating the description of the flow configuration.

The first dimensionless parameter derived by this dimensional analysis is the density ratio $\rho_p^* / \rho_f^*$. The second is the dimensionless gravity $g = g^* L_f^* / U_f^{*2}$ which is equal to the inverse of the square of the Froude number $\text{Fr} = U_f^* / \sqrt{g^* L_f^*}$.

The third parameter often used to characterize gas–solid flows is the mass loading:

$$\eta = \frac{\dot{m}_{p,\text{tot}}^*}{\dot{m}_{f,\text{tot}}^*} = \frac{1}{\Delta T^*} \sum_{i=1}^{N_p} 1/6 \pi d_p^{*3} \rho_{p,i}^* \int \rho_f^* u_f^* dA^*$$. \hspace{1cm} (2.1)

Here $\dot{m}_{p,\text{tot}}^*$ denotes the total mass flux of the particles through the averaging surface $A^*$, i.e., the total particle mass passing the surface $A^*$ during the time period $\Delta T^*$. $\dot{m}_{f,\text{tot}}^*$ denotes the fluid mass flux through the same surface $A^*$. This parameter describes the influence of the disperse phase on the carrier phase: With increasing mass loading the carried momentum by the disperse phase rises and hence also the influence of the disperse
phase on the continuous phase increases. Instead of the mass loading $\eta$, the volume fraction

$$\Phi = \frac{V_{p,tot}^*}{V_{tot}^*} = \frac{\sum_{i=1}^{N_p} 1/6 \pi d_{p,i}^3}{V_{f,tot}^* + V_{p,tot}^*}$$

(2.2)

is often used which defines the ratio of the total volume occupied by the particles $V_{p,tot}^*$ to the total domain volume $V_{tot}^*$, i.e., the sum of the total fluid volume $V_{f,tot}^*$ and the total particle volume $V_{p,tot}^*$. This parameter is used to quantify the importance of inter–particle collisions: With increasing total particle volume the mean spacing between the particles diminishes and hence the probability of the particles to collide increases.

For the fourth dimensionless parameter different definitions mostly depending on the research field can be found. The most common used is the Stokes number:

$$St = \frac{\tau_p^*}{\tau_{cf}^*}.$$  (2.3)

Here $\tau_{cf}^*$ denotes a characteristic fluid time scale depending on the research field and $\tau_p^*$ is the particle relaxation time:

$$\tau_p^* = \frac{\rho_p^* d_p^{*2}}{18 \mu_f^*}.$$  (2.4)

The particle relaxation time $\tau_p^*$ describes the time frame a particle initially at rest needs to reach about 63% of the fluid velocity in the Stokes flow regime (Sommerfeld, 2000). The Stokes number describes the class of eddies which predominantly influence the dynamic behavior of the particles: Eddies with a characteristic time of $\tau_{cf}^* \ll \tau_p^*$ are not able to influence the particle dynamics since the particles do not respond to their motion. On the other hand for eddies with a characteristic time of $\tau_{cf}^* \gg \tau_p^*$ in a turbulent flow a lot of smaller eddies exist influencing the local particle trajectory. This would be, e.g., the case if the particle relaxation time is of the order of the Kolmogorov time. In this case it seems reasonable to assume that the eddies belonging to the inertial regime would not substantially influence the dynamics of such small particles. That means that particles with a small relaxation time $\tau_p^*$ do not ”see” the eddies with a large characteristic time $\tau_{cf}^*$. Hence, it seems reasonable to assume that eddies with $\tau_{cf}^* \approx \tau_p^*$ are the one which mostly effect the particle motion.

With the above considerations we get the often cited map of Elghobashi (1994) (see Fig. 2) defining the interaction regimes between particles and turbulence. Elghobashi (1994) used the Stokes number $St = \tau_p^*/\tau_{\eta}^*$ defined with the Kolmogorov time scale $\tau_{\eta}^*$ and the volume fraction $\Phi$ to characterize the different flow regimes appearing in gas–solid flows for a constant Reynolds number, constant density ratio and negligible influence of gravity.

For $\Phi \leq 10^{-6}$ the influence of the particles on the turbulence is negligible and hence the particle motion is only determined by the carrier phase. This regime is called one–way coupling regime since the interaction between turbulence and particles goes only in one direction.

For $10^{-6} \leq \Phi \leq 10^{-3}$ the momentum transfer from the particle to the fluid is large enough to alter the structure of the turbulent flow. This regime is called two–way coupling regime because of the mutual influence between the particles and the carrier–phase. Depending on the Stokes number the two–way coupling regime is further divided into an area where the particles attenuate the turbulence and an area where the particles lead to a production of turbulence. Elghobashi (1994) argued that for larger $\tau_p^*$ and hence also
larger particle diameters $d_p^*$ (of course $\rho_p^*$ and $\mu_f^*$ have to be taken as constant for this consideration) vortex shedding takes place behind the particles leading to an additional source of turbulence.

The next flow regime defined by Elghobashi (1994) starts at $\Phi \geq 10^{-3}$ when the spacing between the particles is low enough to turn the inter–particle collisions to an important mechanism influencing the particle dynamics. This regime is called four–way coupling regime since the interaction takes place between the fluid and the particles (two directions) and between the particles themselves (additional two directions).

For a further increase of $\Phi$ the role of the fluid on the particle trajectories decreases reaching for $\Phi \approx 1$ the granular flow regime.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{interaction_regimes.png}
\caption{Map of interaction regimes between particles and turbulence (Elghobashi, 1994).}
\end{figure}

As a concluding remark in Table 1 a list of different definitions of the Stokes number is given to emphasize the difficulties that sometimes arise when comparing the results of different authors. Since in different research fields the focus is set on different time scales (in DNS the smallest time scales are resolved while in RANS only the mean field is important) also the chosen characteristic time scales for the fluid $\tau_{cf}^*$ varies with the research field and therewith associated also the value of the St number (see eq. (2.3)). Hence, special care has to be taken when comparing the particle statistics with a given St number of two different authors. For example, in the DNS of isotropic turbulence typically the Kolmogorov time $\tau_{\eta}^*$ is used as the characteristic fluid time scale while in wall–bounded (channel or pipe) DNS the viscous time $\tau_{vis} = \nu^*/u_f^2$ is usually taken. In LES the large–eddy turn over time $\tau_e = L_f^*/U_f$ is often used as the characteristic time. For particle–laden flow simulations using RANS no unambiguous definition of the fluid time scale has been asserted by the author since a lot of different definitions for this quantity are used in the literature. For this reason it is omitted in these considerations.
<table>
<thead>
<tr>
<th>Dimensionless parameter</th>
<th>Definition</th>
<th>Research field</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \text{St} )</td>
<td>( \tau_p^* / \tau_\eta^* = \tau_p^* / (\nu^* / \epsilon^*)^{(1/2)} )</td>
<td>DNS of isotropic turbulence (e.g., Wang and Maxey, 1993; Sundaram and Collins, 1997)</td>
</tr>
<tr>
<td>( \text{St}, \tau^+, \tau_p^+ )</td>
<td>( \tau_p^* / \tau_{vis}^* = \tau_p^* / (\nu^* / u_T^2) )</td>
<td>DNS of wall–bounded flow (e.g., Marchioli and Soldati, 2002; Dritselis and Vlachos, 2008; Marchioli et al., 2008c; Nasr et al., 2009)</td>
</tr>
<tr>
<td>( \text{St} )</td>
<td>( \tau_p^* / \tau_{\text{le}} = \tau_p^* / (L_f^* / U_f^*) )</td>
<td>LES, e.g., Apte et al. (2003b); Breuer et al. (2006); Oefelein et al. (2007)</td>
</tr>
</tbody>
</table>

Table 1: Definition of Stokes numbers found in the literature.

2.2 Literature Review on Simulation Methods for Gas–Solid Flows

Depending on the position in the map of interactions (see Fig. 2 and Elghobashi (1994)) Balachandar and Eaton (2010) drew a map of applicability of different computational approaches to treat disperse gas–solid flows (see Fig. 3). Note that the map shown in Fig. 3 was drawn for cases where the carrier phase is treated by means of DNS or LES, since the review article of Balachandar and Eaton (2010) from where the map is extracted is focused on these methodologies to treat the carrier phase. Furthermore, the scale of the abscissa in Fig. 3 extracted from Balachandar and Eaton (2010) differ from the scale of Fig. 2 extracted from Elghobashi (1994). The reason is probably that the point–particle approach is only capable the describe turbulence attenuation by particles and not turbulence production by particles (Sundaram and Collins, 1996; Vreman, 2007). Hence, beyond \( \tau_p^*/\tau_\eta^* > 10^2 \) only the fully–resolve approach can be applied which resolves the full flow field around the particle. That means, that it is not necessary to extend the scale in Fig. 3 to the same range of the scale in Fig. 2. For that reason it can describe both, turbulence attenuation and also production by particle (For a description of the computational methodologies and the assumptions made see below). However, in the view of the author of this thesis even if the fluid is treated by another computational approaches (LES, DES or RANS) it represents a good overview on how single computational methodologies are marked off. In case of LES or RANS the ratio \( d_p^*/\eta_k^* \) should be replaced by the ratio particle diameter to the grid spacing \( d_p^*/\Delta_g^* \). In this way Fig. 3 can also be used to roughly mark of the validity of the methods used to threat the disperse phase: For particles of the order of the grid size the point–particle approach is not any more valid and the finite size has to by considered. For particles much smaller as the grid size the amount of particle becomes to high (of course for a given mass loading) an the point–particle approach is not any more affordable. Hence, an other modeling approach has to be chosen ( Again, for a description of the computational methodologies and the assumptions made see below). The different modeling strategies can be divided into two different branches: (i) The particles are treated in a Lagrangian frame of reference (the fully resolved and the point–particle approach), i.e., each particle is tracked individually in the computational domain by solving Newton’s second law; (ii) The particles are
treated in an Eulerian frame of reference (the Euler–Euler, Equilibrium Euler and the dusty gas approach), i.e., their field quantities are averaged in a continuum and their spatial and temporal evolution are described by partial differential equations similar to the continuous flow. The left–hand side limit of each approach arises due to the computational costs (i.e., the fully resolved approach could be extended until tiny particles but the computational costs would be tremendous). The right–hand side border of each approach in the map drawn by Balachandar and Eaton (2010) arises from the validity of the modeling assumptions. The explanations concerning this topic will be given along with the description of the single methods. Furthermore, it is worth to mention, that the Euler–Euler, the Lagrangian point–particle and the fully resolved approach can be applied also in the four–way coupled regime, whereas the map drawn by Balachandar and Eaton (2010) is misleading concerning this point.

Figure 3: Map of applicability of different computational approaches (Balachandar and Eaton, 2010).

In the following section a brief overview of these computational approaches is given and the basic assumptions made are recalled in order to underline the limitations and advantages of the single methodologies. Furthermore, the usual application areas of the described modeling strategies are elucidated and some methods used to compute granular flows are also included in the literature review to complete the picture of available procedures to treat flows containing solid particles.

2.2.1 Fully Resolved Euler–Lagrange Approach

The fully resolved approach is the one with the fewest assumptions among the methods presented in this thesis. The flow field around each particle is fully resolved and
the forces displacing the particle can be calculated by evaluating the components of the pressure and the stress tensor at the particle surface. Note that the definition “Fully Resolved Approach” found in the literature denominate the methodologies where all flow scales around a particle are resolved. Hence, only simulation methods where the carrier phase is fully resolved (DNS) belong to this definition. After calculating the forces and moments acting on the particle surface, the trajectory is predicted by Newton’s second law. Since the flow field around each particle is fully resolved, this method can accurately capture the physics governing the interaction between the particles and the turbulent flow with great detail. Unfortunately, due to the high computational costs and the rather low maximum treatable Reynolds number (DNS reaches nowadays only bulk Reynolds numbers of $Re \approx O(10^4)$) this methodology is restricted to academic research.

The most commonly used technique to compute the flow field around a particle is the Immersed Boundary Method (IBM) (see, e.g., Kajishima et al., 2001; Uhlmann, 2005; Lucci et al., 2010; Kempe and Fröhlich, 2012a) which allows the continuous phase to be treated on a simple Cartesian grid and imposing the no-slip and impermeability boundary condition at the particle surface without deforming the grid around the particles. The IBM uses two different kinds of grid points: one are denoted Eulerian grid points (see Fig. 4) where the fluid quantities are stored and the others are denoted Lagrangian grid points which are moving attached to the particle surface. The no-slip and the impermeability condition are achieved by additional force terms added to the Navier–Stokes equations. These force terms, however, are only applied to the Eulerian grid points in the vicinity of the particle surface (see Fig. 4) in order to force the fluid velocity stored at the Eulerian grid points interpolated to the Lagrangian points to be equal to the particle velocity at the solid surface. Hence, this method is capable to accurately describe the one-way and two-way coupling regime without modeling assumptions. This fact implicates another big advantage against the point-particle approach, since in principle both, turbulent attenuation and turbulence production by particles, can be described (see Fig. 2). Contrarily, the piece-wise constant source terms used in the point-particle approach to model the two-way coupling have been shown to be able to describe only turbulence attenuation (Sundaram and Collins, 1996; Vreman, 2007). However, since the Eulerian grid size using the fully resolved approach is imposed by the particle size, the problem becomes quickly intractable for smaller particles.

According to the detailed review of Kempe and Fröhlich (2012b) there are three com-
Commonly used methods to treat the particle–particle and particle–wall collisions in the framework of IBM. The first is the same hard–sphere collision model (HSM) as described in § 4.3.1 (particle–wall collisions) and § 5.4.1 (particle–particle collisions). The second model is a soft–sphere model (SSM) where the collision is resolved in time by using a spring–damping system describing the particle dynamics during the contact. The third approach is to define a somehow ad–hoc repulsive force (RFM) as a function of the distance between two colliding particles or the particle and the wall. The scope is to prevent the overlapping of two particles or of a particle with bounding walls. Usually the repulsive force is switched on if the distance between two particles or between a particle and the wall is less than two Eulerian grid points (see also Uhlmann, 2008; Lucci et al., 2010; Kempe and Fröhlich, 2012a). Kempe and Fröhlich (2012b) identified for each of the above mentioned models shortcomings, if applied in the framework of IBM. The HSM leads to an overestimation of the viscous forces because of the strong particle acceleration during the collision. The SSM leads to an unaffordable reduction of the time step size in order to provide accurate results since the collision process needs to be resolved. The collision time is typically much shorter than the time step to advance the continuous phase. Furthermore, the collision process needs to be resolved with at least a few time steps, which yields to a drastic increase of the computational resources if many particles are tracked throughout the domain (Kempe and Fröhlich, 2012b). The RFM contains an arbitrarily chosen constant of proportionality to adjust the repulsive force used to prevent the overlapping of two particles or the particle and the wall, which is a major disadvantage.

To reduce the above mentioned shortcomings, Kempe and Fröhlich (2012b) proposed to divide the collision process into three parts. The first part comes into play when the distance between two particles or a particle and the wall is too small in order to resolve the flow field by means of the Eulerian grid. In this case a lubrication model is applied to account for the liquid film squeezed out of the gap between two colliding particles or the particle and the wall. The second part of the model comes into play during the contact period. Similar to the HSM the normal and the tangential component of the particle motion are decoupled from each other. For the normal component an ordinary differential equation is solved similar to the SSM, but the contact time is imposed to be ten times the time step size used to advance the fluid (Kempe and Fröhlich, 2012b). The factor ten was chosen since it led to better agreement of the results obtained by the model with experimental data as using smaller factors (five and seven). In this way a too expensive time step reduction and an overestimation of the viscous force due to the strong particle acceleration is avoided. However, to achieve a quantitatively correct result for the normal post–collision velocity, the stiffness and the damping constants are adjusted in order that the post-collisional velocity is equal to the one predicted by a HSM. The tangential motion is calculated by setting the tangential force proportional to the normal force in case of sliding. In case of sticking the tangential force is calculated in order to fulfill the no–slip condition, i.e., the particle rolls during the collision. After the collision process the lubrication model is applied again to account for the liquid entrained into the gap between the two colliding particles or the particles and the wall until the flow field in the gap can again be resolved by the Eulerian grid. With these measures good agreement with experimental data from the literature were achieved by Kempe and Fröhlich (2012b).

Until now with the IBM only problems involving $O(10^3)$ particles in simple geometries could be solved because of the huge computational costs. For example, the particle motion in isotropic turbulence was computed by Lucci et al. (2010) with a maximum of $N_p =$
6400. Uhlmann (2008) computed a downward directed channel flow with a bulk Reynolds number of $\text{Re}_{\text{bulk}} = 2700$ involving $N_p = 4086$ particles. Shao et al. (2012) investigated a horizontal channel flow with $\text{Re}_{\text{bulk}} = 5000$ involving 2160 particles. Kajishima (2004) investigated the motion of 2048 particles settling down under the influence of gravity. Chan-Braun et al. (2011) fully resolved the flow in a transitionally rough channel flow at $\text{Re}_{\text{bulk}} = 2900$. The wall roughness was modeled by squared packed spheres having a diameter of 10 and 50 viscous length scales, respectively. For the smaller roughness the influence of 9216 wall spheres on the fluid was accounted by the method described by Uhlmann (2005).

### 2.2.2 Euler–Lagrange Approach using Point Particles

The point–particle approach treats the fluid in the usual Eulerian frame of reference while the particles are modeled as point masses. In contrary to the fully resolved approach for this methodology no restrictions concerning the modeling of the continuous phase are given and hence DNS and also all commonly used modeling strategies for the Navier–Stokes equations, i.e., LES, DES and RANS can be applied. The change of the translational velocity and angular velocity is described by Newton’s second law, where the fluid forces and torques acting on the particle are calculated as a function of the fluid quantities interpolated at the particle position. With this assumption the equations of motion for a single particle are reduced to simple ordinary differential equations:

\begin{align}
\frac{m_p^*}{\Delta t} \frac{\text{d} u_p^*}{\text{d} t} &= \sum F_p^* \\
I_p^* \frac{\text{d} \omega_p^*}{\text{d} t} &= \sum T_p^*.
\end{align}

Here $m_p^*$ is the particle mass, $I_p^*$ is the particle moment of inertia, $F_p^*$ are the forces acting on a single particle and $T_p^*$ is the torque acting on a single particle. By this way only the set of ordinary differential equations (2.5) has to be solved allowing to simultaneously track millions of particles (e.g., $1.4 \times 10^7$ as done in § 8.6) through the computational domain with rather low computational costs. Another big advantage of this method compare to the Euler–Euler method is that polydisperse flows can be treated without limitations of the size classes considered. Furthermore, the most relevant physical mechanisms influencing the particle motion, i.e., drag, gravity and lift forces, influence of the unresolved fluid scales, two–way coupling, particle–particle and particle–wall collisions can easily be modeled leading to an approach capable to realistically describe the particle trajectories. A detailed description of these modeling assumptions is provided in § 4. The limitations of this approach are essentially given by the particle size. The particle size is restricted on the one hand by the grid spacing since the particles should be smaller than the grid spacing in order not to violate the point–particle assumption. This point–particle assumption implicates that the particle size is small enough in order that the disturbances inflicted on the carrier phase decay within the range of the grid spacing. If the particle size is of the same order or even greater than the spacing between two computational nodes, this precondition is violated and the point–particle assumption does not hold any more. On the other hand the approach is restricted by the computational resources, i.e., if the particles are very small their amount increases drastically in order to fulfill a certain prescribed mass loading.
Because of the above mentioned advantages, the Euler-Lagrange approach using point particles has a vast application area going from engineering applications to fundamental investigations. In the following an overview of applications of the point-particle approach found in the literature is given. The applications are grouped based on the modeling strategies commonly adopted to solve the continuous phase, i.e., DNS, LES and RANS. The scope is to elucidate the shortcomings and strength of the different modeling strategies for the two-phase flow.

2.2.2.1 DNS

In DNS the turbulent flow is fully resolved and hence no modeling is required regarding the influence of the carrier phase on the disperse phase in the frame of the point particle approach. The advantage against the other two modeling approaches adopted for the continuous phase (LES and RANS) is quite obvious since no modeling uncertainties are introduced in the description of the fluid flow. This also implies that no modeling is required in the range of validity of the point-particle approach to account for the influence of the unresolved scales on the particles and vice versa. Hence, the interaction between the particles and turbulence can be studied in great detail outlining the physical mechanisms influencing this interplay. Unfortunately, the application of DNS are restricted to rather low Reynolds numbers because of the very high resolutions needed. For unladen flows the maximum computed Reynolds numbers reach about $O(10^4)$ in very simple geometries such as channel flows ($Re_B \approx 43,000$, Hoyas and Jiménez, 2006, 2008) and pipe flows ($Re_B \approx 20,000$, Wu and Moin, 2008). DNS studies reported in the literature concerning particle-laden flows are carried out at even lower Reynolds numbers, i.e., about $Re_B \approx 4000$ in channel flows (Bijlard et al., 2010) and about $Re_B \approx 2000$ in pipe flows (Vreman, 2007). Furthermore, DNS studies are confined to simple geometries because of the difficulties to adopt highly accurate discretization procedures mandatory for DNS (e.g., spectral methods or compact finite differences) on complex grids. For that reason DNS combined with the point-particle approach is still only adopted for fundamental research.

Since no models are required for the continuous phase, the modeling strategies are restricted to the interaction mechanisms between the particles and the fluid, the particle themselves and between the particles and the bounding walls. As already mentioned, the interaction regimes between the particles and the turbulent flow can be divided into one-way coupling and two-way coupling. If inter-particles collisions play a role the four-way coupling regime is reached.

Regarding the one-way coupling regime the modeling strategies adopted concern the fluid forces acting on the particles. For cases for large density ratios $\rho_p^*/\rho_f^*$ mostly drag, gravity and lift forces due to linear shear are considered (see, e.g., Rouson and Eaton, 2001; Marchioli and Soldati, 2002; Marchioli et al., 2007b). From the literature reviewed no study which includes the lift force due to the particle rotation (Magnus lift) could be asserted. The reason is probably the lag on DNS considering the change of the particle momentum parallel to the wall. Specially for rough-wall impacts the particles acquire high rotational velocities (Hussainov et al., 1996; Yamamoto et al., 2001; Sommerfeld, 2003; Alletto and Breuer, 2013) and the Magnus lift force should be considered.

In order to describe the influence of the particles on the continuous phase (two-way coupling), the commonly used procedure is the application of the particle-source in cell (PSIC) method originally described in Crowe et al. (1977). Crowe et al. (1977) accounted for the effect of the disperse phase on the fluid by summing up all forces related to the
fluid flow acting on all particles in a control volume, inverting the sign and adding the resulting contribution to the equation describing the fluid motion. The procedure can be seen as Newton’s third law “actio equals reactio”. Usually in DNS combined with a point–particle approach only the drag force is considered for the two–way coupling because it is assumed to be the force with the largest magnitude (see, e.g., Elghobashi and Truesdell, 1993; Boivin et al., 1998; Bijlard et al., 2010).

In the framework of DNS combined with the point–particle approach the interaction between particles is described by deterministic hard–sphere collisions. Since inter–particles collisions are local phenomena, the collision detection is limited to neighboring particles in order to break down the computational effort. The effect of collisions on the particle motion is investigated by DNS in simple flow configurations like isotropic turbulence (see, e.g., Sundaram and Collins, 1997), downward channel flows (see, e.g., Li et al., 2001; Dritselis and Vlachos, 2008; Nasr et al., 2009; Dritselis and Vlachos, 2011a) or downward pipe flows (Rani et al., 2004; Vreman, 2007). From the literature reviewed it can be judged that no stochastic particle–collision model was applied. In the view of the author of the present thesis the reason why no stochastic collision models are found in the framework of DNS is based on consistency. In case of DNS all fluid scales are resolved and therefore the particle trajectory are supposed to be calculated very accurately. For that reason applying a stochastic model (which is not as accurate as a deterministic model) for the inter–particles collision seems to be not consistent with the accuracy demands of DNS.

### 2.2.2.2 LES

In LES the large energy–carrying eddies are resolved in space and time while the influence of the small more isotropic scales on the large scales is modeled. The disadvantage against DNS is the inherent uncertainties arising by the subgrid–scale modeling and hence the method can not be assumed to be as exact as DNS. However, since the resolutions required are not as fine as in DNS, the computational cost is lower allowing to compute flows at higher Reynolds numbers compared with DNS. Especially, if the near–wall layer is not resolved and the influence of this region on the bulk flow is model by wall functions, rather high Reynolds numbers can be reached for the single phase flow (channel flow, \( \text{Re}_B \approx 8 \times 10^9 \) (\( \text{Re}_T \approx 2 \times 10^9 \)) Chung and McKeon, 2010). Concerning particle laden flows the reachable Reynolds numbers are also higher compared to DNS, e.g., for wall–resolved downward channel flows for example \( \text{Re}_B \approx 11,000 \) (see, e.g., Fukagata et al., 1999; Yamamoto et al., 2001; Fugakata et al., 2001; Breuer and Alletto, 2012b) and \( \text{Re}_B \approx 22,000 \) for wall–resolved horizontal channel flows (Konan et al., 2011; Breuer et al., 2012; Mallouppas and van Wachem, 2013). Fairweather and Yao (2009) and Yao and Fairweather (2010) simulated the one–way coupled particle laden flow in a square duct flow at \( \text{Re}_B \approx 250,000 \) with a no–slip boundary condition at the wall. However, for both simulations the wall–normal resolution (\( \Delta y^+ = 6.39 \)) seem a bit to coarse to justify the no–slip boundary condition. If the wall layer is modeled the simulated Reynolds number can reach values of (\( \text{Re}_B \approx 60,000 \), Alletto and Breuer, 2013, or § 8.6). For these reasons it seems to be obvious that one of the big advantages against DNS is the higher range of explorable Reynolds numbers. Furthermore, the methodology can be adopted also in complex geometries since the demand on highly accurate numerical schemes is not as restricting as in DNS and finite–volume methods working on structured (see, e.g., Breuer, 2002) or unstructured grids (see, e.g., Mahesh et al., 2004; Riber et al., 2009) can be applied. For this reason LES combined with a point–particle approach was successfully
applied in configuration like cyclone separators (see, eg., Derksen, 2003; de Souza et al., 2012; Derksen et al., 2006, 2008), the cold flow in a model combustion chamber (see, e.g., Riber et al., 2009; Alletto and Breuer, 2012; Berrouk, 2012; Breuer and Alletto, 2012b), in particle–laden swirling flows (see, e.g., Apte et al., 2003b; Oefelein et al., 2007), the particle deposition in respiratory systems (see, e.g., Breuer et al., 2007; Kleinstreuer and Zhang, 2010; Lambert et al., 2011), the particle dispersion in ventilated rooms (see, e.g., Wang et al., 2012) and the particle–laden flow in square ducts (see, e.g., Winkler et al., 2004; Fairweather and Yao, 2009; Yao and Fairweather, 2010). Furthermore, Escauriaza and Sotiropoulos (2011) analyzed the mechanisms leading to the onset of scour around circular piles and Derksen (2003b) computed the flow in a stirred tank were solid particle are suspended in water. Although the last two examples belong to the class of liquid–solid flows, they are mentioned here to show the vast application area of LES combined with a point–particle approach. Hence, in contrast to DNS, LES combined with a point particle approach can already be applied in practical relevant configurations.

Following the division into one–way and two–way coupling adopted in the former section, for both interaction regimes models have to be introduced to account for the influence of the unresolved scale on the particles and the influence of the particles on the unresolved scales. In the one–way coupling regime the effect of the unresolved scales on the motion of tiny particles has to be modeled. In the two–way coupling regime the effect of the particles on the subgrid–scale stress has to be considered. Regarding the four–way coupling usually the same deterministic hard–sphere collision model as used in DNS is applied. From the literature reviewed it can be judged that no stochastic particle–collision model was applied in the framework of LES.

Regarding the forces acting on the particles the majority of investigation reviewed considered only the drag and gravity forces (see, e.g., Apte et al., 2003b; Derksen, 2003; Kuerten and Vreman, 2005; Derksen et al., 2006; Kuerten, 2006; Oefelein et al., 2007; Derksen et al., 2008; Riber et al., 2009; Marchioli et al., 2008b; Fairweather and Yao, 2009; Konan et al., 2011; Alletto and Breuer, 2012; Berrouk, 2012; Breuer and Alletto, 2012b; de Souza et al., 2012). LES studies including lift forces due to linear shear and particle rotation are still rare (see, e.g., Yamamoto et al., 2001; Winkler et al., 2004; Yao and Fairweather, 2010; Breuer et al., 2012; Alletto and Breuer, 2013).

As already mentioned, in LES only the large scales are resolved and the small scales are modeled. In order to account the effect of the unresolved scales on the particle motion different modeling strategies can be found in the literature reviewed. A method to estimate the full turbulent scales is applying an approximate deconvolution to the LES velocity field (see, e.g., Shotorban and Mashayek, 2005; Kuerten, 2006). The intention is to try to reconstruct the full velocity field (i.e., the one which would be obtained by DNS) by applying an inverse filter to the velocity field predicted by LES. The fluid velocity field obtained is casted into the equations used to calculate the fluid forces acting on the particles. Another class of models often employed are of Langevin–type. In this class of equations a random contribution due to the unresolved scales is added to the equation describing the particle motion, i.e., the forces displacing the particles consist of a deterministic part and a stochastic part due to the subgrid scales (see, e.g., Fede et al., 2006; Bini and Jones, 2007; Pozorski and Apte, 2009; Jin et al., 2010a). Both classes of models reproduce reliably the particle turbulent kinetic energy compared with DNS data, i.e., the models can successfully add the influence of the turbulent kinetic energy of the unresolved scale on the particle motion (Shotorban and Mashayek, 2005; Fede et al., 2006;
Pozorski and Apte, 2009; Jin et al., 2010a). If tested in a channel flow (which belongs to the class of wall–bounded flows examined in this thesis), unfortunately, both, the approximate deconvolution and the Langevin–type model, predict for small particles in turbulent channel flows an augmentation of the velocity fluctuations in all directions (see Kuerten, 2006; Marchioli et al., 2008b). It is known that in LES of turbulent channel flows, the streamwise velocity fluctuations are typically overpredicted with respect to DNS data and underpredicted in the other two directions. The same observation can be made also for small particles, i.e., the particle streamwise fluctuations are overpredicted compared to the particle fluctuations obtained by DNS and underpredicted in the other two directions (Kuerten, 2006). Hence, the presented models reproduce the right trend compared to DNS in spanwise and wall–normal direction but do not achieve the correct effect in streamwise direction. From this observation it is obvious that the development of subgrid–scale models for the particles accounting for anisotropy effects have still a great potential. An other disadvantage of this model are the computational costs since either the inverse filter operation has to be applied (Shotorban and Mashayek, 2005; Kuerten, 2006) or a stochastic differential equation has to be solved for the subgrid–scale velocity (Fede et al., 2006; Jin et al., 2010a).

A simplified version of the above described Langevin model is to assume the full velocity field as the sum of the filtered velocity field and a random component due to the subgrid scales (see Segura, 2004; Bini and Jones, 2008; Pozorski and Apte, 2009, and § 5.2). In this case the subgrid scales are assumed to be isotropic and Gaussian distributed. Difference between the models found in Segura (2004); Bini and Jones (2008); Pozorski and Apte (2009) and the one adopted in this thesis arise in the estimation of the amplitude of the subgrid–scale velocity fluctuations. An advantage of this models is clearly the simplicity: They solely require an estimation of the subgrid–scale kinetic energy and are thus cheap to compute. However, since they assume an isotropic distribution of the subgrid–scales they lead to an increase of the particle velocity fluctuation in all direction (see also § 8.1) and can not account for anisotropy effects.

In the view of the author of the present thesis an other still open question is how to model the influence of the unresolved scales on the preferential concentration of tiny particles. Preferential concentration is the known accumulation of particles in high–strainrate and low–vorticity region of the flow field (Elghobashi, 1994). By comparing DNS with LES it turns out that filtering reduces the preferential concentration of small particles but leads to denser particle clusters for larger particles (Pozorski and Apte, 2009; Ray and Collins, 2011). Pozorski and Apte (2009), however, pointed out that a diffusion–type subgrid–scale model (models which enhance the particle diffusion by adding turbulent kinetic energy to the fluid displacing the particles) is only able to reproduce the randomization effect of the small scale on larger particles but not the concentration effect on small particles. Especially in the view of considering particle agglomeration, another crucial aspect which has to be carefully addressed when modeling the effect of the unresolved scales on the particle motion, is the reduction of the particle collision frequency by filtering (Jin et al., 2010b). The error is much more pronounced for tiny particles leading a reduction of the collision frequency up to 60% for St = 0.5 (for details see, Jin et al., 2010b). Jin et al. (2010b) found that for tiny particles the filtering leads to an underprediction of the relative velocity between the particles and also an underprediction of the radial distribution function (a measure of particle clustering in isotropic turbulence, for details, see, Jin et al., 2010b, and references therein). Hence, it can be concluded
from the analysis of Jin et al. (2010b) that filtering leads to a reduction of the relative velocity between tiny particles and also to a reduction of particle clustering. Therefore, a strong reduction of the collision frequency with increasing filter width can be observed. That means that for tiny particles, which most likely tend to agglomerate, the errors in predicting the collision frequency introduced by the filtering procedure are expected to be most significant. Note, however, that for particles with a relaxation time much larger than the smallest resolved scales in LES (which are similar to the largest unresolved scales) the influence of the subgrid scales can be neglected.

Regarding the two-way coupling, in LES the same PSIC method described by Crowe et al. (1977) as used in DNS is applied. However, in contrast to DNS, where the influence of the particles on the full turbulent spectrum is accounted for by this method, in LES only the influence on the resolved scales is captured. That means that the source term accounting for the momentum exchange between the phases is casted into the equation of the large-scale motion of the fluid and the influence of the particles on the subgrid scales is usually disregarded (see, e.g., Boivin et al., 2000; Riber et al., 2009; Wang, 2010). To the author’s best knowledge Lei et al. (2002) were the only study which proposed a modification of the turbulent viscosity to account for the influence of the particles on the subgrid scales in the framework of gas–solid flows. Besides the lag of models accounting for the subgrid–scale coupling, another still open question is how to describe the turbulence production by solid particles (see Fig. 2). This effect is relevant for large particles where the wake behind the particles is responsible for the turbulence production. Sundaram and Collins (1996) showed that piecewise-constant point forces as applied in the PSIC method have a globally dissipative character, i.e., it results in a sink term in the global turbulent kinetic energy balance (see also Vreman, 2007). In the view of the author this issue would be a crucial aspect in order to extend the point–particle approach towards wall–bounded flows at high bulk Reynolds numbers loaded with rather inertial particles. Since inertial particles do not fulfill the no–slip condition at the wall, the velocity difference between inertial particles and the fluid in the vicinity of the wall is very high (see, e.g., Kussin and Sommerfeld, 2002; Sommerfeld and Kussin, 2004; Breuer et al., 2012). For high bulk Reynolds number flows this leads also to high particle Reynolds numbers in this region and probably the additional vortices generated in the wake of the particles would cause a substantial alteration of the wall turbulence. This alteration of the wall turbulence by the vortex shedding taking place behind particles at high $Re_p$ is presumably not predictable by simple source terms.

From the literature reviewed (the focus was set in the industrial application of LES) it can be stated that most large-eddy simulations combined with a point–particle approach employ a deterministic hard–sphere collision model to account for the momentum exchange between the particle. Hence, modeling–intrinsic differences between the investigations made by the research groups can only be found in the components of the collision force: For example, Geurts and Vreman (2006); Dritselis and Vlachos (2011b); Konan et al. (2011); Breuer and Alletto (2012b) accounted for the momentum exchange only in collision–normal direction and, e.g., Yamamoto et al. (2001); Vreman et al. (2009); Breuer et al. (2012) considered both, the momentum exchange in collision–normal and also in tangential direction. Furthermore, different collision detection algorithms can be found. Regarding the collision detection basically two different types of algorithms are employed in order to break down the computational costs from a brute force approach ($O(N_p)^2$, where $N_p$ is the number of particles inside the domain) to more tractable com-
putational costs. The first method stores for each particle a list of neighboring particles. That means, that for particle A all neighboring particles within a certain distance are stored. The collision occurrence is only checked between the particle A and his neighbors. In order to save computational time the list of neighboring particles is only updated every 4 to 10 time steps. The details of the algorithm are described in Hoomans et al. (1996) and is adopted in Geurts and Vreman (2006); Vreman et al. (2009). The second collision–detection algorithm found in LES is based on search cells, i.e., the computational domain is divided into three–dimensional cells and basically only particles located inside this search cells are checked for collisions (see, e.g. Jin et al., 2010b; Breuer et al., 2012; Mallouppas and van Wachem, 2013). If only particles located inside such search cells are check for collision, potentially colliding particles on the border of two cells cannot be detected. To circumvent this shortcoming two different methods are asserted. The first method includes also adjacent search cells into the collision detection procedure which is adopted in Jin et al. (2010b). The details of the algorithm are described in Wang et al. (1998). The second method repeats the collision detection a second time on a slightly modified search grid (see, Breuer and Alletto, 2012b, and also § 6.2.3). Note that the above mentioned approaches to treat the inter–particles collisions are independent of model of the carrier phase. In this section only the methods to handle the hard–sphere collision in the framework of LES using a point–particle approach are discussed.

In the view of the author of the present thesis the reasons why mostly deterministic hard sphere collision model can be found instead of stochastic models are basically twofold. The first question which arise is whether to take a hard–sphere or a soft–sphere model. Since hard–sphere collisions are instantaneous events the collision processes has not to be resolve in time. Thus, the computational costs are much cheaper than a soft sphere collision where the impacts between particles has to be resolved in time. Because of this reason a deterministic soft–sphere collision model could only be found in Mallouppas and van Wachem (2013). However, soft–sphere models are potentially more accurate than hard–sphere models since only material constants are incorporated (Mallouppas and van Wachem, 2013). The second question which arise is whether to take a stochastic or a deterministic model. In case of LES the most energetic fluid scales are resolved and therefore the particle trajectory are supposed to be calculated very accurately. For that reason applying a stochastic model (which is not as accurate as a deterministic model) for the inter–particles collision seems to be not consistent with the accuracy demands of LES. Of course, this argument is even much more decisive in case where the fluid motion is directly resolved by DNS.

Nevertheless, some stochastic–collision models exist in the framework of LES combined with a point–particle approach. They are however applied in topics related with atmospheric science and for details it is referred to the specialized literature. For example, Vinkovic et al. (2006) simulated the saltating particle in turbulent boundary layers applying the stochastic model of Sommerfeld (2001).

2.2.2.3 RANS

The RANS approach is based on the statistical treatment of turbulence introduced by Osborne Reynolds. Due to the division of the flow field in a mean value and the superposed fluctuations, the well–known closure problem of turbulence is introduced into the governing equations. Hence, the influence of the whole turbulence spectrum on the mean flow has to be modeled with the inherent difficulties. For that reason RANS simulations
are commonly accepted to be less accurate than DNS and LES in predicting complicated flow phenomena occurring in technical applications like transition, curved streamlines, recirculation regions, precessing vortex cores, etc. Furthermore, adding particles to the flow configuration requires supplementary modeling of the particulate phase in all interaction regimes. That means that in the one–way coupling regime the influence of the whole turbulent scales on the particle motions has to be considered. In the two–way coupling regime the influence of the particles on the full spectrum of turbulent eddies has to be modeled. In the four way–coupling regime usually stochastic models are adopted.

However, RANS simulations are still the most common engineering practices because of the lower computational costs among the methods described in this section. The reasons for the reduced computational costs are the coarser resolution usually applied compared to LES and DNS. Furthermore, no time averaging is required (except for URANS) since the equations of motion for the mean quantities are solved and symmetries emerging in the flow configuration can be used to reduce the computational domain. In order to reduce the computational costs of treating the disperse phase, the parcel method is often applied. In this case a group of particles are tracked through the domain with the same response to the fluid as the individual but with the same influence on the carrier phase as the sum of the particles contained in a parcel (for details see below). Another advantage with respect to DNS and LES is that for RANS no restriction regarding the Reynolds number is given. For that reason the method is applied in a vast application area like swirling flows (Sommerfeld and Qiu, 1993), horizontal conveying of solids (Huber and Sommerfeld, 1998; Lain and Sommerfeld, 2008, 2012), cyclone separators (Ho, 2004), cold flows in model combustion chambers (Minier et al., 2004), particle transport in respiratory systems (see, e.g., the review of Kleinstreuer and Zhang, 2010), the particle dispersion in ventilated rooms (see, e.g., Wang et al., 2012), the particle conveying in pipe loops (Pirker et al., 2010), the sand erosion in compressors (Suzuki and Yamamoto, 2011) and the particle–laden flow in a stirrer vessel (see, e.g., Decker, 2004; Sommerfeld and Decker, 2004).

Differences to eddy–resolving methods are not only found in the modeling of the continuous phase but also in the method to obtain a converged solution for the fluid and the solid phase. In contrast to LES and DNS where the solution of both, the continuous and the disperse phase, are advanced in time simultaneously, for RANS simulations only the particle phase is resolved in time. The general sequential procedure is the following (Sommerfeld et al., 2008):

(i) The time–averaged solution of the continuous phase is calculated without considering particles.

(ii) A large amount of particles or parcels are tracked through the domain without considering two–way coupling and inter–particle collisions to gain converged particle–phase statistics. Two–way and four–way coupling is not considered in this stage of the interaction because for the calculation of the source terms for the two–way coupling and for the stochastic treatment of the collisions converged particulate phase statistics are required.

(iii) If two–way coupling is considered the source terms in the conservation equations modeling the influence of the disperse on the continuous phase are calculated and the solution of the Eulerian part is calculated again taking the source terms into account.
The particles are again tracked through the computational domain considering the recently predicted continuous flow field and also inter-particle collisions.

Step (iii) and (iv) are repeated until a converged solution is achieved. Hence, the computational costs solving the two-phase flow is considerably increased with respect to the single-phase flow.

Regarding the forces considered in the momentum equation for the particles, in this branch of the Euler–Lagrangian approach using point-particles the forces due to linear shear and the particle rotation were accounted for much earlier than in DNS and LES (see, e.g., Sommerfeld, 1992; Lun and Liu, 1997; Huber and Sommerfeld, 1998). Furthermore, the researchers payed attention at particle–wall collisions at rough surfaces much earlier then the groups which treat the carrier phase with DNS and LES. To the best knowledge of the author the first investigation which studied the influence of rough wall impacts on the particle motion in the framework of RANS was Huber (1997); Huber and Sommerfeld (1998). Hence, it was almost twenty years earlier than the first investigation considering the rough–wall impacts in the framework of eddy–resolving techniques (see, Squires and Simonin, 2006; Vreman, 2007; Konan et al., 2011; Breuer et al., 2012).

In contrast to LES and DNS where the turbulent motion of the fluid is resolved in time, in RANS the turbulent eddies responsible for the particle dispersion are only captured by their statistical representation (e.g. the turbulent kinetic energy $k$ or the components of the Reynolds stress term $\langle u'_i u'_j \rangle$). Hence, without modeling two particles released at the same source would follow exactly the same trajectory. This observation is in striking contrast to the random nature of turbulence. For that reason in the framework of RANS combined with a point–particle approach the influence of the turbulent vortices on the particle dispersion has to be taken into account by an appropriate model.

The most simple models to account for the particle dispersion in the framework of RANS are the so called "eddy – lifetime models" (for details, see, Crowe et al., 1998). For this class of models the fluid velocity at particle position is decomposed in the mean velocity and the superposed fluctuations. The fluctuations are assumed to be proportional to the square root of the turbulent kinetic energy multiplied by a Gaussian distributed random number with unit variance and zero mean. In order to account for the eddy–crossing effect (a particle displacing in a turbulent flow needs a certain amount of time to cross a turbulent eddy) the computed velocity fluctuations is kept constant during the interaction time. The interaction time is calculated taking the minimum of the residence time (a turbulence length scale divided by the relative velocity between the particle and the fluid, for details see Crowe et al., 1998) and the eddy life time (a turbulence length scale divided by the square root of two thirds of the turbulent kinetic energy, for details see Crowe et al., 1998). After the elapse of interaction time the velocity fluctuations are recomputed as described before. Crowe et al. (1998) pointed out two main shortcomings of this class of models, i.e., the obtained fluid velocity field do not satisfy the continuity equation and this class of models are not able to describe the preferential concentration of particles.

A slightly more sophisticated model can by found in Sommerfeld et al. (2008) valid for isotopic turbulence. Sommerfeld et al. (2008) described the evolution of the fluid velocity fluctuations at the particle position as a deterministic part and a stochastic part. The deterministic part describes the correlation of the fluid velocity fluctuation at two subsequent time steps and therefore decays to zero if the time step size is large compared the the Lagrangian time scale. The stochastic part accounts for the random nature of
turbulence and is proportional to the square root of the turbulent kinetic energy multiplied by a random number of zero mean and unit variance for time step sizes large compared with the Lagrangian time scales. Furthermore, the stochastic part vanishes if the time step size is much smaller than the Lagrangian time scales. That means that for small time step sizes the evolution of the velocity fluctuations are purely deterministic and for large time step sizes purely random.

Even more sophisticated models describe the temporal evolution of the fluid velocity fluctuations by means of a stochastic differential equations (called also Langevin–type equations). In this case it is assumed that the change of the fluid velocity fluctuations seen by a Lagrangian particle along his trajectory can model by a deterministic part and a stochastic part which accounts for the randomness of turbulence. The deterministic part models the eddy–crossing effect on the velocity fluctuations seen by a Lagrangian particle and takes into account anisotropy effects (see, e.g., Minier, 1998; Iliopoulos and Hanratty, 1999; Iliopoulos et al., 2003; Minier et al., 2004). The stochastic part is usually modeled by random numbers with zero mean (Minier, 1998; Iliopoulos and Hanratty, 1999; Minier et al., 2004; Iliopoulos et al., 2003). In the view of the author a drawback of the models used to take into account the particle dispersion in the framework of RANS is that they contain a certain number of model constants. Furthermore, they require turbulent statistics like the turbulent kinetic energy $k$, the turbulent dissipation rate $\epsilon$ or components of the Reynolds stress term $\langle u_i' u_j' \rangle$. Hence, in addition to the known shortcomings of RANS in predicting the aforementioned turbulent quantities, additional modeling uncertainties are introduced in accounting for the turbulent dispersion of solid particles.

Since the particles do not only modify the mean flow but also turbulence, this effect has to be quantified in the RANS equations. For that purpose in the two-way coupling regime source terms are not only inserted into the equation of motion of the average velocity, but also in the equations modeling the influence of the turbulent eddies on the mean flow, i.e., into the conservation equations of $k$, $\epsilon$ or the components of the Reynolds stress $\langle u_i' u_j' \rangle$. Formally, the influence of the particles on the transport equations of $k$, $\epsilon$ and $\langle u_i' u_j' \rangle$ can be derived from the modified Navier–Stokes equations including the particle source term. However, by this procedure additional unclosed terms arise (see, e.g., Meyer, 2012). For that reason different models for the source terms in the $k$ and $\epsilon$ equations (see, e.g., Crowe, 2000; Sommerfeld et al., 2008; Alvandifar et al., 2011) or in the $\langle u_i' u_j' \rangle$ equations (see, e.g., Lain and Sommerfeld, 2012; Meyer, 2012) have been proposed. However, even if the models achieve a reasonable agreement of the attenuation by particles observed in experiments (Lain and Sommerfeld, 2008) or DNS (Meyer, 2012) or even can predict reasonably turbulent augmentation by particles observed in experiments (Alvandifar et al., 2011) still modeling uncertainties remain.

Thematically connected with the two–way coupling assumption is the often employed parcel method. In order to save computational costs, particles are grouped into parcels with the same response to the carrier flow as the individual in the group (see, e.g., Sommerfeld et al., 2008). However, the influence of the particle on the carrier phase (i.e., the source terms in the transport equations) is multiplied by the number of particles grouped in a parcel. In this way, the influence of the solid phase with a given mass loading $\eta$ on the carrier phase can be modeled without the need to track each individual particle through the domain. On the other hand, if too much particles are grouped into a parcel (that means that the amount of parcels tracked diminishes) it should be difficult to obtain
statistically converged solutions of the particulate phase. Furthermore, Sommerfeld and Decker (2004) (see also the references therein) pointed out that for high mass loadings the convergence rate of the continuous phase solver is diminished because of the stochastic nature of the source terms (the source term is different in every computational cell and not homogeneously distributed). Hence, for a smaller amount of parcels (the source term "attached" at each parcel increases) the convergence difficulties to solve the coupled problem flow should probably increase.

In the four-way coupling regime stochastic collision models are often applied in contrast to the research fields where the carrier phase is calculated by eddy-resolving methods (DNS or LES). As already mentioned above, the reason why stochastic methods are preferred instead of deterministic methods is probably due to consistency reasons. In the view of the author it is not reasonable to save computational time and therefore accept the loss of accuracy by applying RANS methods instead of DNS or LES and after worth adopting costly deterministic collision models. An often employed stochastic collision model was developed by Sommerfeld (2001). Every time step and for each real particle contained in the computational domain, Sommerfeld (2001) sampled a fictive particle which can potentially collide with the real particle. The velocity fluctuations of the fictive particle (in order to collide and allow a momentum exchange, particles must have a velocity difference) is modeled by a correlation based on the Stokes number. That means, that for very small particles ($St \to 0$) the velocity of the fictive particle is equal to the velocity of the real particles. For large particles ($St \to \infty$) the velocities of both particles are completely decorrelated and the velocity fluctuations of the fictive particle is obtained by random numbers with zero mean and variance equal to the velocity fluctuations of the real particle. After ensuring a velocity difference between the real and the fictive particle, the collision probability is calculated by an expression derived for heavy particles unresponsive to the fluid, i.e., it is solely proportional to the velocity difference of the particles, the particle concentration and the particle projected surface. The influence of the surrounding fluid on the collision probability is neglected. If the random number generated is less than the calculated collision probability, the real and the fictive particle collide and the post-collisional velocity of the real particle is calculated by a standard hard-sphere collision model. The advantage is that no time-consuming algorithms for the collision detection have to be applied in contrast to a deterministic treatment of the particle-particle impacts. Furthermore, the methods is applicable also for the parcel concept since the collision frequency is determined by a model expression and not explicitly by checking if two particles collide or not. A clear disadvantage is that an additional model uncertainties is introduced.

\subsection*{2.2.3 Euler–Euler Approach}

In the Euler–Euler approach both phases, fluid and particles, are described in an Eulerian frame of references (two-fluid model). This implies the presence of a sufficiently large number of particles in order to justify the continuum assumption. To derive the equations of motion the concept of two interpenetrating continua is used (see Fig. 5). That means that the infinitesimal volume $dV$ over which the field quantities of both phases experience an infinitesimal change is split into two separate volumes (red and blue in Fig. 5). Then the equations of motion of both phases are derived separately. The continuous flow can be described as usual by means of the Navier–Stokes equations (DNS) and its filtered forms (LES and RANS). The equations of motion for the disperse phase take a form similar
to the compressible Navier–Stokes equations (see, e.g., Fevrier et al., 2005; van der Hoef et al., 2008; Michaelides, 2013):

\[
\frac{\partial n_p^*}{\partial t^*} + \frac{\partial}{\partial x_i^*}(n_p^* u_{p,i}^*) = 0 \quad (2.6a)
\]

\[
n_p^* \frac{\partial u_{p,i}^*}{\partial t^*} + n_p^* u_{p,j}^* \frac{\partial u_{p,i}^*}{\partial x_j^*} = F_{f,pi}^* - \frac{\partial}{\partial x_j^*}(n_p^* \sigma_{p,ij}^*) - n_p^* g_i^* \quad (2.6b)
\]

\(n_p^*\) is the particle number density and \(\sigma_{p,ij}^*\) the particle kinetic stress tensor which describes the interaction between the particles. The above system of four partial differential equations for each particle class considered describes the evolution of the four field quantities \(u_{p,i}^*\) and \(n_p^*\). To close the system some relation for the stress tensor has to be found. The coupling between the phases is achieved by the forces \(F_{f,pi}^*\) and \(F_{p,fi}^* = -F_{f,pi}^*\) (one is the force exerted by the fluid on the particles and the other is the force exerted by the particles on the fluid). \(F_{p,fi}^*\) is obviously casted into the carrier phase equations. The proposed equation of motion for the particles found in the literature differ from each other in the modeling of the rather abstract particle stress tensor \(\sigma_{p,ij}^*\) and in the forces considered \(F_{f,pi}^*\).

**Figure 5:** Euler–Euler approach: Concept of two interpenetrating continua.

Fevrier et al. (2005), e.g., took only the drag force: \(F_{f,pi}^* = -n_p(u_{p,i}^* - u_{f,i}^*)/\tau_p^*\) into account and proposed an additional transport equation for the trace of \(\sigma_{p,ij}^*\). Riber et al. (2009), e.g., used the filtered form of the equation proposed by Fevrier et al. (2005) neglecting the particle stress tensor to compute a disperse flow in a model combustion chamber. Young and Leeming (1997) considered in addition to the drag and the gravity also the Saffman lift force and substituted the particle stress tensor with a relation for
the partial particle pressure associated with the random motion of the particles. In the
description of the Euler–Euler approach of Brennen (2005) the particle stress tensor $\sigma_{\ast p,ij}$ is
completely neglected.

Inter–particle collisions, i.e., the momentum transfer among the solid phase, are consid-
ered by modeling the particle stress tensor $\sigma_{\ast p,ij}$. For this purpose the particle stress tensor
is modeled in a similar way as the fluid stress tensor, i.e., it is assumed to be equal to the
gradient of the solid pressure and to the solid viscosity multiplied by the deformation
tensor of the particles (Van Wachem et al., 2001; van der Hoef et al., 2008).

The Euler–Euler approach is clearly advantageous compared to the point–particle ap-
proach if a large number of monosized particles is present in the computational domain
which are impossible to be tracked individually. However, for polydisperse flows a set
of four partial differential equations has to be solved for each size class and the system
can quickly become intractable. Another shortcoming compared with the Euler–Lagrange
approach is that considering the effect of particle motion is quite difficult (Pirker et al.,
2010). For dense flows, where inter–particle collisions play a role, constitutive relations
for the particle stress $\sigma_{\ast p,ij}$ (see, e.g., Van Wachem et al., 2001; van der Hoef et al., 2008)
have to be introduced with the inherent modeling uncertainties. Furthermore, if the equa-
tions of motion for the particulate phase are time averaged (RANS) (see, e.g., Young and
Leeming, 1997) or filtered in space (see, e.g., Riber et al., 2005) the same closure problems
as for the continuous phase arise.

A further source of uncertainty for Euler–Euler approach is the specification of the
particle–wall boundary conditions since the no slip condition does not hold for the solid
phase (Michaelides, 2013). Typical boundary conditions for the Euler–Euler approach
specify the gradient of the particle velocity in wall–normal direction (see, e.g., Li et al.,
2010; Zhong et al., 2012, and references therein). The major disadvantage if this boundary
condition used for the Euler–Euler approach that it contains a constant which depends
on the roughness of the wall and ranges between zero for a free slip boundary condition
and one for a no–slip boundary condition (Zhong et al., 2012). However, the connection
between the parameter in the wall boundary condition and texture of the wall–roughness
is not clear.

Typical applications of the Euler–Euler approach are for example the flow in a model
combustion chamber (see, e.g., Fede and Simonin, 2010), conveying of solids (see, e.g.,
Kartushinsky et al., 2011; Strömgren et al., 2011) or fluidized beds (see, e.g., van der Hoef
et al., 2008; Li et al., 2010; Zhong et al., 2012).

### 2.2.4 Equilibrium–Euler Approach

The equilibrium Euler method assumes only one–way coupling and that the particles are
sufficiently small to almost perfectly follow the carrier phase (see Fig. 3). Furthermore, it is
also assumed that the particles can be described in a Eulerian frame of reference. Based on
this constraints Ferry and Balachandar (2001) and Ferry et al. (2003) obtained for particles
with a small relaxation time an analytical relation between the fluid and the particle
velocity, i.e., the particle velocity at a certain position in the domain is only a function
of the fluid velocity at the same position. The clear advantage of this method against
the Euler–Euler approach is its numerical simplicity, i.e., that instead of a set of partial
differential equations only a set of algebraic equations has to be solved for the particles.
The solution is, however, only valid for small particle relaxation times and gives fairly
accurate results provided $\tau_p/\tau_\eta \leq 0.2$ (Balachandar and Eaton, 2010). The applications
are still restricted to very simple flow configuration, i.e., isotropic turbulence (Balachandar and Eaton, 2010). Consequently, the equilibrium Euler method is inappropriate for the applications considered in the present thesis.

2.2.5 Dusty Gas Approach

Similar to the afore described Euler–Euler and Equilibrium–Euler approach also in the dusty gas approach the particles are treated as a continuum. In his review Balachandar and Eaton (2010) pointed out that the dusty gas approach deals with flows where the particles perfectly follow the fluid. For these reason the flow can be treated as a single phase flow with the fluid density depending also on the local mass fraction of the particles. In this way analytical solutions of one–dimensional compressible particle–laden flows can be obtained by solving the compressible Navier–Stokes equations with a modified gas density due to the presence of the particles (Marble, 1970).

Despite the comments found in Balachandar and Eaton (2010), the terminology ”dusty gas” do not appear only in flows where the particles perfectly follows the fluid but also in flows with more general modeling assumptions (see, e.g., Saffman, 1962; Asmolov and Manuilovich, 1998; Hernández, 2001, and references therein). The latter investigations treat two–dimensional laminar flows for which the particle Reynolds number $R_{ep}$ is assumed to be small so that the forces displacing the particles can be approximated by the Stokes drag. For this reason, the coupling term accounting for the influence of the particles on the fluid appearing in the fluid momentum equation, depends linearly of the particle velocity. Furthermore, inter–particle collisions are neglected. Hence, in the investigations of Saffman (1962); Asmolov and Manuilovich (1998); Hernández (2001) the modeling assumptions made associated with the terminology dusty gas are more similar to a Euler–Euler approach valid only for two–dimensional laminar flows and small particle Reynolds numbers. However, despite of the different modeling assumptions associated with the terminology dusty gas approach (either particles perfectly following the fluid or two–dimensional laminar flows with small particle Reynolds numbers), the method is not appropriate for the applications considered in this thesis.

An application of the dusty gas approach belonging to the class of two–dimensional laminar flows, is to study the stability of simple two–dimensional laminar flows where solutions can be obtained by analytical methods or very accurate numerical schemes. For example, Saffman (1962) and Asmolov and Manuilovich (1998) studied the stability of laminar boundary layers where the particles perfectly follow the carrier phase. Hernández (2001) investigated the stability of two–dimensional fluidized beds with a non–uniform particle concentration distribution. That means, that in the initial conditions the particle concentration solely varied from bottom to top and the particles were kept at rest by the equilibrium between the drag force exerted by the constant gas velocity and the gravity.

An advantage of investigating simple configurations by means of analytical or very accurate numerical tools is that fundamental understanding of some basic physical mechanism (e.g., the onset of instabilities) can relatively easily be gathered. Of course due to the above mentioned simplifications the parameter space in which the dusty gas approach can be applied is rather narrow and accurate solution can be only obtained for simple configurations.
2.2.6 Methods to treat Collision Dominated Particulate Flows

With increasing volume fraction $\Phi$ the interaction between particles gains importance in the behavior of particulate flows until the dynamics of the system is entirely dominated by inter–particle collisions, i.e., the granular flow state is reached (see Fig. 3). Here two methods to deal with this flow state should be shortly described: The Discrete Element Method (DEM) for granular flows which treats the particles in a Lagrangian frame of reference and a continuum mechanics approach to treat granular flows. Note that the scope of this section was just to give a brief overview of the existing methods to treat collision dominated particulate flows and therefore no completeness is claimed in the application areas nor in the references cited.

2.2.6.1 Discrete Element Method for Granular Flows

In the discrete element method (DEM) the particle displacement is calculated by Newton’s second law. The main forces acting on a particle arise from the contact with the surrounding particles. They are derived from the Hertzian contact law and its extensions (Bierwisch, 2009), i.e., they arise due to the deformation of the particles (soft–sphere model). To account for the dissipation of energy also dissipation forces and friction between the particles are considered. The gravity and the Stokes drag (the surrounding fluid is assumed to be at rest) are modeled as point forces (Bierwisch, 2009). Summing up, the main difference compared to the point–particle approach is that the collisions between particles are resolved in time and are not treated as discrete events. Furthermore, multiple collisions are allowed while in the point–particle approach collisions are assumed to be binary.

Typical application areas are the design of industrial devices used to process solids. This are, e.g., screens used to separate particles of different sizes, mixing of solids in the food industry, conveying of particle on belts, grinding mills or fluidized beds (Cleary, 2009). Limitations of this approach arise from the computational resources available, i.e., the number of particles simulated and the degree of accuracy of the models of the physical phenomena included into the simulation (Cleary, 2009).

2.2.6.2 Continuum Mechanics Approach for Granular Flows

Concerning the continuum mechanics treatment of dense granular flows the research is still at a very fundamental level because of the difficulties in obtaining constitutive equations. Following Forterre and Pouliquen (2008) the reason is the appearance of three flow regimes: A solid state where the particles are at rest or the system containing the particles exhibit quasi–static deformations. A liquid state where the particles are interacting by collisions and friction and a gaseous state where the particles interact by predominantly binary collisions. For the gaseous state constitutive equations already exist (see, Campbell, 1990; Goldhirsch, 2003) but the range of applicability is rather narrow (Forterre and Pouliquen, 2008). These equations are derived from gas kinetic theory assuming binary collisions of spherical particles and have a similar form as the compressible Navier–Stokes equation. Note that the influence of the gaseous phase enclosed between the particles is completely neglected. For the liquid phase still the research is ongoing to derive a set of closed equations (Forterre and Pouliquen, 2008).

The advantage of the continuum mechanics approach over the DEM is that the number of particles is not restricted by the computational costs. However, the applications are restricted to purely academic research in case of the gaseous state because the assumption...
of binary collisions of spherical particles without taking into account the interstitial fluid leads to a narrow application field.

2.3 Summary

In this section commonly applied simulation methods to treat gaseous flows laden with solid particles are reviewed. Three methodologies were identified to be able to treat gas–particle flows considering one–, two– and four–way coupling, i.e., the fully resolved approach, the point–particle approach and the Euler–Euler approach.

In the fully resolved approach the flow field around each particle is fully resolved and the modeling assumptions are restricted to the treatment of the inter–particle collisions. Hence, it is the most accurate approach among the methods present. However, the applications are restricted to purely academic research because of the huge computational costs and low Reynolds numbers treatable.

On the other hand, in the Euler–Euler approach a lot of modeling assumptions have to be made in order to get a closed set of equations if particle–particle collisions have to be accounted for. Furthermore, the proper boundary conditions for the solid phase at the walls is still an open question (Michaelides, 2013). For that reason, in the view of the author this approach should be used only if the computational costs is too high in order to track each particle individually, e.g., in designing large scale industrial devices.

The point–particle approach represents a compromise between computational costs and accuracy and is applicable in a wide parameter space. Among the methods to treat the continuous phase and the inherent modeling procedures for the particle phase, DNS, LES and RANS have to be distinguished. DNS resolves all turbulent scales and is still restricted to low Reynolds number flows and simple geometries. RANS models mimic all turbulent scales and because of that also the interaction between the particles and the fluid in all turbulent scales has to be modeled with the intrinsic difficulties. LES resolves the most energy–carrying scales and models the small more isotropic scale. Hence, accounting for the interaction between the particles and the unresolved scales is much easier than for RANS simulations leading to more reliable results. Furthermore, the methodology presented in this thesis has already been successfully tested in industrial applications. For this reason it seems to be reasonable to assume that in the near future with growing computational power LES can complement and partially also replace RANS simulations in the standard engineering practice. Moreover, with increasing performance of the computers the methodology favored (i.e., LES with a point–particle approach) is able to advance into the parameter space yet reserved for the Euler–Euler approach. Thus a broadening application field is expected for the foreseeable future.
3 Theoretical Background of Large-Eddy Simulation

In the following section the governing equations for the continuous phase are described. Since the major effort was spent to extend the particle side of the computational code \textit{LESOCC} \textsuperscript{3}, the theoretical considerations about the continuous phase are only briefly addressed here. For a more detailed overview of the theoretical background of LES presented in this section the interested reader is referred to Breuer (1998, 2002) or Sagaut (2006). The main objective of this section is to provide the governing equations and the different boundary conditions applied for the continuous phase.

3.1 Derivation of the Governing Equations for the Continuous Phase

Starting point for the derivation of the equations used to describe the fluid motion in the framework of Large–Eddy Simulations (LES) are the incompressible Navier–Stokes equations. They read in the common dimensionless form:

\[
\frac{\partial u_j}{\partial x_j} = 0 \quad (3.1a)
\]

\[
\frac{\partial u_i}{\partial t} + \frac{\partial (u_i u_j)}{\partial x_j} = -\frac{\partial p}{\partial x_i} - \frac{1}{Re} \frac{\partial \tau_{ij}^{mol}}{\partial x_j} \quad (3.1b)
\]

\[
\tau_{ij}^{mol} = -2 \mu S_{ij} \quad \text{where} \quad S_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \quad (3.1c)
\]

\(u_i\) is the fluid velocity described in an Eulerian frame of reference, \(p\) the pressure, \(x_j\) represents the three spatial directions and \(\tau_{ij}^{mol}\) the viscous stress tensor assuming a Newtonian fluid. Since the topics considered in this thesis consider solely isothermal flows with constant fluid properties the solution of the energy equation is not required and is therefore omitted.

The above equations are widely accepted to be valid for laminar and turbulent flows and constitute the foundation the whole fluid mechanics is build on. Their solution can be computationally quite expensive (especially for high–Re number flows, Breuer, 2002) if all turbulent scales have to be resolved (direct numerical simulation). Hence, for practically relevant CFD simulations some averaging has to be applied in order to avoid resolving all turbulent scales.

In case of LES a spatial filter is applied to the above equations (for an overview of the different filtering approaches see, e.g., Piomelli and Chasnov, 1996; Breuer, 2002; Sagaut, 2006). The basic idea is to resolve the large energy–carrying scales and to model the small more isotropic scales. Filtering the above equations leads to:

\[
\frac{\partial \overline{u}_i}{\partial x_j} = 0 \ , \quad (3.2a)
\]

\[
\frac{\partial \overline{u}_i}{\partial t} + \frac{\partial (\overline{u}_i \overline{u}_j)}{\partial x_j} = -\frac{\partial \overline{p}}{\partial x_i} - \frac{1}{Re} \frac{\partial \overline{\tau}_{ij}^{mol}}{\partial x_j} \ . \quad (3.2b)
\]

\textsuperscript{3}The original CFD code \textit{LESOCC} is accurately described in Breuer (1998, 2002) and Breuer et al. (2006).
Here the overline denotes the filtering operation. The final form of the LES equations are obtained by the definition of the subgrid–scale stress tensor \( \tau_{ij}^{SGS} \) (see, also Piomelli and Chasnov, 1996):

\[
\tau_{ij}^{SGS} = \overline{u_i u_j} - \overline{u_i} \overline{u_j}.
\]  

(3.3)

By decomposing the full velocity field in a filtered \( \overline{u_i} \) and the subgrid scale contribution \( u'_i \), i.e., \( u_i = \overline{u_i} + u'_i \) the subgrid scale tensor can be written as follows (see, e.g., Piomelli and Chasnov, 1996; Breuer, 2002; Sagaut, 2006):

\[
\tau_{ij}^{SGS} = \overline{u_i u_j} - \overline{u_i} \overline{u_j} = \underbrace{\overline{u_i u_j}}_{\mathcal{L}_{ij}} - \overbrace{\overline{u_i u'_j} + \overline{u'_i u_j}}^{\mathcal{C}_{ij}} + \overbrace{\overline{u'_i u'_j}}_{\mathcal{R}_{ij}}.
\]  

(3.4)

\( \mathcal{L}_{ij}, \mathcal{C}_{ij} \) and \( \mathcal{R}_{ij} \) are called Leonard, cross–term and Reynolds stress tensors which represent the interaction among the large scales, the cross–scale interaction between large and small scales and the interaction between small scales, respectively. For the specific modeling issues of the three terms representing the subgrid scale tensor see, e.g., Breuer (2002). Note that according to Piomelli and Chasnov (1996) the decomposition (3.4) has been abandoned since neither \( \mathcal{L}_{ij} \) nor \( \mathcal{C}_{ij} \) are Galilean invariant.

The final form of the LES equations used in this thesis read:

\[
\frac{\partial \overline{u_j}}{\partial x_j} = 0 , \quad \text{(3.5a)}
\]

\[
\frac{\partial \overline{u_i}}{\partial t} + \frac{\partial (\overline{u_i u_j})}{\partial x_j} = - \frac{\partial \overline{p}}{\partial x_i} - \frac{1}{Re} \frac{\partial \tau_{ij}^{mol}}{\partial x_j} - \frac{\partial \tau_{ij}^{SGS}}{\partial x_j}, \quad \text{(3.5b)}
\]

\[
\tau_{ij}^{mol} = -2 \mu \overline{S}_{ij} \quad \text{where} \quad \overline{S}_{ij} = \frac{1}{2} \left( \frac{\partial \overline{u_i}}{\partial x_j} + \frac{\partial \overline{u_j}}{\partial x_i} \right). \quad \text{(3.5c)}
\]

\( \tau_{ij}^{SGS} \) arises from the decomposition of the non–linear convective term in known and unknown quantities and describes the effect of the small unresolved scales on the large scales of a turbulent flow. Note that in this thesis no explicit filter is applied. That means that the grid spacing \( h_i \) is equal to the filter width \( \Delta_i \), i.e., \( \Delta_i = h_i \) (implicit filtering). For that reason the resolved velocity field \( \overline{u_i} \) can be seen as the mean of the full velocity field \( u_i \) over the computational cell. This procedure was applied in order reduce the required computational points. The reason is that the smallest resolved scales are proportional to the filter width \( \Delta_i \). For an explicit filtering the filter width is usually chosen to be approximately twice the grid spacing \( \Delta_i \approx 2h_i \) (Breuer, 2002). Hence, for \( \Delta_i = 2h_i \) in order to resolve the same scales of the turbulent flow by applying an explicit filter requires eight times more grid point than using an implicit filter. The widely accepted drawback of this procedure is the matter that physical modeling and numerical discretization are not fully separated.

Since \( \tau_{ij}^{SGS} \) is unknown for LES some closure has to be found to obtain a closed set of equations for the filtered velocity components \( \overline{u_i} \) and for the filtered pressure \( \overline{p} \). The subgrid–scale stress tensor is usually decomposed in an anisotropic part \( \tau_{ij}^{ani} \) and an isotropic part \( \tau_{ij}^{iso} \):

\[
\tau_{ij}^{SGS} = \tau_{ij}^{ani} + \tau_{ij}^{iso} = \tau_{ij}^{ani} + \frac{1}{3} \delta_{ij} \tau_{kk}^{SGS}. \quad \text{(3.6)}
\]
The isotropic part is then added to the pressure and forms a new variable:

\[ P = \bar{p} + \frac{1}{3} \tau_{kk}^{SGS}. \]  

(3.7)

The reason is to be consistent with often used eddy–viscosity models which establish a relation between the subgrid–scale tensor and the trace–free deformation tensor \( \mathbf{S}_{ij} \). Hence, also the subgrid–scale tensor has to be trace–free.

### 3.2 Subgrid–scale Modeling

In this section the subgrid–scale models used to close eq. (3.5) relevant for this thesis are described. The interested reader is again referred to Breuer (2002) or Sagaut (2006) for a more detailed description of available subgrid–scale models.

#### 3.2.1 Smagorinsky Model

The most commonly used approach to model \( \tau_{ani}^{\text{m}} \) relies on the eddy–viscosity concept which dates back until 1877 to Boussinesq (1877). It assumes an analogy between \( \tau_{ani}^{\text{m}} \) and the viscous stress tensor. The model of Smagorinsky (1963) relies on the same analogy:

\[ \tau_{ani}^{\text{m}} = -2 \mu_T \mathbf{S}_{ij}. \]  

(3.8)

\( \mu_T \) is the turbulent eddy–viscosity and is not a constant as the molecular viscosity but has to be derived as a function of the known flow quantities. The relation between the turbulent eddy–viscosity and known field quantities is established by a dimensional analysis. Assuming an analogy between the viscosity of the fluid \( \mu^* \) and the turbulent eddy–viscosity \( \mu_T^* \) the dimension of the latter can be established (Breuer, 2002):

\[ \mu_T^* \sim \rho_c^* l_c^* u_c^*. \]  

(3.9)

\( \rho_c^* \) is a characteristic density which is constant for the incompressible flows considered here. \( l_c^* \) is a characteristic length scale of the subgrid scales and \( u_c^* \) is a characteristic velocity of the subgrid scales. Note that the superscript * represent dimensional quantities. The characteristic length of the subgrid scales is easy to obtain since the biggest not resolved scales are of the order of the filter width \( \Delta_i \) (Note that in this thesis the filter width is equivalent to the grid spacing):

\[ l_c^* = C_s \Delta_i^* = C_s \sqrt[3]{\Delta V \text{ol}^*}. \]  

(3.10)

Since in the general case the computational grid of industrially relevant configurations have not the same grid spacing in all three Cartesian directions, the cubic root of the volume of the computational cell \( \sqrt[3]{\Delta V \text{ol}^*} \) is taken as a characteristic filter width. The proportionality constant \( C_s \) is called Smagorinsky constant and usually lies between 0.065 \( \leq C_s \leq 0.1 \) (Breuer, 2002). In order to determine the characteristic velocity scale \( u_c^* \) the characteristic length \( l_c^* \) is multiplied with the absolute value of the strain–rate tensor \( |\mathbf{S}_{ij}^*| \):

\[ u_c^* = l_c^* |\mathbf{S}_{ij}^*|, \quad \text{with} \quad |\mathbf{S}_{ij}^*| = \sqrt{2 \mathbf{S}_{ij}^* \mathbf{S}_{ij}^*}. \]  

(3.11)
The final and dimensionless form of the turbulent eddy–viscosity reads:

\[ \mu_T = \ell_c^2 |\mathbf{S}_{ij}| = C_s^2 \Delta^2 |\mathbf{S}_{ij}|. \]  

(3.12)

Hence, the anisotropic part of the subgrid–scale tensor can be expressed as

\[ \tau_{ani}^{ij} = -2 C_s^2 \Delta^2 |\mathbf{S}_{ij}| \mathbf{S}_{ij} \]  

(3.13)

Relation (3.8) has some drawbacks since it can not reproduce the right asymptotic behavior of the subgrid–scale stress close to the wall (\( \mathbf{S}_{ij} \) is usually not equal to zero while the subgrid–scale stress has to vanish asymptotically towards the wall due to the no–slip condition). To ensure the correct asymptotic behavior of the subgrid–scale stresses, the Van Driest damping function (Van Driest, 1956) is introduced:

\[ l_c = C_s \Delta \left[ 1 - \exp \left( -\frac{y^+}{25} \right) \right]^{0.5}, \quad y^+ = \frac{y u^*_s}{v_f}. \]  

(3.14)

The second drawback of the Smagorinsky model regards the simulation of transitional flows. For laminar flows the subgrid–scale tensor \( \tau_{ani}^{ij} \) has to be equal to zero because of the absence of turbulent fluctuations. The Smagorinsky model, however, predicts a non–zero value of \( \tau_{ani}^{ij} \) even in laminar flows since the strain rate tensor is not equal to zero. This shortcoming is circumvented by the introduction of a trigger function which is equal to zero for laminar boundary layers and equal to one for turbulent boundary layer. The trigger function is then multiplied by \( l_c \) defined in eq. (3.10). For the details see Breuer (2002) and the references therein.

A further disadvantage of the Smagorinsky model is that it can not model the backscatter–effect, i.e., the energy transfer from the small scales to the large scales (Leslie and Quarini, 1979). That means that only the dissipation effect of the small scales on the large scales can be accounted for by this model.

The advantage of the Smagorinsky is its simplicity and the stabilizing effect on the numerical procedure due to its dissipative properties (Breuer, 2002).

### 3.2.2 Dynamic Model of Germano

The basic concept of the SGS model proposed by Germano et al. (1991) is to automatically adjust the Smagorinsky constant in space and in time in order to adapt the model to the local structure of turbulence (Sagaut, 2006). Note that in principle the procedure described here can be adopted also to order models. Here, only the application to the Smagorinsky model is shown since the dynamic model used in this thesis relies on the Smagorinsky model.

The basic idea of the model proposed by Germano et al. (1991) is to introduce a second test filter \( \tilde{\Delta} \) which has a wider filter width than the filter used to derive the LES equations (see, eq. (3.2) and eq. (3.5)). The tilde denotes the quantities filtered with the test filter and the overline denotes the quantities filtered with the primary LES filter. If the momentum equation eq. (3.1b) is filtered first with the primary filter \( \Delta \) and than a second time with the test filter \( \tilde{\Delta} \), the momentum equation for the doubly filtered velocity field \( \tilde{u}_i \) is obtained:

\[ \frac{\partial \tilde{u}_i}{\partial t} + \frac{\partial (\tilde{u}_i \tilde{u}_j)}{\partial x_j} = - \frac{\partial \tilde{p}}{\partial x_i} - \frac{1}{\text{Re}} \frac{\partial \tilde{\tau}_{mol}^{ij}}{\partial x_j}. \]  

(3.15)
From the above equation it is easy to see that the new subgrid–scale tensor $T_{ij}^{SGS}$ can be expressed as:

$$T_{ij}^{SGS} = \tilde{u}_i \tilde{u}_j - \tilde{u}_i \tilde{u}_j.$$  \hfill (3.16)

After that Germano et al. (1991) introduced the resolved turbulent stress tensor $L_{ij}$ defined as

$$L_{ij} = \tilde{u}_i \tilde{u}_j - \tilde{u}_i \tilde{u}_j .$$  \hfill (3.17)

It represents the scales lying between the test filter $\tilde{\Delta}$ and the original filter $\Delta$. The components of the above tensor are known quantities since they can be calculated based on the filtered velocity field $\tilde{u}_i$. Finally, the Germano identity is introduced which relates the new subgrid–scale tensor $T_{ij}^{SGS}$ and the original one $\tau_{ij}^{SGS}$ in the following manner:

$$L_{ij} = \tilde{u}_i \tilde{u}_j - \tilde{u}_i \tilde{u}_j = \tilde{u}_i \tilde{u}_j - (\tilde{u}_i \tilde{u}_j - \tilde{u}_i \tilde{u}_j).$$  \hfill (3.18)

$\tilde{\tau}_{ij}^{SGS}$ represents the subgrid–scale stress $\tau_{ij}^{SGS}$ filtered with the test filter. The identity (3.18) can now be exploited to dynamically adjust the Smagorinsky constant, i.e., to determine $C_s = C_s(x_i, t)$. $L_{ij}$ can be calculated directly since it depends solely on known quantities. At the right-hand side of eq. (3.18) the Smagorinsky model (see, eq. (3.13)) obtained from the filtered velocity field $\tilde{u}_i$ and the doubly filtered velocity field $\tilde{\tilde{u}}_i$ can be inserted to establish a relation for $C_s(x_i, t)$:

$$L_{ani}^{ani} = L_{ij} - \frac{1}{3} \delta_{ij} L_{kk} = -2 C_s^2 \frac{\tilde{\Delta}^2}{\tilde{\Delta}^2} |S_{ij}| S_{ij} + 2 C_s^2 \frac{\Delta^2}{\tilde{\Delta}^2} |S_{ij}| S_{ij} .$$  \hfill (3.19)

Note that only the anisotropic part $L_{ani}^{ani}$ of the tensor $L_{ij}$ is calculated since the strain rate tensor $S_{ij}$ is trace free. If $C_s \Delta$ is factored out of the above equation (Note that it is only an approximation since $C_s(x_i, t)$ is not any more a constant) we obtain:

$$L_{ani}^{ani} = -2 (C_s \Delta)^2 \left[ \frac{\tilde{\Delta}^2}{\Delta^2} |S_{ij}| S_{ij} - |S_{ij}| S_{ij} \right] = -2 (C_s \Delta)^2 M_{ij}. $$  \hfill (3.20)

The above system of equations is overdetermined since it consists of five independent relations for the unknown $C_s(x_i, t)$ (not six since both tensors $L_{ani}^{ani}$ and $M_{ij}$ are symmetric and trace free and one component of the diagonal can be expressed as a function of the other two). Different methods are applied in the literature to obtain values for $(C_s \Delta)^2$ which are not discussed in this thesis. The interested reader is referred to Breuer (2002) or Sagaut (2006) for an overview. The method applied in this thesis is the one proposed by Lilly (1992) which suggested to determine $(C_s \Delta)^2$ by the least square approach. The residual $Q$ of eq. (3.20) reads:

$$Q = L_{ani}^{ani} + 4 (C_s \Delta)^2 L_{ani}^{ani} M_{ij} + 4 (C_s \Delta)^4 M_{ij} .$$  \hfill (3.21)

$(C_s \Delta)^2$ is determined by minimizing the above residual, i.e., setting $\partial Q/\partial (C_s \Delta)^2 = 0$. From the solution of this equation (i.e., taking the derivative of eq. (3.21) with respect to...
\[(C_s \Delta)^2 \text{ and setting it to zero) Lilly (1992) obtained the relation for } (C_s \Delta)^2 \]

\[
(C_s \Delta)^2 = -\frac{1}{2} \frac{L_{ani}^{M_{ij}}}{M_{nn}M_{nn}}.
\]

(3.22)

Local evaluations of eq. (3.22) determined large and also negative values for the turbulent viscosity \(\mu_T\) (Breuer, 2002). For that reason in the code developed by Breuer (1998, 2002) the numerator and the denominator of eq. (3.22) can be averaged in homogeneous directions. That means that \((C_s \Delta)^2\) is predicted as an average which is constant along the homogeneous directions as for example in channel and pipe flows. Of course, it remains a function of time and of the inhomogeneous directions. For totally inhomogeneous flows a low-pass filter is applied:

\[
(C_s \Delta)^2_{\text{filtered}} = (1 - \epsilon)(C_s \Delta)^2 + \epsilon(C_s \Delta)^2_{n+1}
\]

(3.23)

Here the superscript \(n\) denotes the value at the time step \(n\) and the superscript \(n + 1\) the value at the time step \(n + 1\). For values of \(\epsilon \approx 10^{-3}\) the high frequency oscillations of \((C_s \Delta)^2\) are filtered out and only the low frequencies are retained (Breuer, 2002). In this thesis a value of \(\epsilon = 10^{-3}\) is adopted. \((C_s \Delta)^2_{\text{filtered}}\) is the square of the length scale adopted to compute the turbulent eddy–viscosity \(\mu_T\). Finally, in order to prevent negative values of the turbulent eddy–viscosity which lead to a destabilization of the numerical procedure to solve the conservation equations (Breuer, 2002), either the total viscosity \(\mu_{\text{total}} = \mu_T + 1/Re\) or the turbulent eddy–viscosity \(\mu_T\) can be set to zero in case of negative values resulting from the above relations.

Compared to the Smagorinsky model the dynamic model has a few advantages:

- The value of \(C_s\) has not to be determined empirically but is adjusted automatically accounting for the local flow structure.

- Close to the wall the subgrid–scale stress vanishes (Germano et al., 1991) reflecting the right behavior near surfaces. Since the tensor \(L_{ani}^{M_{ij}}\) contains only filtered velocities which in LES predictions have to fulfill the no–slip condition also each component of \(L_{ani}^{M_{ij}}\) vanishes at the wall. Hence, also the turbulent length scale \((C_s \Delta)^2\) vanishes since the numerator of eq. (3.22) turns to zero at the wall.

- For transitional flows no trigger function is required since for laminar flows \(L_{ani}^{M_{ij}}\) also vanishes.

- The only remaining parameter which can be varied remains the width of the test filter \(\tilde{\Delta}\) which is set equal to \(\tilde{\Delta}/\Delta = 2\).

### 3.3 Boundary Conditions for the Continuous Phase

Because of the elliptical character in space of eq. (3.5) boundary conditions at all domain boundaries are required to get a unique solution. In the following sections it is distinguished between physical boundary conditions, i.e., boundary conditions at the solid wall, and artificial boundary conditions which arise from delimiting the computational domain in order to save computational costs, i.e., the inflow and outflow conditions and periodic boundary conditions. The artificial boundary conditions have to be chosen very carefully.
to get a reliable solution since they always consist in an approximation of the conditions which prevail at the cutting plane (Breuer, 2002).

3.3.1 Conditions at the Wall

3.3.1.1 No–Slip Boundary Condition

The no–slip boundary condition relies on the assumption that the fluid moves with zero relative velocity to the wall, i.e., that the molecules adjacent to the wall stick at it. Mathematically it reads:

\[ u_i(x_w, y_w, z_w) = u_w. \]  

\( x_w, y_w \) and \( z_w \) are the coordinates and \( u_w \) is the velocity of the wall. In the framework of LES applying the no–slip condition means that the velocity field in the vicinity of the wall is completely resolved including the viscous sublayer, i.e., the steep linear velocity gradient observed in attached flows in the region \( 0 \leq y^+ \leq 5 \). This thin region has to be resolved with at least a few grid points in order to obtain an adequate prediction of the turbulent flow. Accordingly also the buffer layer and the log–layer above the viscous sublayer require an adequate resolution. Especially for high–Re number flows this implies a very high grid resolution of the wall region which is not always practicable. The resolution requirements for wall–resolved LES scale with \( \text{Re}^2 \) (Baggett et al., 1997) which is only slightly below the resolution requirements of DNS, i.e., \( \text{Re}^{9/4} \). \( \text{Re}^2 = u^*_r L_f / \nu^* \) is the Reynolds number based on the friction velocity \( u^*_r \). Hence, for high–Re number flows some modeling of the wall region has to be achieved to circumvent the necessity of too fine resolutions at the wall.

3.3.1.2 Wall Model of Schumann

The wall model of Schumann (1975) assumes a phase coincidence between the instantaneous wall shear stress and the velocity component tangential to the wall and was developed for channel and annular flows. For a plane wall, where the wall–normal direction points towards the \( y \)-axis and the streamwise velocity \( u \) points towards the \( x \)-axis, it reads in dimensionless form (Schumann, 1975):

\[ \tau_{12,w}(x, y, t) = \frac{\langle \tau \rangle}{\langle \tau(y) \rangle} \Delta \pi(x, y_2, z, t) \]  

\[ \tau_{22,w}(x, y, t) = 0 \quad \text{with} \quad \tau_w(x, z, t) = 0 \]  

\[ \tau_{32,w}(x, y, t) = \frac{1}{\text{Re}} \frac{\Delta \pi(x, y_2, z, t)}{\Delta y_2} \]  

The brackets \( \langle \dots \rangle \) denote the temporal averages of the quantities. If there are homogeneous directions, the averaging can be also applied in these directions. \( \Delta y_2 \) is the wall distance of the cell center of the first cell adjacent to the wall and \( \Delta \pi(x, y_2, z, t) \) the difference of the spanwise velocity in wall–normal direction. Note that for the derivation of the wall shear stress \( \tau_{32,w}(x, y, t) \) Schumann (1975) assumed a linear spanwise velocity distribution over the first cell. The left–hand side of eq. (3.25) is used as boundary condition for the momentum equation (3.5) discretized by a finite–volume method. \( \langle \tau(y) \rangle \) is obtained directly by averaging the streamwise velocity. \( \langle \tau_w \rangle \) however, is still unknown and has to be specified iteratively by assuming a universal velocity distribution of the
averaged flow \( \langle \overline{u}(y^+) \rangle \) close to the wall:

\[
\begin{align*}
\langle \overline{u}^+ \rangle &= y^+ & \text{for: } & 0 \leq y^+ \leq 5 & (I) \\
\langle \overline{u}^+ \rangle &= 5.0 \cdot \ln(y^+) - 3.05 & \text{for: } & 5 \leq y^+ \leq 30 & (II) \\
\langle \overline{u}^+ \rangle &= 2.5 \cdot \ln(y^+) + 5.2 & \text{for: } & 30 \leq y^+ \leq 500 & (III)
\end{align*}
\]

The above velocity distributions represent the velocity profiles found in a canonical boundary layer (see, also Sagaut, 2006). (I) represents the viscous sublayer where the velocity profile is well accepted to be linear (the linear velocity profile can also be derived analytically, see, e.g., Schlichting and Gersten, 2000). (II) represents the velocity profile in the buffer layer and it is chosen in a way to have a continuous transition of the velocity profile (I) and (II) and the profiles (III) and (III). (III) is the velocity profile in the log–layer which general relationship can be determined analytically from matched asymptotic expansions (Schlichting and Gersten, 2000), where the constants \( 1/\kappa = 2.5 \) and \( C = 5.2 \) are determined experimentally.

Inserting the definitions for \( \langle \overline{u}^+ \rangle = \langle \overline{u}^* \rangle / \langle u^*_* \rangle \) and \( y^+ = \Delta y^* u^*_* / \nu^* \) with \( u^*_* = \sqrt{\langle \tau_w^\ast \rangle / \rho^*} \) in the above equations we get the conditional equations for the dimensionless wall shear stress \( \tau_w = \tau_w^* / U_f^2 \rho_f^* \):

\[
\begin{align*}
\langle \overline{u}^+ \rangle / \sqrt{\langle \tau_w^\ast \rangle} &= \Delta y \ Re \sqrt{\langle \tau_w^\ast \rangle} & \text{for: } & 0 \leq y^+ = \Delta y Re \sqrt{\langle \tau_w^\ast \rangle} \leq 5 & (3.27a) \\
\langle \overline{u}^+ \rangle / \sqrt{\langle \tau_w^\ast \rangle} &= 5.0 \cdot \ln(\Delta y Re \sqrt{\langle \tau_w^\ast \rangle}) - 3.05 & \text{for: } & 5 \leq y^+ = \Delta y Re \sqrt{\langle \tau_w^\ast \rangle} \leq 30 & (3.27b) \\
\langle \overline{u}^+ \rangle / \sqrt{\langle \tau_w^\ast \rangle} &= 2.5 \cdot \ln(\Delta y Re \sqrt{\langle \tau_w^\ast \rangle}) + 5.2 & \text{for: } & 30 \leq y^+ = \Delta y Re \sqrt{\langle \tau_w^\ast \rangle} \leq 500. & (3.27c)
\end{align*}
\]

Note that the superscript \( \ast \) represents dimensional quantities and all other quantities are dimensionless. From the above relations it becomes clear that an iterative method has to be adopted to find the correct value of \( \langle \tau_w \rangle \) which fulfills eq. (3.27). Note that only \( \langle \overline{u}^+ \rangle \) is known from the simulation. Briefly summarized the iterative method to obtain the averaged wall shear stress at the new time step \( \langle \tau_w^{n+1} \rangle \) works as follows: Starting from the wall shear stress computed at the old time step \( \langle \tau_w^n \rangle \) the value of \( y^{+n} \) at the old time step can be determined. After that a guess for the wall shear stress \( \langle \tau_w^{n+1, \text{guess}} \rangle \) can be obtained from eq. (3.27), i.e., by solving either eq. (3.27a), eq. (3.27b) or eq. (3.27c). The choice of the equation to be solved depends on the value of \( y^{+,n} \). Using \( \langle \tau_w^{n+1, \text{guess}} \rangle \) a new value of \( y^{+,n+1} \) can be computed. If both \( y^{+,n} \) and \( y^{+,n+1} \) lie in the same region (I), (II) or (III) \( \langle \tau_w^{n+1, \text{guess}} \rangle \) corresponds to the right wall shear stress and the iterative procedure can be interrupted. Otherwise the iterative procedure has to be repeated starting from \( \langle \tau_w^{n+1, \text{guess}} \rangle \). Based on \( \langle \tau_w \rangle \) the wall shear stress applied in the momentum equation can be predicted with help of eq. (3.25).

For curvilinear computational grids the velocity vector is decomposed in a streamwise and a wall–normal component. After that for the streamwise velocity component the boundary condition eq. (3.25a) and for the wall–normal velocity component the boundary condition eq. (3.25c) can be applied.

Note that for flow configurations with recirculation regions problems can arise applying the model of (Schumann, 1975). Since for separation points the mean velocity \( \langle \overline{u}(y_d) \rangle \) and also the mean wall shear stress \( \langle \tau_w \rangle \) tend to zero. Therefore, eq. (3.25a) is undefined (Breuer, 2002) leading to numerical problems. The reason is that the law of the wall (eq. (3.26)) is solely valid for attached flows with a mild adverse pressure gradient.
3.3.1.3 Wall Model of Werner and Wengle

An alternative proposal to model the wall region in LES was made by Werner (1991) and Werner and Wengle (1993) who also assumed a phase coincidence between the instantaneous wall shear stress and the velocity component tangential to the wall. They divided the wall region into two regions:

\[ u^+ = y^+ \quad \text{for:} \quad 0 \leq y^+ \leq 11.81 \]  
\[ u^+ = A (y^+)B \quad \text{for:} \quad 11.81 \leq y^+ \leq 1000. \]

The constants stand for \( A = 8.3 \) and \( B = 1/7 \). By adopting the above velocity distributions they assumed that the time–averaged universal velocity profile found in attached boundary layers is also valid for the instantaneous realization of the flow. This assumption is questionable but adopting the wall model of Werner and Wengle produced to some degree feasible results in practically relevant cases (Breuer, 2002). An analytical expression for the instantaneous wall shear stress \( \tau_w \) in dimensionless form can be obtained by integrating the above equation over the first computational cell and calculating the mean velocity at the first cell center adjacent to the wall:

\[ \tau_w = \frac{1}{Re} \frac{\overline{u}(x, y, z, t)}{\Delta y_2} \quad \text{for:} \quad 0 \leq y^+ \leq 11.81 \]  
\[ \tau_w = \left[ \frac{1}{2} (1 - B) A^{1+B} \frac{1}{(2\Delta y_2 \text{Re})^{1+B}} + \frac{1 + B}{A} \frac{\overline{u}(x, y, z, t)}{(2\Delta y_2 \text{Re})^B} \right] \Delta y^2 \quad \text{for:} \quad 11.81 \leq y^+ \leq 1000. \]

Here again \( \Delta y_2 \) denotes the wall distance of the first cell center. An advantage of this model is that the averaged velocity \( \langle \overline{u} \rangle \) and the averaged wall shear stress \( \langle \tau_w \rangle \) are not required and no iterative method has to be applied to obtain the wall shear stress. Another advantage is that from the numerical point of view no problems arise in flow configuration with recirculation regions. However, the assumed velocity distributions (3.28) in such flow regions are highly questionable (Breuer, 2002) owing to the same reason as for the Schumann wall model.

3.3.2 Periodic Boundary Conditions

If the problem to be solved has one or more homogeneous directions, a way to circumvent the difficulty to set appropriate inflow and outflow conditions is to apply periodic boundary conditions. For example for a channel flow (see § 7.1–S 7.3) with homogeneous directions in \( x \) and \( z \) direction they read:

\[ \overline{u}_i(x, y, z, t) = \overline{u}_i(x + L_x, y, z, t) \]  
\[ \overline{u}_i(x, y, z, t) = \overline{u}_i(x, y, z + L_z, t). \]

\( L_x \) and \( L_z \) are the extensions of the channel in \( x \) and \( z \) direction, respectively. The extensions of the computational domain have to be chosen in order that the two–point correlations decay to zero until \( L_x/2 \) and \( L_z/2 \). That means that the greatest structures have to be resolved by the computational domain in order to get reliable results.

For problems with a mean pressure gradient in one homogeneous direction, e.g., channel
or pipe flows (see § 7.1–§ 7.3 and § 7.4–§ 7.6), the forcing term:

\[ F_{n+1} = F_n - \frac{\alpha}{\Delta t} \left( U_{0\text{mean}} + U_{\text{mean}} - 2U_{1\text{mean}} \right) \]  \hspace{1cm} (3.32)

proposed by Benocci and Pinelli (1990) is applied in the corresponding momentum equation to ensure a constant mean velocity. \( \alpha \) is an under–relaxation factor which is chosen to be equal to \( \alpha = 0.3 \) in the present thesis. \( U_{0\text{mean}} \) is the mean velocity desired, \( U_{\text{mean}} \) is the mean velocity calculated at the old time step and \( U_{1\text{mean}} \) the mean velocity of the new time step. \( F_n \) is the forcing term of the previous time step and \( F_{n+1} \) is the forcing term casted into eq. (3.5b) to regulate the mass flow.

3.3.3 Inflow Conditions

When generating the inflow conditions it has to be done with special care since they can significantly effect the simulations even far downstream from the location where they are applied (Breuer, 2002). In this thesis three different methods to generate inflow conditions are used. For alternative methods the interested reader is referred to Breuer (2002) or Sagaut (2006).

3.3.3.1 Generation with Support of a Simulation with Periodic Boundary Conditions

If the flow at the inflow boundary can be assumed to be fully developed (see, the cold flow in a combustion chamber in § 7.7), a method to produce realistic inflow conditions is to run a supplementary simulation with periodic boundary conditions (e.g., a channel, a pipe or an annular ring flow). The whole velocity field is then extracted every time step in a plane parallel to the mean flow direction. Of course, in order to reproduce reliably the inflow conditions the time step of the simulation used to extract the flow field has to be equal to the one used in the main simulation. Furthermore, the grid at the extracting plane has to be equal to the grid at the inflow boundary. The extracted data are then directly applied as boundary conditions at the domain inlet. A disadvantage of this method is that besides the additional CPU–time for the periodic simulation it requires quite a lot of disc space (\( O(\text{TBs}) \)). Therefore, problems related with handling huge amounts of data like transferring the files from one computer to another or the possible corruption (the possibility of an inversion of a bit is higher in bigger files) of the file can arise. An alternative is to run both simulations in parallel and thus avoiding to store huge amount of data.

3.3.3.2 Experimental Mean Profiles with Imposed Fluctuations

This method was used to further improve the inflow velocity field for the cold flow in a model combustion chamber (see § 7.7). The reason of the choice of this method to generate the inflow conditions was that it was not possible to reproduce the experimentally measured mean velocity profile and the second–order fluid and particle statistics by a four–way coupled turbulent pipe flow simulation with wall roughness seen by the particles and applying periodic boundary conditions. The four–way coupled simulation with periodic boundary conditions predicted almost vanishing fluid velocity fluctuations while the experiments of Borée et al. (2001) did not show this phenomenon. Furthermore, for
the annular flow (for a detailed description of the numerical setup see § 7.7) a simulation with periodic boundary condition does not reproduce the asymmetric mean velocity profile found in the experiments of Borée et al. (2001). The reason for the discrepancies observed are presumably that in the experiments the developing length $L_d$ of the annular flow was not long enough to ensure a fully developed profile ($L_d/(R_a - R_i) = 54$). Here $R_a$ and $R_i$ denote the outer and inner radius of the annular ring, respectively. This conjecture is further reinforced by the observation that in the experiments of Borée et al. (2001) the radial velocity very close to the chamber entrance has a non-zero value (5% of the bulk velocity). For this reason an alternative method to generate the inflow data described in § 3.3.3.1 is realized as follows. The mean streamwise and radial velocity of the experiments is imposed at the inlet. In order to produce a realistic instantaneous velocity field at the inlet this mean profile is superimposed by velocity fluctuations. The amplitude of the fluctuations are simultaneously adjusted to a value which reasonably match the measured one:

\[
\begin{align*}
    u_{x,inflow}(x, y, z, t) &= \langle u_{x,exp}(x_n, y_n, z_n) \rangle + C_x \left( u_x(x, y, z, t) - \langle u_x(x, y, z) \rangle \right) \\
    u_{y,inflow}(x, y, z, t) &= \langle u_{y,exp}(x_n, y_n, z_n) \rangle + C_y \left( u_y(x, y, z, t) - \langle u_y(x, y, z) \rangle \right) \\
    u_{z,inflow}(x, y, z, t) &= \langle u_{z,exp}(x_n, y_n, z_n) \rangle + C_z \left( u_z(x, y, z, t) - \langle u_z(x, y, z) \rangle \right)
\end{align*}
\]

$\langle u_x(x, y, z) \rangle$, $\langle u_y(x, y, z) \rangle$ and $\langle u_y(x, y, z) \rangle$ are the simulated mean velocities in $x$-, $y$- and $z$-direction at the cell center located at the point $(x, y, z)$. $\langle u_{x,exp}(x_n, y_n, z_n) \rangle$, $\langle u_{y,exp}(x_n, y_n, z_n) \rangle$ and $\langle u_{z,exp}(x_n, y_n, z_n) \rangle$ are the corresponding measured mean velocities approximated by a spline with 100 supporting points. $(x_n, y_n, z_n)$ are the coordinates of the supporting points next to a cell center located at $(x, y, z)$. The resulting velocities with the superscript inflow denote the finally applied inflow data. The constants $C_x$, $C_y$ and $C_z$ are the factors used to adjust the magnitude of the simulated velocity fluctuations to the magnitude of the measured velocity fluctuations. Note that although the constants $C_x$, $C_y$ and $C_z$ should have the same value to fulfill the continuity condition, they are chosen to have a different value in the different directions in order to obtain a better agreement between simulated and measured velocity profiles at the inlet. For the details, see § 7.7.

### 3.3.3.3 Imposed Mean Profile

An alternative method to obtain an inflow boundary condition is to impose a mean velocity profile valid for attached boundary layers. This method was used to generate the inflow conditions for the cyclone separator (see § 7.8). For example, Reichardt (1951) obtained an empirical correlation valid for turbulent pipe and channel flows:

\[
\langle u^+(y^+) \rangle = C_{infl} \left[ \frac{1}{\kappa} \ln(1 + \kappa y^+) + 7.8 \left( 1 - e^{-y^+/11} - \frac{y^+}{11} e^{-0.33y^+} \right) \right].
\] (3.34)

Since for a rectangular inlet at a given point of the cross-section two different distances from the wall exist, the shortest distance from the wall was chosen to calculate the value of $y^+$. The constant $C_{infl} = 0.297$ is used to adjust the mass flow to the value obtained from the measurements. $C_{infl}$ was introduced since the integration of eq. (3.34) over a rectangular cross-section does not automatically lead to the desired mass flow. Note that eq. (3.34) solely describes a mean flow without any fluctuations. Gronald and Derksen (2011) mentioned that in their finite-volume LES predictions of the same cyclone config-
uration as described in § 7.8 the velocity fluctuations applied at the inlet had no influence on the cyclone flow. Based on their own observations Gronald and Derksen (2011) chose to not apply any artificial or natural fluctuations at the inlet. Therefore, in this thesis it was decided to also omit any perturbation of the velocity profile (3.34). The choice of this specific boundary condition is further motivated by the lag of detailed information about the design of the experimental setup upstream of the cyclone inlet. That means that if no information about the upstream condition are available, every boundary condition applied results is a conjecture. Therefore, the computationally cheapest method is applied. Furthermore, the predicted velocity profile in the inlet section of the cyclone (see, also § 7.8) was examined at a distance upstream of the circular part equal to the radius of the barrel. The evaluation of the simulated data showed that the velocity fluctuations (root–mean square values) in all three direction have already reached values of more than 10 % of the bulk velocity. Hence, the mean velocity profile (3.34) is sufficiently destabilized to guarantee a reasonably turbulent velocity field entering the body of the cyclone.

3.3.4 Outflow Conditions

Similar to the inflow also for the outflow special care has to be taken since it always represents an artificial boundary of the problem treated. To minimize the effect of the outflow boundary on the flow region of interest, it should be always set far enough downstream. Furthermore, it should be ensured that no backflow is present at this boundary (Breuer, 2002). In DNS and LES a so–called convective boundary conditions was proven to be adequate:

\[
\frac{\partial u_i}{\partial t} + U_{\text{conv}} \frac{\partial u_i}{\partial \chi} \bigg|_{\text{outflow}} = 0.
\]  

(3.35)

\(\frac{\partial}{\partial \chi}\) is the gradient in the direction of the convective velocity \(U_{\text{conv}}\). The convective velocity has to be chosen in accordance with the flow configuration. In all simulations performed \(U_{\text{conv}}\) is chosen to be equal to the mean velocity at the outflow which is calculated by means of the mass conservation \(U_{\text{conv}} = \langle u_{\text{inflow}} \rangle A_{\text{inflow}} / A_{\text{outflow}}\). \(\langle u_{\text{inflow}} \rangle\) is the mean time–averaged velocity at the inflow, \(A_{\text{inflow}}\) and \(A_{\text{outflow}}\) are the surface areas of the inflow and the outflow cross–section, respectively. For DNS and LES it was shown that the above boundary condition avoids the reflection of pressure waves towards the inside of the domain and therewith connected also the error propagation towards the interior of the domain (Breuer, 2002). Furthermore, applying the above boundary condition ensures that the turbulent eddies can leave the computational domain nearly undisturbed and without being reflected.

3.3.5 Initial Conditions

Because of the parabolic character of the Navier–Stokes equations in time also initial conditions have to be set to get an unique solution. For turbulent flows the initial conditions are in many cases, however, of minor importance since it is assumed that the statistical stationary state is always reached independently of the initial field (Breuer, 2002). This assumption is, however, not proven and relies only on observations (Rotta, 1972). Note that in statistically unsteady flows not considered in this thesis the situation is completely different.

Nevertheless, the initial conditions for statistically stationary flows can be chosen in a manner to speed up the development towards the statistical stationary state. For the
channel and pipe flow (§ 7.1–§ 7.3 and § 7.4–§ 7.6) the velocity profile (3.34) was superposed by analytical and random disturbances in order to accelerate the destabilization of the initial profile.

For the combustion chamber flow (§ 7.7) the initial velocity in the entire integration domain was set equal to the mean velocity at the outflow. No destabilization of this profile was necessary since the inflow velocity field was already turbulent.

For the cyclone separator (§ 7.8) the velocity field at the inlet was initialized by the profile (3.34) and the velocity field in the circular part of the cyclone was initialized according to a rigid–body vortex. In this case the velocity at the wall is set to zero to ensure the no–slip condition.
Theoritical Background of the Point-Particle Approach

The scope of this section is to present the governing equations for the solid phase in the framework of the point–particle approach in the most general way possible, i.e., independently of the modeling assumptions for the continuous phase (DNS, LES or RANS). In order to elucidate the concept of the point–particle approach in § 4.1 the assumptions made and the formalism adopted to derive the governing equations for the disperse phase are pointed out. In § 4.2 the governing equations for the solid phase used in this thesis are presented explicitly. Afterwards, in § 4.3 the interaction of the solid phase with the domain boundaries is described. For this case the influence of physical boundaries (i.e., solid walls) and artificial boundaries (inlet, outlet and periodic boundaries) has to be distinguished. The specific modeling issues in the framework of LES and also the coupling procedure (one–way, two–way and four–way coupling) between the continuous phase and the particles are described in a separate section, i.e., in § 5.

As a concluding remark, note that the governing equations for the solid phase are represented in vector notation in contrast to the governing equations for the continuous phase which are represented in tensor notation. The scope is to visually distinguish the frame of references in which the equations are described, i.e., in the Eulerian frame of reference for the fluid and in the Lagrangian frame of reference for the particles.

4.1 Derivation of the Governing Equations for the Disperse Phase

The basic assumption to derive the fluid forces displacing the particles is that the particles are much smaller than the grid spacing, i.e., \( d_p \ll \Delta_g \). This assumption implicates that the fluid velocity at the particle position varies only moderately within a range of \( O(d_p) \) and hence the fluid forces can be taken either from analytical solutions or empirical correlations of bodies moving in a flow where the bulk flow remains undisturbed at a large distance from the body. This means that the point–particle approach is strictly only valid if the distance \( r \) (see Fig. 6) where the disturbance of the particle on the surrounding fluid decays to zero is much smaller than the grid spacing \( \Delta_g \), i.e., the range where the fluid velocity changes. Furthermore, it is also assumed that the forces acting on a particle can be superimposed which is strictly only valid for \( Re_p \ll 1 \), where the Navier–Stokes equations reduce to the Stokes equation and thus are still linear. With this assumption the equation of motion for a single particle can be described by Newton’s second law and thus is reduced to a set of ordinary differential equations:

\[ m_p^* \frac{d \mathbf{u}_p^*}{dt^*} = \sum \mathbb{F}_p^* \]  
\[ I_p^* \frac{d \mathbf{\omega}_p^*}{dt^*} = \sum \mathbb{T}_p^* \]

Here \( m_p^* \) is the particle mass, \( I_p^* \) is the particle moment of inertia, \( \mathbf{u}_p^* \) and \( \mathbf{\omega}_p^* \) are the particle translational and angular velocities, \( \mathbb{F}_p^* \) represents the force acting on a single particle and \( \mathbb{T}_p^* \) is the torque acting on a single particle. Note that as already mentioned before, the superscript \( ^* \) denotes dimensional quantities. Because of the rather simple to obtain expressions for the forces and the torques acting on a particle, most studies in the literature assume a spherical shape of the particles. The first who rigorously derived the
equations of motion for small spherical particles moving in a non–homogeneous flow were Gatignol (1983) and Maxey and Riley (1983). In their works they accounted for the effect of the viscous Stokes drag, the pressure gradient of the undisturbed flow, the added–mass force, the Basset history term and the buoyancy. The added–mass effect describes the force required by the particle to accelerate or decelerate the fluid surrounding the particle, i.e., it is an inertial force. The Basset force can be also traced back to the acceleration of the particle and is caused by the retardation of the boundary layer development on the particle with changing relative velocity (Sommerfeld, 2000). As already mentioned the equations derived by Gatignol (1983) and Maxey and Riley (1983) are only valid for \( \text{Re}_p \ll 1 \). In order to extend the point–particle approach towards higher particle Reynolds numbers basically the same procedure as adopted by Gatignol (1983) and Maxey and Riley (1983) is applied, i.e., the superposition of forces originating by different aerodynamic effects. The forces displacing the particles are then replaced by empirical relations valid also for \( \text{Re}_p > 1 \). The reason why the superposition of the forces is applied also for particle Reynolds numbers greater than unity, is to avoid to resolve the flow field around each particle and the huge computational costs associated with this procedure (see, § 7). Especially when millions of particles are tracked throughout the domain, the full resolution of the flow field around each particle is completely intractable. Of course, the point–particle procedure has to be validated carefully since it represents only an approximation of the ”real” forces and torques acting on the particles.

In the following sections the extensions of the equations employed in the Lagrangian point–particle approach towards higher \( \text{Re}_p \) are discussed. Furthermore, some considerations about the importance of the relevant forces and torques for gas–solid flows which model the effect of the carrier phase on the particle motion are made. The scope is to illustrate the importance of the aerodynamic forces considered in this thesis.

4.1.1 Drag Force

Probably the most important force is the drag force which consists in the friction exerted on a sphere and the pressure difference arising between the stagnation point in front of
the sphere and the rear end. It is commonly calculated as follows:

\[ F_D^* = C_D \frac{\rho_f^*}{2} |u^*_f - u^*_p| (u^*_f - u^*_p) A_p^*. \]  

(4.2)

Here \( u^*_f \) denotes the fluid velocity at the particle position, \( A_p^* \) is the projection of the particle surface in the direction of the incoming flow and \( C_D \) is the drag coefficient. A frequently used expression for \( C_D \) is an empirical correlation derived for spheres in an uniform flow (Schiller and Naumann, 1933):

\[ C_D = \frac{24}{Re_p} (1 + 0.15 Re_p^{0.687}), \quad Re_p = \frac{d^* p |u^*_f - u^*_p|}{\nu_f^*}. \]  

(4.3)

The correlation fits the experimentally measured data of a rigid sphere reasonable well until \( Re_p = 800 \). Considering only the drag force in the equation of motion should give reasonable agreements with experiments in flow configurations with weak velocity gradients (see, e.g., Apte et al., 2003b; Oefelein et al., 2007; Riber et al., 2009; Alletto and Breuer, 2012; Breuer and Alletto, 2012b, for LES combined with a point–particle approach). In this kind of flows the influence of the lift force due to linear shear described in the next section can be disregarded. If only the drag force is considered, it should be also ensured that the particle relaxation time is much smaller than the time between two subsequent wall collisions of a particle in order to guarantee that the influence of the wall roughness and the influence of the lift force due to the particle rotation is small (a particle hitting a rough surface acquires high rotation rates). Of course also the gravity should have a negligible influence which is the case for small particles where the gravity is aligned with the mean flow direction. Furthermore, also the ratio of the particle density to the fluid density should be \( \rho_p^*/\rho_f^* \ll 1 \) in order to that neglecting the buoyancy, the added–mass and the Basset force is justified (Sommerfeld, 2000).

### 4.1.2 Lift Force due to Linear Shear

A particle displacing with a relative velocity with respect to a linearly sheared flow generates different velocity distributions on the two particle hemispheres. Hence, an asymmetric pressure and shear stress distribution arises which leads to a net force normal to the incoming flow.

To the best of the author’s knowledge, Saffman (1964) was the first who obtained an analytical solution of a spherical particle displacing in a linear shear flow. The solution was obtained by means of matched asymptotic expansions and is valid for Stokes flows (i.e., \( Re_p \ll 1 \)) and additionally requiring \( Re_p \ll Re_G^{1/2} \) (the definition of the shear Reynolds number \( Re_G \) is provided below).

McLaughlin (1991) extended the work of Saffman (1964) with the scope to remove the restriction \( Re_p \ll Re_G^{1/2} \). By employing a Fourier transformation of the creeping flow McLaughlin (1991) obtained an analytical solution for the lift force acting on a spherical particle in a linear shear flow:

\[ F_L^{McL} = \frac{9}{4\pi} \mu_f^* d_p^2 (u^*_f - u^*_p) \text{sign}(G^*) \left[ \frac{|G^*|}{\nu_f^*} \right]^{1/2} J^* u^* \]  

(4.4)
with
\[ J^*u = f(\epsilon), \quad \epsilon = \text{sign}(G^*) \frac{|G^*| \nu^*_f}{u^*_p - u^*_f} \, . \] (4.5)

\( f(\epsilon) \) is given in McLaughlin (1991) based on an analytical relation. For \( |\epsilon| \ll 1 \) the function \( J^*u \) can be expressed as \( J^*u = -32\pi^2 \epsilon^5 \ln(1/\epsilon^2) \). For \( |\epsilon| \gg 1 \) the function \( J^*u \) is defined as \( J^*u = 2.255 - 0.6463/\epsilon^2 \). For values of \( \epsilon \approx O(1) \) the function \( J^*u \) is given in tabular form.

\( G^* = \nabla^* u^*_f \) is the fluid velocity gradient tensor. In order to derive the above equation McLaughlin (1991) made the following assumptions: (i) the velocity disturbance of the particle decays at infinity and (ii) the particle Reynolds number \( \text{Re}_p \) and the shear Reynolds number \( \text{Re}_G = |G^*| d^2_p/\nu^*_f \) are smaller than unity since the above equation is derived in a Stokes flow regime.

Although not applied in the present thesis, in the following the available extensions of the lift force due to linear shear towards \( \text{Re}_p \geq 1 \) found in the literature are briefly described for the sake of completeness. In order to derive a relation for the lift force valid for higher particle Reynolds numbers, typically a lift coefficient is introduced (see, e.g., Crowe et al., 1998; Sommerfeld, 2000):

\[ F^*_L = \frac{\beta_f \pi}{2} d^3_p C_{LS} \left( (u^*_f - u^*_p) \times \omega^*_f \right) . \] (4.6)

\( \omega^*_f = \nabla^* \times u^*_f \) is the fluid rotation. Based on numerical simulations different relations of \( C_{LS} \) based on the particle Reynolds number \( \text{Re}_p \) and the Reynolds number of the shear flow \( \text{Re}_S \) can be found. The Reynolds number of the shear flow is defined as (Sommerfeld, 2000):

\[ \text{Re}_S = \frac{d^2_p |\omega^*_f|}{\nu^*_f} . \] (4.7)

One expression for \( C_{LS} \) found in the literature is based on the numerical calculation of Dandy and Dwyer (1990) (see, also Crowe et al., 1998; Sommerfeld, 2000):

\[ C_{LS} = \frac{4.1126}{\sqrt{\text{Re}_S}} \left( (1 - 0.3314 \beta^{0.5}) \exp(-0.1 \text{Re}_p) + 0.3314 \beta^{0.5} \right) \quad \text{for } \text{Re}_p \leq 40 \] (4.8a)

\[ C_{LS} = \frac{4.1126}{\sqrt{\text{Re}_S}} 0.0524 (\beta \text{Re}_p)^{0.5} \quad \text{for } \text{Re}_p \geq 40 \] (4.8b)

with \( \beta = 0.5 \frac{\text{Re}_S}{\text{Re}_p} \) (4.8c)

The above correlations for \( C_{LS} \) are valid for \( 0.1 \leq \text{Re}_p \leq 100 \) and \( 0.005 \leq \beta \leq 0.4 \) (Dandy and Dwyer, 1990). Another expression for \( C_{LS} \) found in the literature was obtained by Kurose and Komori (1999) based on three–dimensional numerical simulations for \( 1 \leq \text{Re}_p \leq 100 \) and \( 0 \leq \beta \leq 0.4 \):

\[ C_{LS} = \frac{\text{Re}_p}{\text{Re}_S} \left[ K_0 \left( \frac{\text{Re}_S}{2 \text{Re}_p} \right)^{0.9} + K_1 \left( \frac{\text{Re}_S}{2 \text{Re}_p} \right)^{1.1} \right] . \] (4.9)

\( K_0 \) and \( K_1 \) are found in Kurose and Komori (1999) in tabular form as functions of \( \text{Re}_p \).
Marchioli et al. (2007b) systematically studied the influence of the lift force on one-way coupled upward and downward channel flows at $Re_B = 2100$ based on the extension for the lift force towards higher $Re_p$ proposed by Kurose and Komori (1999). The main outcomes were:

(i) The lift force basically effects only the particle concentration at the wall while other statistics are almost unaffected.

(ii) The lift force leads to a reduction of the concentration at the wall for the upward channel flow (the same results are found also in an upward pipe flow, Marchioli et al., 2003).

(iii) The lift force leads to an increase of the particle concentration at the wall for a downward channel flow.

(iv) The effect of the lift force is more pronounced for smaller particles.

### 4.1.3 Lift Force due to Rotation (Magnus Lift)

Similar to a particle moving in a linear shear flow also a rotating particle in an uniform flow generates an asymmetric pressure and shear stress distribution along the particle surface. Hence, the fluid exerts a force on the particle surface which is normal to the incoming fluid flow. Similar to the lift force due to linear shear also for the lift force due to rotation it is possible to derive an analytical solution for $Re_p \ll 1$ (Rubinow and Keller, 1961):

$$F^*_{Mag} = \pi \frac{d'^3}{8} \rho_f^* \omega_p^* \times u_p^*.$$  \hspace{1cm} (4.10)

Rubinow and Keller (1961) derived the above equation considered a particle translating with the velocity $u_p^*$ and rotating with the angular velocity $\omega_p^*$ in a surrounding fluid at rest. In order to consider the fluid rotation in the calculation of the lift force the relative rotation of the particles $\Omega_{rel}^*$ has to be introduced (see, Sommerfeld, 2000):

$$\Omega_{rel}^* = \frac{1}{2} \nabla^* \times u_f^* - \omega_p^*.$$ \hspace{1cm} (4.11)

Note that the factor $1/2$ in the definition of the relative rotation $\Omega_{rel}^*$ derives from the fact that for a solid body rotation the angular velocity of the fluid $\omega_{sb}^*$ is exactly one half of the vorticity $\omega_{sb}^* = 1/2 \nabla^* \times u_{sb}^* = 1/2 \omega_f^*$. The final relation found in Sommerfeld (2000) considering the relative rotation and the relative particle velocity reads:

$$F^*_{Mag} = \pi \frac{d'^3}{8} \rho_f^* \left( \Omega_{rel}^* \times (u_f^* - u_p^*) \right).$$ \hspace{1cm} (4.12)

Recently, however, Oesterlé and Bui Dinh (1998) introduced an empirical correlation valid until $Re_p < 140$ leading to the following expression for the Magnus lift:

$$F^*_{Mag} = C_{LR} \rho_f^* \frac{d'^3}{8} \pi |u_f^* - u_p^*| \Omega_{rel}^* \times (u_f^* - u_p^*) \frac{\Omega_{rel}^*}{|\Omega_{rel}^*|}.$$ \hspace{1cm} (4.13)
The coefficient $C_{LR}$ is defined by:

$$C_{LR} = 0.45 + \left( \frac{Re_r}{Re_p} - 0.45 \right) \exp (-0.05684 \cdot Re_p^{0.4} Re_r^{0.3}) .$$

(4.14)

The Reynolds number of the particle rotation $Re_r$ is defined as:

$$Re_r = \frac{\rho_t^* d_p^2 |\Omega_{rel}|}{\mu_f^*} .$$

(4.15)

Unfortunately, no systematic studies on the effect of the Magnus force on dilute particle-laden flows are known to the author. However, a few authors underlined the importance of considering this force due to the high angular velocities acquired by particles hitting rough walls (Hussainov et al., 1996; Yamamoto et al., 2001; Sommerfeld, 2003; Alletto and Breuer, 2013). Note that in this thesis the formulation (4.13) with the lift coefficient of Oesterlé and Bui Dinh (1998) is used to account for the Magnus lift force.

4.1.4 Gravity and Buoyancy Force

The gravitational force arises from the attraction of two bodies and acts in the direction of the gravitational acceleration $g^*$. As will be shown in §8.6, this force becomes especially important if $g^*$ is not aligned with the mean flow direction. The gravity leads to indirect changes in the flow characteristics by the influence of the two-way coupling induced by the settling of the particles at the bottom part of the horizontal pipe.

The buoyancy force found by Archimedes arises from the pressure difference between the bottom and top part of a body immersed in a fluid. This force is directed against the gravitational acceleration $g^*$. Note that for the high density ratios $\rho_p^*/\rho_f^* \gg 1$ considered in this thesis it is not relevant but nevertheless it is retained in the predictions because it is computationally cheap. The sum of the two forces reads:

$$F_{GB}^* = m_p^* g^* \left( 1 - \frac{\rho_f^*}{\rho_p^*} \right) .$$

(4.16)

Note that both forces described above are not aerodynamic forces in contrast to all other forces mentioned in this section.

4.1.5 Added–mass, Pressure Gradient and Basset Force

In the Lagrangian point–particle approach the added–mass, the pressure gradient and the Basset force mentioned in Gatignol (1983) and Maxey and Riley (1983) are commonly assumed to be negligible compared to the drag for high density ratio flows, i.e., if $\rho_p^*/\rho_f^* \gg 1$. This assumption is supported by various numerical and theoretical studies. For example, Armenio and Fiorotto (2001) studied the relative importance of the drag, the added–mass, the pressure gradient and the Basset force compared to the drag force for density ratios ranging from $\rho_p^*/\rho_f^* = 2.65$ to $\rho_p^*/\rho_f^* = 2650$ in a one–way coupled DNS of a turbulent channel flow at a Reynolds number based on the friction velocity of $Re_f = 175$. The main outcome was that the added–mass force was at least two orders of magnitudes smaller than the drag force for all density ratios. The pressure gradient was found to be important only for the smallest density ratio considered. The ratio of the Basset force to
the drag force was shown to decrease from 0.25 for $\rho_p/\rho_f^* = 2.65$ to 0.096 for $\rho_p/\rho_f^* = 2650$. Despite of the not completely neglectable magnitude of the Basset force compared to the drag force, Armenio and Fiorotto (2001) mentioned that only small differences in the particle dispersion occur between the computations performed considering only the drag force and the computations considering the drag force, the added–mass, the pressure gradient and the Basset force. The differences between the two different simulations amounted to only 1.6% for $\rho_p/\rho_f^* = 2.65$ and 0.97% for $\rho_p/\rho_f^* = 265$.

The results of Armenio and Fiorotto (2001) are further supported by the findings of Hjelmfelt and Mockros (1966) who analytically studied the relative importance of the drag, the added–mass, the pressure gradient and the Basset force in an oscillating flow. For this purpose Hjelmfelt and Mockros (1966) evaluated the response of the particles to an oscillatory fluid flow (the analytical solutions were obtained by expressing the fluid and the particle velocity in terms of Fourier integrals). Hjelmfelt and Mockros (1966) computed the ratio of the amplitudes of the particle velocity to the fluid velocity and the phase shift between the fluid and particle velocity as function of the fluid frequency. Four different solution are compared to each other: One was obtained by considering only the drag, the second was obtained by considering the drag and the pressure gradient force, the third was computed by considering the drag, the pressure gradient and the added–mass force and the forth was obtained by considering the drag, the pressure gradient, the added–mass and the Basset force. The main outcome was that for heavy particles (copper and glass in air) no difference between the four solutions regarding the dependency of the velocity amplitude ratio as a function of the fluid frequency could be asserted. For high frequencies (strong accelerations) however, a small phase shift between the solution obtained by considering only the drag force and the solution obtained by considering all forces could be observed. Note that the added–mass and the pressure gradient had almost no influence on the solutions.

Based on the findings of Hjelmfelt and Mockros (1966) and Armenio and Fiorotto (2001) mentioned above, the state of the art procedure (neglecting the added–mass, the pressure gradient and the Basset force) of the Lagrangian point–particles approach for high density ratio flows ($\rho_p/\rho_f^* \gg 1$) is adopted. Therefore, only the influence of the drag, the lift forces, the gravity and buoyancy are considered in the equation of motion of the particles.

### 4.1.6 Torque acting on a Spherical Particle

For small particle Reynolds numbers $Re_p$, Rubinow and Keller (1961) derived an analytical solution for the torque acting on a spherical particle:

$$T^*_{p} = -\pi \mu_f^* d_p^3 \rho_p^* \omega_p^*.$$  \hspace{1cm} (4.17)

As for the lift force due to the particle rotation also for the viscous torque the relative rotation $\Omega^*_{rel}$ has to be introduced to account for the fluid rotation:

$$T^*_{p} = \pi \mu_f^* d_p^3 \Omega^*_{rel}.$$  \hspace{1cm} (4.18)

For higher $Re_p$ no analytical solution for the torque is available and hence some empirically or numerically determined relations for the torque has to be found in the following
form (Sommerfeld, 2000):

\[ T_p^* = C_R \rho_f^* \left( \frac{d_p^*}{2} \right)^5 |\Omega_{rel}^*| \Omega_{rel}^*. \] (4.19)

Dennis et al. (1980) obtained a correlation for \( C_R \) by numerically calculating the torque acting on a particle rotating with constant angular velocity in an incompressible liquid at rest:

\[ C_R = \frac{12.9}{Re_r^{0.5}} + \frac{128.4}{Re_r}, \quad \text{for} \quad 32 < Re_r < 1000. \] (4.20)

For smaller \( Re_r \), the expression obtained by Rubinow and Keller (1961) can be used (Sommerfeld, 2000). Note that in the present thesis eq. (4.18) is used to calculate the torque acting on the particles.

### 4.1.7 Corrections due to the Presence of Walls and other Particles

As already mentioned, the equations of motion presented above are derived assuming that the disturbance of the particle decays to a negligible amount at a distance which is small compared to the grid spacing. For the cases where this assumption is violated different corrections are available in the literature.

For example, Brenner (1961) and Goldman et al. (1967) derived a correction of the Stokes drag coefficient for a particle moving towards and parallel to a flat wall, respectively. Both corrections are valid for large distances from the wall compared to the particle diameter \( d_p \). Because of the difficulty of deriving analytical or empirical corrections of the lift and drag forces in the vicinity of a wall at finite Reynolds numbers, more recent trends are to compute correlations for the lift and drag coefficient by means of DNS (see, e.g., Zeng et al., 2005; Lee and Balachandar, 2010). In this thesis no correlation of the forces displacing the particles due to the presence of solid walls is applied. The corrections require the wall–normal distance which is not trivial to compute for general curvilinear grids and are therefore neglected. Furthermore, Arcen et al. (2006) pointed out that in their one–way coupled DNS of a particle–laden channel flow at a bulk Reynolds number of \( Re_B = 2800 \) the drag correction due to the presence of the wall has a negligible influence on the first and second–order moments of the particles and also on the concentration profile. A similar comment is found also in the one–way coupled DNS of Armenio and Fiorotto (2001) (\( Re_r = 175, Re_B \approx 2800 \)). They pointed out that their simulations were insensitive to the corrections of the Stokes drag parallel and normal to the wall.

When the distance between the particles becomes smaller the assumption of an undisturbed incoming flow for which the drag coefficient in eq. (4.2) is derived may not hold anymore. For this case correction factors of the drag coefficient as a function of the volume fraction \( \Phi \) can be found in the litterature (see, e.g., Li and Kuipers, 2003, and references therein). Since the volume fractions \( \Phi \) considered in this thesis are of \( \Phi \approx O(10^{-3}) \) the correction of the drag coefficient due to the presence of other particles is neglected.

### 4.2 Equations of Motion used in the Thesis

In this work six relevant effects appearing in particle–laden flows bounded by rough walls are considered:
(i) The drag force arising from a relative velocity between the particle and the fluid is considered by means of eq. (4.2) using the drag coefficient given by eq. (4.3).

(ii) The lift force acting on a particle in a linear shear flow is accounted for by eq. (4.4). This specific choice of the lift force is made since no particular attention is set on the role of the lift force. For that reason, the formulation of the lift force originally implemented in the code LÉSÖCC (see, Breuer et al., 2007) was retained instead of using the relations valid for higher particle Reynolds numbers described in § 4.1.2.

(iii) The lift force due to the particle rotation is incorporated by means of eq. (4.13) using the relation (4.14) for the coefficient $C_{LR}$. Since particles hitting a rough wall acquire a high angular velocity, this effect is also included in the governing equations.

(iv) The gravity force which can significantly influence the particle motion especially in flow configurations where the gravitational acceleration is not aligned with the mean flow direction (see, e.g., § 8.6). Therefore, it is taken into account.

(v) The buoyancy force is also considered since it is cheap to calculate. For the cases considered in the present thesis assuming $\rho_p^*/\rho_f^* \gg 1$ its physical influence can be neglected.

(vi) The decrease of the particle angular velocity due to the viscous torque is accounted for by eq. (4.18). Since the evaluation of this equation leads to an analytical relation for the time evolution of $\omega_p^*$, it is easily computed. Thus, it is preferred with respect to eq. (4.19).

(vii) The added–mass, the pressure gradient and the Basset force are not considered since they are of minor importance for the high density ratio flows (i.e., $\rho_p^*/\rho_f^* \gg 1$) considered in this thesis.

Summarizing the effects (i)–(v) and considering also the influence of the viscous torque on the particle angular velocity, the model equations used in this work to describe the effect of the fluid on the particle motion are obtained:

\[
\frac{d \mathbf{u}_p^*}{dt^*} = \frac{\mathbf{F}_D^*}{m_p^*} + \frac{\mathbf{F}_{GB}^*}{m_p^*} + \frac{\mathbf{F}_{L}^{*McL}}{m_p^*} + \frac{\mathbf{F}_{L}^{*Mag}}{m_p^*} \tag{4.21a}
\]

\[
\frac{d \omega_p^*}{dt^*} = \frac{\mathbf{T}_p^*}{I_p^*} = \frac{10}{m_p^* d_p^* 2} T_p^* = \frac{10}{3 \tau_p^*} \Omega_{rel}. \tag{4.21b}
\]

$\mathbf{F}_D^*$, $\mathbf{F}_{GB}^*$, $\mathbf{F}_{L}^{*McL}$, $\mathbf{F}_{L}^{*Mag}$ and $I_p^*$ are the drag force, the gravity and the buoyancy force, the lift force due to the velocity shear (Saffman force), the lift force due to rotation (Magnus force) and the moment of inertia of the particle, respectively. $\tau_p^*$ is the particle relaxation time and is defined as follows:

\[
\tau_p^* = \frac{\rho_p^* d_p^* 2}{18 \mu_f^*}. \tag{4.22}
\]
The terms on the right–hand side of eq. (4.21a) read:

\[
\frac{F_D^*}{m_p^*} = \frac{u_f^* - u_p^*}{\tau_p/\alpha} \quad \text{with} \quad \alpha = 1 + 0.15 \Re_p^{0.687} \tag{4.23a}
\]

\[
\frac{F_{GB}^*}{m_p^*} = g^* \left( 1 - \frac{\rho_f^*}{\rho_p^*} \right) \tag{4.23b}
\]

\[
\frac{F_{L\text{McL}}^*}{m_p^*} = \frac{27}{2\pi^2 d_p^2 \rho_p^*} \mu_f^* (u_f^* - u_p^*) \text{sign}(G^*) \left[ \frac{|G^*|}{\nu_f^*} \right]^{1/2} J^{su}, \quad J^{su} = f \left( \text{sign}(G^*) \frac{|G^*| \nu_f^*}{u_p^* - u_f^*} \right) \tag{4.23c}
\]

\[
\frac{F_{L\text{Mag}}^*}{m_p^*} = \frac{3}{4 \pi^2 d_p^2 \rho_p^*} C_{LR} |u_f^* - u_p^*| \frac{\Omega_{rel}^* \times (u_f^* - u_p^*)}{|\Omega_{rel}^*|} \tag{4.23d}
\]

The above equations are still in dimensional form. Since the code utilized in the present thesis works with dimensionless variables, eqs. (4.21) and (4.23) have to be rewritten in dimensionless form. For this purpose the dimensionless variables without superscript * are introduced: \( u_p = u_p^* U_f^* \), \( u_f = u_f^* U_f^* \), \( t = t^* U_f^* / L_f^* \), \( G = G^* L_f^*/U_f^* \), \( \Omega_{rel} = \Omega_{rel}^* U_f^* / L_f^* \), \( \omega_p = \omega_p^* U_f^* / L_f^* \), \( g = g^* U_f^*/U_f^* \), \( \rho_p = \rho_p^* / \rho_f^* \). \( U_f^* \) and \( \rho_f^* \) are characteristic fluid velocity and density and \( L_f^* \) is a characteristic length of the geometry. All this quantities are dependent of the flow configuration and have to be chosen accordingly. If we insert the new variables into eq. (4.23) and multiply the equations with \( L_f^*/U_f^* \) we get the dimensionless forces:

\[
\frac{F_D^*}{m_p^* U_f^*} = \frac{u_f^* - u_p^*}{\tau_p/\alpha}, \quad \tau_p = \Re \rho_p d_p^2 / 18, \quad \Re = U_f^* L_f^*/\nu_f^* \tag{4.24a}
\]

\[
\frac{F_{GB}^*}{m_p^* U_f^*} = g^* \left( 1 - \frac{1}{\rho_p} \right) \tag{4.24b}
\]

\[
\frac{F_{L\text{McL}}^*}{m_p^* U_f^*} = \frac{3}{4 \pi^2} \frac{d_p^2 \Re^{1/2}(u_f^* - u_p^*) \text{sign}(G) |G|^{1/2} J^u,}{\tau_p} \tag{4.24c}
\]

\[
\frac{F_{L\text{Mag}}^*}{m_p^* U_f^*} = \frac{3 C_{LR}}{4 \pi^2 d_p^2 \rho_p^*} |u_f^* - u_p^*| \frac{\Omega_{rel}^* \times (u_f^* - u_p^*)}{|\Omega_{rel}^*|}. \tag{4.24d}
\]

Hence, the dimensionless equations for the particle acceleration are obtained in the form which are implemented in the code:

\[
\frac{d u_p}{d t} = \frac{u_f^* - u_p^*}{\tau_p/\alpha} + g^* \left( 1 - \frac{1}{\rho_p} \right) + \frac{3}{4 \pi^2} \frac{d_p^2 \Re^{1/2}(u_f^* - u_p^*) \text{sign}(G) |G|^{1/2} J^u,}{\tau_p} \tag{4.25a}
\]

\[
\frac{d \omega_p}{d t} = \frac{10}{3 \tau_p} \Omega_{rel}. \tag{4.25b}
\]
Finally, the computation of the factor $\alpha$ in the drag coefficient (see, eq. (4.23a)) requires the computation of the particle Reynolds number $Re_p$. In the code it is achieved as follows:

$$Re_p = \frac{d_p |u_f^* - u_p^*|}{\nu_f^*} = d_p |u_f - u_p| Re. \quad (4.26)$$

### 4.3 Interaction with the Domain Boundaries

Since for the particles the computational domain has a finite extension, appropriate boundary conditions have to be chosen also for this phase. Similar to the continuous phase also for the disperse phase the artificial boundary conditions (at the inlet, outlet and at the periodic boundaries) have to be chosen very carefully to get a reliable solution since they always consist in an approximation of the conditions which prevail at the cutting plane. Regarding solid walls imposing a suitable boundary condition is unfortunately not as simple as for the continuous phase where the no-slip condition can be applied. The reason is that the particles can not be assumed to have a zero relative velocity with respect to the wall. Unlike the fluid where the molecules stick at the solid surface, the dynamics of the particles hitting a solid wall is governed by rather complicated contact mechanics (see, e.g., Johnson, 1989, for an introduction into the topic) and hence, some modeling assumptions have to be made in order to keep the computational costs at a reasonable level.

In § 4.3.1 and 4.3.2 these topics are discussed in more detail compared to the other boundaries since the modeling of the interaction of solid particles with smooth and rough walls is one of the key aspects of this thesis. The basic concept of the wall modeling especially for non-smooth walls is as follows: When a particle hits a rough wall (i) the momentum loss has to be accounted for and (ii) the random nature of the wall roughness and the shadow effect (the detailed description of this phenomenon is given in § 4.3.2) has to be mimicked. The model described in the next two sections fulfills both requirements. Requirement (i) is achieved by a standard hard-sphere model which is described in detail in § 4.3.1. Requirement (ii) is accomplished by a randomly inclined wall-normal vector with a mean inclination towards the trajectory of the incoming particles. The detailed description of the model is provided in § 4.3.2. Similar considerations as made in the following two sections can be also found in the already published own article, i.e., in Breuer, Alletto, and Langfeldt (2012). First in § 4.3.1 the interaction of a solid particle with a smooth wall is described. After that, in § 4.3.2 it is discussed how to obtain a simple model to mimic the rebound of solid particles at rough walls. The treatment of the particles at the periodic boundaries, the inlet and the outlet is illustrated in § 4.3.4, § 4.3.5 and § 4.3.6, respectively.

#### 4.3.1 Interaction with a Smooth Wall

The change of the particle translational and angular velocity during the smooth wall impact relies on an inelastic hard-sphere collision model including friction (see, e.g., Crowe et al., 1998). For that purpose, a spherical homogeneous and non-deformable particle and a non-deformable wall are assumed. In this way the deformation of the particle and of the wall is not required to be resolved in time. This assumption is justified as long as the contact time is much smaller than the time step size used in LES. If the contact time is of the same order as the LES time step size, the collision process can not be seen
anymore as an instantaneous event (the hard–sphere model models the collision process as an infinitesimal short event) and other models have to be applied. For cases where the hard–sphere model is not justified, a soft–sphere model must be applied (see, e.g., Hoomans, 2000; Bierwisch, 2009, and references therein) which is computationally more expensive.

The configuration considering at first a hard–sphere collision at a smooth wall is sketched in Fig. 7. The governing equations can be derived from the conservation equations of translational and angular momentum of classical mechanics assuming infinitesimal short contact times and negligible deformations:

\[
\begin{align*}
    m_p (u^+_p - u^-_p) &= \hat{F},^4 \\
    I_p (\omega^+_p - \omega^-_p) &= \mathbf{r} \times \hat{F}.
\end{align*}
\]

\(u^-_p\) and \(u^+_p\) are the particle velocities before and after the wall impact. Accordingly, \(\omega^-_p\) and \(\omega^+_p\) are the angular velocities before and after the wall impact, respectively. \(\mathbf{r}\) denotes the distance vector from the sphere center \(S\) to the contact point \(B\) (see Fig. 7). \(m_p = 1/6\pi \rho_p d^3_p\) is the dimensionless mass and \(I_p\) the dimensionless moment of inertia of the spherical particle given by \(I_p = 0.1 m_p d^2_p\). \(\hat{F}\) stands for the impact force integral defined as the integral of the forces acting on the particle during the entire collision time. The translational \(u^-_p\) and angular velocities \(\omega^-_p\) of the particles before the wall collision are known. To determine these quantities after the wall collision, the impact force integral is required. For that purpose the impact force vector is split up into a component acting in wall–normal direction \(\hat{F}_n\) and a tangential component \(\hat{F}_r\) acting opposite to the direction of the relative velocity \(\mathbf{u}_{pr}\) between the contact point \(B\) on the particle and the surface:

\[
\hat{F} = \hat{F}_n + \hat{F}_r \quad \text{with} \quad \hat{F}_n = \hat{F}_n \mathbf{n}_w = (\hat{F} \cdot \mathbf{n}_w) \mathbf{n}_w.
\]

Since the behavior of the particle in wall–normal direction is completely decoupled from the behavior in the direction of the relative velocity, it can be handled independently. Based on the definition of the wall–normal restitution coefficient:

\[
e_{n,w} = - \frac{u^+_p}{u^-_p} = - \frac{u^+_p \cdot \mathbf{n}_w}{u^-_p \cdot \mathbf{n}_w}.
\]

\(^4\)Since the code \texttt{LESOC} works with dimensionless variables, the following relations are also expressed in dimensionless form. The variable are made dimensionless as follows: \(u_p = u_p/U_j^*\), \(\omega_p = \omega_p U_j^*/L_j^*\), \(m_p = m_p^*/(\rho_j^* L_j^{*3})\), \(I_p = I_p^*/(\rho_j^* L_j^{*3})\), \(r = r^*/L_j^*\) and \(\hat{F} = \hat{F}^*/(\rho_j^* L_j^{*3} U_j^*)\).
the wall–normal velocity component after the collision can be determined. Furthermore, inserting eq. (4.27a) into eq. (4.28) and replacing $u_p^+ \cdot n_w$ via the definition (4.29) of $e_{n,w}$ yields the wall–normal force:

$$\hat{F}_n = -m_p (1 + e_{n,w}) (u_p^- \cdot n_w) n_w. \tag{4.30}$$

The wall–normal force $\hat{F}_n$ is required to determine the force $\hat{F}_r$ in the direction opposite to the relative velocity assuming Coulomb’s law of friction. For an elastic collision process with $e_{n,w} \leq 1$ two cases have to be distinguished: The particle slides along the wall over the entire period of the wall collision (sliding case) or it stops sliding at some instant in time during the collision (non–sliding or rolling case). For the latter, the no–slip condition for the forces:

$$|\hat{F}_r| \leq \mu_{st,w} |\hat{F}_n| \tag{4.31}$$

has to be fulfilled, where $\mu_{st,w}$ denotes the static coefficient of friction. Physically, it means that the particle rolls along the wall after the collision. This condition can be reformulated in terms of the relative velocity $u_{pr}$ at the contact point B between the particle and the wall defined as:

$$u_{pr} = u_p - (u_p \cdot n_w) n_w + \omega_p \times r = u_p - (u_p \cdot n_w) n_w - \frac{d_p}{2} \omega_p \times n_w, \tag{4.32}$$

where $r = -d_p/2 n_w$ denotes the distance from the particle center to the contact point B pointing in the opposite wall–normal direction. If the particle does not slide along the wall but rolls, the relative velocity $u_{pr}^+$ at the contact point after collision has to be zero, i.e.,

$$u_{pr}^+ = u_p^+ - (u_p^+ \cdot n_w) n_w - \frac{d_p}{2} \omega_p^+ \times n_w = 0. \tag{4.33}$$

Introducing eqns. (4.27a), (4.27b), (4.28) and (4.29) into this condition for rolling yields the corresponding force vector:

$$\hat{F}_r = -\frac{2}{7} m_p u_{pr}^- . \tag{4.34}$$

By inserting this relation into the no–slip condition (4.31) and replacing $\hat{F}_n$ via eq. (4.30) leads to a condition for the relative velocity before the collision $u_{pr}^-$:

$$|u_{pr}^-| \leq -\frac{7}{2} \mu_{st,w} (1 + e_{n,w}) u_p^- \cdot n_w = v_{lim}. \tag{4.35}$$

If the above condition is fulfilled, rolling of the particle takes place. Thus, purely based on the relative velocity before collision it can be analyzed, whether the particle will roll on the surface or not.

For a more detailed modeling also a tangential restitution coefficient $e_{t,w}$ defined as

$$e_{t,w} = -\frac{u_{pr}^+}{u_{pr}^-} \tag{4.36}$$

can be introduced. That means that for values of $e_{t,w} > 0$ the particles stop sliding during the collision and additionally the sign of the relative velocity $u_{pr}^+$ is inverted. Negative
values of $e_{t,w}$ are not allowed since it would represent the case where only the magnitude of the relative velocity is reduced without inverting the sign. This scenario is already covered by the sliding collision described above. For $e_{t,w} = 0$ the rolling collision is recovered.

In order to determine the contact force for values of $e_{t,w} > 0$ the definition of $u_{pr}$ described in eq. (4.32) is casted in eq. (4.36):

$$u_p^+ - (u_p^+ \cdot n_w)n_w - \frac{d_p}{2} \omega_p^+ \times n_w = -e_{t,w}u_{pr}^+. \quad (4.37)$$

By using eqs. (4.27) the translational and angular velocities after the collision can be replaced by the contact force $\hat{F}$ and the corresponding velocities before the collision. Furthermore, by using the definition of $e_{n,w}$ described in eq. (4.29) the dot product in eq. (4.37) can also be expressed as a function of the particle velocity before the collision. The result of these operations read:

$$u_p^- + \frac{\hat{F}}{m_p} + e_{n,w}(u_p^- \cdot n_w)n_w - \frac{d_p}{2} \omega_p^- \times n_w + \frac{5}{2} \frac{\omega_p^+ \times n_w}{m_p} \times n_w = -e_{t,w}u_{pr}^- . \quad (4.38)$$

The double vector product in the above equation can be transformed by the Grassmann identity (see, e.g., Merziger and Wirth, 1999):

$$u_p^- - \frac{d_p}{2} \omega_p^- \times n_w + \frac{\hat{F}_n + \hat{F}_r}{m_p} + e_{n,w}(u_p^- \cdot n_w)n_w + \frac{5}{2} \frac{\omega_p^+ \times n_w}{m_p} \times n_w = -e_{t,w}u_{pr}^- . \quad (4.39)$$

Note that in the above equation the decomposition of the contact force in the components in the wall–normal direction and in the direction of the relative velocity are already inserted. It is obvious that the second dot product in the above equation is exactly the definition of the contact force in the wall–normal direction (see, eq. (4.28)). Hence, only $\hat{F}_r$ remains inside the big brackets on the left–hand side of eq. (4.39). Furthermore, the wall–normal contact force in the third term on the left–hand side of the above equation can be replaced by means of eq. (4.30). The result of these operations reads:

$$u_p^- - \frac{d_p}{2} \omega_p^- \times n_w - (u_p^- \cdot n_w)n_w + \frac{\hat{F}_r}{m_p} + \frac{5}{2} \frac{\omega_p^+ \times n_w}{m_p} \times n_w = -e_{t,w}u_{pr}^- . \quad (4.40)$$

After reorganizing the above equation an expression for the force vector $\hat{F}_r$ can be derived:

$$\hat{F}_r = -\frac{2}{7} \frac{m_p (1 + e_{t,w})}{u_{pr}^-} . \quad (4.41)$$

The limiting velocity for the occurrence of a non–sliding (rolling) collision can be obtained by casting eq. (4.41) and eq. (4.30) into eq. (4.31):

$$|u_{pr}^-| \leq -\frac{7}{2} \frac{m_p (1 + e_{n,w})}{(1 + e_{t,w})} \frac{u_p^- \cdot n_w}{v_{lim}} . \quad (4.42)$$

Otherwise a sliding collision takes place. Note that the condition (4.42) reduces to the former condition (4.35), when the tangential restitution coefficient $e_{t,w}$ is set to zero, i.e.,
a tangential restitution coefficient is not taken into account. In case of a sliding collision, i.e., $|\mathbf{u}_{pr}| > v_{lim}$, Coulomb’s law of friction is assumed to hold for the sliding process taking a dynamic coefficient of friction $\mu_{dy,w} \leq \mu_{st,w}$ into account. Then, the tangential contact force is calculated as follows:

$$\hat{\mathbf{F}}_r = -\mu_{dy,w} \frac{|\mathbf{u}_{pr}|}{|\mathbf{u}_{pr}|} \hat{\mathbf{F}}_n. \quad (4.43)$$

Finally, after inserting eqns. (4.41) and (4.30) in eqns. (4.27a) and (4.27b) we get for the post–collision translational and angular velocities in case of non–sliding (rolling):

$$\mathbf{u}^+ = \mathbf{u}^- - \frac{2}{7} \left( (1 + \epsilon_{t,w}) \mathbf{u}_{pr} - (1 + \epsilon_{n,w}) \left( \mathbf{u}_{p} \cdot \mathbf{n}_w \right) \mathbf{n}_w \right) \quad (4.44a)$$

$$\mathbf{\omega}^+ = \mathbf{\omega}^- + \frac{10}{7} \left( (1 + \epsilon_{t,w}) \mathbf{n}_w \times \mathbf{u}_{pr} \right) \quad (4.44b)$$

and in case of sliding using additionally eq. (4.43):

$$\mathbf{u}^+_p = \mathbf{u}_p - \frac{2}{7} \left( (1 + \epsilon_{t,w}) \mathbf{u}_{pr} - (1 + \epsilon_{n,w}) \left( \mathbf{u}_p \cdot \mathbf{n}_w \right) \mathbf{n}_w \right) \cdot \left( \mu_{dy,w} \frac{|\mathbf{u}_{pr}|}{|\mathbf{u}_{pr}|} - \mathbf{n}_w \right) \quad (4.45a)$$

$$\mathbf{\omega}^+_p = \mathbf{\omega}_p - \frac{5}{d_p} \left( (1 + \epsilon_{n,w}) \left( \mathbf{u}_p \cdot \mathbf{n}_w \right) \mu_{dy,w} \frac{|\mathbf{u}_{pr}|}{|\mathbf{u}_{pr}|} \mathbf{n}_w \times \mathbf{u}_{pr} \right). \quad (4.45b)$$

Hence, the wall collision model depends on the tangential $\epsilon_{t,w}$ and normal restitution coefficients $\epsilon_{n,w}$ as well as on the static $\mu_{st,w}$ and dynamic coefficients of friction $\mu_{dy,w}$. Unfortunately, these parameters are typically not constants but depend on the particle–wall material pairing and have to be determined experimentally (see, e.g., Foerster et al., 1994). Above a certain velocity the parameters mentioned above also depend on the impact velocity and angle (Sommerfeld and Huber, 1999). However, for the sake of simplicity and in order to keep the experimentally determined relations to a minimum only the dependence of the parameters $\epsilon_{t,w}, \epsilon_{n,w}, \mu_{st,w}$ and $\mu_{dy,w}$ on the material pairings is retained in the modeling (see, § 7).

### 4.3.2 Interaction with a Rough Wall

#### 4.3.2.1 Characterization of Rough Surfaces

Surfaces of technical devices are manufactured by different production processes (e.g. turning machines, milling cutters or honing tools) which lead to different deviations from the ideal form. According to DIN 4760:1982-06 these form deviations are classified into six categories (see, e.g., Macherauch and Zoch (2011)). Besides a general deviation (first order) and the waviness (second order) in categories 3 and 4 the roughness of the surface is specified (see Fig. 8). According to DIN 4760:1982-06 form deviations (deviation from the ideal form prescribed by the developer of the workpiece) arise from errors in guiding the machine tool, the bending of the machine or of the workpiece, etc. These

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5All standards cited in this thesis can be purchased at different web pages, e.g., http://www.din.de/, (2013) or http://webstore.ansi.org/, (2013). Unfortunately the standards are not available free of charge.

6Categories 5 and 6 denote deviations due to microstructure and the lattice structure on the molecular level. Thus, categories 5 and 6 are not considered in the wall modeling since the scope of the model is to reproduce the effect of the roughness originating by the production process on the particles.
form deviations have a regular form and are therefore not possible to be captured by the model presented below which assumes a random constitution of the surface texture. According to DIN 4760:1982-06 the waviness represents long wave structures arising from, e.g., vibrations of the machine. All waves with a ratio of the amplitude to the wavelength from 100 to 1000 lie within this category. Assuming that the amplitudes of the long waves are of the order of the sand grain roughness \( k_s \) (for the definition see below) for new steel pipes \( (k_s \approx 20 - 100 \mu m, \text{Idelchik, 1986}) \) it results in wave length of 2-10 mm. Note that the test cases with rough walls considered in this thesis have all steel walls. For the cases where the roughness model presented in the following is evaluated, this estimated wave length is of the order of the streamwise grid resolution \( \Delta z^* \) \( (\Delta z^* = 0.86 \text{ mm}, 1.5 \text{ mm and } 1.2 \text{ mm for the horizontal channel, the downward pipe and the horizontal pipe, respectively. For the test case descriptions, see } \S 7.3, \S 7.4 \text{ and } \S 7.6) \). For that reason in principle also the waviness is captured by the model since it is not resolved explicitly by the grid. Generally, roughness is considered to be the high frequency and thus short wavelength component of a measured surface. In practice, waviness and roughness are separated by filtering the scanned profile of a surface with a limiting wave length using a digital Gauss filter. Categories 3 and 4 of the form deviations arise from the direct action of the tool used to finish the workpiece (see, DIN 4760:1982-06), i.e., from the form of the cutting edge (category 3) and due to the chip formation (category 4). Thus, categories 2–4 are modeled since the model aims to represent the influence of all random and non-resolvable surface textures originated by the production process on the rebound behavior of the particles.

Figure 8: First to fourth–order deviations of the surface (DIN 4760:1982-06).

Due to its random nature (two items produced with the same manufacturing process do not show the same three–dimensional surface \( y = f(x, z) \)), it seems rather obvious that some statistical methods have to be adopted to characterize rough surfaces. A detailed description of the surface roughness is given by the power spectrum of the surface, which can be seen as the Fourier transformation of the measured elevations in an isotropic topography (see for example Bhushan; Persson et al., 2005):

\[
P(k_x) = \frac{1}{L} \left| \int_0^L y(x)e^{(ik_x x)}dx \right|^2.
\]

(4.46)

\( k_x \) represents the wave number of the measured surface and \( L \) the measuring distance. For a non–isotropic surface the power spectrum defined above gives a different spectrum depending on the direction where the measuring device is guided along. Hence, at least
a second wave number (e.g., \(k_z\)) has to be defined to account for the dependence on the measuring direction. The power spectrum provides a full description of the length scales characterizing an isotropic rough surface, but modeling the rebound behavior of the particles taking this representation of the surface into account seems to be far from trivial. Furthermore, it would require that \(P(k_z)\) is known which typically is not the case.

Contrarily, in most cases very poor information is available about the structure and the length scales describing the manufactured surfaces. Typically, solely an amplitude parameter is introduced to characterize the rough surface based on the vertical deviations of the high-pass filtered roughness profile from the mean line \(\langle y \rangle\). The most often used parameters defined in DIN EN ISO 4287:2010-07 are:

- **Peak–to–valley roughness** \(R^*_t\): Vertical difference between deepest groove and highest cusp within the entire measuring length.

- **Mean roughness** \(R^*_z\): The measuring length is divided into 5 intervals. In each interval the vertical difference between the deepest groove and the highest cusp is determined. Then \(R^*_z\) results as the average of these five measuring intervals.

- **Arithmetic average roughness** \(R^*_a\):

  \[
  R^*_a = \frac{1}{NM} \sum_{m=1}^{M} \sum_{n=1}^{N} | y^*(x^*_m, z^*_n) - \langle y^* \rangle |
  \]

  Here, \(N\) and \(M\) are the number of scanning points in \(x\)– and \(z\)–direction to measure the roughness, e.g., mechanically by a perthometer. Grooves and peaks are indistinguishable. Furthermore, \(R^*_a\) does not allow to distinguish different profile forms. Owing to the strong averaging this roughness measure is not sensitive to grooves and peaks of the surface texture (see, Fig. 9). From Fig. 9(b) (both roughness structures have the same value of \(R^*_a\)) it is evident that particles hitting the two surfaces presented will have a completely different rebound behavior. Therefore, \(R^*_a\) is not a good measure to characterize the rebound of solid particles at rough walls and should not be used (whenever possible) as a parameter in the model described in the following.

- **Root–mean–squared roughness** \(R^*_q\):

  \[
  R^*_q = \sqrt{\frac{1}{NM} \sum_{m=1}^{M} \sum_{n=1}^{N} (y^*(x^*_m, z^*_n) - \langle y^* \rangle)^2}
  \]

  The definition of \(R^*_q\) is similar to \(R^*_a\). However, \(R^*_q\) is more sensitive to grooves and peaks than \(R^*_a\). Thus, this measure of roughness is generally preferred (whenever provided) in this thesis. In practical applications often solely this quantity is given to characterize the quality of the surface. Unfortunately, the roughness characterization based on an amplitude parameter, i.e., \(R^*_t, R^*_z, R^*_a\) or \(R^*_q\), does not describe the surface topography with sufficient detail, e.g., how it influences the rebound behavior of the particles. No information is provided for example about the spacing between two peaks or about the mean slope of the asperities which influences the particle rebound behavior. As shown
in Fig. 9(a) and 9(b) surfaces with similar $R_a^*$ show a completely different topographical structure. Hence, the same particle hitting a surface with the same $R_a^*$ but a different surface structure will show a different rebound behavior.

Nevertheless, a simple and computationally cheap model using only one of the mean roughness parameters and the particle diameter $d_p^*$ as parameters was developed, which describes the influence of the randomly distributed surface asperities on the rebound behavior of the particles (see also the article published by the author of the present thesis, Breuer et al., 2012).

4.3.2.2 Wall Roughness Model for the Particles

In the following the wall model for the dispersed phase is described. Note that the following considerations are made in dimensionless form in order to be consistent with the implementation in the code LESOCC. As a starting point the classical modeling approach for the continuous phase along rough walls is briefly outlined since the roughness model for the particles relies on a similar idea.

In order to describe the roughness effect on single–phase flows, the sandgrain roughness was introduced a long time ago (Nikuradse, 1933; Schlichting, 1936). In this model it is assumed that the wall is covered by a densely packed layer of sand grains idealized by mono–disperse spheres as sketched in Fig. 10. The diameter of the spheres denotes the sandgrain roughness $k_s$. Each type of roughness appearing in technical applications can be assigned to a so–called equivalent sandgrain roughness by comparing the friction factor of the surface in question with Nikuradse’s sandgrain data, at least for the fully rough regime defined by $k_s^+ \geq 70$. Consequently, solely the influence of the sandgrain roughness on the velocity distribution in the vicinity of the wall (law of the wall) or the friction coefficient has to be considered leading for example to the well–known Nikuradse diagram (Nikuradse, 1933). In order to use these results for practical applications, a relationship between the sandgrain roughness $k_s$ and the measured root–mean–squared roughness $R_q$ of the surface under investigation is required. Shockling et al. (2006) investigated the
roughness effect in turbulent pipe flows for a wide range of Reynolds numbers, where the surface of the pipe was prepared by a honing tool. They found the equivalent sandgrain roughness to be $k_s = C_{\text{surface}} \cdot k_{\text{rms}} = C_{\text{surface}} \cdot R_q$ with $C_{\text{surface}} \approx 3$. This finding is in agreement with previous investigations by Zagarola and Smits (1998) for a surface produced by a similar honing process. For other machined or polished surfaces $C_{\text{surface}}$ may differ, see, e.g., Hama (1954) for a machined surface with an approximately Gaussian distribution of roughness elements yielding $C_{\text{surface}} \approx 5$ and Schlichting (1936) for a wide range of different surface structures. Hence this parameter expresses that an arbitrary surface needs more than one characteristic scale to describe its effect on the near–wall flow (Shockling et al., 2006). Consequently, the sandgrain wall model (for $k_s^+ \gg 1$) relies on two parameters, i.e., the root–mean–squared roughness $R_q$ which can be measured and the factor $C_{\text{surface}}$ which depends on the surface finish.

Before starting with the details of the surface roughness model, the abstraction process is described which is used to derive the sandgrain model for the particles (see, Fig. 10). The rough surface can be seen as a three–dimensional topology with valleys and mountain tops schematically sketched in Fig. 10. In order to determine the post–collision translational and angular velocities by the hard–sphere model described above, the orientation of the wall–normal vector $n_{w\text{rough}}(x, z)$ at every point $(x, z)$ on the surface is required. However, because of the random nature of the wall roughness it is not possible to determine the detailed distribution of $n_{w\text{rough}}(x, z)$. Therefore, some statistical measures have to be adopted in order to describe the topography. As already mentioned above, usually only $R_a$ or $R_q$ are provided in technical applications as the parameters describing the surface roughness. The way how one of these two parameters enters into the model is described below. In the roughness model developed in this thesis the wall inclination $\alpha_R$ is assumed to be Gaussian distributed with a mean value corresponding to the mean inclination of the flat surface and a standard deviation $\sigma_w$. $\alpha_R$ defines the angle between the normal vector $n_w$ describing the nominally smooth surface and the normal vector $n_{w\text{rough}}(x, z)$ at a given point $(x, z)$ of the rough surface. The angles $\gamma$ and $\delta^-$ in Fig. 10 denote the incidence angles of the particle trajectory regarding the wall–normal direction or the wall, respectively. $n_w$ is the normal unit vector of the smooth wall pointing outward the wall. In Fig. 10 the normal vector associated with the smooth wall is denoted as $n_w$. For a better comprehension the wall–normal vectors associated with the minimum inclination $n_1$ (mathematically negative) and also the wall–normal vector associated with the maximum inclination $n_2$ (mathematically positive) are depicted in Fig. 10.

The particles, however, do not see the full topography of the rough surface. First of all, when a particle is approaching a rough surface with an incident angle $\gamma$ (see, Fig. 10) some regions located at the lee side of the mountain are shadowed, i.e., are impossible to be reached by the particles. That means that the minimum inclination seen by the particles $n_{1s}$ is larger than the minimum inclination of the rough surface $n_1$. For that reason the mean wall–normal vector seen by the particles $\langle n_R \rangle$ is not any more equal to the mean wall–normal vector of the nominally smooth surface $n_w$. Note that the brackets $\langle \ldots \rangle$ denote the statistical average. Since the shadowed regions lie at the lee side of the rough topography, $\langle n_R \rangle$ has to be inclined towards the trajectory of the incoming particle. This effect is called shadow effect (Sommerfeld, 2000). Furthermore, also the wall–normal vector associated with the maximum inclination of the wall $n_2$ is not equal to the wall–normal vector associated with the maximum inclination seen by the particles $n_{2s}$. This fact is rather obvious since for a constant roughness small particles compared
with the roughness height (i.e., $d_p \ll R_q$) will experience the full roughness of the surface. Big particles, however, (i.e., $d_p \gg R_q$), are not able to reach the valleys of the roughness topography and hence the inclination seen by the big particles is smaller than the one seen by the small particles. For the limiting case of very big particles the wall seen is smooth.

All these modeling requirements can be satisfied by modeling the surface morphology as a carpet of smooth spheres of constant radius. Thus, the proposed model to capture the influence of the roughness on the motion of the particles is based on a similar idea as employed for the continuous phase. Figure 10 shows the model surface. $R$ denotes the radius of the spheres modeling the surface topography and establishes an analogy to the sandgrain roughness $k_s = 2R$ used to describe the effects of surface roughness on the continuous flow. Following the findings for the fluid flow that depending on the production process a surface parameter $C_{\text{surface}}$ is required to relate the sandgrain roughness $k_s$ to classical roughness parameters such as $R_q$, we obtain for the radius of the wall spheres:

$$R = \frac{k_s}{2} = \frac{1}{2} C_{\text{surface}} R_q.$$  \hspace{1cm} (4.49)

Thus based on a measured or given roughness parameter and a second parameter depending on the surface finish, the geometry of the model surface is well-defined. Instead of $R_q$ sometimes $R_z$ is provided. Owing to the lack of a general relation between both quantities, it is assumed that both are of the same order, i.e., $R_z \approx R_q$. 

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**Figure 10:** Modeling process to derive the sandgrain roughness model.
As already mentioned above the model has to achieve three tasks: First, when approaching the wall the wall–normal vector seen by the particle $\mathbf{n_R}$ not solely depends on the root–mean square roughness (represented by the sphere radius $R$) but also on the particle diameter $d_p$ and the incident angle $\gamma$. This dependency is achieved by appropriately choosing the standard deviation $\sigma_w$ of the random wall inclination. Note that the dependence on $\gamma$ is introduced by modeling the shadow effect. Second, the random nature of the wall roughness has to be accounted for by the model. This requirement is fulfilled by randomly inclining the wall–normal vector seen by the particles $\mathbf{n_R}$. As the third issue, the shadow effect explained above can be taken into account by this model geometry. The details of the realization of this three points are shown below.

The proposed model relies on the ”virtual wall” concept used by Sommerfeld and Huber (1999), Squires and Simonin (2006) and Vreman (2007). In accordance with Sommerfeld and Huber (1999) and Squires and Simonin (2006) the random wall–normal vector $\mathbf{n_R}$ is assumed to be Gaussian distributed with zero mean and a standard deviation $\sigma_w$, but with the essential difference that $\sigma_w$ is derived solely, by model intrinsic geometric relations as will be explained below. Additionally, a new normal vector $\mathbf{n_{R_{new}}}$ is calculated if the particle could not reach a shadowed region. This relation is derived, similar to $\sigma_w$, based on model inherent geometric relations. Briefly outlined, the major steps involved in the model are the following:

(I) Determination of the standard deviation $\sigma_w$ and limiting $3\sigma_w$ to $90^\circ$ for the case $d_p/2 = r_p < R$.

(II) Random inclination of the wall–normal vector $\mathbf{n_R}$ within a cone defined by the cone angle $\alpha_R$. (see Fig. 10)

(III) Check for the shadow effect.

(IV) If the shadow effect occurs, recompute the normal vector based on geometric conditions leading to $\mathbf{n_{R_{new}}}$.

After gaining a rough idea about the basic steps of the model, the single procedures are explained in more detail:

(I): The standard deviation $\sigma_w$ is obtained by casting the particle between two adjacent wall spheres (see Fig. 11). $\sigma_w$ is set equal to the angle between the original normal–vector and the straight line connecting the centers of the particle and the sphere crossing the contact point:

$$\sigma_w = \arcsin \left( \frac{R}{R + d_p/2} \right). \quad (4.50)$$

The standard deviation is limited to $30^\circ$ because $99.7\%$ of the random variables computed using a Gaussian distribution lie within $3\sigma_w$ and hence only a vanishing percentage of the computed wall–normal vectors exceed an inclination angle of $90^\circ$ describing the unrealistic scenario, where the particle hits a vertical asperity. This restriction is only active for the case that the particle is smaller than the wall spheres, i.e., $d_p/2 < R$; otherwise it is not necessary. However, for $d_p/2 < R$ the standard deviation $\sigma_w$ computed by eq. (4.50) becomes larger than $30^\circ$ which for Gaussian
distributed random numbers leads to angles $\alpha_R$ larger than 90°. Hence, in order to avoid the scenario which occurs for values of $\alpha_R \geq 90°$ where the wall–normal vector has a component directed inside the wall, the restriction mentioned above is applied. As will be shown in § 7, in practical applications often the particle radii are much larger than the radii of the wall spheres and thus the restriction is not required in these cases. Furthermore, the above formulation is purely based on geometric conditions and covers all asymptotic cases, i.e., for large particles and small $R$ the computed angles tend to zero, which is equal to the smooth wall case. Contrarily, for small particles and large $R$ the maximum computed angle does not exceed 90°, which is equal to the case where a particle hits a vertical asperity.

As will be shown in § 7, in practical applications often the particle radii are much larger than the radii of the wall spheres and thus the restriction is not required in these cases. Furthermore, the above formulation is purely based on geometric conditions and covers all asymptotic cases, i.e., for large particles and small $R$ the computed angles tend to zero, which is equal to the smooth wall case. Contrarily, for small particles and large $R$ the maximum computed angle does not exceed 90°, which is equal to the case where a particle hits a vertical asperity.

(II): The new normal vector $\mathbf{n}_R$ is computed by inclining $\mathbf{n}_w$ by the Gaussian distributed polar angle $\alpha_R$ with zero mean and standard deviation $\sigma_w$ (see, Fig. 11) and rotating it by the uniformly distributed azimuthal angle $\phi$ (see, Fig. 12) between $[0 - 2\pi]$:

$$\alpha_R = \sigma_w \xi, \quad (4.51a)$$
$$\mathbf{n}_R = \mathbf{n}_w \cos(\alpha_R) + \mathbf{t}_a \sin(\alpha_R) \cos(\phi) + \mathbf{t}_b \sin(\alpha_R) \sin(\phi). \quad (4.51b)$$

$\xi$ represents a Gaussian distributed random number with zero mean and unit standard deviation. $\mathbf{t}_a$ and $\mathbf{t}_b$ are arbitrarily chosen tangential vectors with unit length and normal to $\mathbf{n}_w$ and to each other:

$$\mathbf{t}_a = [0, n_z, -n_y] / \sqrt{n_y^2 + n_z^2}, \quad (4.52a)$$
$$\mathbf{t}_b = \mathbf{n}_w \times \mathbf{t}_a. \quad (4.52b)$$

$n_x, n_y$ and $n_z$ are the components of $\mathbf{n}_w$ in $x$–, $y$– and $z$–direction. The $x$–component of $\mathbf{t}_a$ was set arbitrarily to zero to achieve a simple expression for $\mathbf{t}_a$. The $y$– and $z$–components are chosen in such a way that the dot product $\mathbf{n}_w \cdot \mathbf{t}_a$ turns to zero, i.e., $\mathbf{n}_w \cdot \mathbf{t}_a = 0$. The resulting vector has to be scaled to unity by the factor $1/\sqrt{n_y^2 + n_z^2}$.

The result of this procedure is that $\mathbf{n}_R$ lies within a cone predefined by $\alpha_R$ (see, Fig. 10).

(III): As obvious in Fig. 13(a) a particle originally approaching the wall defined by the wall–normal vector $\mathbf{n}_w$ not always moves towards the randomly inclined surface described by $\mathbf{n}_R$, i.e., the shadow effect occurs. This scenario has to be taken into account.
account if the scalar product between the particle velocity before collision $u_p^-$ and the inclined normal vector $n_R$ is positive:

$$u_p^- \cdot n_R > 0. \quad (4.53)$$

Physically, it means that a certain region of the wall sphere is shadowed and cannot be reached by the particle (see Fig. 13).

(IV): To account for the shadow effect, we recompute $n_R$ by calculating the two possible intersection points between the straight line $x$ given by the particle trajectory and the wall sphere with radius $R$ (see Fig. 13). In the three-dimensional space the straight line $x$ can be described by the following parametric equation:

$$x = x_p + u_p^- t , \quad (4.54a)$$

with:

$$x_p = R n_R . \quad (4.54b)$$

$x_p$ describes the coordinates of the impact point $P$ of the particle on the sphere in the shadow region (see Fig. 13(b)) and $t$ is a free parameter. To obtain the second possible intersection point $S$ of the straight line with the wall sphere, we insert equation (4.54a) into the equation for the wall sphere with radius $R$. For the center of the wall sphere lying in the origin of the coordinate system (see Fig. 13(b)) one obtains:

$$(x_P + u_p^- t)^2 + (y_P + v_p^- t)^2 + (z_P + w_p^- t)^2 = R^2 . \quad (4.55)$$

The above equation has two solutions: One is the trivial solution setting $t_1 = 0$ leading to $x = x_p$. With the second solution we obtain the parameter $t_2$ to calculate the second intersection point $x_S$:

$$t_2 = -2 \frac{x_p u_p^- + y_p v_p^- + z_p w_p^-}{|u_p^-|^2} = -2 \frac{u_p^- \cdot n_R}{|u_p^-|^2} R , \quad (4.56a)$$

with:

$$x_S = x_p + u_p^- t_2 = R n_{R_{\text{new}}} . \quad (4.56b)$$

Finally, we obtain the new normal vector $n_{R_{\text{new}}}$ by dividing the above equation by $R$:

$$n_{R_{\text{new}}} = n_R - 2 \frac{(u_p^- \cdot n_R)}{|u_p^-|^2} u_p^- . \quad (4.57)$$
Thus if the shadow effect occurs, it is assumed that the particle already hits the wall sphere at the front part and consequently the associated new normal vector is predicted.

In the following considerations the notation $\mathbf{n}_R$ denotes the normal vector also in case of the shadow effect.

The above described model has a vast application area, i.e., it can be applied, whenever particle–laden flows are substantially influenced by the bounding wall. Just to mention a few, this application fields concerning gas–solid flows are the pneumatic conveying of solids or cyclone separators. Of course the roughness model can also be applied without restrictions to solid–liquid flows like the transport of sediments in hydro power plants or the flow of solid suspensions in stirred tanks.

### 4.3.3 A–priori Analysis of the Roughness Model for the Particles

In order to verify if the newly developed model fulfills the requirements stated above, i.e., the randomness, the dependence of the standard deviation $\sigma_w$ of the wall–normal vector seen by the particles $\mathbf{n}_R$ on the ratio $r_p/R$ and the reproduction of the shadow effect, the sandgrain roughness model is first analyzed based on an a-priori test without taking the fluid flow and the contact mechanics into account. Particles of different sizes characterized by the particle radius $r_p$ are fired against a flat wall with varying roughness heights defined by the radius of the wall spheres $R$. For the wall model solely the ratio $r_p/R$ between both quantities is of importance. Thus $r_p/R$ is varied between 0.1 for the case of small particles hitting a wall consisting of large roughness elements and 10 for the case of large particles hitting a wall with small roughness elements. As a second essential parameter the impact angle $\delta^-$ between the particle trajectory and the wall (see Fig. 13) is varied between $\delta^- = 10^\circ$ for a shallow path towards the wall and $\delta^- = 90^\circ$ for a perpendicular impact. As the main outcome the wall inclination angle $\alpha_R$ is analyzed which defines the direction of the normal vector $\mathbf{n}_R$ or $\mathbf{n}_{R\text{new}}$, respectively, used for the prediction of the particle path after the impact.

Fig. 14 comprises the main results of the investigation. For each case 50,000 events are evaluated statistically resulting in probability density distributions (PDF) of the wall.
inclination angle $\alpha_R$. For $r_p/R = 1$ and a normal impact (Fig. 14c) a classical Gaussian distribution with a standard deviation of $\sigma_w = 30^\circ$ results and the entire range of possible inclination angles $-90^\circ \leq \alpha_R \leq 90^\circ$ appears. Decreasing the ratio $r_p/R$ towards smaller values does not change the distribution anymore since the angles already spread over the entire possible range. However, increasing the ratio to $r_p/R = 5$ (Fig. 14f) or $r_p/R = 10$ (Fig. 14i) means that for the same roughness surface larger particles are hitting the wall. Regarding the sandgrain model it implies that the range of possible inclination angles has to become narrower as visible in the distributions depicted. For the limiting case of $r_p/R \to \infty$ the Gaussian distribution degenerates into a single peak at $\alpha_R = 0^\circ$ representing a smooth specular wall. The same trend of a narrower distribution with increasing $r_p/R$ is also visible for the other impact angles $\delta^-$ indicating that for arbitrary impact angles the model leads to the smooth wall case for $r_p/R \to \infty$. Furthermore, there are no significant differences between the distributions of the ratio $r_p/R = 5$ for $\delta^- = 30^\circ$ and $90^\circ$ (Fig. 14e and Fig. 14f). The same observation can be made for the ratio $r_p/R$ to 10 (Fig. 14h and Fig. 14i). This result can be explained considering that the shadow effect is only appearing if the maximum inclination of the normal vector $\vec{n}_R$, i.e., $3\sigma_w$, exceeds the impact angle $\delta^-$. This leads to a relation delimiting the maximum impact angle $\delta^\text{max}$ for which the occurrence of the shadow effect is possible:

$$\delta^\text{max}_- < 3\sigma_w < 3 \arcsin \left( \frac{R}{R + d_p/2} \right). \tag{4.58}$$

Inserting the ratio $r_p/R$ in the above inequation, we get $\delta^\text{max}_- = 90^\circ, 28.7^\circ$ and $15.65^\circ$ for $r_p/R = 1, 5$ and 10, respectively.

For flatter impact angles according to $\delta^- < \delta^\text{max}$ the shadow effect appears (see also Fig. 13(b)). Particles can not reach certain parts of the roughness spheres characterized by wall inclination angles $\alpha_R > \delta^-$. Thus the corresponding PDFs end abruptly at this limit as visible for example in Figs. 14a, 14b, 14d, and 14g. According to the wall model suggested, in these cases the impact between the particles and the wall is assumed to appear on the front part of the roughness element, i.e., at the first intersection point between the particle path and the roughness element (Fig. 13(b)). Consequently, the resulting PDFs of $\alpha_R$ are no longer symmetric around $\alpha_R = 0^\circ$. The arithmetic mean angle $\overline{\alpha}_R$ is negative, e.g., $\overline{\alpha}_R = -9.2^\circ$ for $r_p/R = 1$ and $\delta^- = 10^\circ$. Hence the resulting mean normal vector is inclined towards the incoming particle trajectory.

The a–posteriori analysis of the wall model will be presented in the results section. Especially for a horizontal channel flow (see, § 8.3) the model is validated with experimental measurements for a variety of wall roughnesses, particle diameters and mass loadings.

### 4.3.4 Periodic Boundary Conditions

If a particle passes a periodic boundary, it is re–inserted at the opposite side of the computational domain. That means that all particle characteristics (i.e., translational and angular velocity, density, diameter) are kept unchanged and only the coordinates normal to the periodic boundary are modified. Thus the periodicity condition can be completely fulfilled.
4.3.5 Inflow Boundary Conditions

In this thesis three different inflow conditions for the particles are used. The first method to generate inflow conditions for the particles is to run a supplementary simulation, e.g., of a pipe or a channel flow with periodic boundary conditions. Then the particle velocities, the positions in the same extracting plane as used for the fluid and the particle diameters are stored on the hard–disk for a certain time interval. The stored particles are injected at the inflow boundary of the main simulation. Similar to the fluid flow, this choice of generating the inflow boundary conditions for the particles provides a good estimation of

Figure 14: A-priori analysis of the sandgrain roughness model.
the condition at the inflow for fully developed flows. This method of generating the inflow conditions is applied for the combustion chamber flow at both mass loadings $\eta$ considered ($\eta = 22\%$ and $110\%$) computed on a coarse grid and additionally for the flow at the lower mass loading $\eta = 22\%$ computed on a fine grid (for the details of the setup see, § 7.7).

The second method to generate inflow conditions for the particulate phase is analogous to the one already described for the continuous flow in § 3.3.3.2:

$$u_{px, inflow}(x, y, z, t) = u_{px}(x, y, z, t)$$  \(4.59a\)

$$u_{py, inflow}(x, y, z, t) = u_{py}(x, y, z, t)$$  \(4.59b\)

$$u_{pz, inflow}(x, y, z, t) = \langle u_{pz, exp}(x_n, y_n, z_n) \rangle + C_{pz} \left( u_{pz}(x, y, z, t) - \langle u_{pz}(x, y, z) \rangle \right)$$  \(4.59c\)

$\langle u_{pz}(x, y, z) \rangle$ is the simulated mean particle velocity in streamwise direction at the cell center located at the point $(x, y, z)$. $\langle u_{pz}(x, y, z) \rangle$ is obtained by a one–way coupled turbulent pipe flow with the roughness model for the particles described above and with considering also the inter–particle collisions. $\langle u_{pz, exp}(x_n, y_n, z_n) \rangle$ is the measured mean streamwise particle velocity approximated by a spline with 100 supporting points. $(x_n, y_n, z_n)$ are the coordinates of the supporting points next to a cell center located at $(x, y, z)$. This method was used to further improve the inflow particle statistics for the cold flow in a model combustion chamber at $\eta = 110\%$ and using the fine grid (for the details of the setup, see § 7.7). The reason of the choice of this method to generate the inflow conditions was that it was not possible to reproduce the experimentally measured mean particle velocity profiles with appropriate second–order particle statistics by a four–way coupled turbulent pipe flow simulation with wall roughness seen by the particles and applying periodic boundary conditions. This four–way coupled LES prediction with periodic boundary conditions at a mass loading $\eta = 110\%$ showed good agreement between the simulated mean particle velocity profiles and the one measured by Borée et al. (2001). However, since for the four–way coupled simulation the fluid velocity fluctuations completely vanished, the simulated particle velocity fluctuations (especially for the smaller particles of the polydisperse diameter distribution) were to low compared to the measurements of Borée et al. (2001). Therefore, the method defined by eq. (4.59) is applied to improve the inflow condition for the high mass loading combustion chamber flow for the fine grid (see, § 7.7 for the details of the numerical setup). The constant $C_{pz} = 0.75$ is used to adjust the magnitude of the simulated velocity fluctuations in streamwise direction in order to reasonably match the data measured by Borée et al. (2001). The radial velocity fluctuations obtained by the one–way coupled simulation considering the wall roughness and the particle collisions show a good agreement with the measurements and thus have not to be adjusted (Note that no measurements of the circumferential velocity fluctuations are available). As already mentioned, this procedure was applied because it was not possible to reproduce the experimentally measured data at the inflow of the cold combustion chamber flow by a four–way coupled simulation with periodic boundary conditions. Note that the method described above can also be used to obtain particle inflow data for flows not fully developed for which a simulation with periodic boundary conditions is not adequate.

The third method is used to generate the particle inflow for the cyclone separator (see, § 7.8). Here the particles are homogeneously distributed in a volume with extension $L_{in,zy}$ normal to the cyclone inflow boundary and the velocity was set equal to the fluid velocity at the particle position (see, Fig. 15). The origin of the injection volume is set at $0.1 \, db$
downstream from the beginning of the inflow section (see, Fig. 15). $d_b$ denotes the diameter of the cyclone body (for the details of the geometry see, § 7.8). The rectangular inflow section of the cyclone is sketched in Fig. 15. The gray shaded volumes in Fig. 15 represents the volume where the particles are homogeneously distributed. The length $L_{in,zy}$ is chosen to avoid particle–free regions at the inflow section between two subsequent injections. The time span between to subsequent injections is denoted as $\Delta t_{in,zy}$. Assuming that the particles displace in the rectangular section with the constant mean velocity $U_{in}$ the length of the inflow section where the particles are injected can be calculated by $L_{in,zy} = \Delta t_{in,zy} U_{in}$. The choice of this specific boundary condition is motivated by the lag of detailed information about the design of the experimental setup upstream of the cyclone inlet. That means that if no information about the upstream conditions are available, every boundary condition applied results is a conjecture. Therefore, the computationally cheapest method is applied. Of course, also for the particles a sufficiently long developing length before entering the cyclone barrel has to be provided to ensure realistic conditions at the beginning of the zones of interest. Because of the rather small particles injected into the cyclone (for the details of the setup see, § 7.8), at a distance upstream from the cyclone barrel equal to the cyclone radius the root–mean square values of the particle velocity fluctuations reach a similar magnitude of the corresponding fluid quantity (about 10 % of the bulk velocity for each direction). Therefore, the dynamics of the particles at the entrance of the cyclone barrel should be sufficiently realistic for a turbulent flow.

\[ L_{in,zy} = U_{in} \Delta t_{in,zy} \]

**Figure 15:** Volume of the cyclone inflow section where the particles are inserted inside the domain. For the details of the geometry of the cyclone, see § 7.8.

### 4.3.6 Outflow

Since at the outflow boundary it is ensured that no back flow is present, the assumption that the particles pass the domain boundary without been swept back is fully justified. Hence, the particle crossing an outflow boundary are removed from the computational domain.
4.4 Representation of Poly–disperse Particle Size Distributions

4.4.1 Cumulative Distribution Function $Q_r(d_p^*)$ and Distribution Function $q_r(d_p^*)$

Since in practical applications like cyclone separators the disperse phase is always poly–
disperse, a meaningful description of the size distribution of the particles is required. Note
that the quantities described in the following are required in the description of the test
cases of a poly–disperse downward pipe flow (§ 7.4), a poly–disperse horizontal pipe flow
(§ 7.6), a poly–disperse flow in a model combustion chamber (§ 7.7) and a poly–disperse
flow in a cyclone separator (§ 7.8). For that purpose, the cumulative distribution functions
$Q_r(d_p^*)$ and the distribution functions $q_r(d_p^*)$ are defined in the standard DIN ISO 9276-
1:2004-09. The subscript $r$ can take the values $r = 0$, 1, 2 or 3. In Fig. 16 the example
for $Q_r(d_p^*)$ and $q_r(d_p^*)$ taken form DIN ISO 9276-1:2004-09 is shown. $d_{p,\text{min}}^*$ represents
the minimum diameter present in the size distributions $Q_r(d_p^*)$ and $q_r(d_p^*)$ and $d_{p,\text{max}}^*$ the
maximum diameter.

![Figure 16: Cumulative distribution functions $Q_r(d_p^*)$ and the distribution functions $q_r(d_p^*)$ taken from DIN ISO 9276-1:2004-09. $d_{p,\text{min}}^*$ represents the minimum diameter present in the size distributions $Q_r(d_p^*)$ and $q_r(d_p^*)$ and $d_{p,\text{max}}^*$ the maximum diameter.](image)

The number 0 stands for the number of particles, 1 for the length, 2 for the surface and
3 for the volume or mass. Relevant for this thesis are $Q_0(d_p^*)$, $q_0(d_p^*)$ as well as $Q_3(d_p^*)$
and $q_3(d_p^*)$. Furthermore, in the test cases where only $Q_3(d_p^*)$ is provided (see § 7.8.1) a
conversion of $Q_3(d_p^*)$ into $q_0(d_p^*)$ is required since $q_0(d_p^*)$ is essential in order to feed the
correct number of particles into the computational domain. The details of the conversion
are provided in § 7.8.1. The discrete version of $q_0(d_p^*)$ and $q_3(d_p^*)$ can be obtained by
dividing the particles into $N_c$ classes. Each size $i$ is described by a representative particle
diameter $d_{p,i}^*$. By the knowledge of the total number of particles $N_p$ and the number of

---

7All standards cited in this thesis can be purchased at different web pages, e.g., http://www.din.de/, (2013) or http://webstore.ansi.org/, (2013). Unfortunately, the standards are not available free of charge.
Particles $N_{p,i}$ belonging to the size class $i$, $q_0(d^*_p)$ and $q_3(d^*_p)$ can be calculated as follows:

$$q_{0,i}(d^*_p) = \frac{N_{p,i}}{N_p} = \tilde{f}_N(d^*_p) \quad (4.60a)$$

$$q_{3,i}(d^*_p) = \frac{N_{p,i} d^3_{p,i}}{\sum_{j=1}^{N_c} N_{p,i} d^3_{p,j}} = \tilde{f}_M(d^*_p). \quad (4.60b)$$

Note that in the often cited text book of Crowe et al. (1998) $q_{0,i}(d^*_p)$ is also denoted number frequency $\tilde{f}_N(d^*_p)$ and $q_{3,i}(d^*_p)$ is denoted mass frequency $\tilde{f}_M(d^*_p)$. The sum $\sum_{j=1}^{N_c} N_{p,i} d^3_{p,j}$ describes the total volume of the particles analyzed. If the right-hand side of eq. (4.60b) is multiplied by the particle density $\rho^*_p$ (in the following it is assumed that all particles have the same density), the distribution function $q_{3,i}(d^*_p)$ can be interpreted as the mass distribution function. From eq. (4.60a) it is obvious that $q_{0,i}(d^*_p)$ is the number distribution function.

The cumulative distribution functions $Q_0(d^*_p)$ and $Q_3(d^*_p)$ are calculated as follows:

$$Q_{0,i}(d^*_p) = \sum_{k=1}^{i} q_{0,k}(d^*_p) \Delta d^*_p, \quad (4.61a)$$

$$Q_{3,i}(d^*_p) = \sum_{k=1}^{i} q_{3,k}(d^*_p) \Delta d^*_p, \quad \text{with } \Delta d^*_p = d^*_p,k - d^*_p,k-1. \quad (4.61b)$$

For continuous distribution functions $Q_r(d^*_p)$ and $q_r(d^*_p)$, the following relations between these two quantities exist (see also Fig. 16 for the graphical representation):

$$q_r(d^*_p) = \frac{dQ_r(d^*_p)}{dd^*_p} \quad (4.62a)$$

$$Q_r(d^*_p) = \int_{d^*_p,min}^{d^*_p} q_r(d^*_p) \, dd^*_p. \quad (4.62b)$$

$d^*_p,min$ denotes the smallest particle diameter present in the poly-disperse distribution.

According to the definitions of Crowe et al. (1998) the following mean quantities denoted number–averaged $\overline{d^*_{p,N}}$ and mass–averaged diameter $\overline{d^*_{p,M}}$ can be determined:

$$\overline{d^*_{p,N}} = \sum_{i=1}^{N_c} d^*_{p,i} q_{0,i}(d^*_p) = \frac{1}{N_p} \sum_{i=1}^{N_c} d^*_{p,i} N_{p,i}, \quad (4.63a)$$

$$\overline{d^*_{p,M}} = \sum_{i=1}^{N_c} d^*_{p,i} q_{3,i}(d^*_p) = \frac{1}{M^*_p} \sum_{i=1}^{N_c} d^*_{p,i} M^*_{p,i}. \quad (4.63b)$$

$M^*_{p,i}$ denotes the mass of the particles belonging to the size class $i$ and $M^*_p$ is the total mass of the particles.
5 Coupling Mechanism

In the previous two sections the governing equations for the continuous phase (§ 3) and for the disperse phase (§ 4) were presented independently from each other. The scope was to provide a general overview about the modeling strategies used in LES and in the point–particles approach as stand–alone approaches. In this section the specific modeling issues pursued to couple the point particles with the continuous phase and vice versa in the framework of LES are elucidated. Since in this section the coupling mechanism are discussed, also the coupling between the particles themselves (i.e., the inter–particle collisions) are described. Thematically connected with the modeling of the particle–particle collisions, in this section the first steps towards the development of an agglomeration model for frictional particle–particle collisions are presented in § 5.4.2 as the final topic.

5.1 Fluid–Particle (One–way) Coupling

For volume fractions lower than $\Phi \leq 1 \times 10^{-6}$ (see, Fig. 2) it can be assumed that the particles neither substantially influence the fluid motion nor interact among each other. Hence, only the effect of the carrier phase on the disperse phase has to be taken into account and the motion of the particles is described by eq. (4.25). In this thesis, where the continuous phase is modeled by means of LES, the filtered velocity at the particle position $\bar{u}_f$ (of course also the gradients of $\bar{u}_f$ to calculate the lift forces) is used to calculate the aerodynamic forces displacing the particles. Consistent with the explicit time–marching scheme used in this work, first the equations of motion for the continuous phase are solved (see, eq. (3.5)). Afterwards, the fluid velocity and the gradients of the fluid velocity are interpolated at the particle position (for the interpolation schemes used see, § 6.2.1) in order to obtain the forces acting on the particles. Then eq. (4.25a) is integrated twice in time to obtain the new position of the particles in the computational domain. After that, the procedure is repeated again for the next time step. The detailed description of the integration and the numeric involved is provided in § 6.2.

5.2 Influence of the Subgrid–scale Velocity on the Particle Motion

For tiny particles with a relaxation time of the same order as the smallest fluid time scales the unresolved scales in LES become important for the particle motion. Filtering the DNS field leads, e.g., to a reduction of the particle accumulation near the channel walls (Kuerten, 2006; Marchioli et al., 2008a) or to an alteration of the preferential concentration and the particle collisions in isotropic turbulence (Ray and Collins, 2011). Hence, it is important to introduce a model which accounts for the influence of the subgrid scales to accurately reconstruct the effect of the unresolved eddies on the particle motion. As already mentioned in § 2.2.2.2, a variety of more complicated subgrid scale models compared to the one used in the present thesis exist in the literature. They can basically divided into two classes: One type of models aims to reconstruct the subgrid scales with Langevin-type equations (see, e.g., Fede et al., 2006; Bini and Jones, 2007; Pozorski and Apte, 2009; Jin et al., 2010a) and the other type of models use an approximate deconvolution to reconstruct the full (DNS) fluid field (see, e.g., Shotorban and Mashayek, 2005; Kuerten, 2006). Both types of model, however, add turbulent fluctuation in all three
Cartesian direction when applied in a turbulent channel flow (see Kuerten, 2006; Marchioli et al., 2008b). Hence, they are not able to withdraw the anisotropic effect of filtering the turbulent velocity field since it is commonly known that LES simulation predict compared to DNS reduced fluctuations in wall–normal and spanwise direction and enhanced fluctuations in streamwise direction. As similar behavior as the models mentioned above (an enhancement of the turbulent fluctuations in all Cartesian direction) can be observed for the model applied in this thesis (for the results of the model see, § 8.1). Thus, in the view of the similar behavior of the simple model used in this thesis compared to the more complicated approaches mentioned above and the reasonable agreement achieved by the model described below with DNS data (see, § 8.1), the computational cheap model proposed by Pozorski and Apte (2009) is used:

\[
\mathbf{u}_f = \mathbf{\overline{u}}_f + \mathbf{u}'_f \quad \text{with} \quad \mathbf{u}'_f = \sqrt{\frac{2}{3}k_{SGS}} \, \mathbf{\xi}. \tag{5.1}
\]

\(\mathbf{\xi}\) is a random number following a Gaussian distribution with zero mean and unit variance. \(k_{SGS}\) denotes the subgrid–scale kinetic energy, \(\mathbf{\overline{u}}_f\) the filtered velocity at the particle position and \(\mathbf{u}'_f\) the subgrid–scale velocity fluctuations. From the above relation it is obvious that the subgrid–scale velocities are assumed to be isotropic. Hence, in the equation of motion for the particles (eq. (4.25a)) the fluid velocity at the particle position is determined as a superposition of the filtered quantity resulting from the solution of the filtered Navier–Stokes equations and a random contribution mimicking the non–resolved part. For the latter the subgrid–scale kinetic energy \(k_{SGS}\) has to be determined. Some subgrid–scale models deliver this value directly. However, for the static or dynamic Smagorinsky model used here that is not the case. Thus \(k_{SGS}\) has to be estimated. The estimation of \(k_{SGS}\) used in this thesis relies on the similarity approach of Bardina et al. (1980). The similarity approach of Bardina et al. (1980) is based on the observation that the interaction of the subgrid scales and the grid scales prevalently takes place at the border between them. Because of the vicinity of the two interacting scales in the spectral space they are assumed to be similar. In order to derive a relation for the subgrid scale tensor, the full (DNS) velocity field \(\mathbf{u}_f\) is decomposed in the filtered velocity \(\mathbf{\overline{u}}_f\) and the subgrid–scale velocity \(\mathbf{u}'_f\):

\[
\mathbf{u}_f = \mathbf{\overline{u}}_f + \mathbf{u}'_f. \tag{5.2}
\]

For a better comprehension the definition of the subgrid–scale tensor \(\tau_{ij}^{SGS}\) in eq. (3.3) is recalled:

\[
\mathbf{T}^{SGS} = \mathbf{u}_f \mathbf{u}_f^T - \mathbf{\overline{u}}_f \mathbf{\overline{u}}_f^T. \tag{5.3}
\]

If we insert eq. (5.2) in the above equation, we obtain:

\[
\mathbf{T}^{SGS} = \mathbf{\overline{u}}_f \mathbf{\overline{u}}_f^T - \mathbf{\overline{u}}_f \mathbf{\overline{u}}_f^T + \mathbf{u}_f \mathbf{u}_f^T + \mathbf{u}'_f \mathbf{u}_f^T + \mathbf{u}'_f \mathbf{u}'_f^T \tag{5.4}
\]

The subgrid–scale field \(\mathbf{u}'_f\) is defined as:

\[
\mathbf{u}'_f = \mathbf{u}_f - \mathbf{\overline{u}}_f. \tag{5.5}
\]

If the filter operation is applied to the above equation, the greatest unresolved scales are obtained:

\[
\mathbf{\overline{u}}'_f = \mathbf{\overline{u}}_f - \mathbf{\overline{u}}_f. \tag{5.6}
\]
To derive a relation for the smallest resolved scales $\tilde{u}_f$, we subtract the double filtered velocity field from the filtered velocity field:

$$\tilde{u}_f = \tilde{u}_f - \bar{u}_f.$$  \hfill (5.7)

Comparing eq. (5.6) with eq. (5.7) we see they are identical. If we cast eq. (5.5) into equation (5.4) we get under the assumptions $u'_f u'_f T \approx \bar{u}_f T \bar{u}_f T$ and $\bar{u}_f T \bar{u}_f T \approx \bar{u}_f T \bar{u}_f T$:

$$\tau_{SGS} = \left( \bar{u}_f T - \bar{u}_f T \right) \approx O(\Delta^2)$$  \hfill (5.8)

The difference of the first two terms on the right-hand side of the above equation (Leonard term) are of the order $O(\Delta^2)$ (Breuer, 2002). Since the numerical scheme adopted in this work has a truncation error of the same magnitude, the term of $O(\Delta^2)$ can be neglected. If a cut-off filter with the same filter width for both filtering operations is applied, this leads to $\bar{u}_f = \bar{u}_f$. Hence, eq. (5.8) would turn to zero. For this reason a slightly coarser filter width $2\Delta$ is used for the second filtering. Thus the filtered velocity field of the fluid is filtered a second time with a test filter $\Delta = 2\Delta$ yielding the doubly-filtered fluid velocity at the particle position $\bar{u}_f$. The doubly filtered velocity $\bar{u}_f(i, j, k)$ at the cell center with the coordinate $(i, j, k)$ in the computational space (for a brief description of the computational space see, § 6) is calculate by volume averaging over the cell with the coordinate $(i, j, k)$ and all 26 surrounding control volumes:

$$\bar{u}_f(i, j, k) = w_1 \bar{u}_f|_{i,j,k} +$$

$$w_2 \left( \bar{u}_f|_{i+1,j,k} + \bar{u}_f|_{i-1,j,k} + \bar{u}_f|_{i,j+1,k} + \bar{u}_f|_{i,j-1,k} + \bar{u}_f|_{i,j,k+1} + \bar{u}_f|_{i,j,k-1} \right) +$$

$$w_3 \left( \bar{u}_f|_{i+1,j,k+1} + \bar{u}_f|_{i-1,j,k+1} + \bar{u}_f|_{i,j+1,k+1} + \bar{u}_f|_{i,j,k+1} + \bar{u}_f|_{i+1,j,k-1} + \bar{u}_f|_{i-1,j,k-1} + \bar{u}_f|_{i,j+1,k-1} + \bar{u}_f|_{i,j,k-1} \right) +$$

$$w_4 \left( \bar{u}_f|_{i+1,j+1,k+1} + \bar{u}_f|_{i+1,j-1,k+1} + \bar{u}_f|_{i+1,j-1,k+1} + \bar{u}_f|_{i+1,j-1,k+1} + \bar{u}_f|_{i+1,j-1,k+1} + \bar{u}_f|_{i+1,j-1,k+1} \right).$$  \hfill (5.9)

$w_1$, $w_2$, $w_3$ and $w_4$ are weighting factors and are equal to $w_1 = 1/8$, $w_2 = 1/16$, $w_3 = 1/32$ and $w_4 = 1/64$. For the prediction of $k_\text{SGS}$ the trace of eq. (5.8) is taken and multiplied by $1/2$. Hence, the estimation of $k_\text{SGS}$ reads:

$$k_{SGS} = \frac{1}{2} (\bar{u}_f \cdot \bar{u}_f - \bar{u}_f \cdot \bar{u}_f).$$  \hfill (5.10)

Note that presently the values of $k_\text{SGS}$ are not interpolated at the particle position but for each particle contained in a computational cell the value of $k_\text{SGS}$ computed at the cell center is used.

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For volume fractions between $1 \times 10^{-6} \leq \Phi \leq 1 \times 10^{-3}$ (see, Fig. 2) the effect of the disperse phase on the carrier phase becomes important and therefore it has to be taken into account. In order to consider the influence of the particles on the fluid motion, the particle-source-in-cell (PSIC) method described in Crowe et al. (1977) is used. It relies on Newton’s third law (action equals reaction). That means that the forces displacing the particles are calculated following eq. (4.25a) (of course the acceleration has to be multiplied by the particle mass), inverted in the sign and casted into the equations for the continuous phase. This leads to a modified filtered Navier–Stokes equation with an additional source term representing the forces exerted by the particles onto the fluid. In the present version of the code used, only the drag force calculated by means of the filtered fluid and particle velocity is considered. The reason is that all other aerodynamic forces of eq. (4.25a) are typically at least one order of magnitude smaller. This leads to the following dimensionless source term in the momentum equation:

$$f_{PSIC}^i = -\sum_{j=1}^{N_p} I_{parcel} F_{D,ij} \Delta V_{ol} = -\sum_{j=1}^{N_p} I_{parcel} \frac{3 \pi d_p}{\Delta V_{ol} \alpha \Re} (u_{f,ij} - u_{p,ij}). \quad (5.11)$$

In the above equation the index $i$ denotes the Cartesian component of the quantities and $j$ is the summation index. $\Delta V_{ol}$ denotes the volume of the computational cell and $\Re$ the Reynolds number of the fluid. $N_p$ represents the number of parcels contributing to the forces in the cell and $I_{parcel}$ is the number of particles grouped in a parcel. For $I_{parcel} = 1$ the parcel concept is practically switched off and the influence of the momentum carried by the particles on the fluid is predicted directly. Nevertheless, the parcel approach makes sense under certain circumstances. In order to avoid high computational costs associated with tracking a huge number of particles through the computational domain but still accounting for the two–way coupling, $I_{parcel}$ is set to a number greater than unity by keeping the diameter and the density of the particles fixed. In this way the aerodynamic properties of the parcels are equal to the aerodynamic properties of the single particles composing the parcels. Thus, for a sufficiently high number of parcels tracked, the statistical moments of the parcels should be similar to the statistical moments of all particles represented by the parcel. The reason is that by keeping the aerodynamic properties of the parcels unchanged respect to the particles composing it, their response to the turbulent flow should be similar. Hence, also the statistics computed by tracking the parcels through the computational domain should not differ substantially from the statistics computed by tracking each single particle. Thus in the one–way coupled regime no substantial differences can be expect (of course for a sufficiently high number of parcels) between the moments computed by means of the parcel approach and the moments computed by tracking each particle through the domain. Of course if unsteady phenomena are of interest (e.g., the temporal evolution of the particle concentration) the parcel concept is in the view of the author probably not the appropriate method of choice since a parcel is only a statistical ensemble of the particles composing it (see also, Apte et al., 2003a). The influence of the true mass loading is accounted for by the factor $I_{parcel}$ which is multiplied with the force required to displace the parcel. Regarding the two–way coupling regime differences between applying the parcel method and tracking each particle can be expected already in the achieved statistical moments of the fluid. In the view of the author the response of the turbulent eddies to one parcel or the number of particles represented by a parcel
should be different. For example a streamwise vortex located closed to a wall would be influenced in a different way by one parcel rather than, e.g., a few hundreds of particles distributed around the same vortex. Note that in all simulation performed in this thesis except the flow in a cyclone separator (see, § 7.8 for the setup) \( I_{\text{parcel}} \) is set to unity since the amount of particles required to be located in the computational domain in order to achieve the same mass loading as the reference experiment does not constitute a problem from the point of view of the computational costs. This is the result of the very efficient particle tracking scheme. Regarding the amount of particles grouped in a parcel for the cyclone separator see, § 7.8.

In order to calculate the sum in eq. (5.11) the following procedure is adopted: First the fluid velocity is interpolated to the particle position using the interpolation scheme suggested by Marchioli et al. (2007a) in order to calculate the drag force (for the details of the interpolation scheme see, § 6.2.1.2). As a second step the force is distributed to the eight cell centers surrounding the particle by means of a trilinear interpolation in order to achieve a smooth source term distribution (for the details of the trilinear interpolation scheme see, § 6.2.1.1). The smooth source term distribution is introduced in order to avoid the convergence problems associated with isolated large source terms. The resulting momentum equation for the continuous phase can be written as follows:

\[
\frac{\partial \vec{u}}{\partial t} + \frac{\partial (\vec{u} \cdot \vec{u})}{\partial x_j} = -\frac{\partial p}{\partial x_i} - \frac{1}{\text{Re}} \frac{\partial \tau_{ij}^{\text{mol}}}{\partial x_j} - \frac{\partial \tau_{ij}^{\text{SGS}}}{\partial x_j} + f_i^{\text{PSIC}}. \tag{5.12}
\]

### 5.4 Particle–Particle (Four–Way) Coupling

For a volume fraction \( \Phi \geq 10^{-3} \) (see, Fig. 2) the mean spacing between the particles becomes smaller and therewith connected also the time span between two particle–particle interactions decreases. Especially for rather inertial particles which hardly adjust to the fluid motion between two subsequent collisions, accounting for this coupling mechanism is indispensable to obtain reliable results.

#### 5.4.1 Model for the Particle Collisions

The particle–particle collisions are taken into account by a standard hard–sphere collision model including friction as found in text books (see, e.g., Crowe et al., 1998). As for the wall collision model (see § 4.3.1) the particles are assumed to be homogeneous and the contact time to be small compared with the time step used in LES. Furthermore, only binary collisions are considered. The configuration of two colliding smooth spherical particles is sketched in Fig. 17.

With the aforementioned assumptions the governing equations can be derived from the conservation equation of translational and angular momentum of classical mechanics assuming infinitesimal short contact times and negligible deformations:

\[
m_{p,1} (u_{p,1}^+ - u_{p,1}^-) = -\hat{F} \tag{5.13a}
\]

\[
m_{p,2} (u_{p,2}^+ - u_{p,2}^-) = \hat{F} \tag{5.13b}
\]

\[
I_{p,1} (\omega_{p,1}^+ - \omega_{p,1}^-) = -r_1 \times \hat{F} = -\frac{d_{p,1}}{2} (n_c \times \hat{F}) \tag{5.13c}
\]

\[
I_{p,2} (\omega_{p,2}^+ - \omega_{p,2}^-) = r_2 \times \hat{F} = -\frac{d_{p,2}}{2} (n_c \times \hat{F}). \tag{5.13d}
\]
Figure 17: Sketch of the binary particle–particle collision and the definitions used.

\( \hat{F} \) is the integral of the contact force over the collision time. \( \mathbf{r}_1 \) and \( \mathbf{r}_2 \) are the vectors from the center of the first (\( S_1 \)) and second particle (\( S_2 \)) to the contact point \( B \), respectively (see, Fig. 17):

\[
\mathbf{r}_1 = \frac{d_{p,1}}{2} \mathbf{n}_c \\
\mathbf{r}_2 = -\frac{d_{p,2}}{2} \mathbf{n}_c. \tag{5.14a/5.14b}
\]

The collision–normal vector \( \mathbf{n}_c \) is defined as the vector pointing from the center of particle 1 to the center of particle 2 (see Fig. 17):

\[
\mathbf{n}_c = \frac{\mathbf{x}_{p,2} - \mathbf{x}_{p,1}}{|\mathbf{x}_{p,2} - \mathbf{x}_{p,1}|} = \frac{2(\mathbf{x}_{p,2} - \mathbf{x}_{p,1})}{d_{p,1} + d_{p,2}}. \tag{5.15}
\]

\( d_{p,1} \) and \( d_{p,2} \) are the diameters of the first and the second particle, respectively. \( \mathbf{x}_{p,2} \) and \( \mathbf{x}_{p,1} \) are the coordinates of the centers of the two colliding particles at the time of contact.

Since the collision detection procedure and therefore also the determination of the exact coordinates of the particles at the contact time is in the view of the author a numerical issue, the details of the determination of \( \mathbf{x}_{p,2} \) and \( \mathbf{x}_{p,1} \) are described in § 6.2.3. As in § 4.3.1 the superscript – denotes the quantities before the collision and the superscript + denotes the quantities after the collision. At this point eqs. (5.13) are reorganized for a better comprehension of the derivation of the contact force in tangential direction.
described in the following (note that $I_p = 1/10 \ m_p d_p^2$):

\begin{align}
\mathbf{u}_{p,1}^+ & = \mathbf{u}_{p,1} - \frac{\hat{\mathbf{F}}}{m_{p,1}} \quad (5.16a) \\
\mathbf{u}_{p,2}^+ & = \mathbf{u}_{p,2} + \frac{\hat{\mathbf{F}}}{m_{p,2}} \quad (5.16b) \\
\omega_{p,1}^+ & = \omega_{p,1} - \frac{5}{m_{p,1} d_{p,1}} (\mathbf{n}_c \times \hat{\mathbf{F}}) \quad (5.16c) \\
\omega_{p,2}^+ & = \omega_{p,2} - \frac{5}{m_{p,2} d_{p,2}} (\mathbf{n}_c \times \hat{\mathbf{F}}) \quad (5.16d)
\end{align}

For the determination of the post–collision quantities the contact force $\hat{\mathbf{F}}$ has to be expressed as a function of pre–collision (known) quantities. To perceive this goal $\hat{\mathbf{F}}$ is divided into a component normal $\hat{\mathbf{F}}_n$ and a component $\hat{\mathbf{F}}_r$ opposite to the relative velocity $\mathbf{u}_{pr}$ of the contact point $B$ (see, Fig. 17). Decomposing the impact force leads to:

\[ \hat{\mathbf{F}} = \hat{\mathbf{F}}_n + \hat{\mathbf{F}}_r \quad \text{with} \quad \hat{\mathbf{F}}_n \mathbf{n}_c = (\hat{\mathbf{F}} \cdot \mathbf{n}_c) \mathbf{n}_c. \quad (5.17) \]

In a similar way as done for the particle–wall collisions described in § 4.3.1 the normal component of eqs. (5.16a)–(5.16b) can be decoupled from the component in the direction of $\mathbf{u}_{pr}$. This can be achieved by inserting eq. (5.17) into eqs. (5.16a)–(5.16b), reorganizing the resulting equations with respect to $-\hat{F}_n/m_{p,1}$ and $\hat{F}_n/m_{p,2}$. After that the scalar product of both equations with the normal vector $\mathbf{n}_c$ is taken. This procedure leads to the following equations:

\begin{align}
-\frac{\hat{F}_n}{m_{p,1}} & = (\mathbf{u}_{p,1}^+ - \mathbf{u}_{p,1}^-) \cdot \mathbf{n}_c \quad (5.18a) \\
\frac{\hat{F}_n}{m_{p,2}} & = (\mathbf{u}_{p,2}^+ - \mathbf{u}_{p,2}^-) \cdot \mathbf{n}_c. \quad (5.18b)
\end{align}

To get the final expression for the contact force in normal direction, we recall the definition of the normal restitution coefficient:

\[ e_{n,p} = -\frac{(\mathbf{u}_{p,2}^- - \mathbf{u}_{p,1}^-) \cdot \mathbf{n}_c}{(\mathbf{u}_{p,2}^- - \mathbf{u}_{p,1}^-) \cdot \mathbf{n}_c}. \quad (5.19) \]

The values of $e_{n,p}$ lie within the values of zero for a perfectly inelastic collision and unity for a perfectly elastic collision. After subtracting eq. (5.18a) from eq. (5.18b) and using eq. (5.19), we get the contact force in normal direction:

\[ \hat{F}_n = -\frac{m_{p,1} m_{p,2}}{(m_{p,1} + m_{p,2})} (1 + e_{n,p})(\mathbf{u}_{p,2}^- - \mathbf{u}_{p,1}^-) \cdot \mathbf{n}_c. \quad (5.20) \]

In order to calculate $\hat{\mathbf{F}}_r$, the tangential velocity of both particles at the contact point $B$ $\mathbf{u}_{Bt}$ is required. $\mathbf{u}_{Bt}$ is obtained by simple solid body kinematics, i.e., by subtracting the normal component of the particle velocity from the total particle velocity at the contact point.
point $B$:

$$
\mathbf{u}_{Bt,1} = \mathbf{u}_{p,1} + \omega_{p,1} \times \frac{d_{p,1}}{2} \mathbf{n}_c - \left( \frac{\mathbf{u}_{p,1} \cdot \mathbf{n}_c}{\mathbf{n}_c} \right) \mathbf{n}_c \quad (5.21a)
$$

$$
\mathbf{u}_{Bt,2} = \mathbf{u}_{p,2} - \omega_{p,2} \times \frac{d_{p,2}}{2} \mathbf{n}_c - \left( \frac{\mathbf{u}_{p,2} \cdot \mathbf{n}_c}{\mathbf{n}_c} \right) \mathbf{n}_c \quad (5.21b)
$$

Note that in eq. (5.21b) the sign before the angular velocity is inverted with respect to eq. (5.21a) because the normal vector $\mathbf{n}_c$ points in the direction of $\mathbf{r}_1$ but in the opposite direction of $\mathbf{r}_2$ (see eqs. (5.14), eq. (5.15) and also Fig. 17). The relative velocity of the two particles at the contact point $\mathbf{u}_{pr}$ is calculated by subtracting eq. (5.21a) from eq. (5.21b):

$$
\mathbf{u}_{pr} = \mathbf{u}_{Bt,2} - \mathbf{u}_{Bt,1} = \mathbf{u}_{p,2} - \mathbf{u}_{p,1} - \left[ \left( \mathbf{u}_{p,2} - \mathbf{u}_{p,1} \right) \cdot \mathbf{n}_c \right] \mathbf{n}_c - \left( \frac{d_{p,2}}{2} \omega_{p,2} + \frac{d_{p,1}}{2} \omega_{p,1} \right) \times \mathbf{n}_c.
$$

(5.22)

Having defined the two possible directions where the contact forces act, also for the particle–particle collision it has to be distinguished if the particles are sliding throughout the collision period (sliding case) or if they stop sliding at some time during the collision (non-sliding or sticking case).

For the sliding case Coulomb’s law of sliding friction is assumed by introducing a dynamic coefficient of friction $\mu_{dy,p}$. The contact force is therefore assumed to be proportional to normal force $\mathbf{F}_n$ and directed in the opposite direction of the relative velocity before the collision $\mathbf{u}_{pr}$. In this way the contact force $\mathbf{F}_r$ reads:

$$
\mathbf{F}_{r,sl} = -\mu_{dy,p} |\mathbf{F}_n| \frac{\mathbf{u}_{pr}^-}{|\mathbf{u}_{pr}^-|} = \frac{m_{p,1} m_{p,2}}{(m_{p,1} + m_{p,2})} \mu_{dy,p} (1 + e_{n,p}) (\mathbf{u}_{p,2}^- - \mathbf{u}_{p,1}^-) \cdot \mathbf{n}_c \frac{\mathbf{u}_{pr}^-}{|\mathbf{u}_{pr}^-|}. \quad (5.23)
$$

Note that $(\mathbf{u}_{p,2}^- - \mathbf{u}_{p,1}^-) \cdot \mathbf{n}_c$ is per definition negative. For the non-sliding or sticking collision another constitutive relation to determine the contact force in tangential direction has to be found. In this case the tangential restitution coefficient $e_{t,p}$ is introduced:

$$
e_{t,p} = -\frac{\mathbf{u}_{p,2}^-}{|\mathbf{u}_{pr}^-|}. \quad (5.24)$$

The above equation has to be seen as a kinematic condition to determine the contact force $\mathbf{F}_r$ in case of sticking. The values of $e_{t,p}$ lie within zero and unity. For a value of zero it means that the two colliding particle have a zero relative motion after the collision, i.e., the particle are rolling. For values greater than zero the relative velocity of the particle after the collision is inverted in the sign.

With the aid of eq. (5.22) we get by using eq. (5.24):

$$
\mathbf{u}_{p,2}^+ - \mathbf{u}_{p,1}^+ - \left[ \left( \mathbf{u}_{p,2}^+ - \mathbf{u}_{p,1}^+ \right) \cdot \mathbf{n}_c \right] \mathbf{n}_c - \left( \frac{d_{p,2}}{2} \omega_{p,2}^+ + \frac{d_{p,1}}{2} \omega_{p,1}^+ \right) \times \mathbf{n}_c =
$$

$$
-\epsilon_{t,p} \left\{ \mathbf{u}_{p,2}^- - \mathbf{u}_{p,1}^- - \left[ \left( \mathbf{u}_{p,2}^- - \mathbf{u}_{p,1}^- \right) \cdot \mathbf{n}_c \right] \mathbf{n}_c - \left( \frac{d_{p,2}}{2} \omega_{p,2}^- + \frac{d_{p,1}}{2} \omega_{p,1}^- \right) \times \mathbf{n}_c \right\}. \quad (5.25)
$$

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Now, in order to bring the contact force into the above relation, the particle translational and angular velocity after the collision have to be expressed as a function of the same quantities before the collision and the contact force. The difference of the particle translational velocities after the collision \( \mathbf{u}_{p,2}^+ - \mathbf{u}_{p,1}^+ \) are obtained by subtracting eq. (5.16a) from eq. (5.16b):

\[
\mathbf{u}_{p,2}^+ - \mathbf{u}_{p,1}^+ = \frac{m_{p,1} + m_{p,2}}{m_{p,1} m_{p,2}} \left( \mathbf{\hat{F}}_n + \mathbf{\hat{F}}_r \right) + \mathbf{u}_{p,2}^- - \mathbf{u}_{p,1}^-.
\] (5.26)

Note that the decomposition (5.17) of the contact force \( \mathbf{\hat{F}} \) was used to determine the above relation. The term \( d_{p,2}/2 \omega_{p,2}^+ + d_{p,1}/2 \omega_{p,1}^+ \) in eq. (5.25) is obtained by multiplying eq. (5.16c) with \( d_{p,1}/2 \) and multiplying eq. (5.16d) multiplying with \( d_{p,2}/2 \). After that the two equations manipulated in this way are summed. The result reads:

\[
\frac{d_{p,2}}{2} \omega_{p,2}^- + \frac{d_{p,1}}{2} \omega_{p,1}^- = \frac{d_{p,2}}{2} \omega_{p,2}^- + \frac{d_{p,1}}{2} \omega_{p,1}^- - \frac{5}{2} \frac{m_{p,1} + m_{p,2}}{m_{p,1} m_{p,2}} \left( \mathbf{n}_c \times (\mathbf{\hat{F}}_n + \mathbf{\hat{F}}_r) \right).
\] (5.27)

Note that the cross product \( \mathbf{n}_c \times \mathbf{\hat{F}}_n \) is equal to zero since both vectors are parallel.

Equations (5.26) and (5.27) can be inserted into eq. (5.25) and we get:

\[
\frac{m_{p,1} + m_{p,2}}{m_{p,1} m_{p,2}} \left( \mathbf{\hat{F}}_n + \mathbf{\hat{F}}_r \right) + \mathbf{u}_{p,2}^- - \mathbf{u}_{p,1}^- + \left[ (\mathbf{u}_{p,1}^+ - \mathbf{u}_{p,2}^+) \cdot \mathbf{n}_c \right] \mathbf{n}_c \\
- \left( \frac{d_{p,2}}{2} \omega_{p,2}^- + \frac{d_{p,1}}{2} \omega_{p,1}^- \right) \times \mathbf{n}_c + \frac{5}{2} \frac{m_{p,1} + m_{p,2}}{m_{p,1} m_{p,2}} \left( \mathbf{n}_c \times \mathbf{\hat{F}}_r \right) \times \mathbf{n}_c = -\epsilon_{t,p} \mathbf{u}_{p,r}^-.
\] (5.28)

The triple vector product at the left–hand side of the above equation can be further simplified with the aid of the Grassmann identity to \( 5/2 (m_{p,1} + m_{p,2})/(m_{p,1} m_{p,2}) \mathbf{\hat{F}}_r \) (for the definition of the Grassmann identity see, e.g., Merziger and Wirth, 1999, or Appendix A). Furthermore, the velocity difference in normal direction after the collision can be expressed as a function of the velocities before the collision with help of eq. (5.19). The result reads:

\[
\frac{m_{p,1} + m_{p,2}}{m_{p,1} m_{p,2}} \left( \mathbf{\hat{F}}_n + \mathbf{\hat{F}}_r \right) + \mathbf{u}_{p,2}^- - \mathbf{u}_{p,1}^- + \left[ \epsilon_{n,p} (\mathbf{u}_{p,2}^- - \mathbf{u}_{p,1}^-) \cdot \mathbf{n}_c \right] \mathbf{n}_c \\
- \left( \frac{d_{p,2}}{2} \omega_{p,2}^- + \frac{d_{p,1}}{2} \omega_{p,1}^- \right) \times \mathbf{n}_c + \frac{5}{2} \frac{m_{p,1} + m_{p,2}}{m_{p,1} m_{p,2}} \mathbf{\hat{F}}_r = -\epsilon_{t,p} \mathbf{u}_{p,r}^-.
\] (5.29)

The contact force \( \mathbf{\hat{F}}_n \) required in the above equation is obtained by multiplying eq. (5.20) with the normal vector \( \mathbf{n}_c \) (see, also eq. (5.17)). By inserting the so obtained contact force in normal direction in the above equation the normal restitution coefficient \( \epsilon_{n,p} \) can
be eliminated. The result reads:

\[
\frac{m_{p,1} + m_{p,2}}{m_{p,1}m_{p,2}} \vec{F}_r + \vec{u}_{p,2} - \vec{u}_{p,1} - \left( (\vec{u}_{p,2} - \vec{u}_{p,1}) \cdot \vec{n}_c \right) \vec{n}_c - \left( \frac{d_{p,2}}{2} \omega_{p,2} + \frac{d_{p,1}}{2} \omega_{p,1} \right) \times \vec{n}_c \\
+ \frac{5}{2} \frac{m_{p,1} + m_{p,2}}{m_{p,1}m_{p,2}} \vec{F}_r = -\epsilon_{t,p} \vec{u}_{pr}
\]

(5.30)

Note that the summation of the second until the fourth term in the above equation is equal to the definition of the relative velocity in the contact point before the collision \( \vec{u}_{pr} \) (see, eq. (5.22)). After reorganizing the above equations with respect to \( \vec{F}_r \) the contact force in case of sticking \( \vec{F}_{r,st} \) is obtained:

\[
\vec{F}_{r,st} = \frac{2}{l} \frac{m_{p,1}m_{p,2}}{m_{p,1} + m_{p,2}} (1 + \epsilon_{t,p}) \vec{u}_{pr}.
\]

(5.31)

To decide whether a sliding or sticking collision occurs, the condition introduced by Coulomb for static friction is used. Therefore, if the condition

\[
|\vec{F}_{r,st}| \leq \mu_{st,p} |\vec{F}_n|
\]

(5.32)

is fulfilled the particles stop sliding during the collision. By casting eqs. (5.31) and (5.20) into the above expression the range of possible relative velocities

\[
|\vec{u}_{pr}| \leq \frac{7}{2} \mu_{st,p} \frac{1 + \epsilon_{n,p}}{1 + \epsilon_{t,p}} (\vec{u}_{p,2} - \vec{u}_{p,1}) \cdot \vec{n}_c
\]

(5.33)

for the occurrence of a sticking collision is obtained. Note that the minus sign in the above equation can be retained since \((\vec{u}_{p,2} - \vec{u}_{p,1}) \cdot \vec{n}_c\) is per definition negative for two approaching particles. Non–approaching particles are disregarded a–priori by the collision detection algorithm (see, § 6.2.3). Therefore, it is not required to apply the modulus operation to the right–hand side of eq. (5.33) since the value is always positive.

Briefly summarized the collision model for the particle works as follows:

(I) After ensuring that two particles collide (for the collision detection algorithm see § 6.2.3) condition (5.33) is checked.

(II) If condition (5.33) is fulfilled a sticking collision occurs and contact forces \( \vec{F}_{r,st} \) (see, eq. (5.31)) and \( \vec{F}_n \) (see, eq. (5.20)) are inserted into eq. (5.16) in order to determine
the particle post-collisional translational and angular velocities:

\[
\begin{align*}
\mathbf{u}^+_{p,1} & = \mathbf{u}_{p,1} + \frac{m_{p,2}}{m_{p,1} + m_{p,2}} \left\{ (1 + e_{n,p}) \left[ (\mathbf{u}^-_{p,2} - \mathbf{u}^-_{p,1}) \cdot \mathbf{n}_c \right] \mathbf{n}_c + \frac{2}{7} (1 + e_{t,p}) \mathbf{u}_{p,pr} \right\} \\
\mathbf{u}^+_{p,2} & = \mathbf{u}^-_{p,2} - \frac{m_{p,1}}{m_{p,1} + m_{p,2}} \left\{ (1 + e_{n,p}) \left[ (\mathbf{u}^-_{p,2} - \mathbf{u}^-_{p,1}) \cdot \mathbf{n}_c \right] \mathbf{n}_c + \frac{2}{7} (1 + e_{t,p}) \mathbf{u}_{p,pr} \right\} \\
\omega^+_{p,1} & = \omega^-_{p,1} + \frac{10}{7 \, d_{p,1}} \frac{m_{p,2}}{(m_{p,1} + m_{p,2})} (1 + e_{t,p}) \left( \mathbf{n}_c \times \mathbf{u}_{p,pr} \right) \\
\omega^+_{p,2} & = \omega^-_{p,2} + \frac{10}{7 \, d_{p,2}} \frac{m_{p,1}}{(m_{p,1} + m_{p,2})} (1 + e_{t,p}) \left( \mathbf{n}_c \times \mathbf{u}_{p,pr} \right).
\end{align*}
\] (5.34a, 5.34b, 5.34c, 5.34d)

(III) If condition (5.33) is not fulfilled a sliding collision occurs and contact force \( \hat{\mathbf{F}}_{r,sl} \) (see, eq. (5.23)) and \( \hat{\mathbf{F}}_{n} \) (see, eq. (5.20)) are inserted into eq. (5.16) in order to determine the particle post-collisional state:

\[
\begin{align*}
\mathbf{u}^+_{p,1} & = \mathbf{u}_{p,1} + \frac{m_{p,2}}{m_{p,1} + m_{p,2}} (1 + e_{n,p}) \left[ (\mathbf{u}^-_{p,2} - \mathbf{u}^-_{p,1}) \cdot \mathbf{n}_c \right] \left( \mathbf{n}_c - \mu_{dy,p} \frac{\mathbf{u}_{p,pr}}{|\mathbf{u}_{p,pr}|} \right) \\
\mathbf{u}^+_{p,2} & = \mathbf{u}^-_{p,2} - \frac{m_{p,1}}{m_{p,1} + m_{p,2}} (1 + e_{n,p}) \left[ (\mathbf{u}^-_{p,2} - \mathbf{u}^-_{p,1}) \cdot \mathbf{n}_c \right] \left( \mathbf{n}_c - \mu_{dy,p} \frac{\mathbf{u}_{p,pr}}{|\mathbf{u}_{p,pr}|} \right) \\
\omega^+_{p,1} & = \omega^-_{p,1} - \frac{5}{d_{p,1}} \mu_{dy,p} \frac{m_{p,2}}{(m_{p,1} + m_{p,2})} (1 + e_{n,p}) \left[ (\mathbf{u}^-_{p,2} - \mathbf{u}^-_{p,1}) \cdot \mathbf{n}_c \right] \left( \mathbf{n}_c \times \frac{\mathbf{u}_{p,pr}}{|\mathbf{u}_{p,pr}|} \right) \\
\omega^+_{p,2} & = \omega^-_{p,2} - \frac{5}{d_{p,2}} \mu_{dy,p} \frac{m_{p,1}}{(m_{p,1} + m_{p,2})} (1 + e_{n,p}) \left[ (\mathbf{u}^-_{p,2} - \mathbf{u}^-_{p,1}) \cdot \mathbf{n}_c \right] \left( \mathbf{n}_c \times \frac{\mathbf{u}_{p,pr}}{|\mathbf{u}_{p,pr}|} \right).
\end{align*}
\] (5.35a, 5.35b, 5.35c, 5.35d)

Note that the coefficients \( e_{n,p}, e_{t,p}, \mu_{dy,p} \) and \( \mu_{st,p} \) are empirical constants and have to be determined experimentally (see, e.g., Foerster et al., 1994; Serway and Vuille, 2006).

### 5.4.2 Agglomeration Model

Many industrial applications deal with the turbulent transport of tiny particles, e.g., the transport of powders by means of pneumatic conveying systems, fluidized bed combustion or the separation of solids from the gaseous phase in cyclone separators. Especially for particle ranging from about 1–10 \( \mu \text{m} \) (diameter) the agglomeration of particles is an important mechanism influencing the particle dynamics (Ho and Sommerfeld, 2002). Particle agglomeration can have a beneficial effect during the operation of industrial devices. For example, in cyclone separators agglomeration lead to greater particle diameters and
therefore the separation efficiency can be enhanced (Obermair et al., 2005). On the other hand, avalanching effects (the sudden onset of motion of powders) and oscillating mass flow rates associated with particle agglomeration lead to feeding and dosing problems in apparatuses conveying powders (Tomas, 2007). Therefore, in order to exploit the beneficial or prevent the negative effects of particle agglomeration in industrial devices, it is important to reliably predict this phenomenon in turbulent flows.

In this section the first steps in developing an agglomeration model valid for the general case of frictional collisions between spherical particles is described. The model involving only collisions without friction is first described in § 5.4.2.3 and is preceded by a brief introduction into the van–der–Waals forces in § 5.4.2.1 and the special case of agglomeration during head–on collisions in § 5.4.2.2. The scope of the aforementioned sections is to give the reader an overview about the methodology used to derive the criterion for the occurrence of an agglomeration between solid particles. Finally, in § 5.4.2.5 a first proposal of a model to define a criterion of the occurrence of agglomeration for the general case of collisions with friction is given. The basic assumptions made in this stage of the development of the model are the following:

(I) Only particle–particle collisions of spherical particles are considered.

(II) Only van–der–Waals forces are responsible for the sticking of two dry particles after a collision. The influence of other forces such as electrostatic charges or the formation of liquid bridges between particles are neglected.

(III) Only small deformations of the particles are allowed.

(IV) The criterion to decide whether an agglomeration occurs or not can be stated by purely energetic considerations.

(V) The dissipated energy can be described using the relations derived in § 5.4.1. That means that it can be expressed solely by pre–collision quantities and is independent of the van–der–Waals forces.

5.4.2.1 Van der Waals Interaction

In this section the theoretical foundation of the van–der–Waals interaction and the derivation of the attractive forces between two bodies required in § 5.4.2.2 are briefly described. For an extended overview see, for example, Israelachvili (2011).

The attractive energy (or potential) $e^{vW}_*\lambda$ between two molecules due to the van–der–Waals force is assumed to be proportional to the distance between the molecules to the power of minus six:

$$e^{vW}_* = -\frac{\lambda}{\delta^6}.$$  \hspace{1cm} (5.36)

$\lambda$ is the London–van–der–Waals constant which depends on the material (see, e.g., Israelachvili, 2011) and $\delta$ defines the distance between two molecules. The attractive energy or van–der–Waals energy between two bodies with the volumes $V_1^*$ and $V_2^*$ can be calculated as follows (see, e.g., Hamaker, 1937):

$$E^{vW}_* = \int_{V_1^*} \int_{V_2^*} \frac{q^2 \lambda}{\delta^6} dV_1^* dV_2^*.$$  \hspace{1cm} (5.37)
Here \( q \) defines the number of molecules contained in the infinitesimal volumes \( dV_1^* \) and \( dV_2^* \) (It is assumed that the two bodies are made of the same material). In order to calculate the van–der–Waals energy, the above integral has to be solved which is far from trivial for complex shaped bodies. The van–der–Waals force is calculated by taking the derivative of the above equation with respect to \( \delta^* \) (Israelachvili, 2011). For simple geometries the attractive forces between two homogeneous solids can be found in the literature. Relevant for this thesis are the forces acting between two spheres at a short distance \( \delta^* \) from each other, i.e., \( \delta^* \ll r_1^*, \delta^* \ll r_2^* \) (Israelachvili, 2011):

\[
F_{vW,sp}^* = \frac{H^*}{6 \delta^* r_1^*} \frac{r_1^*}{r_2^*} + \frac{r_2^*}{r_1^*}.
\]  

(5.38)

The second force required in this thesis is the one between two bodies with the flat contact area \( A_{con}^* \) at the distance \( \delta^* \) from each other (Israelachvili, 2011):

\[
F_{vW,fl}^* = \frac{H^*}{6 \delta^*^3} A_{con}^*.
\]  

(5.39)

\( H^* \) is the Hamaker constant which depends on the material of the two interacting bodies and the material present in the interstitial space between the two bodies. Common values can be found in the literature (see, e.g., Israelachvili, 2011) and are of the order of \( 10^{-20} - 10^{-19} \) J. For example, for silica (SiO\(_2\)) in vacuum the Hamaker constant is \( 6.3 \times 10^{-20} \) J (Israelachvili, 2011) or for limestone in vacuum it is \( 3.8 \times 10^{-20} \) J (Tomas, 2007).

The last point to clarify in this section is how to obtain the dimensionless form of the van–der–Waals forces since the code used in this thesis works with dimensionless variables. For this scope, eq. (5.39) can be made dimensionless by means of the fluid density \( \rho_f^* \), the characteristic velocity of the fluid \( U_f^* \) and the characteristic length of the fluid \( L_f^* \):

\[
F_{vW,fl} = \frac{H^*}{6 \pi \delta^*^3} A_{con}^* L_f^*.
\]  

(5.40)

Hence, after dividing the above equation by \( \rho_f^* U_f^* L_f^* \), we obtain the dimensionless van–der–Waals force for a flat surface which is used in the following considerations:

\[
F_{vW,fl} = \frac{H^*}{\rho_f^* U_f^* L_f^*} A_{con}^* = \frac{H}{6 \pi \delta^*^3} A_{con}^*.
\]  

(5.41)

Here \( H \) is the dimensionless Hamaker constant. The dimensionless form of the van–der–Waals force acting between two spheres is derived in the same manner and is written as follows:

\[
F_{vW,sp} = \frac{H}{6 \delta^*^2} \frac{r_1}{r_1^*} + \frac{r_2}{r_2^*}.
\]  

(5.42)

Although not used in this section, the dimensionless yield pressure \( \sigma^* \) (see, eq. (5.61) and eq. (5.62)) is defined at this point since the equations presented in the following are all in dimensionless form:

\[
\sigma^* = \frac{\sigma}{\rho_f^* U_f^*}.
\]  

(5.43)
\( \sigma^* \) is the yield pressure including dimensions.

5.4.2.2 Head–on Collision

In order to provide a first introduction of the procedure to derive a relation for the occurrence of agglomeration, the case of a head–on collision is considered. Note that the considerations made in this section can be found in similar form also in Löfller and Muhr (1972), Hiller (1981), Ho and Sommerfeld (2002), Ho (2004) and Jürgens (2012). In case of a head–on collision the velocity vectors of the approaching particles are collinear (see Fig. 18). Although the case described in this section is a quite crude assumption for particles displacing in a turbulent flow, it is taken as an introductory example of the method used to derive the agglomeration condition for the more general cases described in the next section.

The starting point for the derivation of a suitable relation for the occurrence of agglomeration is the energy balance made for different stages of the collision process (see Fig. 18). All balances made are considered in a coordinate system which is displacing at the constant velocity \( \mathbf{u}^c \). \( \mathbf{u}^c \) is defined as the velocity of the center of mass of the two particles involved:

\[
\mathbf{u}^c = \frac{\mathbf{u}_{p,1}m_{p,1} + \mathbf{u}_{p,2}m_{p,2}}{m_{p,1} + m_{p,2}} = \frac{\mathbf{u}_{p,1}^+m_{p,1} + \mathbf{u}_{p,2}^+m_{p,2}}{m_{p,1} + m_{p,2}} = \mathbf{u}^{c+} = \mathbf{u}^c. \tag{5.44}
\]

Note that also in this section the superscript \(-\) denotes quantities before and the superscript \(+\) quantities after the collision. The equality of the center of mass velocity expressed by quantities before the collision \( \mathbf{u}^{c-} \) and the center of mass velocity expressed by quantities after the collision \( \mathbf{u}^{c+} \) follows from the momentum conservation. Therefore, since \( \mathbf{u}^c \) is constant (it does not change over the collision process), the frame of reference moving with this constant velocity \( \mathbf{u}^c \) is an inertial frame of reference. All particle velocities, however, are represented by the corresponding quantities described in a fixed coordinate system at rest. The reason is that the code works with variables defined in such a reference frame. The vector \( \mathbf{u}_c \) displayed in Fig. 18 denotes the collision–normal vector and the vector \( \mathbf{t}_{ag} \) denotes the collision–tangential direction. The definition of \( \mathbf{t}_{ag} \) is supplied in § 5.4.2.3 since it is no required in this section.

As a first step the kinetic energy expressed in a coordinate system displacing with the constant velocity \( \mathbf{u}^c \) is derived. The scope is to facilitate the verification of the expressions presented in the following since the agglomeration criterion presented relies on energy balances expressed in a frame of reference moving with \( \mathbf{u}^c \). The velocity of the center of the two colliding particles expressed in a frame of reference moving with constant \( \mathbf{u}^c \) (\( \mathbf{u}^c_{p,1,0} \) and \( \mathbf{u}^c_{p,2,0} \)) reads:

\[
\mathbf{u}^c_{p,1,0} = \mathbf{u}_{p,1} - \mathbf{u}^c = \mathbf{u}_{p,1} \frac{m_{p,1} + m_{p,2}}{m_{p,1} + m_{p,2}} - \frac{\mathbf{u}_{p,1}m_{p,1} + \mathbf{u}_{p,2}m_{p,2}}{m_{p,1} + m_{p,2}} = -\frac{m_{p,2}}{m_{p,1} + m_{p,2}}(\mathbf{u}_{p,2} - \mathbf{u}_{p,1}) \tag{5.45a}
\]

\[
\mathbf{u}^c_{p,2,0} = \mathbf{u}_{p,2} - \mathbf{u}^c = \mathbf{u}_{p,2} \frac{m_{p,1} + m_{p,2}}{m_{p,1} + m_{p,2}} - \frac{\mathbf{u}_{p,1}m_{p,1} + \mathbf{u}_{p,2}m_{p,2}}{m_{p,1} + m_{p,2}} = \frac{m_{p,1}}{m_{p,1} + m_{p,2}}(\mathbf{u}_{p,2} - \mathbf{u}_{p,1}) \tag{5.45b}
\]

The subscript 0 denotes that the velocities are expressed in a coordinate system where the axes are aligned with the Cartesian axes. The superscript \( \mathbf{c} \) denotes the velocities.
expressed in a moving coordinate system. The subscript is introduced in order to allow an unambiguous distinction to the velocities expressed in a coordinate system where two axes are aligned with the collision–normal and the collision–tangential direction and the third axis is defined to be normal to the former two (for details see, § 5.4.2.5). The total kinetic energy of the two particles expressed in a frame of reference moving at constant $\mathbf{u}^c$ can be written as

$$E_{\text{rel}}^{\text{kin}} = \frac{1}{2} m_{p,1} \mathbf{u}_{p,1}^c \cdot \mathbf{u}_{p,1}^c + \frac{1}{2} m_{p,2} \mathbf{u}_{p,2}^c \cdot \mathbf{u}_{p,2}^c. \quad (5.46)$$

Note that the rotational kinetic energy is not considered since for the relations derived here it is assumed that the particles do not change their angular velocity during the collision. Therefore, the angular velocity is assumed to be zero throughout the whole simulation. If eqs. (5.45) are inserted in the above equation, we get:

$$E_{\text{rel}}^{\text{kin}} = \frac{1}{2} \frac{m_{p,1} m_{p,2}^2}{(m_{p,1} + m_{p,2})^2} \left( \mathbf{u}_{p,1} \cdot \mathbf{u}_{p,1} - 2 \mathbf{u}_{p,1} \cdot \mathbf{u}_{p,2} + \mathbf{u}_{p,2} \cdot \mathbf{u}_{p,2} \right) + \frac{1}{2} \frac{m_{p,2}^2 m_{p,1}}{(m_{p,1} + m_{p,2})^2} \left( \mathbf{u}_{p,1} \cdot \mathbf{u}_{p,1} - 2 \mathbf{u}_{p,1} \cdot \mathbf{u}_{p,2} + \mathbf{u}_{p,2} \cdot \mathbf{u}_{p,2} \right). \quad (5.47)$$

If the term $1/2 m_{p,1} m_{p,2}/(m_{p,1} + m_{p,2})$ is factored out of the above expression, the final form of the relative kinetic energy is obtained:

$$E_{\text{rel}}^{\text{kin}} = \frac{1}{2} \frac{m_{p,1} m_{p,2}}{m_{p,1} + m_{p,2}} (\mathbf{u}_{p,2} - \mathbf{u}_{p,1})^2. \quad (5.48)$$

The next step for the derivation of the agglomeration criterion is an energy balance involving four stages during the particle–particle collision. The starting point of the energy balance is the state where the particles start to deform, i.e., just before the onset of the compression of the two particles (state 1 in Fig. 18(a)). In this case the total energy is defined as the relative kinetic energy of the two colliding particles plus the integral of the van–der–Waals force $F_{vW}$ before the collision. The integral can be interpreted as the work of the van–der–Waals force acting on the moving spheres, i.e., it is the van–der–Waals energy. The van–der–Waals force before the collision is the attractive force of two spheres since the particle are not deformed during the approaching period. The second state of the energy balance is the state at the end of the compression of the two particles (state 2 in Fig. 18(a)). $\delta_0$ is the minimum separation of the particles during the contact and is introduced to avoid the singularity in the calculation of the van–der–Waals forces (see eq. (5.41) and eq. (5.42)). From a physical point of view it can be seen as the distance where the repulsive forces between the electron shells of the atoms of the two approaching bodies start to act preventing a complete contact. At this state the particles are assumed to have reached the velocity of the center of mass. Thus the relative kinetic energy is zero, which demonstrates the advantage to work in the coordinate system moving with the center of mass. In this case only the energy due to the elastic deformation of the two particles is left. However, in order to balance state 1 and state 2, also the energy due to the irreversible plastic deformation has to be considered. The balance equation reads:

$$\frac{1}{2} \left( \frac{m_{p,1} m_{p,2}}{m_{p,1} + m_{p,2}} \right) (\mathbf{u}_{p,2} - \mathbf{u}_{p,1})^2 + \int_{\delta_0}^\infty F_{vW} \, dx = E_{\text{el}} + E_{\text{pl}}. \quad (5.49)$$
Figure 18: (a) Energy balance of the particles before the collision (b) Energy balance of the particles after the collision.

Note that \( dx \) in the above equation defines the differential distance between the two particles. It means that the total energy at the onset of the compression of the two particles is completely transformed in elastic and plastic deformation. In the next step we have to balance the energies of state 3 and 4 (Fig. 18(b)). State 3 also represents the state of the collision at the end of the compression period, however, only the energy due to the elastic deformation is left. \( E_{el} \) is transformed into the kinetic energy after the collision and the work required to escape from the action of the attractive van–der–Waals force after the collision \( F_{vW}^{+} \). Note that the van–der–Waals force after the particle collision is different from the van–der–Waals force before the collision, since the particles are plastically deformed. The balance of state 3 and state 4 reads:

\[
E_{el} = \frac{1}{2} \left( \frac{m_{p,1} m_{p,2}}{m_{p,1} + m_{p,2}} \right) (u_{p,2}^{+} - u_{p,1}^{+})^2 - \int_{\delta_{0}}^{\infty} F_{vW}^{+} dx. \tag{5.50}
\]

The minus sign before the integral expresses that the force is directed in the opposite
direction respect to the particle displacement. In the next step we assume that the particles agglomerate after the collision. In this case both particles displace with the same velocity, i.e., the velocity of the center of mass. Therefore, the first term at the right–hand side of the above equation turns to zero and \( E_{el} \) can be expressed solely by the work of the van–der–Waals forces after the collision. Inserting eq. (5.50) into eq. (5.49) yields:

\[
\frac{1}{2} \left( \frac{m_{p,1} m_{p,2}}{m_{p,1} + m_{p,2}} \right) (u_{p,2} - u_{p,1})^2 + \int_{\delta_0}^{\infty} F_{vW}^- \, dx = - \int_{\delta_0}^{\infty} F_{vW}^+ \, dx + E_{pl}. \quad \text{(5.51)}
\]

The remaining unknown in the above equation is the energy dissipated during the plastic deformation of the particles since the van–der–Waals forces depend solely on the geometry. An estimation for \( E_{pl} \) can be obtained assuming that the whole dissipated kinetic energy is transformed into plastic deformation. If the agglomeration and also the van–der–Waals forces are neglected, the kinetic energy transformed into plastic deformation is equal to the difference between the relative kinetic energy before and after the collision:

\[
E_{pl} = E_{rel}^{rel-} - E_{kin}^{rel+}. \quad \text{(5.52)}
\]

Here \( E_{kin}^{rel+} \) denotes the relative kinetic energy after the collision calculated with the standard hard–sphere model described in § 5.4.1, i.e., without considering agglomeration and the van–der–Waals forces. By recalling the definition of the normal restitution coefficient defined by eq. (5.19) and squaring it, we obtain the ratio of the relative kinetic energies before and after the collision. Inserted into the above equation, we obtain:

\[
E_{pl} = E_{kin}^{rel-} - e_{n,p}^2 E_{kin}^{rel-} = \frac{1}{2} \left( 1 - e_{n,p}^2 \right) \left( \frac{m_{p,1} m_{p,2}}{m_{p,1} + m_{p,2}} \right) (u_{p,2}^- - u_{p,1}^-)^2. \quad \text{(5.53)}
\]

Thus neglecting the agglomeration and the van–der–Waals forces, the energy dissipated due to the plastic deformation can be expressed in terms of quantities before the collision using eq. (5.53). For the case with agglomeration the above considerations are only an approximation since the relative kinetic energy after the collision is equal to zero and the influence of the van–der–Waals force generally have to be considered. Therefore, the definition of \( E_{pl} \) used in eq. (5.52) is not exact for the agglomeration case. Nevertheless, eq. (5.53) is borrowed and inserted into (5.51) to close the system. The expression reads:

\[
e_{n,p}^2 \frac{1}{2} \left( \frac{m_{p,1} m_{p,2}}{m_{p,1} + m_{p,2}} \right) (u_{p,2}^- - u_{p,1}^-)^2 = \int_{\delta_0}^{\infty} F_{vW}^+ \, dx - \int_{\delta_0}^{\infty} F_{vW}^- \, dx \quad \text{(5.54)}
\]

In order to calculate the difference of the van–der–Waals forces before and after the particle collision, a shape of the deformed bodies has to be assumed. Note that the van–der–Waals force before the collision \( F_{vW}^- \) can be calculated by eq. (5.42) since the particles are assumed to be spherical before the impact. In order to obtain a simple expression for the van–der–Waals forces after the collision, the contact area of the deformed particles is assumed to be flat. Hence, the van–der–Waals force after the collision can be calculated by means of eq. (5.41). Therefore, the term on the right–hand side of eq. (5.54) reads:

\[
\int_{\delta_0}^{\delta_0} F_{vW}^+ \, dx - \int_{\delta_0}^{\delta_0} F_{vW}^- \, dx = - \frac{H}{6 \delta_0} \frac{r_1 r_2}{r_1 + r_2} + \frac{H}{12\pi \delta_0^3} A_{con}. \quad \text{(5.55)}
\]
Figure 19: Definition of the depths $h_{pl,1}$ and $h_{pl,2}$ of the plastic deformation.

Note that the first term on the right–hand side (the van–der–Waals energy of two spheres) can be neglected with respect to the second term on the right–hand side (the van–der–Waals energy of two flat surfaces). This is possible since the minimal contact distance $\delta_0$ is usually very small and is of the order $O(\text{nm})$ (Hiller, 1981; Israelachvili, 2011) and hence the term of $O(1/\delta_0^2)$ prevails.

After the aforementioned simplifications eq. (5.54) can be expressed as follows:

$$e_{n,p}^2 \frac{1}{2} \left( \frac{m_{p,1} m_{p,2}}{m_{p,1} + m_{p,2}} \right) (u_{p,2} - u_{p,1})^2 = \frac{H}{12 \pi \delta_0^2} A_{con}. \quad (5.56)$$

The contact area $A_{con}$ can be easily calculated by the formula of the circular area of a spherical cap $A_{cap}$:

$$A_{cap} = \pi (d_{p,1} h_{pl,1} - h_{pl,1}^2) = \pi (d_{p,2} h_{pl,2} - h_{pl,2}^2). \quad (5.57)$$

The assumed deformation of the two colliding particle is sketched in Fig. 19. $h_{pl,1}$ and $h_{pl,2}$ are the depths of the plastic deformation and $A_{cap}$ is the surface of the circular contact area. Thus for small deformations (i.e., $h_{pl,1} \ll d_{p,1}$ and $h_{pl,2} \ll d_{p,2}$) the contact area $A_{con}$ is obtained by the following expression:

$$A_{con} = \pi d_{p,1} h_{pl,1} = \pi d_{p,2} h_{pl,2}. \quad (5.58)$$

Hence, the integral of the van–der–Waals force after the collision can be written as

$$\frac{H}{12 \pi \delta_0^2} A_{con} = \frac{H}{12 \delta_0^2} d_{p,1} h_{pl,1} = \frac{H}{12 \delta_0^2} d_{p,2} h_{pl,2}. \quad (5.59)$$

---

8 The formula can be found in, e.g., http://en.wikipedia.org/wiki/Spherical\_cap
and we obtain for equation (5.54)
\[ \epsilon_{n,p}^2 \frac{1}{2} \left( \frac{m_{p,1} m_{p,2}}{m_{p,1} + m_{p,2}} \right) (u_{p,2} - u_{p,1})^2 = \frac{H}{12} \frac{d_{p,1}}{\delta_0^2} h_{pl,1} = \frac{H}{12} \frac{d_{p,2}}{\delta_0^2} h_{pl,2}. \]  
(5.60)

\( h_{pl,1} \) and \( h_{pl,2} \) are obtained by the work required to deform a ductile material (see, e.g., Antonyuk, 2006):
\[ E_{pl} = \pi \int_0^{h_{pl,1}} \sigma \, d_{p,1} \, h_1 \, dh_1 + \pi \int_0^{h_{pl,2}} \sigma \, d_{p,2} \, h_2 \, dh_2. \]  
(5.61)

\( \sigma \) is the mean yield stress depending on the material. As pointed out by Antonyuk (2006), the micro–yield stress (the stress where the particles start to plastically deform) is higher than the yield stress \( \sigma_{F,l} \) obtained by an uni–axial tensile test. For ductile materials with a Poisson’s ratio of \( \nu = 0.3 \), e.g., the mean yield stress can be found to be \( \sigma = 1.6 \sigma_{F,l} \) (Johnson, 1989). Of course, the above relation is a very crude simplification of the work required to plastically deform the two spheres. The evaluation of the above expression using eq. (5.58) gives:
\[ E_{pl} = \frac{1}{2} \pi \frac{\sigma}{\mathcal{p}} d_{p,1} h_{pl,1}^2 \left( 1 + \frac{d_{p,1}}{d_{p,2}} \right). \]  
(5.62)

In order to get the plastic deformation \( h_{pl,1} \) as a function of quantities before the collision, we insert eq. (5.53) in the above relation:
\[ \frac{1}{2} (1 - \epsilon_{n,p}^2) \left( \frac{m_{p,1} m_{p,2}}{m_{p,1} + m_{p,2}} \right) (u_{p,2} - u_{p,1})^2 = \frac{1}{2} \pi \frac{\sigma}{\mathcal{p}} h_{pl,1}^2 \left( 1 + \frac{d_{p,1}}{d_{p,2}} \right). \]  
(5.63)

After reorganizing, we get:
\[ h_{pl,1} = \left[ (1 - \epsilon_{n,p}^2) \left( \frac{m_{p,1} m_{p,2}}{m_{p,1} + m_{p,2}} \right) (u_{p,2} - u_{p,1})^2 \right]^{1/2} \frac{1}{\pi \sigma (d_{p,1} + d_{p,2}^2)}. \]  
(5.64)

After inserting the above equation in eq. (5.60), we get the relation for the limiting velocity for the occurrence of agglomeration in case of a head–on collision:
\[ |u_{p,2} - u_{p,1}|_{lim} = \frac{H d_{p,1}}{6 \delta_0^2} \frac{1}{\epsilon_{n,p}^2} \left( \frac{m_{p,1} + m_{p,2}}{m_{p,1} m_{p,2}} \right) \frac{1}{\pi \sigma (d_{p,1} + d_{p,2}^2)} \left( \frac{d_{p,2}}{d_{p,1}} \right)^{1/2}. \]  
(5.65)

By expressing the particle mass \( m_p \) as a function of the particle density \( \rho_p \) and the particle diameter \( d_p \), the above relation can be further simplified. The final result reads:
\[ |u_{p,2} - u_{p,1}|_{lim} = \frac{H}{6 \delta_0^2} \frac{1}{\epsilon_{n,p}^2} \frac{6}{\pi^2 \rho_p \sigma} \frac{d_{p,1}^3 + d_{p,2}^3}{d_{p,1}^2 d_{p,2}^2 (d_{p,1} + d_{p,2})} \left( \frac{d_{p,2}}{d_{p,1}} \right)^{1/2}. \]  
(5.66)

Thus agglomeration takes place if the relative velocity of the two particles involved is smaller than this limiting value. Otherwise, the kinetic energies of the particles are sufficiently large to overcome the van–der–Waals forces.

The last issue to clarify is what happens if the relative velocity of the two colliding
particles is slightly greater than the limiting relative velocity. Note that similar considerations are also made by Hiller (1981). In this case it is reasonable to assume that the particles can hardly escape the attractive van–der–Waals force and for that reason only slowly separate from each other. However, in the current formulation the post–collision velocities of the particles are calculated without considering the effect of the van–der–Waals force on the particles at all. To overcome this shortcoming the energy balance in case of non–agglomerating particles is considered again:

$$E_{\text{kin}}^{\text{rel}^{-}} + \int_{\delta_{0}}^{\delta} F_{vW}^{-}\,dx = - \int_{\delta}^{\infty} F_{vW}^{+}\,dx + E_{\text{pl}} + E_{\text{kin}}^{\text{rel}^{+}}. \quad (5.67)$$

The above relation is similar to eq. (5.51) with the difference that the particles separate after the collision. For that reason the relative kinetic energy after the collision $E_{\text{kin}}^{\text{rel}^{+}}$ is retained in the energy balance. If we insert eq. (5.41), (5.42) and (5.53) in the above relation and additionally neglect the contribution of the van–der–Waals force of the undeformed spheres, we obtain:

$$E_{\text{kin}}^{\text{rel}^{-}} = \frac{H}{12 \, \delta_{0}} \, d_{p,1} \, h_{pl,1} + (1 - \varepsilon_{n,p}^{2}) E_{\text{kin}}^{\text{rel}^{-}} + E_{\text{kin}}^{\text{rel}^{+}}. \quad (5.68)$$

After inserting eq. (5.64), reorganizing with respect to the relative kinetic energy after the collision $E_{\text{kin}}^{\text{rel}^{+}}$ and dividing by $E_{\text{kin}}^{\text{rel}^{-}}$, the expression reads:

$$\frac{E_{\text{kin}}^{\text{rel}^{+}}}{E_{\text{kin}}^{\text{rel}^{-}}} = \varepsilon_{n,p}^{2} - \frac{1}{12 \, \delta_{0}} \, d_{p,1} \left[ (1 - \varepsilon_{n,p}^{2}) \left( \frac{m_{p,1} m_{p,2}}{m_{p,1} + m_{p,2}} \right) \frac{1}{\pi \, \sigma} (d_{p,1} + d_{p,2}^3) \right]^{1/2}. \quad (5.69)$$

Taking the definition of the normal restitution coefficient (5.19) into account, the left–hand side of the above equation can be interpreted as the square of a modified coefficient $\tilde{\varepsilon}_{p,n}$. If we insert the definition of the relative kinetic energy before the collision in the above equation, the modified normal restitution coefficient can be expressed in terms of known quantities:

$$\tilde{\varepsilon}_{p,n}^{2} = \varepsilon_{n,p}^{2} - \frac{1}{12 \, \delta_{0}} \, d_{p,1} \left[ (1 - \varepsilon_{n,p}^{2}) \left( \frac{m_{p,1} m_{p,2}}{m_{p,1} + m_{p,2}} \right) \frac{1}{\pi \, \sigma} (d_{p,1} + d_{p,2}^3) \right]^{1/2}. \quad (5.70)$$

By expressing the particle mass $m_{p}$ as a function of the particle density $\rho_{p}$ and the particle diameter $d_{p}$, the above relation can be further simplified. The final result reads:

$$\tilde{\varepsilon}_{p,n}^{2} = \varepsilon_{n,p}^{2} - \frac{1}{12 \, \delta_{0}} \, d_{p,1} \left[ (1 - \varepsilon_{n,p}^{2}) \frac{6}{\rho_{p} \, \sigma} \left( \frac{d_{p,1}^{3} + d_{p,2}^{3}}{d_{p,1}^2 \, d_{p,2}^2} \right) \right]^{1/2}. \quad (5.71)$$

It is obvious that $\tilde{\varepsilon}_{p,n}$ takes into account the decelerating effect of the van–der–Waals forces since it is always smaller than $\varepsilon_{p,n}$.

Briefly summarized the procedure of agglomeration detection is as follows: In case of a head–on collision the relative velocity of the two colliding particles is checked. If it is less than the limiting relative velocity defined by eq. (5.66) the two particles agglomerate and they are displacing with the same velocity, i.e., the velocity of the center of mass defined by eq. (5.44). If the two particles do not agglomerate, the normal restitution
coefficient is modified according to eq. (5.71) and the collision process it treated as a standard hard–sphere collision without friction. Note, however, that the case presented in this section is not implemented in the multiphase code LESOCC. The scope of this section is to introduce the reader into the methodology adopted to derive a more general condition for the case, where the particles also possess a relative tangential velocity. The derivation of this more general criterion is described in the next section.

5.4.2.3 Collision with Relative Tangential Velocity

In this section a more general condition than in the former section is derived, i.e., the relative velocity of the approaching particles has not to be collinear. Note that friction is still not considered during the collision. The procedure to derive an agglomeration condition is the same as described in the former section, i.e., it is based on energetic considerations. Also in this instance the scenario is analogous to the case of the head–on collision: The particles approach each other (stage 1 in Fig. 18(a)) and elastically and plastically deform (stage 2 in Fig. 18(a)). After the compression period only the elastic energy is left (stage 3 in Fig. 18(b)). The elastic energy is transformed into kinetic energy and into work required by the particles to escape from the potential well of the modified van–der–Waals force (stage 4 in Fig. 18(b)). Hence, the energy balance derived for the scenario where the two particles agglomerate still holds (see, eq. (5.51)). This equation means that in the limiting case of an agglomeration the kinetic energy of the two particles before the collision is equal to the difference of the van–der–Waals forces arising due to the deformation of the particles plus the dissipated energy due to the plastic deformation. As already mentioned, the kinetic energy of the two particles is represented in a coordinate system which moves with the velocity of the center of mass. Therefore, also in this case the kinetic energy of the two particles after the collision displacing at the same velocity vanishes. Note that for the energy balance made in the case of agglomeration the rotation of the agglomerate is still not considered. For a relative tangential velocity of the particles the conservation of the angular momentum balance (see, eq. (5.109)) leads to an angular velocity of the agglomerate although no tangential forces are allowed for a frictionless collision. In order to remove this conflict, the rotation of the agglomerate is completely disregarded in this section.

Also in this case the plastic deformation takes solely place because of the relative velocity of the two particles in collision–normal direction. Since for a frictionless collision the momentum can only be transferred in collision–normal direction, this assumption is consistent with the case already considered. Again it is assumed that the whole dissipated energy is transformed in plastic deformation. As in the previous section the energy due to the plastic deformation is calculated by the difference of the relative kinetic energy before and after the collision neglecting agglomeration and the van–der–Waals forces:

\[
E_{pl} = E_{\text{kin,rel}}^{rel} - E_{\text{HS,rel}}^{rel} = \frac{1}{2} \left( \frac{m_{p,1} m_{p,2}}{m_{p,1} + m_{p,2}} \right) \left[ (u_{p,2} - u_{p,1})^2 - (u_{p,2}^{HS} - u_{p,1}^{HS})^2 \right]. \tag{5.72}
\]

Here \(u_{p,1}^{HS}\) and \(u_{p,2}^{HS}\) are the particle velocities calculated by the standard hard–sphere model described in § 5.4.1, i.e., without considering agglomeration and the van–der–Waals forces. \(E_{\text{kin,rel}}^{rel}\) is the resulting relative kinetic energy. With eqs. (5.35a)-(5.35b) (Note that in the frictionless case no velocity change in the collision–tangential direction occurs) the difference of the post–collision velocity can be expressed in terms of the velocities
before the collision. It can then be easily verified that the above equation reads:

\[ E_{pl} = E_{kin}^{rel} - E_{kin}^{HS,rel} = \frac{1}{2} (1 - \epsilon_{n,p}^2) \left( \frac{m_{p,1} m_{p,2}}{m_{p,1} + m_{p,2}} \right) \left( (u_{p,2} - u_{p,1}) \cdot n_c \right)^2. \]  

(5.73)

In this case the plastic deformation takes place only in collision–normal direction and therefore only the velocity difference in this direction enters into the above equation to calculate the energy dissipated due to the plastic deformation. Note that for the head–on collision discussed in the former section, \( E_{pl} \) is based on the total velocity difference (see, eq. (5.53)) and therefore the dissipated energy during a head–on collision should be larger than during a collision where also a relative tangential velocity component of the particles is existing.

In order to solve the energy balance (5.51) the difference of the van–der–Waals force before \( F_{vW}^- \) and after the collision \( F_{vW}^+ \) is required. As in the previous section the influence of the van–der–Waals force exerted by two undeformed spheres is neglected and only the effect of the flattened surfaces is retained. Hence, a relation for the height of the plastic deformation \( h_{pl,1} \) has to be found (see eq. (5.59)). The relation for \( h_{pl,1} \) is obtained by combining eq. (5.73) with eq. (5.62) which means that the dissipated energy is equal to the work required to plastically deform the two particles. After rearranging with respect to \( h_{pl,1} \), we obtain:

\[ h_{pl,1} = \left[ (1 - \epsilon_{n,p}^2) \left( \frac{m_{p,1} m_{p,2}}{m_{p,1} + m_{p,2}} \right) \left( (u_{p,2} - u_{p,1}) \cdot n_c \right)^2 \right] \frac{1}{\pi \sigma \left( d_{p,1} + \frac{d_{p,1}^2}{d_{p,2}} \right)} \right]^{1/2}. \]  

(5.74)

Comparing the above relation with the plastic deformation \( h_{pl,1} \) obtained in the former section (eq. (5.64)), it is obvious that the two expressions are almost identical. The only difference is that the relative velocity of the particles before the collision in eq. (5.64) is replaced by its component in collision–normal direction in eq. (5.74). With the above relation the van–der–Waals force after the collision defined by eq. (5.59) can be expressed as follows:

\[ -\int_{\delta_0}^{\infty} F_{vW}^+ dx = \frac{H}{12 \sigma_0^2} \left[ (1 - \epsilon_{n,p}^2) \left( \frac{m_{p,1} m_{p,2}}{m_{p,1} + m_{p,2}} \right) \left( (u_{p,2} - u_{p,1}) \cdot n_c \right)^2 \right] \frac{1}{\pi \sigma \left( d_{p,1} + \frac{d_{p,1}^2}{d_{p,2}} \right)} \right]^{1/2}. \]  

(5.75)

At this point of the analysis we can express the relation for the limiting case (see, eq. (5.51)) where agglomeration takes place, solely as a function of known (pre–collision) quantities:

\[ \frac{1}{2} \left( \frac{m_{p,1} m_{p,2}}{m_{p,1} + m_{p,2}} \right) \left( u_{p,2} - u_{p,1} \right)^2 = \frac{H}{12 \sigma_0^2} \left[ (1 - \epsilon_{n,p}^2) \left( \frac{m_{p,1} m_{p,2}}{m_{p,1} + m_{p,2}} \right) \left( (u_{p,2} - u_{p,1}) \cdot n_c \right)^2 \right] \frac{1}{\pi \sigma \left( d_{p,1} + \frac{d_{p,1}^2}{d_{p,2}} \right)} \right]^{1/2} + \]

(5.76)

\[ \frac{1}{2} \left( \frac{m_{p,1} m_{p,2}}{m_{p,1} + m_{p,2}} \right) \left( u_{p,2} - u_{p,1} \right)^2 \left( 1 - \epsilon_{n,p}^2 \right). \]

In order to obtain a relation to determine whether an agglomeration of two colliding
particles occurs or not, in the above equation the equal sign has to be replaced by a greater–than or a less–than sign. The sign to choose becomes quite obvious if the dissipated energy is shifted to the left–hand side of eq. (5.76). The relative kinetic energy before the collision subtracted by the dissipated energy is exactly the elastic energy left in order to overcome the van–der–Waals energy. Hence in eq. (5.76) the equal sign has to be replaced by a less–than sign to establish the relation for the occurrence of agglomeration:

\[
\frac{1}{2} \left( \frac{m_{p,1} m_{p,2}}{m_{p,1} + m_{p,2}} \right) (u_{p,2} - u_{p,1})^2 - \frac{1}{2} \left( \frac{m_{p,1} m_{p,2}}{m_{p,1} + m_{p,2}} \right) \left[ (u_{p,2} - u_{p,1}) \cdot n_c \right]^2 \leq \left(1 - e_{n,p}^2\right) \sigma \pi \left( d_{p,1} + \frac{d_{p,2}^3}{d_{p,2}^2} \right)^{1/2}
\]

The above expression means that, if the elastic energy after the compression period of the collision (the residual potential energy or elastic energy) is less than the work required to overcome the van–der–Waals forces, agglomeration occurs. After expressing the left–hand side of eq.(5.77) solely as a function of the relative particle velocity before the collision and the normal–restitution coefficient \( e_{n,p} \), the result reads:

\[
\frac{(u_{p,2} - u_{p,1})^2 - [(u_{p,2} - u_{p,1}) \cdot n_c]^2(1 - e_{n,p}^2)}{(u_{p,2} - u_{p,1}) \cdot n_c} \leq \frac{H}{6 \frac{d_{p,1}^2}{\delta_0}} \left[ (1 - e_{n,p}^2) \left( \frac{m_{p,1} + m_{p,2}}{m_{p,1} m_{p,2}} \right) \frac{1}{\pi \sigma (d_{p,1} + \frac{d_{p,2}^3}{d_{p,2}^2})} \right]^{1/2}.
\]

The final relation to determine if agglomeration occurs or not, is obtained by expressing the particle masses \( m_p \) in the above equation by means of the diameter \( d_p \) and the density \( \rho_p \):

\[
\frac{(u_{p,2} - u_{p,1})^2 - [(u_{p,2} - u_{p,1}) \cdot n_c]^2(1 - e_{n,p}^2)}{(u_{p,2} - u_{p,1}) \cdot n_c} \leq \frac{H}{6 \frac{d_{p,1}^2}{\delta_0}} \left[ (1 - e_{n,p}^2) \frac{6}{\pi^2 \rho_p \sigma} \frac{d_{p,1}^3 + d_{p,2}^3}{d_{p,1}^2 d_{p,2}^2 (d_{p,1} + d_{p,2})} \right]^{1/2}.
\]

It is easy to verify that the above inequation can be transformed into the condition of agglomeration in case of a head–on collision (the relative velocity \( u_{p,2} - u_{p,1} \) for a head–on collision is aligned with the collision–normal vector \( n_c \)). In this case the dot product \( (u_{p,2} - u_{p,1}) \cdot n_c \) is replaced by the absolute value of the relative velocity \( |u_{p,2} - u_{p,1}| \) and therefore eq. (5.66) is obtained.

The last issue to clarify in this section is how to consider the change of the post–collision particle velocities due to the modification of the van–der–Waals forces in case that no agglomeration occurs. The reason why this issue should be addressed is quite clear: If the threshold (5.79) is only slightly missed, it seems to be reasonable to assume that the particles should only slowly separate from each other. Therefore, a suitable condition has to be derived to accomplish this requirement. The derivation of this requirement is presented in the following.

Starting point for the analysis is the energy balance (5.67). Furthermore, the relative
velocity is decomposed into a normal and a tangential component:

\[
\mathbf{u}_{p,2} - \mathbf{u}_{p,1} = \frac{[ (\mathbf{u}_{p,2} - \mathbf{u}_{p,1}) \cdot \mathbf{n}_c ] \mathbf{n}_c}{\mathbf{u}_n} + \frac{[ (\mathbf{u}_{p,2} - \mathbf{u}_{p,1}) \cdot \mathbf{u}_t ] \mathbf{u}_t}{\mathbf{u}_n}
\] (5.80)

With the above relation the relative kinetic energy can be decomposed into a normal \(E_{kin,n}^{rel}\) and tangential component \(E_{kin,t}^{rel}\):

\[
E_{kin}^{rel} = \frac{1}{2} \left( \frac{m_{p,1} m_{p,2}}{m_{p,1} + m_{p,2}} \right) (\mathbf{u}_{p,2} - \mathbf{u}_{p,1})^2 = \frac{1}{2} \left( \frac{m_{p,1} m_{p,2}}{m_{p,1} + m_{p,2}} \right) \begin{bmatrix} \mathbf{u}_n \cdot \mathbf{u}_n + 2\mathbf{u}_n \cdot \mathbf{u}_t + \mathbf{u}_t \cdot \mathbf{u}_t \end{bmatrix}
\] (5.81)

\[
E_{kin,n}^{rel} + E_{kin,t}^{rel}.
\]

After this operation eq. (5.67) can be expressed as follows:

\[
E_{kin,n}^{rel-} + E_{kin,t}^{rel-} + \int_{\delta_0}^{\delta_1} F_w^- dx = - \int_{\delta_0}^{\infty} F_w^+ dx + E_{pl} + E_{kin,n}^{rel+} + E_{kin,t}^{rel+}.
\] (5.82)

Of course, at this point some assumptions (the above scalar equation contains the two unknowns \(E_{kin,n}^{rel+}\) and \(E_{kin,t}^{rel+}\)) how the action of the van–der–Waals forces is partitioned between the components of the relative kinetic energy in normal \(E_{kin,n}^{rel+}\) and in tangential direction \(E_{kin,t}^{rel+}\) has to be undertaken. Here, two different scenarios are considered: (i) the van–der–Waals force only influences the normal component of the relative kinetic energy \(E_{kin,n}^{rel+}\) (with \(E_{kin,t}^{rel+} = E_{kin,t}^{rel-}\)) and (ii) both, \(E_{kin,n}^{rel+}\) and \(E_{kin,t}^{rel+}\) are affected.

After inserting eq. (5.73) into eq. (5.82) and expressing the work exerted by the van–der–Waals force by means of eq. (5.59), the energy balance for case (i) reads:

\[
E_{kin,n}^{rel-} = \frac{H}{12 \delta_0^2} d_{p,1} h_{pl,1} + (1 - e_{n,p}^2) E_{kin,n}^{rel-} + E_{kin,n}^{rel+}.
\] (5.83)

After reorganizing with respect to \(E_{kin,n}^{rel+}\), dividing by \(E_{kin,n}^{rel-}\) and using eq. (5.74), we obtain:

\[
\frac{E_{kin,n}^{rel+}}{E_{kin,n}^{rel-}} = e_{n,p}^2 - \frac{1}{E_{kin,n}^{rel-}} \frac{H}{12 \delta_0^2} d_{p,1} \left( 1 - e_{n,p}^2 \right) \left( \frac{m_{p,1} m_{p,2}}{m_{p,1} + m_{p,2}} \right) \left( \mathbf{u}_{p,2} - \mathbf{u}_{p,1} \right) \cdot \mathbf{n}_c \frac{1}{\pi \sigma \left( d_{p,1} + \frac{d_{p,2}^3}{d_{p,1}^2} \right)} \right)^{1/2}.
\] (5.84)

Based on the definition of the relative kinetic energy in normal direction defined by eq. (5.81) and comparing the above relation with the definition of the normal restitution coefficient (5.19), a modified normal restitution coefficient \(\tilde{e}_{n,p}\) is obtained (Note that as done before, the particle masses are expressed by the corresponding diameters and the density):

\[
\tilde{e}_{n,p}^2 = e_{n,p}^2 - \frac{1}{(\mathbf{u}_{p,2} - \mathbf{u}_{p,1}) \cdot \mathbf{n}_c} \frac{H}{6 \delta_0^2} \left[ (1 - e_{n,p}^2) \frac{6}{\pi^2 \rho_p \sigma} \frac{d_{p,1}^3 + d_{p,2}^3}{d_{p,1}^2 d_{p,2} (d_{p,1} + d_{p,2})} \right]^{1/2}.
\] (5.85)

It is easy to verify that in case of a head–on collision (\( (\mathbf{u}_{p,2} - \mathbf{u}_{p,1}) \) and \(\mathbf{n}_c\) are parallel)
expression (5.71) is obtained.

Case (ii) is only considered, if \( e_{n,p}^2 \) is found to be less than zero. That means that the particles separate only due to the particle velocity difference in tangential direction. In this case eq. (5.67) can be formulated as follows (\( E_{kin,n}^{rel+} = 0 \)):

\[
E_{kin,n}^{rel-} + E_{kin,t}^{rel-} = \frac{H}{12 \, \delta_0} \, d_{p,1} \, h_{pl,1} + (1 - e_{n,p}^2) E_{kin,n}^{rel-} + E_{kin,t}^{rel+}.
\]

After reorganizing the above equation with respect to \( E_{kin,t}^{rel+} \) and dividing by \( E_{kin,t}^{rel-} \), we obtain

\[
e_{t,p}^{\tilde{\epsilon}} = \frac{E_{kin,t}^{rel+}}{E_{kin,t}^{rel-}} = \frac{u_{t}^2}{u_{t}^2 - \frac{e_{n,p}^2}{u_{n}^2} \frac{H}{12 \, \delta_0} \, d_{p,1} \, h_{pl,1}} + 1. \tag{5.87}
\]

The above relation can be interpreted as a modified tangential restitution coefficient \( e_{t,p}^{\tilde{\epsilon}} \). This can be easily recognized if the definition of the tangential restitution coefficient \( e_{t,p} \) is recalled (see, eq. (5.24)). It defines the ratio of the relative velocity before and after the collision \( u_{pr.p}^+, u_{pr.p}^- \). Since in the case considered in this section no angular velocity is allowed, the absolute value of the relative velocity found in § 5.4.1 (see eq. (5.22)) is identical to the absolute value of the tangential velocity defined in this section (see eq. (5.80)) i.e., \( |u_{pr}| = |u_t| \). Hence, eq. (5.87) can be written by using eq. (5.74) and (5.81) as follows:

\[
e_{n,p}^2 u_n^{-2} - \frac{H}{6 \, \delta_0} d_{p,1} \left( 1 - e_{n,p}^2 \right) \left( \frac{m_{p,1} + m_{p,2}}{m_{p,1} m_{p,2}} \right) u_n^{-2} \frac{1}{\pi \, \sigma \left( d_{p,1} + d_{p,2} \right)} \right)^{1/2} + 1. \tag{5.88}
\]

Finally, after expressing the particle masses as a function of the density and the diameter the above equations reads:

\[
e_{n,p}^2 u_n^{-2} - \frac{H}{6 \, \delta_0} d_{p,1} \left( 1 - e_{n,p}^2 \right) \left( \frac{m_{p,1} + m_{p,2}}{m_{p,1} m_{p,2}} \right) u_n^{-2} \frac{1}{\pi \, \sigma \left( d_{p,1} + d_{p,2} \right)} \right)^{1/2} + 1. \tag{5.89}
\]

The difference between the modified tangential restitution coefficient \( e_{t,p}^{\tilde{\epsilon}} \) and the tangential restitution coefficient defined in § 5.4.1 it that \( e_{t,p}^{\tilde{\epsilon}} \) does not lead to an inversion of the sign of the tangential velocity after the collision. Thus \( e_{t,p}^{\tilde{\epsilon}} \) is used to reduce the total kinetic energy in order to fulfill the energy balance (5.82).

The post–collision velocities of the two particles are calculated in a analogous way as in § 5.4.1. Also in this section the contact force \( F_{n,ag} \) is divided into a normal component \( F_{n,ag} \) and a tangential component \( F_{t,ag} \). In order to compute the momentum balance of the particles over the collision process, it is assumed that \( F_{t,ag} \) acts at the center of each particle, respectively. For that reason \( F_{t,ag} \) can be interpreted as a volume force acting at the center of the particles. The assumption about the location of the point of action of the contact force \( F_{t,ag} \) is made in order not to contradict the frictionless particle–particle collision. Since for a collision without friction no angular velocity change is allowed, the only possible point of action of \( F_{t,ag} \) which reproduces the correct result (no angular velocity changes) is the center of the particles.

The normal component of the contact force \( F_{n,ag} \) is obtained by inserting \( F_{n,ag} \) and \( F_{t,ag} \)
in eq. (5.16a) and (5.16b), taking the dot product of both equations with the collision–normal vector \( n_c \) and subtraction eq. (5.16b) from eq. (5.16a). By using the definition of the modified normal restitution coefficient \( \tilde{e}_{n,p} \) (see, eq. (5.85), the final form of \( F_{n,ag} \) reads:

\[
F_{n,ag} = -\frac{m_{p,1}m_{p,2}}{m_{p,1} + m_{p,2}} (1 + \tilde{e}_{n,p}) \left( u_{p,2}^- - u_{p,1}^- \right) \cdot n_c \quad n_c
\]

(5.90)

The tangential component of the contact force \( F_{t,ag} \) is directed towards \( u_t \) and the tangential unit vector \( t_{ag} \) is defined as follows:

\[
t_{ag} = \frac{u_t^-}{|u_t^-|}.
\]

(5.91)

By inserting the contact forces \( F_{n,ag} \) and \( F_{t,ag} \) in eq. (5.13a) and (5.13b), taking the dot product of both equations with \( t_{ag} \) and afterwards subtracting eq. (5.13b) from eq. (5.13a), we obtain a scalar equation for the absolute value of the contact force in the tangential direction:

\[
|u_t^+| - |u_t^-| = \frac{m_{p,1} + m_{p,2}}{m_{p,1} m_{p,2}} |F_{t,ag}|.
\]

(5.92)

Note that the dot product can be substituted by the absolute value since \( u_t^- \), \( u_t^+ \) and \( F_{t,ag} \) are aligned per definition with \( t_{ag} \). Furthermore, the post–collision tangential velocity \( u_t^+ \) can be replaced as a function of the tangential velocity before the collision by means of the definition of \( \tilde{e}_{t,p} \) (eq. (5.87)):

\[
|F_{t,ag}| = \frac{m_{p,1} m_{p,2}}{m_{p,1} + m_{p,2}} (1 - \tilde{e}_{t,p}) |u_t^-|.
\]

(5.93)

Note that the contact force in normal direction \( F_{n,ag} \) is not calculated explicitly in this section, since the procedure to calculate it is the same as in § 5.4.1. Finally, the velocities of the two colliding particles for case (ii) setting \( \tilde{e}_{n,p} = 0 \) are obtained:

\[
\begin{align*}
  u_{p,1}^+ &= u_{p,1}^- + \frac{m_{p,2}}{m_{p,1} + m_{p,2}} \left\{ \left[ (u_{p,2}^- - u_{p,1}^-) \cdot n_c \right] n_c + (1 - \tilde{e}_{t,p}) u_t^- \right\} \\
  u_{p,2}^+ &= u_{p,2}^- - \frac{m_{p,1}}{m_{p,1} + m_{p,2}} \left\{ \left[ (u_{p,2}^- - u_{p,1}^-) \cdot n_c \right] n_c + (1 - \tilde{e}_{t,p}) u_t^- \right\}
\end{align*}
\]

(5.94a)

(5.94b)

5.4.2.4 Summary of the Model in Case of Collisions without Friction

Briefly summarized, the agglomeration model implemented in the code \( \mathcal{LESOC}C \) works as follows:

(i) First, it is checked if two particles collide as shown in § 6.2.3.

(ii) For two colliding particles, criterion (5.79) is evaluated.

(iii) If criterion (5.79) is fulfilled, the particles agglomerate. Hence, the velocities of the two particles are set equal to the velocity of the center of mass (see, eq. (5.44)).

In the following steps of the simulation the agglomerate is treated as a spherical

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The equivalent diameter is derived by the mass conservation, i.e., the mass of the two agglomerated particles has to be equal to the mass of the representative sphere:

\[ \frac{1}{6} \pi \rho d_{\text{res}}^3 = \frac{1}{6} \pi \rho_p \left( d_{p,1}^3 + d_{p,2}^3 \right). \]  

That means that the agglomerate moves through the computational domain as a sphere having the same volume as the two agglomerated particles. The idealization of the agglomerate as a sphere has the big advantage that the collision detection is much easier to accomplish than for a configuration of two spheres stuck together. Furthermore, the aerodynamic forces on the particles can still be calculated by eq. (4.25).

(iv) If criterion (5.79) is not fulfilled, the modified normal restitution coefficient \( \tilde{e}_{p,n} \) is computed (see, eq. (5.85)). For predicted values greater than zero it is assumed that the van–der–Waals force due to the plastic flattening of the particles influences only the collision–normal motion. Hence, the post–collision particle velocities are calculated as follows:

\[ u_{p,1}^+ = u_{p,1}^- + \frac{m_{p,2}}{m_{p,1} + m_{p,2}} \left\{ (1 + \tilde{e}_{n,p}) \left[ (u_{p,2}^- - u_{p,1}^-) \cdot n_c \right] n_c \right\}, \]  

\[ u_{p,2}^+ = u_{p,2}^- - \frac{m_{p,1}}{m_{p,1} + m_{p,2}} \left\{ (1 + \tilde{e}_{n,p}) \left[ (u_{p,2}^- - u_{p,1}^-) \cdot n_c \right] n_c \right\}. \]  

(v) For values of \( \tilde{e}_{p,n} \) less than zero, it is assumed that the van–der–Waals forces also influence the tangential motion of the two particles. In this case the particles separate only due to the relative velocity in tangential direction. Hence, \( \tilde{e}_{p,n} \) is set to zero and a modified tangential restitution coefficient \( \tilde{e}_{t,p} \) according to eq. (5.89) is predicted. Based on that the post–collision particle velocities are calculated as follows:

\[ u_{p,1}^+ = u_{p,1}^- + \frac{m_{p,2}}{m_{p,1} + m_{p,2}} \left\{ (u_{p,2}^- - u_{p,1}^-) \cdot n_c \right\} n_c + (1 - \tilde{e}_{t,p}) u_t \]  

\[ u_{p,2}^+ = u_{p,2}^- - \frac{m_{p,1}}{m_{p,1} + m_{p,2}} \left\{ (u_{p,2}^- - u_{p,1}^-) \cdot n_c \right\} n_c + (1 - \tilde{e}_{t,p}) u_t \]  

5.4.2.5 Extention of the Model towards Collisions with Friction

In this section the possible extension of the agglomeration model towards collisions with friction is discussed.

The derivation of a condition for the occurrence of an agglomeration in case of inter–particle collisions with friction at the contact point can be based on energy balances as done in the previous sections. Since friction during the collision implies a contact
force which acts at the contact point, the particles change their angular velocity over the impact. Hence, also the rotational kinetic energy has to be considered when balancing the energies before and after the collision:

\[ E_{\text{rel}}^{-} + E_{\text{rot,ntz}}^{-} + \int_{\delta_0}^{\infty} F_{vW}^{-} \, dx = E_{\text{rel}}^{+} + E_{\text{rot,ntz}}^{+} + E_{\text{dis,ntz}} - \int_{\delta_0}^{\infty} F_{vW}^{+} \, dx \]  

(5.99)

The above energy balance means that the sum of the translational and the rotational kinetic energies and the work exerted by the van–der–Waals force before the collision \((E_{\text{kin,ntz}}^{-}, E_{\text{rot,ntz}}^{-}, \int_{\delta_0}^{\infty} F_{vW}^{-} \, dx, \) respectively) has to be equal to the sum of the same quantities after the collision \((E_{\text{kin,ntz}}^{+}, E_{\text{rot,ntz}}^{+}, \int_{\delta_0}^{\infty} F_{vW}^{+} \, dx, \) respectively) plus the dissipated energy \(E_{\text{dis,ntz}}.\)

The superscript \(\text{rel}\) denotes again that the energies are calculated in a coordinate system displacing with the constant center of mass velocity \(u_{c}\). The subscript \(\text{ntz}\) denotes that the above energy balance is furthermore expressed in a coordinate system where one axis is aligned in collision–normal direction \(n_{c}\), the second axis in collision–tangential direction \(t_{ag}\) and the third axis \(z_{ag}\) is normal to \(n_{c}\) and \(t_{ag}\) (see, Fig. 20). The computation of \(z_{ag}\) is described below. \(a_{1}\) and \(a_{2}\) in Fig. 20 are the vectors pointing from the center of mass of the agglomerate \(S_{ag}\) to the center \(S_{1}\) of the particle 1 and the vector pointing from the center of mass of the agglomerate \(S_{ag}\) to the center \(S_{2}\) of the particle 2, respectively. The advantage of expressing the balance in such a coordinate system is that the inertial tensor of the agglomerate (two spheres stuck together) has only diagonal elements since the deviatoric moments of an axisymmetric body vanish if one coordinate axis is aligned with the axis of rotation. This becomes true if the collision–normal vector (it describes the line connecting the centers of the two colliding spheres) is chosen as one axis of the coordinate system in which the inertial tensor is expressed.

**Figure 20:** Coordinate system attached to the center of mass and aligned to the collision–normal and collision–tangential direction.

At the first glance it can be supposed that choosing the coordinate system in such a
manner is disadvantageous from the computational point of view since the translational and angular velocities required for the computation of the kinetic energies have to be transformed from the fixed coordinate system in which the translational and angular velocities of the particles are expressed in the code (the $x$-$y$-$z$ system in Fig. 20) to the coordinate system attached to the two spheres (the $n_c$-$t_{ag}$-$z_{ag}$ system in Fig. 20). However, it is shown afterwards that the computation of all energies involved in the balance except the rotational energy of the agglomerate does not require a transformation of the velocities and angular velocity from the $x$-$y$-$z$ system to the $n_c$-$t_{ag}$-$z_{ag}$ system. This is quite intuitive since the kinetic energy is a scalar quantity and should not depend on the orientation of the coordinate system but only on the chosen inertial frame of reference.

The dissipated energy $E_{dis,ntz}$ can be divided into the energy transformed in plastic deformation $E_{pl}$ and new contributions, i.e., the heat $Q$ produced by the friction. However, the distinction between the way how the energy is dissipated is unimportant for the agglomeration criterion derived in the following. If agglomeration occurs, the relative kinetic energy after the collision vanishes, i.e., $E_{rel,ntz} = 0$. However, the rotational energy after the collision $E_{rot,ntz}^{rel}$ is not zero since the agglomerate keeps a finite angular velocity $\omega_{ag,ntz}$. Hence, the above energy balance can be written in case of agglomeration:

$$E_{rel,ntz}^{rel} + \frac{1}{2} I_{p1} \cdot (\omega_{p1,ntz}^-)^2 + \frac{1}{2} I_{p2} \cdot (\omega_{p2,ntz}^-)^2 + \int_{\delta_0}^{\infty} F_{vW}^- dx =$$

$$- \frac{1}{2} I_{ag,ntz} \cdot \omega_{ag,ntz}^2 + E_{dis,ntz} - \int_{\delta_0}^{\infty} F_{vW}^+ dx.$$  \hspace{1cm} (5.100)

$I_{p1}$ and $I_{p2}$ are the inertial tensors of the two particles. The inertial tensor of the spherical particle 1 can be expressed as follows:

$$I_{p1} = \begin{pmatrix}
0.1 m_{p,1} d_{p,1}^2 & 0 & 0 \\
0 & 0.1 m_{p,1} d_{p,1}^2 & 0 \\
0 & 0 & 0.1 m_{p,1} d_{p,1}^2
\end{pmatrix}.$$  \hspace{1cm} (5.101)

To calculate the inertial tensor of particle 2 the subscript 1 in the above equation has to be replaced by the subscript 2. $I_{ag,ntz}$ is the inertial tensor of the agglomerate described in a coordinate system where one axis is aligned with the collision–normal direction (see, Fig. 20). $\omega_{p1,ntz}^-$, $\omega_{p2,ntz}^-$ and $\omega_{ag,ntz}$ are the particle angular velocities before the collision and the angular velocity of the agglomerate expressed in the new coordinate system shown in Fig. 20. For the computation of the total (translatory and rotatory) kinetic energy the reader is referred to standard text books such as, e.g., Balke (2011) or appendix B. As already mentioned, the coordinate system in which the energy balance is expressed is chosen in a way that one axis is aligned with the collision–normal direction $n_c$ and one with the tangential vector $t_{ag}$ (see, Fig. 20). The third axis $z_{ag}$ is obtained by calculating the vector product of the first two axes mentioned:

$$z_{ag} = n_c \times t_{ag}.$$  \hspace{1cm} (5.102)

By choosing the coordinate system in such a way, only the diagonal elements of the inertial tensor $I_{ag,ntz}$ of the agglomerate are retained since the deviatoric moments vanish.
for axisymmetric bodies where one coordinate axis is aligned with the axis of rotation. The inertial tensor of the agglomerate can be described by the sum of the inertial tensors of the two particles expressed in a coordinate system located at the center of mass plus the components resulting from the parallel shift of the axes. Hence, applying the parallel-axis or Huygens–Steiner theorem (see, e.g., Balke, 2011) leads to the following expression for the inertial tensor of the agglomerate \( I_{ag,\text{nts}} \):

\[
I_{ag,\text{nts}} = \begin{pmatrix}
0.1 m_{p,1}d_{p,1}^2 + 0.1 m_{p,2}d_{p,2}^2 & 0 & 0 \\
0 & m_{p,1}(0.1 d_{p,1}^2 + a_1^2) + m_{p,2}(0.1 d_{p,2}^2 + a_2^2) & 0 \\
0 & m_{p,2}(0.1 d_{p,2}^2 + a_2^2) & m_{p,2}(0.1 d_{p,2}^2 + a_2^2)
\end{pmatrix}.
\]

The angular velocity of the agglomerate can be easily calculated by the conservation of angular momentum:

\[
I_{ag,\text{nts}} \cdot \omega_{ag,\text{nts}} = I_{p1,\text{nts}} \cdot \omega_{p1,\text{nts}} - a_1 \mathbf{n}_{\text{nts}} \times m_{p,1} \mathbf{u}_{p1,\text{nts}} + I_{p2,\text{nts}} \cdot \omega_{p2,\text{nts}} + a_2 \mathbf{n}_{\text{nts}} \times m_{p,2} \mathbf{u}_{p2,\text{nts}}.
\]

\( \mathbf{u}_{p1,\text{nts}} \) and \( \mathbf{u}_{p2,\text{nts}} \) are the velocities of the particles expressed in a coordinate system moving with the constant center of mass velocity \( \mathbf{u}^c \) (see, eq. (5.44)) and additionally oriented as shown in Fig. 20. \( \mathbf{n}_{\text{nts}} = (1 \ 0 \ 0)^T \) is the normal vector expressed in the coordinate system shown in Fig. 20. \( a_1 \) and \( a_2 \) are the distances from the center of mass of the agglomerate \( S_{ag} \) (see, Fig. 20) to the center of the particles:

\[
a_1 = \frac{d_{p,1} + d_{p,2}}{2} \frac{m_{p,2}}{m_{p,1} + m_{p,2}} \quad (5.105a)
\]
\[
a_2 = \frac{d_{p,1} + d_{p,2}}{2} \frac{m_{p,1}}{m_{p,1} + m_{p,2}} \quad (5.105b)
\]

The velocities appearing in the two vector products of eq. (5.104) can be expressed in a frame of reference fixed with the geometry but still oriented as shown in Fig. 20 by the following relations (see, also eq. (5.45)):

\[
\mathbf{u}_{p1,\text{nts}} = - \frac{m_{p,2}}{m_{p,1} + m_{p,2}}(\mathbf{u}_{p2,\text{nts}} - \mathbf{u}_{p1,\text{nts}}) \quad (5.106a)
\]
\[
\mathbf{u}_{p2,\text{nts}} = \frac{m_{p,1}}{m_{p,1} + m_{p,2}}(\mathbf{u}_{p2,\text{nts}} - \mathbf{u}_{p1,\text{nts}}). \quad (5.106b)
\]

After inserting the above relation in the vector product appearing in eq. (5.104), the result reads:

\[
- a_1 \mathbf{n}_{\text{nts}} \times m_{p,1} \mathbf{u}_{p1,\text{nts}} + a_2 \mathbf{n}_{\text{nts}} \times m_{p,2} \mathbf{u}_{p2,\text{nts}} =
- a_1 m_{p,1} \mathbf{n}_{\text{nts}} \times \frac{m_{p,2}}{m_{p,1} + m_{p,2}}(\mathbf{u}_{p1,\text{nts}} - \mathbf{u}_{p2,\text{nts}}) + a_2 m_{p,2} \mathbf{n}_{\text{nts}} \times \frac{m_{p,1}}{m_{p,1} + m_{p,2}}(\mathbf{u}_{p2,\text{nts}} - \mathbf{u}_{p1,\text{nts}}) =
- a_1 m_{p,1} \mathbf{n}_{\text{nts}} \times \mathbf{u}_{p1,\text{nts}} (m_{p,2} + m_{p,2} a_2/a_1) + a_2 m_{p,2} \mathbf{n}_{\text{nts}} \times \mathbf{u}_{p2,\text{nts}} (m_{p,1} + m_{p,1} a_1/a_2)
\]

\( m_{p,1} + m_{p,2} \quad (5.107) \)
At this point of the transformation the ratios \(a_2/a_1\) and \(a_1/a_2\) can be computed by means of eq. (5.105). The results of this manipulation reads:

\[
\begin{align*}
-a_1 m_{p,1} \mathbf{u}_{p1,ntz} \times \mathbf{u}_{p1,ntz} (m_{p,2} + m_{p,2} a_2/a_1) + a_2 m_{p,2} \mathbf{u}_{p2,ntz} \times \mathbf{u}_{p2,ntz} (m_{p,1} + m_{p,1} a_1/a_2) &= \\
-a_1 m_{p,1} \mathbf{u}_{p1,ntz} \times \mathbf{u}_{p1,ntz} (m_{p,2} + m_{p,1}) + a_2 m_{p,2} \mathbf{u}_{p2,ntz} \times \mathbf{u}_{p2,ntz} (m_{p,1} + m_{p,2}) &= \\
- a_1 m_{p,1} \mathbf{u}_{p1,ntz} + a_2 m_{p,2} \mathbf{u}_{p2,ntz} =
\end{align*}
\]

(5.108)

\(\mathbf{u}_{p1,ntz}\) and \(\mathbf{u}_{p2,ntz}\) are the particle velocities expressed in a coordinate system oriented as displayed in Fig. 20 but fixed with the geometry of the computational domain, i.e., not displacing with the constant center of mass velocity \(\mathbf{u}^e\). With this transformation the equation describing the balance of the angular momentum before and after the impact can be written as follows:

\[
\mathbf{I}_{ag,ntz} \cdot \mathbf{\omega}_{ag,ntz} = -a_1 m_{p,1} \mathbf{u}_{p1,ntz} \times \mathbf{u}_{p1,ntz} + a_2 m_{p,2} \mathbf{u}_{p2,ntz} \times \mathbf{u}_{p2,ntz}.
\]

(5.109)

Note that the observation that the angular momentum balance is identical when expressed in a coordinate system moving with \(\mathbf{u}^e\) (see, eq. (5.104)) or in a laboratory (or fixed) coordinate system (see, eq. (5.109)) follows from the fact that both frames are inertial frames of reference. The advantage of a representation of the angular velocities and the tensors of inertia in a coordinate systems as displayed in Fig. 20 is obvious by analyzing eq. (5.109). Since the inertial tensor of the agglomerate has only diagonal elements, no matrix inversion is required to solve eq. (5.109) and an analytic expression for the angular velocity of the agglomerate can be obtained:

\[
\begin{align*}
\omega_{ag,n} &= \frac{0.1 m_{p,1} d_{p,1}^2 \omega_{p1,n}^n + 0.1 m_{p,2} d_{p,2}^2 \omega_{p2,z}^n}{0.1 m_{p,1} d_{p,1}^2 + 0.1 m_{p,2} d_{p,2}^2} \\
\omega_{ag,t} &= \frac{0.1 m_{p,1} d_{p,1}^2 \omega_{p1,t}^t + a_1 m_{p,1} u_{p1,z} + 0.1 m_{p,2} d_{p,2}^2 \omega_{p2,t}^t - a_2 m_{p,2} u_{p2,\text{ag},z}}{0.1 m_{p,1} d_{p,1}^2 + a_1^2 m_{p,1} + 0.1 m_{p,2} d_{p,2}^2 + a_2^2 m_{p,2}} \\
\omega_{ag,z} &= \frac{0.1 m_{p,1} d_{p,1}^2 \omega_{p1,z}^z - a_1 m_{p,1} u_{p1,\text{ag},z} + 0.1 m_{p,2} d_{p,2}^2 \omega_{p2,z}^z + a_2 m_{p,2} u_{p2,t}^t}{0.1 m_{p,1} d_{p,1}^2 + a_1^2 m_{p,1} + 0.1 m_{p,2} d_{p,2}^2 + a_2^2 m_{p,2}}
\end{align*}
\]

(5.110a, 5.110b, 5.110c)

Note that eq. (5.110a) has no contribution of the vector product appearing in eq. (5.109) since the collision–normal vector \(\mathbf{n}_{ntz}\) has no components in collision–tangential nor in \(\mathbf{z}_{ag}\)–direction, i.e., \(\mathbf{n}_{ntz} = (1\ 0\ 0)^T\). Therefore, the first component of the vector products appearing in eq. (5.109) is always equal to zero. \(\omega_{ag,n}, \omega_{ag,t}\) and \(\omega_{ag,z}\) are the components of the angular velocity of the agglomerate in \(\mathbf{n}_{ag}, \mathbf{t}_{ag}\) and \(\mathbf{z}_{ag}\)–direction, respectively. Of course, the components of the particle velocities \((u_{p1,\text{ag},t}^- , u_{p2,\text{ag},t}^- \text{ and } u_{p1,\text{ag},z}^- , u_{p2,\text{ag},z}^-)\) and the angular velocities \((\omega_{p1,n}^- , \omega_{p1,t}^- , \omega_{p1,z}^- \text{ and } \omega_{p2,n}^- , \omega_{p2,t}^- , \omega_{p2,z}^-)\) before the collision have to be expressed in the same coordinate system and can be calculated by forming the dot product between the translational or angular velocity and the vectors \(\mathbf{n}_{ag}, \mathbf{t}_{ag}\) and \(\mathbf{z}_{ag}\). The operation is shown exemplarily for the angular velocity of particle 1 (for all other
quantities required the procedure is analogous):

\( \omega_{p_1,n} = \omega_{p_1} \cdot n_c \)  \hspace{1cm} (5.111a)

\( \omega_{p_1,t} = \omega_{p_1} \cdot t_{ag} \)  \hspace{1cm} (5.111b)

\( \omega_{p_1,z} = \omega_{p_1} \cdot z_{ag} \)  \hspace{1cm} (5.111c)

The last point to clarify in order to close the relation (5.100) is how to express the dissipated kinetic energy \( E_{\text{dis,ntz}} \) in terms of known (pre–collision) quantities and how to calculate the difference of the van–der–Waals force. Assuming that the major deformation of the particles occurs in collision–normal direction, the difference of the van–der–Waals forces can be calculated as in § 5.4.2.3. In order to derive an expression for the dissipated energy \( E_{\text{dis,ntz}} \) as a function of known (or pre–collision) quantities, the same assumption is made as in the former two sections: It is assumed that \( E_{\text{dis,ntz}} \) can be calculated by the difference of the total (translational and rotational) kinetic energies before and after the collision without considering any agglomeration or the van–der–Waals force:

\[
E_{\text{dis,ntz}} = \frac{1}{2} \left( \frac{m_{p_1} m_{p_2}}{m_{p_1} + m_{p_2}} \right) \left[ (u_{p_2,ntz} - u_{p_1,ntz})^2 - (u_{p_2,ntz}^H - u_{p_1,ntz}^H)^2 \right] + \frac{1}{2} I_{p_1} \cdot (\omega_{p_1,ntz})^2 - \frac{1}{2} I_{p_1} \cdot (\omega_{p_1,ntz}^H)^2 + \frac{1}{2} I_{p_2} \cdot (\omega_{p_2,ntz})^2 - \frac{1}{2} I_{p_2} \cdot (\omega_{p_2,ntz}^H)^2
\]

Following the same assumption as in § 5.4.2.3, the quantities with the superscript HS in the above expression can be calculated as follows: In case of a sliding collision eq. (5.35) has to be used. On the other hand, if a sticking collision occurs eq. (5.34) has to be applied. Hence, the condition for the occurrence of agglomeration (see, eq. (5.100)) can be extended:

\[
E_{\text{rel,ntz}} - k_{\text{in,ntz}} + \frac{1}{2} \left( \frac{m_{p_1} m_{p_2}}{m_{p_1} + m_{p_2}} \right) \left[ (u_{p_2,ntz} - u_{p_1,ntz})^2 - (u_{p_2,ntz}^H - u_{p_1,ntz}^H)^2 \right] \leq \frac{1}{2} I_{ag,ntz} \cdot \omega_{ag,ntz}^2 + E_{\text{dis,ntz}} + \frac{H}{12 \delta_0} d_{p_1} \left[ (1 - e_{n,p}^2) \left( \frac{m_{p_1} m_{p_2}}{m_{p_1} + m_{p_2}} \right) \left( \frac{u_{p_2} - u_{p_1}}{n_c} \right) \right]^2 \frac{1}{\pi \sigma (d_{p,1} + d_{p,2})^{1/2}}.
\]

Note that the difference of the van–der–Waals energy is calculated as done in § 5.4.2.3 (see, eq.(5.77)) since the particles are assumed to deform plastically only in collision–normal direction. The final relation to determine agglomeration can be obtained by further simplifying the above expression. First, the dissipated energy defined by eq. (5.112) is inserted into eq. (5.113). By performing this operation the rotational and translational kinetic energies before the collision is eliminated from eq. (5.113) and only the corresponding quantities after the collision calculated with a standard hard–sphere model remain. Furthermore, in order to calculate the translational and rotational kinetic energies of the two particles (not the agglomerate) the translational and angular velocities do not need to be transformed into the coordinate system displayed in Fig. 20. This becomes obvious by
the following equation:

\[
\frac{1}{2} \mathbf{I}_{p1} \cdot \omega_{p1,ntz}^2 = \frac{1}{20} m_{p1} d_{p1,1}^2 \omega_{p1,ntz}^2 = \frac{1}{20} m_{p1} d_{p1,1}^2 \omega_{p1,1}^2
\]

\[
(u_{p2,ntz}^- - u_{p1,ntz}^-)^2 = (u_{p2}^- - u_{p1}^-)^2.
\] (5.114b)

The above equalities follow from the fact that the dot product of a vector with itself provides the square of the magnitude of the vector. Since the magnitude of a vector does not change by switching its representation from one orientation of the coordinate system to another, the kinetic energies are also independent of the orientation of the coordinate system. The rotational kinetic energy of particle 2 is calculated in an analogous manner. Hence, the final relation to determine agglomeration can be written as follows:

\[
\frac{1}{2} \mathbf{I}_{ag,ntz} \cdot \omega_{ag,ntz}^2.
\]

The above relation means that if the total (rotational and translational) kinetic energy after the collision calculated by the standard hard–sphere approach is less than the kinetic energy of the agglomerate plus the work required to overcome the van–der–Waals force, agglomeration occurs.

Concerning the post–collisional treatment of the agglomerate some care has to be taken in order not to violate the energy conservation. In the case discussed in § 5.4.2.3 no angular momentum change is allowed over the collision process and therefore the angular velocity of the particles is zero (of course the moments exerted by the viscous forces have to be neglected). In this case, if the agglomerate is treated as a volume–equivalent sphere without rotation, no problems concerning the energy balance arise. That means that the kinetic energy of the agglomerate (two spheres stuck together) is the same as the kinetic energy of a volume–equivalent sphere since the translational kinetic energy depends beside on the velocity only on the mass of the agglomerate. Note that the velocity of the volume–equivalent sphere is not changed with respect to the velocity of the the center of mass. Therefore, if the mass is conserved by the definition of the equivalent diameter \( d_{ves} \) (see, eq. (5.96)) no energy differences arise between the configuration of two spheres stuck together and the volume–equivalent sphere. Furthermore, the conservation of momentum is achieved by the definition of the post–collision velocity of the center of mass (see, eq. (5.44)).

Problems arise if friction is allowed during the collision. In this case the particles do not possess a vanishing angular velocity. Hence, the rotational kinetic energy of the agglomerate (two spheres stuck together) has to be equal to the rotational kinetic energy of the equivalent sphere in order to avoid artificial source or sink terms in the global energy balance. However, the condition can not be fulfilled since the tensors of inertia of a volume–equivalent sphere and two spheres stuck together (see, Fig. 20) are not the
same. In order to remove this inconsistency in the energy balance, the agglomerate is treated as a porous sphere with a diameter $d_{ps}$ and a homogeneous density $\rho_{ps}$ which is different from the particle density $\rho_p$. The moment of inertia of a porous sphere $I_{ps}$ is calculated by:

$$I_{ps} = \begin{pmatrix} 
\frac{1}{60} \pi \rho_{ps} d_{ps}^5 & 0 & 0 \\
0 & \frac{1}{60} \pi \rho_{ps} d_{ps}^5 & 0 \\
0 & 0 & \frac{1}{60} \pi \rho_{ps} d_{ps}^5 
\end{pmatrix}.$$

(5.116)

In order not to violate the energy balance, the rotational energy of the agglomerate and the rotational energy of the porous sphere have to be equal:

$$\frac{1}{2} I_{ps} \cdot \omega_{ps,ntz}^2 = \frac{1}{2} I_{ag,ntz} \cdot \omega_{ag,ntz}^2.$$

(5.117)

Here $\omega_{ps,ntz}$ denotes the angular velocity of the porous sphere which is determined by means of the angular momentum balance:

$$I_{ps} \cdot \omega_{ps,ntz} = I_{ag,ntz} \cdot \omega_{ag,ntz}.$$

(5.118)

Rearranging the above equation with respect to $\omega_{ps,ntz}$ leads together with eq. (5.116) to the following result:

$$\omega_{ps,ntz} = \frac{I_{ag,ntz} \cdot \omega_{ag,ntz}}{1/60 \pi \rho_{ps} d_{ps}^5}.$$

(5.119)

The required inertial moment of the porous sphere is determined by inserting the above definition of $\omega_{ps,ntz}$ in the energy balance (5.117). The result of this operation reads:

$$\frac{(I_{ag,ntz} \cdot \omega_{ag,ntz})^2}{1/60 \pi \rho_{ps} d_{ps}^5} = I_{ag,ntz} \cdot \omega_{ag,ntz}^2.$$

(5.120)

Hence, the inertial moment of the porous sphere can be determined:

$$\frac{1}{60} \pi \rho_{ps} d_{ps}^5 = \frac{(I_{ag,ntz} \cdot \omega_{ag,ntz})^2}{I_{ag,ntz} \cdot \omega_{ag,ntz}^2}.$$

(5.121)

The above relation still has the two unknowns $d_{ps}$ and $\rho_{ps}$. The last relation to obtain the diameter of the porous sphere $d_{ps}$ is the mass conservation. The mass of the porous sphere has to be equal to the mass of the two agglomerating particles:

$$\rho_{ps} \frac{1}{6} \pi d_{ps}^3 = \frac{1}{6} \pi (\rho_{p,1} d_{p,1}^3 + \rho_{p,2} d_{p,2}^3).$$

(5.122)

That yields the density of the porous sphere $\rho_{ps}$:

$$\rho_{ps} = \frac{\rho_{p,1} d_{p,1}^3 + \rho_{p,2} d_{p,2}^3}{d_{ps}^3}.$$

(5.123)
If we insert $\rho_{ps}$ in eq. (5.121) a constitutive equation for the diameter $d_{ps}$ is achieved:

$$d_{ps} = \left( \frac{60 \pi (\rho_{p,1} d_{p,1}^3 + \rho_{p,2} d_{p,2}^3)}{\mathbf{I}_{ag,ntz} \cdot \omega_{ag,ntz}^2} \right)^{1/2}.$$  

(5.124)

The last issue considered in this section is how to proceed in the cases where no agglomeration occurs. This matter has to be considered since the post–collisional translational and angular velocities calculated by the standard hard–sphere model described in § 5.4.1 have to be modified in order to take into account the influence of the van–der–Waals forces. Starting point of the analysis is eq. (5.99) which balances the kinetic energy and the work done by the van–der–Waals forces before the collision with the same quantities after the collision plus the dissipated energy. The scope of the considerations made in the following is to derive relations for the relative translational $E^{rel+}_{kin}$ and the relative rotational kinetic energies $E^{rel+}_{rot}$ after the collision for the cases where no agglomeration occurs. Note that the subscript $ntz$ is omitted since the energy balance is independent of the orientation of the frame of reference and therefore it can also be expressed in a Cartesian coordinate system. Since only spherical particles are involved in the following observation, the inertial tensor of the particles is also independent of the orientation of the coordinate systems. In order to derive a relation for $E^{rel+}_{kin}$ and $E^{rel+}_{rot}$ for the case where no agglomeration occurs, these two quantities are expressed as follows:

$$E^{rel+}_{kin} = E^{HS,rel+}_{kin} - \Delta E^{rel}_{kin}$$  
$$E^{rel+}_{rot} = E^{HS,rel+}_{rot} - \Delta E^{rel}_{rot}.$$  

(5.125a, b)

$E^{HS,rel+}_{kin}$ and $E^{HS,rel+}_{rot}$ are the translational and rotational kinetic energies after the collision calculated with a standard–hard sphere model, i.e., without considering agglomeration and the van–der–Waals force. These two quantities can be calculated as a function of the pre–collision quantities by means of eqs. (5.35) and (5.34) depending on whether a sliding or sticking collision occurs. $\Delta E^{rel}_{kin}$ and $\Delta E^{rel}_{rot}$ denote the differences between the post–collision energies calculated by the standard–hard sphere model and the one considering also the influence of the van–der–Waals forces. After inserting eq. (5.125) into eq. (5.99), the resulting expression reads:

$$E^{rel-}_{kin} + E^{rel-}_{rot} + \int_0^{\delta_0} F^{-}_{vW} dx = E^{HS,rel-}_{kin} - \Delta E^{rel}_{kin} + E^{HS,rel+}_{rot} - \Delta E^{rel}_{rot} + E_{dis} - \int_\delta^{\infty} F^{+}_{vW} dx.$$  

(5.126)

The dissipated energy $E_{dis}$ is calculated by the same assumption as made in the former section: It can be expressed by the difference of the total energy before and after the collision calculated by the standard hard–sphere model, i.e., without considering agglomeration and the van–der–Waals forces:

$$E_{dis} = E^{rel-}_{kin} - E^{HS,rel+}_{kin} + E^{rel-}_{rot} - E^{HS,rel+}_{rot}.$$  

(5.127)

By inserting the above equation into eq. (5.126), the following relation is obtained (here the work exerted by the van–der–Waals forces before the collision is already neglected
with respect to the same quantity after the collision):

\[- \int_{\delta_0}^{\infty} F_{vW}^+ \, dx = \Delta E_{\text{kin}}^+ + \Delta E_{\text{rot}}^+ = E_{\text{HS,rel}}^+ - E_{\text{kin}}^+ + E_{\text{rot}}^+ - E_{\text{rot}}^+. \quad (5.128)\]

The above equation means that the total kinetic energy computed by the standard hard–sphere model has to be reduced by the amount of the work exerted by the van–der–Waals force (see, eq. (5.75) for the definition) in order to obtain the total kinetic energy after the collision. Finally, after dividing the relative kinetic energies \( E_{\text{HS,rel}}^+ \) and \( E_{\text{kin}}^+ \) into a component in normal and tangential direction as done in § 5.4.2.3, we obtain:

\[- \int_{\delta_0}^{\infty} F_{vW}^+ \, dx = E_{\text{HS,rel}}^+ - E_{\text{kin,n}}^+ + E_{\text{HS,rel}}^+ - E_{\text{kin,n}}^+. \quad (5.129)\]

Of course, at this point further assumptions similar to the ones used in § 5.4.2.3 have to be made since the above scalar equation has three unknowns, i.e., \( E_{\text{kin,n}}^+ \), \( E_{\text{kin,t}}^+ \) and \( E_{\text{rot}}^+ \). Here three different cases are distinguished:

(i) In the first case it is assumed that the work done by the van–der–Waals forces influences only the relative kinetic energy in normal direction, whereas the relative kinetic energy in tangential direction and the rotational kinetic energy remain unaffected, i.e., \( E_{\text{HS,rel}}^+ = E_{\text{kin,t}}^+ \) and \( E_{\text{rot}}^+ = E_{\text{rot}}^+ \). With this assumption eq. (5.129) reads:

\[- \int_{\delta_0}^{\infty} F_{vW}^+ \, dx = E_{\text{HS,rel}}^+ - E_{\text{kin,n}}^+ \quad 9. \quad (5.130)\]

By rearranging the above equation with respect to \( E_{\text{kin,n}}^+ \) and dividing the result by \( E_{\text{HS,rel}}^+ \), a modified normal restitution coefficient \( k_{n,p}^2 \) is obtained:

\[ k_{n,p}^2 = \frac{E_{\text{kin,n}}^+}{E_{\text{HS,rel}}^+} = \frac{u_n^+}{(u_n^{\text{HS}+})^2} = 1 - \frac{- \int_{\delta_0}^{\infty} F_{vW}^+ \, dx}{E_{\text{HS,rel}}^+}. \quad (5.131)\]

Note that the integral in the above expression can be calculated by means of eq. (5.75). \( u_n^+ \) is the relative velocity in collision–normal direction (see, eq. (5.80) for the determination) of the particles after the collision considering also the influence of the van–der–Waals forces. \( u_n^{\text{HS}+} \) is the relative velocity in collision–normal direction calculated by the standard hard–sphere model, i.e., by means of eqs. (5.34a) and (5.34b) for a sticking collision or by means of eqs. (5.35a) and (5.35b) for a sliding collision, respectively. In order to calculate the post–collision velocities the momentum balance in collision–normal direction between the hard–sphere model and the model including the van–der–Waals force can be used (see, also Fig. 21 for

\[ \text{Note that for a frictionless collision the following equality holds:} \quad E_{\text{HS,rel}}^+ = e_{n,p}^2 E_{\text{kin,n}}^+. \quad \text{Therefore, the balance (5.83) made to obtain the modified normal restitution coefficient } \tilde{e}_{n,p}^2 \text{ in the former section can be restored in the limiting case of a frictionless collision.} \]
the definition of $\hat{F}_{\text{ag}}$):

$$
\mathbf{u}_{p,1}^+ \cdot \mathbf{n}_c = \mathbf{u}_{p,1}^{HS+} \cdot \mathbf{n}_c - \frac{\hat{F}_{\text{ag}}}{m_{p,1}} \cdot \mathbf{n}_c
$$

(5.132a)

$$
\mathbf{u}_{p,2}^+ \cdot \mathbf{n}_c = \mathbf{u}_{p,2}^{HS+} \cdot \mathbf{n}_c + \frac{\hat{F}_{\text{ag}}}{m_{p,2}} \cdot \mathbf{n}_c
$$

(5.132b)

$\hat{F}_{\text{ag}}$ can be interpreted as a force originating by the van–der–Waals interaction. At this point it has to be decided, which of the two possible solutions of eq. (5.131) is taken to calculate the relative velocity $\mathbf{u}^+_n$ in collision–normal direction after the collision. Since the aim of the present consideration is to reduce $\mathbf{u}^+_n$ with respect to $\mathbf{u}_{n}^{HS+}$ and not to invert its sign, the solution delivering the same sign is taken. Therefore, $k_{n,p}$ reads as follows:

$$
k_{n,p} = \frac{\mathbf{u}^+_n}{\mathbf{u}_{n}^{HS+}}.
$$

(5.133)

By subtracting eq. (5.132a) from eq. (5.132b) and using the above definition, a relation for the collision–normal component of $\hat{F}_{\text{ag}}$ can be obtained:

$$
\hat{F}_{\text{ag}} \cdot \mathbf{n}_c = -\frac{m_{p,1} m_{p,2}}{m_{p,1} + m_{p,2}} (1 - k_{n,p}) \left( \mathbf{u}_{p,2}^{HS+} - \mathbf{u}_{p,1}^{HS+} \right) \cdot \mathbf{n}_c
$$

(5.134)

The above force can be inserted in eq. (5.132) to calculate the normal component of the particles’ post–collision velocities. For the limiting case of a vanishing van–der–Waals force $k_{n,p}$ is equal to unity (see, eq. (5.131)). Therefore, $\hat{F}_{\text{ag}} \cdot \mathbf{n}_c$ is equal to zero and the post–collision particle velocities are equal to the ones calculated by the standard hard–sphere model.

(ii) The second case is considered if $k_{n,p}^2$ is found to be less than zero. In this case the normal relative kinetic energy after the collision $E_{kin,n}^{rel+}$ is set to zero. Therefore, eq. (5.129) reads:

$$
- \int_{\delta_0}^{\infty} F_{vW}^+ dx = E_{HS,rel+}^{kin,n} + E_{HS,rel+}^{kin,t} - E_{HS,rel+}^{kin,t}.
$$

(5.135)

Note that it is assumed that the rotational kinetic energy is still unaffected. After rearranging with respect to $E_{kin,t}^{rel+}$ and dividing by $E_{kin,t}^{HS,rel+}$ a modified tangential restitution coefficient $k_{t,p}^2$ is obtained:

$$
k_{t,p}^2 = \frac{E_{kin,t}^{rel+}}{E_{kin,t}^{HS,rel+}} = \frac{u_t^+}{u_t^{HS+}} = 1 - \frac{- \int_{\delta_0}^{\infty} F_{vW}^+ dx - E_{HS,rel+}^{kin,n}}{E_{kin,t}^{HS,rel+}}.
$$

(5.136)

$u_t^+$ is the relative velocity in collision–tangential direction (see, eq. (5.80) for the

---

Note that for a frictionless collision the following equalities hold: $E_{kin,n}^{HS,rel+} = e_{n,p}^2 E_{kin,n}^{rel-}$ and $E_{kin,t}^{HS,rel+} = E_{kin,t}^{rel-}$. Therefore, in the limit of a frictionless collision the balance (5.86) made to obtain the modified tangential restitution coefficient $e_{t,p}^2$ described in the former section can be restored.
determination) of the particles after the collision considering also the van–der–Waals forces. $u_{t}^{HS+}$ is the relative velocity in collision–tangential direction calculated by the standard hard–sphere model, i.e., by means of eqs. (5.34a) and (5.34b) for a sticking collision or by means of eqs. (5.35a) and (5.35b) for a sliding collision, respectively. In order to calculate the post–collision velocities the momentum balance in collision–tangential direction between the hard–sphere model and the model including the van–der–Waals force can be used (see, also Fig. 21 for the definition of $\hat{F}_{ag}$):

\begin{align}
    u_{p,1}^{+} \cdot t_{ag} &= u_{p,1}^{HS+} \cdot t_{ag} - \frac{\hat{F}_{ag}}{m_{p,1}} \cdot t_{ag} \\
    u_{p,2}^{+} \cdot t_{ag} &= u_{p,2}^{HS+} \cdot t_{ag} + \frac{\hat{F}_{ag}}{m_{p,2}} \cdot t_{ag}
\end{align}

(5.137a) \hspace{1cm} (5.137b)

Note that here it is assumed that $\hat{F}_{ag}$ acts at the center of each particle since the angular velocity of the particles should not be affected in this case. At this point it has to be decided, which of the two possible solution of eq. (5.136) it is taken to calculate the relative velocity in collision–tangential direction after the collision $u_{t}^{+}$. Since the aim of the present consideration is to reduce $u_{t}^{+}$ with respect to $u_{t}^{HS+}$ and not to invert its sign, the positive solution is taken. Therefore, $k_{t,p}$ reads as follows:

\[
k_{t,p} = \frac{u_{t}^{+}}{u_{t}^{HS+}}.
\]

(5.138)

By subtracting eq. (5.137a) from eq. (5.137b) and using the definition (5.138) of the
coefficient \(k_{t,p}\), a relation for the tangential component of \(\hat{F}_{ag}\) can be obtained:

\[
\hat{F}_{ag} \cdot t_{ag} = -\frac{m_{p,1} m_{p,2}}{m_{p,1} + m_{p,2}} (1 - k_{t,p}) \left( u_{p,2}^{\text{HS}+} - u_{p,1}^{\text{HS}+} \right) \cdot t_{ag} \tag{5.139}
\]

The above force can be inserted in eq. (5.137) to calculate the tangential component of the particles post–collision velocities.

(iii) The third case is considered if both \(k_{n,p}^2\) and \(k_{t,p}^2\) are less than zero. In this case the relative kinetic energy (normal and tangential) is set to zero and the rotational kinetic energy has to be reduced to fulfill the energy balance (5.129). Equation (5.129) reads in the third case considered:

\[
-\int_{\delta_0}^{\infty} F_{eW} dx = E_{\text{kin},n}^{\text{rel},+} + E_{\text{kin},t}^{\text{rel},+} + E_{\text{rot},+}^{\text{rel},+} - E_{\text{rel},+}^{\text{rot}}. \tag{5.140}
\]

After rearranging with respect to the difference of the rotational kinetic energy \(E_{\text{rot},+}^{\text{rel},+} - E_{\text{rot},+}^{\text{rel}}\), the above equation reads:

\[
\frac{1}{2} I_{p,1} \cdot (\omega_{p,1}^{\text{HS}+})^2 - (\omega_{p,1}^{\text{HS}+})^2 + \frac{1}{2} I_{p,2} \cdot (\omega_{p,2}^{\text{HS}+})^2 = -\int_{\delta_0}^{\infty} F_{eW} dx - E_{\text{kin},n}^{\text{rel},+} - E_{\text{kin},t}^{\text{rel},+} \tag{5.141}
\]

\((\omega_{p,1}^{\text{HS}+})^2\) and \((\omega_{p,2}^{\text{HS}+})^2\) are the particle angular velocities after the collision calculated by a standard hard–sphere model, i.e., by means of eqs. (5.34c) and (5.34d) for a sticking collision or by means of eqs. (5.35c) and (5.35d) for a sliding collision, respectively. In the cases (i) and (ii) the momentum balance delivers two additional equations to determine the post–collision particle velocities in collision–normal and collision–tangential direction. Unfortunately, the angular momentum balance can not be used for this case since this requires two moments acting in opposite sense on each particle (Since no external moment acts on the particles, the sum of the moments has to be zero.). For two particles having the same sense of rotation, this would lead to an acceleration of one particle and only a slow down of the other particle. Therefore, no simultaneously compliance of the energy and angular momentum balance can be achieved by the method proposed. Since the agglomeration criterion is based on energetic considerations, the fulfillment of the energy balance is preferred.

Therefore, at this point another assumption has to be made since the the above equation still contains the two unknowns \((\omega_{p,1}^{+})^2\) and \((\omega_{p,2}^{+})^2\). Thus the question arise how the right–hand side of the above equation is distributed amongst the two colliding particles.

This is achieved by introducing the factor \(\beta\):

\[
\beta = \frac{1/2 \ I_{p,1} \cdot (\omega_{p,1}^{\text{HS}+})^2}{1/2 \ I_{p,1} \cdot (\omega_{p,1}^{\text{HS}+})^2 + 1/2 \ I_{p,2} \cdot (\omega_{p,2}^{\text{HS}+})^2} \tag{5.142}
\]

In this way one equation for each particle which defines the difference of the rotational energy calculated by means of the standard hard–sphere model and the model
considering also the van–der–Waals forces can be obtained:

$$\frac{1}{2} I_p^1 \cdot \left( (\omega_{p,1}^{HS+})^2 - (\omega_{p,1}^+)^2 \right) = \beta \left( - \int_{\delta_0}^{\infty} F_{vW}^+ dx - E_{HS,rel}^{HS,rel} - E_{kin,t}^{HS,rel} \right)$$

(5.143a)

$$\frac{1}{2} I_p^2 \cdot \left( (\omega_{p,2}^{HS+})^2 - (\omega_{p,2}^+)^2 \right) = (1 - \beta) \left( - \int_{\delta_0}^{\infty} F_{vW}^+ dx - E_{HS,rel}^{HS,rel} - E_{kin,t}^{HS,rel} \right).$$

(5.143b)

The summation of eq. (5.143a) and (5.143b), of course, restores eq. (5.141). Finally, after rearranging the above equations, two factors defining the ratios $\omega_{p,1}^+/(\omega_{p,1}^{HS+})^2$ and $(\omega_{p,2}^+)^2/(\omega_{p,2}^{HS+})^2$ are derived:

$$k_{\omega,1}^2 = \frac{(\omega_{p,1}^+)^2}{(\omega_{p,1}^{HS+})^2} = 1 - \frac{2\beta}{I_p^1 \cdot (\omega_{p,1}^{HS+})^2} \left( - \int_{\delta_0}^{\infty} F_{vW}^+ dx - E_{HS,rel}^{HS,rel} - E_{kin,t}^{HS,rel} \right)$$

(5.144a)

$$k_{\omega,2}^2 = \frac{(\omega_{p,2}^+)^2}{(\omega_{p,2}^{HS+})^2} = 1 - \frac{2(1 - \beta)}{I_p^2 \cdot (\omega_{p,2}^{HS+})^2} \left( - \int_{\delta_0}^{\infty} F_{vW}^+ dx - E_{HS,rel}^{HS,rel} - E_{kin,t}^{HS,rel} \right).$$

(5.144b)

5.4.2.6 Summary of the Model in Case of Collisions Involving Friction

Briefly summarized, the agglomeration model implemented in the code LESOCC in case of collisions involving friction works as follows:

(i) First, it is checked if two particles collide as shown in § 6.2.3.

(ii) $u_{p,1}^{HS+}$, $u_{p,2}^{HS+}$, $\omega_{p,1}^{HS+}$, and $\omega_{p,2}^{HS+}$ required for the following steps of the model are computed by means of eqs. (5.34) in case of a sticking collision or by means of eqs. (5.35) in case of a sliding collision.

(iii) For two colliding particles, criterion (5.115) is evaluated.

(iv) If criterion (5.115) is fulfilled, the particles agglomerate. Hence, the velocities of the two particles are set equal to the velocity of the center of mass (see, eq. (5.44)). In the following steps of the simulation the agglomerate is treated as a porous sphere with the diameter $d_{ps}$ defined by eq. (5.124) and the density $\rho_{ps}$ defined by eq. (5.123). The angular velocity of the porous sphere $\omega_{ps,ntz}$ is obtained by the angular momentum balance (5.118) and therefore is calculated by eq. (5.119). The idealization of the agglomerate as a porous sphere has the big advantage that the collision detection is much easier to accomplish than for a configuration of two or more spheres stuck together. Furthermore, the aerodynamic forces on the particles can still be calculated by eq. (4.25). Since eq. (5.119) defines the components of the angular velocity of the porous sphere $\omega_{ps,ntz}$ in the frame of reference depicted in Fig. 20, the angular velocity of the agglomerate has to be transformed back to the
Cartesian coordinate system in which the particle variables are stored:

$$\omega_{ps} = \omega_{ps,n} n_c + \omega_{ps,t} t_{ag} + \omega_{ps,z} z_{ag}.$$ (5.145)

(v) If criterion (5.115) is not fulfilled, the post–collisional translational and angular velocities are calculated by the following relation:

$$u_{p,1}^+ = u_{p,1}^{HS^+} + \frac{m_{p,2}}{m_{p,1} + m_{p,2}} \left( (1 - k_{n,p}) u_n^{HS^+} + (1 - k_{t,p}) u_t^{HS^+} \right)$$ (5.146a)

$$u_{p,2}^+ = u_{p,2}^{HS^+} - \frac{m_{p,1}}{m_{p,1} + m_{p,2}} \left( (1 - k_{n,p}) u_n^{HS^+} + (1 - k_{t,p}) u_t^{HS^+} \right)$$ (5.146b)

$$\omega_{p,1}^+ = k_{\omega,1} \omega_{p,1}^{HS^+}$$ (5.146c)

$$\omega_{p,2}^+ = k_{\omega,2} \omega_{p,2}^{HS^+}.$$ (5.146d)

The post–collisional velocities can be calculated by inserting the values of $k_{n,p}$ and $k_{t,p}$ in the definitions of the contact force in collision–normal (eq. (5.134)) and collision–tangential direction (eq. (5.139)). After inserting the contact forces in the respective momentum balances (eq. (5.132) and eq. (5.137)) the above relations for the post–collisional translational velocities are obtained. $k_{\omega,1}$ and $k_{\omega,2}$ are the positive solutions of eqs. (5.144a) and (5.144b). This specific choice is taken since the sense of rotation of the two particles when considering also the van–der–Waals forces is assumed to be the same as the one obtained by the standard hard–sphere model. At this point the coefficients $k_{n,p}$, $k_{t,p}$, $k_{\omega,1}$ and $k_{\omega,2}$ have to be computed depending on whether case (i), (ii) or (iii) occurs. For case (i) $k_{n,p}$ is computed by eq. (5.131) and all other coefficients are set to unity. For case (ii) $k_{t,p}$ is computed by eq. (5.136), $k_{n,p}$ is set to zero and $k_{\omega,1}$ and $k_{\omega,2}$ are set to unity. For case (iii) only $k_{\omega,1}$ and $k_{\omega,2}$ are computed by means of eq. (5.144) and the other two coefficients are set to zero.

5.4.2.7 A–priori Analysis of the Agglomeration Model for Frictionless Collisions

At first, the agglomeration criterion (5.79) in case of frictionless collisions with relative tangential velocity is analyzed. The scope is to visualize the limiting relative particle velocity $|u_{p,2x}^{*}|_{lim}$ (see Fig. 22 for the configuration) in case of a frictionless collision as a function of the two particle diameters $d_{p,1}^*$ and $d_{p,2}^*$. The particle sizes analyzed range from 1 to 100 µm. For that purpose, the two–dimensional configuration depicted in Fig. 22 is considered. Here the particle 1 is at rest while the second particle has only a velocity component in $x$–direction. The angular velocities $\omega^{*}_{p,1z}$ and $\omega^{*}_{p,2z}$ are set to zero since they have no influence on the agglomeration criterion (5.79) in case of frictionless collisions. Four different scenarios are examined. The first case is a head–on collision. In the other three cases the angle $\alpha$ between the velocity $u_{p,2x}^{*}$ of the particle 2 before the collision and the collision–normal vector $n_c$ is set to achieve the following values: $\alpha = 30^\circ$, $60^\circ$ and $89^\circ$.

For the four simple configurations depicted in Fig. 22 criterion (5.79) reads in dimen-
The following observations can be made:

Figure 22: Configurations of the particles before the impact to analyze the agglomeration criterion in case of a collision with and also without friction.

\[
\frac{(u_{p,2x}^-)^2 - (u_{p,2x} n_{c,x})^2 (1 - \epsilon_{n,p}^2)}{u_{p,2x}^- n_{c,x}} \leq \frac{H^*}{6 \delta_0^2} \left[ (1 - \epsilon_{n,p}^2) \frac{6}{\pi^2} \frac{\rho_p^* \bar{\sigma}}{d_{p,1}^3 + d_{p,2}^3} \right]^{1/2}
\]

(5.147)

\(n_{c,x}\) is the \(x\)-component of the collision–normal vector \(n_c\). The \(y\)-component of the collision normal vector \(n_c\) does not appear in the above relation since the second particle in the configurations depicted in Fig. 22 has only a velocity in \(x\)-direction and particle 1 is fixed. After rearranging the above expression with respect to \(u_{p,2x}^\rightarrow\) the following result is obtained in dimensional form:

\[
u_{p,2x}^\rightarrow \leq \frac{n_{c,x}}{1 - n_{c,x}^2 (1 - \epsilon_{n,p}^2) 6 \delta_0^2} \left[ (1 - \epsilon_{n,p}^2) \frac{6}{\pi^2} \frac{\rho_p^* \bar{\sigma}}{d_{p,1}^3 + d_{p,2}^3} \right]^{1/2}
\]

(5.148)

The above relation is given in dimensional form since the crucial parameters for the occurrence of agglomeration are dimensional sizes of the particles and not the dimensionless diameters \(d_{p,1} = d_{p,1}/L_f^*\) and \(d_{p,2} = d_{p,2}/L_f^*\). The evaluation of the above function for the different collision–normal vectors is shown in Fig. 23 and is performed with the software gnuplot. The results are illustrated in dimensional form in order to quantify the particle diameter sizes relevant for the occurrence of agglomeration. The material constants required to evaluate eq. (5.148) are listed in Table 2 including the constants required for the agglomeration with friction. The constant \(H^*, \rho_p^*, \delta_0^*\) and \(\bar{\sigma}^*\) are chosen for limestone particles and can be found in Tomas (2007). The normal restitution coefficient \(\epsilon_{n,p}\) is taken from Ho and Sommerfeld (2002) also for limestone particles.

Fig. 23 shows the limiting velocity \(|u_{p,2x}^\rightarrow|_{\text{lim}}\) for the occurrence of agglomeration as a function of the particle diameters \(d_{p,1}^*\) and \(d_{p,2}^*\) for the four cases depicted in Fig. 22. The following observations can be made:

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### Table 2: Constants required for the agglomeration criterion without friction and with friction.

The additional constants required for the agglomeration with friction are listed below the second double line.

<table>
<thead>
<tr>
<th>constant</th>
<th>value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hamaker constant $H^*$</td>
<td>$3.8 \times 10^{-20}$ J</td>
</tr>
<tr>
<td>particle density $\rho_p^*$</td>
<td>2710 kg/m$^3$</td>
</tr>
<tr>
<td>minimal contact distance $\delta_0^*$</td>
<td>$3.36 \times 10^{-10}$ m</td>
</tr>
<tr>
<td>mean yield stress $\overline{\sigma}^*$</td>
<td>$3.0 \times 10^8$ Pa</td>
</tr>
<tr>
<td>normal restitution coefficient $e_{n,p}$</td>
<td>0.4</td>
</tr>
<tr>
<td>tangential restitution coefficient $e_{t,p}$</td>
<td>0.44</td>
</tr>
<tr>
<td>dynamic coefficient of friction $\mu_{dy,p}$</td>
<td>0.6</td>
</tr>
<tr>
<td>static coefficient of friction $\mu_{st,p}$</td>
<td>0.85</td>
</tr>
</tbody>
</table>

(i) For all cases $|u_{p,2x}^-|_{lim}$ tends to zero if the diameter of both particles approach about 100 $\mu$m and has a maximum for the smallest particles diameter considered, i.e., $d_{p,1}^* = d_{p,2}^* = 1 \mu$m. The values of $|u_{p,2x}^-|_{lim}$ for $d_{p,1}^* = d_{p,2}^* = 1 \mu$m as a function of $\cos \alpha$ are shown in Fig. 24.

(ii) $|u_{p,2x}^-|_{lim}$ decreases for increasing angle $\alpha$. This observation is reasonable since for a frictionless collision no force can be exerted in collision–tangential direction. Furthermore, it is obvious from eq. (5.79) that the van–der–Waals energy is proportional to the component of the relative velocity of the two particles in collision–normal direction. For values of $\alpha$ close to 90° the van–der–Waals energy vanishes and therefore the probability of the two particles to agglomerate is close to zero. This is obvious from the small values of $|u_{p,2x}^-|_{lim}$.

### 5.4.2.8 A–priori Analysis of the Agglomeration Model for Collisions with Friction

As the second point in this a–priory analysis, the agglomeration criterion (5.115) in case of a collision with friction is analyzed. For that purpose, the two–dimensional configuration depicted in Fig. 22 is considered again. At first, the angular velocities of both particles $\omega_{p,1z}$ and $\omega_{p,2z}$ are set to zero. For this case the same four angles $\alpha$ as done in the previous section are analyzed. As in the previous section, the limiting relative velocity of the second particle $|u_{p,2x}^-|_{lim}$ is evaluated as a function of the particle diameters $d_{p,1}^*$ and $d_{p,2}^*$. In order to analyze the influence of the angular velocity of the particles on the occurrence of agglomeration, two angular velocity pairs are examined: $\omega_{p,1z}^* = -5$ s$^{-1}$, $\omega_{p,2z}^* = 5$ s$^{-1}$ and $\omega_{p,1z}^* = -50$ s$^{-1}$, $\omega_{p,2z}^* = 50$ s$^{-1}$. Also for this setup the limiting relative velocity $|u_{p,2x}^-|_{lim}$ can be visualized as a function of the particle diameters $d_{p,1}^*$ and $d_{p,2}^*$. Finally, the density $\rho_{ps}^*$ and the diameter $d_{ps}^*$ of the porous sphere used to simplify the geometry of the agglomerate are also evaluated as a function of the particle diameters $d_{p,1}^*$ and $d_{p,2}^*$. That means that, when a limiting relative velocity $|u_{p,2x}^-|_{lim}$ is reached for a given diameter pair $d_{p,1}^*$ and $d_{p,2}^*$ which satisfies criterion (5.115), the density of the porous sphere $\rho_{ps}^*$ is calculated by means of eq. (5.123) and the diameter $d_{ps}^*$ of the porous sphere is obtained by eq. (5.124). As shown in the following, for the simple two–dimensional
Figure 23: Limiting relative particle velocity $|u_{p,2x}^-|_{\text{lim}}$ for the occurrence of agglomeration in case of a frictionless collision as a function of the two particle diameters $d_{p,1}$ and $d_{p,2}$ and different angles $\alpha$. Note the different scaling of the $|u_{p,2x}^-|_{\text{lim}}$ axis.

Figure 24: Values for $|u_{p,2x}^-|_{\text{lim}}$ for the occurrence of agglomeration in case of a frictionless collision for $d_{p,1} = d_{p,2} = 1 \mu\text{m}$ as a function of $\cos \alpha$.

configuration considered here, both aforementioned quantities are independent of $\alpha$ and therefore the case for $\alpha = 0^\circ$ is taken.

The material constants required for the evaluation of eq. (5.115) are summarized in Table 2. The same constants $H^*$, $\rho_p^*$, $\delta_0^*$, $\sigma^{*}$ and $\epsilon_{n,p}$ as in the former section are used.
The static $\mu_{st,p}$ and dynamic coefficient of friction $\mu_{dy,p}$ are taken from the review of experimental results published by Byerlee (1978). For the tangential restitution coefficient the same value as used in § 7.4 and 7.6 for glass–glass inter–particle collisions is chosen since no measured values are found.

Figure 25 shows the evaluation of the agglomeration criterion (5.115) for a zero initial angular velocity of both particles and different angles $\alpha$. In contrast to the previous section the calculation of the limiting relative velocity $|u_{p,2x}^*|_{lim}$ is performed numerically since the derivation of an analytical solution is not trivial. Furthermore, the equations to solve eq. (5.115) are already disposable in the code. By defining the initial configuration, the quantities denoted by the superscript HS (eq. (5.34) for a sliding and eq. (5.35) for a sticking collision) and the kinetic energy of the agglomerate $1/2 I_{ag,ntz} \cdot \omega_{ag,ntz}^2$ in eq. (5.115) can easily be calculated. For a given particle diameter pair $d_{p,1}^*$ and $d_{p,2}^*$ the velocity $u_{p,2x}^*$ of the second particle is reduced successively from an initial value of $u_{p,2x} = 1.0$ m/s until condition (5.115) is fulfilled. The results of this calculation are presented in Fig. 25. The following observations can be made:

(i) As expected, for the head–on collision ($\alpha = 0^\circ$) with zero angular velocities of the particles visualized in Fig. 25(a) the same dependency of $|u_{p,2x}^*|_{lim}$ from the particle diameter $d_{p,1}^*$ and $d_{p,2}^*$ as for the frictionless collision is found (see Fig. 23(a)). For a head–on collision the angular velocities $\omega_{p,1}^{HS+}$ and $\omega_{p,2}^{HS+}$ and the angular velocity of the agglomerate $\omega_{ag,ntz}$ are zero. Furthermore, changes of the translational velocity can only occur in collision–normal direction (see eq. (5.34) and (5.35) for the computation of the post–collisional state). Therefore, eq. (5.115) reduces to eq. (5.79) and Fig. 23(a) and Fig. 25(a) are identical.

(ii) For large diameters $d_{p,1}^*$ and $d_{p,2}^*$ of both particles, $|u_{p,2x}^*|_{lim}$ decreases towards zero, i.e., agglomeration is impossible.

(iii) $|u_{p,2x}^*|_{lim}$ decreases for increasing angles $\alpha$ since the van–der–Waals energy (the first term on the right–hand side of eq. (5.115)) tends to zero for increasing $\alpha$.

(iv) The local maxima for the cases $\alpha \neq 0^\circ$ appearing for $d_{p,1}^* = d_{p,2}^*$ can be explained as follows: The analysis of the numerical data show that the rotational kinetic energy of the agglomerate $1/2 I_{ag,ntz} \cdot \omega_{ag,ntz}^2$ and the van–der–Waals energy have a local maximum for equal–sized diameters, i.e., $d_{p,1}^* = d_{p,2}^*$. Therefore, also the right–hand side of eq. (5.115) has a local maximum for this diameter pairing and the limiting relative velocity $|u_{p,2x}^*|_{lim}$ can reach higher values than for $d_{p,1}^* \neq d_{p,2}^*$. (see the local maximum in Fig. 25(b)-(d)). Of course for $\alpha = 0^\circ$ the rotational kinetic energy is equal to zero and therefore this explanation does not hold any more. The peak values visible for small equal–sized particles ($d_{p,1}^* = d_{p,2}^* = d_p^*$) derives from the fact that the van–der–Waals energy in condition (5.115) is proportional to $d_p^3$, the translational kinetic energy is proportional to $d_p^5$ and the other two remaining terms are proportional to $d_p$. Therefore, for small particle diameters the van–der–Waals energy has a larger value compared to the other terms in condition (5.115) allowing larger limiting velocities $|u_{p,2x}^*|_{lim}$.

Figures 26 and 27 shows the evaluation of the agglomeration criterion (5.115) for two different pairs of the initial angular velocity and different angles $\alpha$. In order to do not
Figure 25: $|\omega_{p,1z}^-| = 0$ and $|\omega_{p,2z}^-| = 0$: Limiting relative particle velocity $|u_{p,2x}^*-\lim|$ for the occurrence of agglomeration in case of a collision with friction as a function of the two particle diameters $d_{p,1}^*$ and $d_{p,2}^*$ and different angles $\alpha$. Note the different scaling of the $|u_{p,2x}^*-\lim|$ axis.

reduce too much the size of the subfigures, it is chosen to represent the eight different cases in two separated figures. The following observations can be made:

(i) For small rotation rates all configuration with angles $\alpha \leq 89^\circ$ only a marginal influence on the limiting relative velocity $|u_{p,2x}^*-\lim|$ can be found (compare Fig. 25(a)-(c) with Fig. 26(a) and (a) and Fig. 27(a)). The configuration $\alpha = 89^\circ$ delivers similar $|u_{p,2x}^*-\lim|$ values for the cases with zero rotation rates and small rotation rates. However, in contrast to the other orientations of the collision–normal vector no solution of criterion (5.115) is found for particles with a diameter around 10 $\mu$m or larger (Note the different ranges of the $d_{p,1}^*$ and $d_{p,2}^*$ axis in Fig. 25(d) and Fig. 27(c) and (d)).

(ii) High rotation rates lead to a sudden jump of $|u_{p,2x}^*-\lim|$ to zero. That means that for a given particle diameter pair $d_{p,1}^*$ and $d_{p,2}^*$ and an angular velocity pair $\omega_{p,1z}^-$ and $\omega_{p,2z}^-$ eq. (5.115) has no solution. The transition to the parameter space where eq. (5.115) has no solution is discontinuous. The explanation for the discontinuous transition is provided below.
(iii) The agglomeration criterion (5.115) is marginally influenced by the rotation rate if one of the two particles involved in the agglomeration is small. That means that under this condition, \( |u_{agg}^{\ast,2z}|_{lim} \) is similar for the small and the high rotation rotation rate (compare Fig. 26(a) with (b), Fig. 26(c) with (d) and Fig. 27(a) with (b) and Fig. 27(c) with (d) in the region where one of the two particles is small).

Figure 26: Variation of \( |\omega_{agg}^{\ast,1z}| \) and \( |\omega_{agg}^{\ast,2z}| \): Limiting relative particle velocity \( |u_{agg}^{\ast,2z}|_{lim} \) for the occurrence of agglomeration in case of a collision with friction as a function of the two particle diameters \( d_{p,1}^{\ast} \) and \( d_{p,2}^{\ast} \) and angles angles \( \alpha = 0^\circ \) and \( 30^\circ \). Note the different scaling of the \( |u_{agg}^{\ast,2z}|_{lim} \) axis.

In the following, an explanation is provided why for rotating particles a sudden jump of \( |u_{agg}^{\ast,2z}|_{lim} \) from a finite value to zero is observed. For that purpose the development of the left–hand side and the right–hand side of eq. (5.115) is depicted in Fig. 28 as a function of the velocity \( u_{agg}^{\ast,2z} \) of the second particle. The case where the rotation rates of the two particles are set to \( \omega_{agg}^{\ast,1z} = -50 \, \text{s}^{-1} \) and \( \omega_{agg}^{\ast,2z} = 50 \, \text{s}^{-1} \) and the head–on collision (see Fig. 26(b)) is taken as an example. For a better overview the abscissa is multiplied by -1. In Fig. 28 \( E_{tot}^{HS+} \) denotes the left–hand side of eq. (5.115) and \( E_{W} + E_{agg} \) the right–hand side. Figures 28(a) and (b) depict \( E_{tot}^{HS+} \) and \( E_{W} + E_{agg} \) as a function of \( u_{agg}^{\ast,2z} \) for the diameter pair \( d_{p,1}^{\ast} = 42 \, \mu m \) and \( d_{p,2}^{\ast} = 41 \, \mu m \). In Figs. 28(c) and (d) the same function is shown but for the parameter pair \( d_{p,1}^{\ast} = 42 \, \mu m \) and \( d_{p,2}^{\ast} = 42 \, \mu m \).
The reason is that the particle velocities before the collision in collision–normal direction are independent of the translational velocity of the particles before the collision. In the case of a head–on collision, the sum of the van–der–Waals energy \(E_{vW}^{agg}\) present in eq. (5.115) for the computation of \(E_{tot}\) and the kinetic energy of the agglomerate \(E_{agg}\) (i.e., \(E_{vW} + E_{agg}\)), decrease with decreasing velocity of the second particle. For the special case of a head–on collision \(E_{vW} + E_{agg}\) shows a linear dependence from \(u_{p,2x}^{-}\). The linear dependence of the van–der–Waals energy from \(u_{p,2x}^{-}\) is rather obvious since the factor \(((u_{p2}^{-} - u_{p1}^{-}) \cdot n_c)^2\) present in eq. (5.115) for the computation of \(E_{vW}\) can be extracted from the square–root. For the case of a head–on collision \(1/2 \mathbf{I}_{agg,nts} \cdot \omega_{agg,nts}^2\) present in eq. (5.115) is independent of the translational velocity of the particles before the collision. The reason is that the particle velocities before the collision in collision–normal direction have no influence on the calculation of \(\omega_{agg,nts}\) (see eq. (5.110)). Therefore, the red lines shown in Fig. 28(b) show a linear decrease for decreasing \(u_{p,2x}^{-}\) with a value greater than zero for \(u_{p,2x}^{-} = 0\). However, for the special case chosen here, the minimum lies in the order of \(\mathcal{O}(10^{-20})\) above the zero axis and is not visible in the figure. The reason
is that both particles are almost equal–sized and have an opposite rotation rate. This
results in a very small rotation rate of the agglomerate and therefore also a small value
of \( \frac{1}{2} I_{ag,ntz} \cdot \omega_{ag,ntz}^2 \).

As shown in Fig. 28(b) \( E_{HS+}^{tot} \) shows a parabolic dependence of \( u_{p,2x}^- \) with a minimum
with greater than zero. The minimum greater than zero is reached since for rotating
particles the total kinetic energy in case of a standard hard–sphere collision \( E_{HS+}^{tot} \) still has
a rotational component even if the translational kinetic energy is zero. For the parameter
space shown in Figs. 28(a) and (b) the blue and the red line cross each other and an
agglomeration is found.

On the other hand, for the case where no solution is found (see, Figs. 28(c) and (d))
the minimum of \( E_{HS+}^{tot} \) is shifted slightly in the direction of the positive ordinate and the
red line is slightly shifted in the direction of the negative ordinate and therefore the blue
and the red lines are not crossing each other. For this scenario no agglomeration occurs.

From a physical point of view the above findings can be interpreted as follows: For
the second case discussed above (where no agglomeration is found) the particles approach
each other, impact and dissipate energy during the collision process. However, the residual
energy left after the collision process is still sufficient to prevent agglomeration. For the

Figure 28: Development of the left–hand side (\( E_{HS+}^{tot} \)) and the right–hand side (\( E_{vW} + E_{agg} \))
of eq. (5.115) as a function of \( u_{p,2x}^- \).
first case discussed above (where agglomeration is found) the particles have dissipated too much energy over the collision process and they remain trapped in the potential well of the van–der–Waals forces leading to agglomeration.

Finally, Fig. 29 shows the dependence of the normalized diameter \( d_{ps}^* / d_{eq}^* = d_{ps}^* / (d_{p,1}^* + d_{p,2}^* / 3)^{1/3} \) and the normalized density \( \rho_{ps}^* / \rho_{eq}^* \) of the porous sphere from the two particle diameters \( d_{p,1}^* \) and \( d_{p,2}^* \). For high rotation rates the functions displayed in Fig. 29(b) and (d) are truncated for large particle diameters \( d_{p,1}^* \) and \( d_{p,2}^* \) since no solution of criterion (5.115) is found. The diameter of the porous sphere \( d_{ps}^* \) is normalized by the diameter of a volume–equivalent sphere \( d_{eq}^* = (d_{p,1}^* + d_{p,2}^* / 3)^{1/3} \). It is evident that \( d_{ps}^* / (d_{p,1}^* + d_{p,2}^* / 3)^{1/3} \) shows a local maximum when both particles involved in the agglomeration process have the same diameter (see Fig. 29(a) and (b)). The analysis of the equation (5.124) defining the diameter \( d_{ps}^* \) of the porous sphere provides a simple explanation of this observation for the simplified configuration considered here. For the two–dimensional case analyzed in this section, the angular velocity of the agglomerate \( \omega_{ag,ntz} \) has only a component in \( z \)–direction. Hence, the expression (5.124) is independent of the angular velocity of the agglomerate and solely depends on the densities and diameters of the two particles involved. If the densities of the two particles \( \rho_{p,1}^* \) and \( \rho_{p,2}^* \) are equal (as considered here), eq. (5.124) reduces solely to a function of the diameter \( d_{p,1}^* \) and \( d_{p,2}^* \) of the two particles involved in the agglomeration. The final expression reads (Since the single steps to derive the equation involve only simple algebraic manipulations they are not shown for the sake of brevity):

\[
d_{ps}^* = \left[ \frac{10}{d_{p,1}^* + d_{p,2}^*} \left( 0.1 d_{p,1}^* + d_{p,2}^* \right)^2 + \frac{d_{p,1}^* d_{p,2}^*}{(d_{p,1}^* + d_{p,2}^*)^2} + 0.1 d_{p,2}^* \right]^{1/2}.
\]

(5.149)

The maximum of the above function is obtained when both particles have the same diameter \( d_{p,1}^* = d_{p,2}^* = d_p^* \). For this case the above expression can be further simplified to:

\[
d_{ps}^* = \sqrt{\frac{7}{2}} d_p^*.
\]

(5.150)

Since Fig. 29(a) and (b) shows the same red color for \( d_{p,1}^* = d_{p,2}^* \), the above relation can also be found in the numerical data. Finally, the maximum of the ratio of the diameter \( d_{ps}^* \) of the porous sphere to the diameter \( d_{eq}^* \) of a volume–equivalent sphere for the case where both particles have the same diameter can be derived as follows:

\[
\frac{d_{ps}^*}{d_{eq}^*} = \frac{\sqrt{7}}{\sqrt{2}} \approx 1.48.
\]

(5.151)

This value is exactly the value of the maximum shown in Fig. 29(a) and (b). That means that for particles with the same diameters \( d_{p,1}^* = d_{p,2}^* = d_p^* \) the diameter \( d_{ps}^* \) of the porous sphere calculated by expression (5.124) is about 1.5 times higher than the diameter \( d_{eq}^* \) of a volume–equivalent sphere. For large differences in the particle sizes the two expressions \( d_{ps}^* \) and \( d_{eq}^* \) are similar (see Fig. 29(a) and (b)). The explanation why the maximum of the diameter \( d_{ps}^* \) of the porous sphere occurs when both particles have the same diameter is rather simple. Supposing we have the two configurations depicted in Fig. 30. For both configurations we have an agglomerate
consisting of two particles with the centers $S_1$ and $S_2$. Furthermore, the agglomerate rotates with $\omega_{agg,z}$ around the $z$–axis of the coordinate system depicted in Fig. 30. The origin of the coordinate system is at the position of the center of mass CM of the two spheres stuck together. For both configurations the sum of the masses of the two particles constituting the agglomerate should be equal, i.e., both agglomerates depicted in Fig. 30 should have the same mass. Furthermore, the angular velocity $\omega_{agg,z}$ of the agglomerate should be the same. For this simple configuration it is obvious that the agglomerate on the left–hand side of Fig. 30 has the larger inertial moment around the $z$–axis than the agglomerate on the right–hand side. For this reason ($\omega_{agg,z}$ is equal) for configuration 1 the rotational kinetic energy of the agglomerate is higher than for configuration 2. Since the porous sphere model guarantees the conservation of energy, configuration 1 leads to a larger diameter $d_{ps}^*$ of the porous sphere than configuration 2.

The differences found between $d_{eq}^*$ and $d_{ps}^*$ explains also the minimum of $\rho_{ps}^*/\rho_p^*$ observed in Fig. 29(c) and (d). Since the mass $m_{eq}^*$ of a volume–equivalent sphere and the mass $m_{ps}^*$ of the porous sphere are equal ($m_{eq}^* = m_{ps}^*$), this leads to a minimum of the ratio $\rho_{ps}^*/\rho_p^*$ of about 0.31 (Note that for a volume–equivalent sphere the density is equal to the
Figure 30: Left: Configurations for which the maximum diameter of the porous sphere occurs; Right: Configurations for which the minimum diameter of the porous sphere occurs.

particle density $\rho_p^*$:

$$\frac{\rho_{ps}^*}{\rho_p^*} = \left( \frac{d_{eq}^*}{d_{ps}^*} \right)^3 \approx \frac{1}{3.27} = 0.31. \quad (5.152)$$
6 Numerical Methods

In the previous three sections the modeling strategies for the continuous phase, the disperse phase and the procedures adopted to couple both phases were described. The scope of these sections was to provide the governing equations which describe the temporal evolution of the two-phase flow. In order to obtain reliable numerical solutions of these equations in an affordable amount of time, efficient and robust numerical methods have to be employed. The scope of this section is to provide an overview of the numerical methods adopted. The numerical methods used for the continuous phase are elucidated in § 6.1 and the one applied for the disperse phase are described in § 6.2. Finally, the determination of the statistics is explained in § 6.3.

6.1 Numerical Methods for the Continuous Phase

In this section the numerical methods employed to solve the LES equations are briefly described. Since the major effort in this thesis was spent to extend the disperse phase part of the code, here only a general overview is provided. Note that the scope of this section is to give the reader a short introduction of the methodologies adopted in the code LESOCC to obtain a numerical solution of the LES equations (5.12) and not to go into the details of the implementation. For the details, see Breuer (1998, 2002); Breuer et al. (2006); Breuer (2013) and the references therein.

In order to numerically solve eq. (5.12) the following steps are performed: First eq. (5.12) has to be transformed to a body-fitted coordinate systems since the equations of motion for the continuous phase are solved in this space. After integrating the resulting equations over the control volume, the LES equations in integral form have to be discretized. This is achieved by the finite-volume method which is presented in § 6.1.2. Note that the transformation to a body-fitted coordinate system and the discretization of the surface integrals are shown exemplarily by means of the convective terms. Since its discretization strongly affects the quality of the LES solution (Breuer, 2002), they are taken as an illustrative example. The discretization of the viscous fluxes and the pressure is only briefly described for the sake of brevity. Finally, the resulting linear system of equations has to be solved. The strategy to achieve a numerical solution of the linear system of equations and the employed solver are explained in § 6.1.3–6.1.5.

6.1.1 Transformation to a Body-fitted Coordinate System

In this section it is shown exemplarily how to transform the convective terms in eq. (5.12) from a Cartesian coordinate system to a curvilinear coordinate system as shown in Fig. 31(a). Since the diffusive terms contain second derivatives, the transformation is quite laborious but can be achieved by the same methodology as shown here. The complete description of the transformation is illustrated in Breuer (2011). The final form of the transformed differential equation can be also found in Ferziger and Perić (2002).

As already mentioned, the code LESOCC works on a curvilinear body-fitted coordinate system (see, Fig. 31(a)). In order to increase the complexity of the representable geometries, the computational domain can furthermore be decomposed into single blocks (see, Fig. 31(b)). Each block is represented by a single curvilinear coordinate system. This results in a discretization of the computational domain by block-structured body-fitted
grids. By dividing the computational domain into blocks, the parallelization is achieved in a natural way.

This discretization method represents a compromise between the flexibility of unstructured grids (in principle every geometry is reproducible) and the efficiency and accuracy of orthogonal (Cartesian) grids. An advantage over orthogonal grids can be seen when the discretization of a circle as depicted in Fig. 31(b) is taken as an example: Using a polar grid for the discretization of the circle results in a degeneration of the rectangles to a triangle in the center. This singularity is avoided by using block-structured curvilinear grids. A disadvantage over orthogonal grids is that the resulting equations are more complicated and therefore it results in a loss of efficiency. Another disadvantage with respect to Cartesian grids it that the reliability of the solution is strongly affected by the quality
of the grid. Especially for strongly deformed grids the computation of the diffusive fluxes is complicated. This can even lead to serious convergence problems (Breuer, 2011).

A characteristic property which curvilinear and orthogonal grids have in common, is that each grid point is uniquely defined by an index triple \((i, j, k)\). Furthermore, an explicit relation exists between the index of the linear array where the corner points are stored and the index of the coordinate line \(i, j\) and \(k\):

\[
ii = i + (j - 1) \times ni + (k - 1) \times ni \times nj.
\] (6.1)

Here \(ni\) and \(nj\) denote the total number of coordinate lines in \(\xi–\) and \(\eta–\)direction. Note that the same relation as described above is also valid to determine the index of the array where the variables (e.g., the fluid velocity) defined at the center of the control volume are stored. In this case \(ni\) and \(nj\) in eq. (6.1) describe the number of control volumes in \(i–\) and \(j–\)direction. For the details of the implementation, see Breuer (2013). Therefore, the indices of the neighboring cells required to discretize the governing equations have not to be stored explicitly. They are required, e.g., to approximate the fluxes over the surfaces of the control volume. Furthermore, very efficient algorithms exist to invert the band matrices obtained from the discretization on structured grids (Breuer, 2011).

The aforementioned advantages of the direct addressing of the control volume centers are completely lost on unstructured grids. Here, the indices of the neighboring cells have to be stored in lists. This indirect addressing of neighboring points results in a efficiency loss (Breuer, 2011). Furthermore, the matrices obtained from the discretization have no regular structure and therefore the solver employed to solve the linear system is not as efficient as for band matrices. A further disadvantage of unstructured grids over block–structured grids is the larger discretization error.

In order to transform the differential equation (5.12), which is described in a Cartesian coordinate system (the physical or \(p–\)space), to a curvilinear coordinate system (the computational or \(c–\)space), the derivatives with respect to the three Cartesian directions \((x, y\) and \(z)\) have to be expressed as a function of the derivatives with respect to the coordinate lines \(\xi(x, y, z)\), \(\eta(x, y, z)\) and \(\zeta(x, y, z)\). Applying the chain rule it is easy to show that the derivatives \(\partial/\partial x_i\) can be written as follows:

\[
\frac{\partial}{\partial x} = \frac{\partial}{\partial \xi} \frac{\partial \xi}{\partial x} + \frac{\partial}{\partial \eta} \frac{\partial \eta}{\partial x} + \frac{\partial}{\partial \zeta} \frac{\partial \zeta}{\partial x}
\] (6.2a)

\[
\frac{\partial}{\partial y} = \frac{\partial}{\partial \xi} \frac{\partial \xi}{\partial y} + \frac{\partial}{\partial \eta} \frac{\partial \eta}{\partial y} + \frac{\partial}{\partial \zeta} \frac{\partial \zeta}{\partial y}
\] (6.2b)

\[
\frac{\partial}{\partial z} = \frac{\partial}{\partial \xi} \frac{\partial \xi}{\partial z} + \frac{\partial}{\partial \eta} \frac{\partial \eta}{\partial z} + \frac{\partial}{\partial \zeta} \frac{\partial \zeta}{\partial z}
\] (6.2c)

After applying the above differential operators to the convective terms \(\partial(\overline{u}_i\overline{u}_j)/\partial x_j\), it is
easy to show that these terms in eq. (5.12) can be written as follows:

\[
\frac{\partial \overline{u_i}}{\partial x_j} = \frac{1}{J} \left[ \frac{\partial (\overline{u_i U J^{-1}})}{\partial \xi} + \frac{\partial (\overline{u_i V J^{-1}})}{\partial \eta} + \frac{\partial (\overline{u_i W J^{-1}})}{\partial \zeta} \right]
\]

(6.3a)

\[
\frac{\partial \overline{v_i}}{\partial x_j} = \frac{1}{J} \left[ \frac{\partial (\overline{v_i U J^{-1}})}{\partial \xi} + \frac{\partial (\overline{v_i V J^{-1}})}{\partial \eta} + \frac{\partial (\overline{v_i W J^{-1}})}{\partial \zeta} \right]
\]

(6.3b)

\[
\frac{\partial \overline{w_i}}{\partial x_j} = \frac{1}{J} \left[ \frac{\partial (\overline{w_i U J^{-1}})}{\partial \xi} + \frac{\partial (\overline{w_i V J^{-1}})}{\partial \eta} + \frac{\partial (\overline{w_i W J^{-1}})}{\partial \zeta} \right]
\]

(6.3c)

\[U, V \text{ and } W \text{ are the contravariant velocities and are defined as follows:}
\]

\[
U = \xi_x \overline{u} + \xi_y \overline{v} + \xi_z \overline{w}
\]

(6.4a)

\[
V = \eta_x \overline{u} + \eta_y \overline{v} + \eta_z \overline{w}
\]

(6.4b)

\[
W = \zeta_x \overline{u} + \zeta_y \overline{v} + \zeta_z \overline{w}
\]

(6.4c)

\[\xi_x, \xi_y, \ldots \text{ are the metric terms.} \text{ } J \text{ and } J^{-1} \text{ are the determinant of the Jacobian and the inverse Jacobin matrix, respectively:}
\]

\[
J = \begin{vmatrix} \xi_x & \xi_y & \xi_z \\ \eta_x & \eta_y & \eta_z \\ \zeta_x & \zeta_y & \zeta_z \end{vmatrix}, \quad J^{-1} = \begin{vmatrix} x_\xi & x_\eta & x_\zeta \\ y_\xi & y_\eta & y_\zeta \\ z_\xi & z_\eta & z_\zeta \end{vmatrix}.
\]

(6.5)

Note that the following relations between the Jacobian determinant \(J^{-1}\) and the differential volume \(\Delta V ol\) in the p–space and the determinant \(J\) and the differential volume \(\Delta V c\) in the c–space exist (Merziger and Wirth, 1999; Ferziger and Perić, 2002):

\[\Delta V ol = J^{-1} \Delta \xi \Delta \eta \Delta \zeta, \quad \Delta V c = \Delta \xi \Delta \eta \Delta \zeta = J \Delta x \Delta y \Delta z.
\]

(6.6)

Since the grid spacing in the c–space is arbitrary, typically \(\Delta \xi = \Delta \eta = \Delta \zeta = 1\) is set. Therefore, \(J^{-1}\) and \(J\) have not to be computed explicitly and can be replaced by \(\Delta V ol\) or 1/\(\Delta V ol\), respectively.

The equivalent but more compact form of the transformed convective terms (6.3) reads:

\[
\frac{\partial \overline{u_i}}{\partial x_j} = J \frac{1}{\partial \xi_j} \frac{\partial (\overline{u_i U J^{-1}})}{\partial x_j},
\]

(6.7)

where \(\xi_i = (\xi, \eta, \zeta)\) for \(i = 1, 2, 3\). After applying the methodology described above to all derivatives present in eq. (5.12), the transport equation for the velocities \(\overline{u_i}\) in a curvilinear coordinate system can be derived and has the final form (see, e.g., Ferziger and Perić, 2002; Breuer, 2011):

\[
\frac{\partial (U_j J^{-1})}{\partial \xi_i} = 0
\]

(6.8a)

\[
J^{-1} \frac{\partial \overline{u_i}}{\partial t} + \frac{\partial}{\partial \xi_j} \left[ U_j \frac{\partial \overline{u_i}}{\partial x_j} J^{-1} \right] = - \frac{\partial \overline{\mu}}{\partial \xi_j} \frac{\partial \overline{u_i}}{\partial x_j} J^{-1} + \frac{\partial}{\partial \xi_j} \left( \mu + \frac{1}{Re} \left( \frac{\partial \overline{u_i}}{\partial \xi_m} J B_{mj} \right) \right) + J^{-1} f_i^{PSIC}
\]

(6.8b)
\[ f_i^{PSIC} \] are the source terms in the momentum equation. The matrix \( B_{mj} \) is defined as \( B_{mj} = \beta_{mi} \beta_{ji} \) and with \( \beta_{kj} = J^{-1} \frac{\partial \xi_j}{\partial x_j} \). Finally, the integral of eq. (6.8) over the volume of the computational space can be taken to obtain a form suitable for the finite–volume discretization:

\[
\int_{V_c} J^{-1} \frac{\partial \bar{u}_i}{\partial t} dV_c + \int_{S_c} \left[ U_j \frac{\partial \bar{u}_i}{\partial x_j} \right] n_{c,j} dS_c = -\int_{S_c} p \frac{\partial \xi_j}{\partial x_j} J^{-1} n_{c,j} dS_c + \int_{V_c} J^{-1} f_i^{PSIC} dV_c \quad (6.9a)
\]

\[
\int_{V_c} J^{-1} \frac{\partial \bar{u}_i}{\partial t} dV_c + \int_{S_c} \left[ \left( \mu_T + \frac{1}{Re} \right) \frac{\partial u_i}{\partial \xi_m} J B_{mj} \right] n_{c,j} dS_c + \int_{S_c} p \frac{\partial \xi_j}{\partial x_j} J^{-1} n_{c,j} dS_c + \int_{V_c} J^{-1} f_i^{PSIC} dV_c \quad (6.9b)
\]

\( n_{c,j} \) is the normal vector with respect to \( dS_c \). The transformation of the volume integral into a surface integral is obtained by the Gauss’s theorem. Note that in the discrete version \( \Delta V_c = 1 \) and \( \Delta S_c = 1 \) since \( \Delta \xi = \Delta \eta = \Delta \zeta = 1 \) is set.

### 6.1.2 Finite–Volume Method and Discretization of the Fluxes

In order to achieve a numerical solution of eq. (6.9) it has to be discretized. In the code \( \mathcal{L}E\mathcal{S}OCC \) the equations of motion for the fluid are discretized by a 3D finite–volume method on arbitrary non–orthogonal block–structured grids with a colocated variable arrangement. The resulting algebraic equations are solved to obtain a solution for the flow quantities stored at the cell center \( P \) of the control volume (see, Fig. 32). Note that the following considerations are made on a 2D grid to simplify the issue. The extrapolation to 3D grid is straightforward. The approximation of the volume integrals in eq. (6.9) is shown explicitly. In order to illustrate the discretization of the surface integrals, the method is shown only for the convective terms in eq. (6.9) for the sake of brevity. The approximation of all other surface integrals are achieved in a similar manner and are only briefly discussed.

The integrand of the volume integral is approximated by its average over the control volume. Hence, the value at the cell center \( P \) (see, Fig. 32) can be directly calculated without involving neighboring control points (denoted E, W, S and N in Fig. 32):

\[
\int_{V_c} J^{-1} \frac{\partial \bar{u}_i}{\partial t} dV_c \approx J^{-1} \frac{\partial \bar{u}_i^P}{\partial t}, \quad \int_{V_c} J^{-1} f_i^{PSIC} dV_c \approx J^{-1} f_i^{PSIC} \quad (6.10)
\]

Note the the volume \( \Delta V_c \) of the control volume in the \( c–space \) is equal to \( \Delta V_c = 1 \) since \( \Delta \xi = \Delta \eta = \Delta \zeta = 1 \). The above approximation of the volume integral is denominated as midpoint rule and is second–order accurate (Ferziger and Perić, 2002). In order to describe the position of the neighboring cells with respect to the cell center \( P \), the commonly used geographical notation is adopted, i.e., E stand for east, W for west, S for south and N for north.

The surface integrals in eq. (6.9) are first split into the sum of the four integrals over the faces. After that each integral over the face is approximated by the midpoint rule, i.e., instead of integrating the variable quantity over the surface of the control volume, its average at the midpoints of the corresponding sides of the control volume (the blue points denotes with e, w, n and s in Fig. 32) is taken. This approximation is second–order accurate (Breuer, 2002). Taking the convective term of eq. (6.9) as an illustratory
example, this approximation reads:

$$\int_{S_c} \tilde{u}_i \mathbf{U}_j J^{-1} n_{e,j} dS_e \approx \int_{S_e} \tilde{u}_{i,e} U_{e}^{cor} J_e^{-1} S_e - \tilde{u}_{i,w} U_{w}^{cor} J_w^{-1} S_w + \tilde{u}_{i,n} V_{n}^{cor} J_n^{-1} S_n - \tilde{u}_{i,s} V_{s}^{cor} J_s^{-1} S_s.$$

(6.11)

$U_{e}^{cor}$, $U_{w}^{cor}$, $V_{n}^{cor}$ and $V_{s}^{cor}$ are the corrected contravariant velocities at the east, west, north and south face of the control volume, respectively. The correction is performed in order to avoid the pressure–velocity decoupling due to the colocated variable arrangement. The way how it is achieved is explained in the following. The minus signs derive from the different orientation of the normal vectors. $S_e$, $S_w$, $S_n$ and $S_s$ are the surfaces of the faces and $\tilde{u}_{i,e}$, $\tilde{u}_{i,w}$, $\tilde{u}_{i,n}$ and $\tilde{u}_{i,s}$ are the values of the velocity $\tilde{u}_i$ at the faces of the control volume. Note that the surface of the faces in the computational space are equal to $S_e = S_w = S_n = S_s = 1$ since $\Delta \xi = \Delta \eta = \Delta \zeta = 1$.

In a colocated arrangement of the variables only the values at the cell centers are known (denoted by the points with the capital letters P, E, W, S and N in Fig. 32). Therefore, the values at faces of the control volume (denoted by the points with the lowercase letters e, w, s and n in Fig. 32) have to be approximated. In the following the interpolation of the contravariant velocity $U_{e}^{cor}$ and the velocities $\tilde{u}_{i,w}$ at the west side are shown exemplarily. The procedure applied to interpolate the velocities $\tilde{u}_i$ and the contravariant velocities $U_{e}^{cor}$ at all other faces of the control volume is achieved in a similar way. Of course, the points involved in the interpolation of the velocity and the interpolation factors are different for each face of the control volume.

In order to linearly interpolate the variables from the cell centers to the center of the cell face $w$, the interpolation factor $f_{x,P}$ is defined:

$$f_{x,P} = |\mathbf{x}_w - \mathbf{x}_P|/|\mathbf{x}_W - \mathbf{x}_P| = l_{wW}/l_{PW}$$

(6.12)
\( f_{x,P} \) is the ratio of the distance in the p–space between the points \( w \) and \( W \) \( |x_w - x_W| \) and the distance between the points \( W \) and \( P \) \( |x_W - x_P| \) (see, Fig. 31a). With the above defined interpolation factor, e.g., the velocities \( \overline{u}_{i,w} \) can be obtained with second–order accuracy:

\[
\overline{u}_{i,w} = f_{x,P} \overline{u}_{i,P} + (1 - f_{x,P}) \overline{u}_{i,W}. \tag{6.13}
\]

The contravariant velocity \( U^\text{cor}_w \), however, is not interpolated linearly to the west face of the computational cell. The reason is that \( U^\text{cor}_w \) is adjusted in order to avoid unphysical pressure oscillations caused by the decoupling of the pressure and the velocity for the collocated arrangement of the variables. Note that \( \rho_f U^\text{cor}_w J^{-1} S_w \) corresponds to the mass flux over the west face. In order to correct the mass flux over the faces of the computational cell, a similar method as employed by Rhie and Chow (1983) (the original method was conceived for steady flows) is adopted in the code \( \mathcal{E}SOCC \):

\[
\overline{u}^\text{cor}_{i,w} = \overline{u}_{i,w} - \left[ \overline{p}_P - \overline{p}_W - 0.5(\overline{p}_e - \overline{p}_{ww}) \right] \Delta t \frac{\partial \xi}{\partial x_i}. \tag{6.14}
\]

\( \overline{p}_e \) and \( \overline{p}_{ww} \) is the pressure interpolated at the east and the west–west side of the control volume (see, Fig. 32) using an analogous operation as defined in eq. (6.13). This procedure leads to a non–vanishing pressure term in eq. (6.14) in case of an oscillating pressure field. In turn, this pressure term in eq. (6.14) leads to an additional mass flux over the control volume faces. This additional mass flux causes in the next iteration an enhanced (oscillation–free) pressure field (Breuer, 2011). The contravariant velocity at the west side \( U^\text{cor}_w \) is calculated by means of the corrected velocity field \( \overline{u}^\text{cor}_{i,w} \):

\[
U^\text{cor}_w = \overline{u}^\text{cor}_{j,w} \frac{\partial \xi}{\partial x_j}. \tag{6.15}
\]

Finally, in order to obtain the momentum flux over the control volume at the west side, \( U^\text{cor}_w \) hast to be multiplied by the interpolated velocity \( \overline{u}_{i,w} \):

\[
\overline{u}_{i,w} U^\text{cor}_w J_w^{-1} S_w = \left( f_{x,P} \overline{u}_{i,P} + (1 - f_{x,P}) \overline{u}_{i,W} \right) U^\text{cor}_w J_w^{-1} S_w. \tag{6.16}
\]

Note that the derivatives present in the viscous fluxes are approximated by a finite difference method of second–order accuracy (for details, see Breuer, 1998, 2002; Breuer et al., 2006; Breuer, 2013). The pressure term in eq. (6.9) is interpolated linearly to the cell faces of the control volume which also leads to a second–order approximation.

The result of the finite–volume method of the momentum equation is an ordinary differential equation with a remaining derivative in time:

\[
\frac{\partial \overline{u}_{i,P}}{\partial t} = \frac{1}{J^{-1}} \left( \mathcal{R}(\overline{u}_i) - \mathcal{F} \left( \overline{p} \frac{\partial \xi_j}{\partial x_i} \right) \right). \tag{6.17}
\]

\( \mathcal{R}(\overline{u}_i) \) is a nonlinear function of the velocities at the point P and of the neighboring points which depends on the discretization of the convective and the viscous fluxes. \( \mathcal{F} \left( \overline{p} \frac{\partial \xi_j}{\partial x_i} \right) \) is a function of the pressure gradient and is the result of the discretization of the surface integral in eq. (6.9) containing the pressure. The discretization of the continuity equation
6.1.3 Time Integration

The finite–volume discretization of eq. (6.9) results in the nonlinear differential equation (6.17) in time. The time integration of eq. (6.17) is performed by a low–storage multi–stage Runge–Kutta method with three sub–steps. It is second–order accurate in time (Binninger, 1989). The sub–steps are calculated as follows:

\[
\begin{align*}
\bar{u}^{(1)}_{i,P} &= \bar{u}^{(n)}_{i,P} + \alpha_1 \frac{\Delta t}{J-1} \left( \mathcal{R}(\bar{u}^{(n)}_i) - \mathcal{F} \left( \frac{\partial \xi_j}{\partial x_i} \right)^{(n)} \right) \quad \text{with} \quad \alpha_1 = \frac{1}{3} \\
\bar{u}^{(2)}_{i,P} &= \bar{u}^{(n)}_{i,P} + \alpha_2 \frac{\Delta t}{J-1} \left( \mathcal{R}(\bar{u}^{(1)}_i) - \mathcal{F} \left( \frac{\partial \xi_j}{\partial x_i} \right)^{(n)} \right) \quad \text{with} \quad \alpha_2 = \frac{1}{2} \\
\bar{u}^{(3)}_{i,P} &= \bar{u}^{(n)}_{i,P} + \alpha_3 \frac{\Delta t}{J-1} \left( \mathcal{R}(\bar{u}^{(2)}_i) - \mathcal{F} \left( \frac{\partial \xi_j}{\partial x_i} \right)^{(n)} \right) \quad \text{with} \quad \alpha_3 = 1 \\
\bar{u}^{(*)}_{i,P} &= \bar{u}^{(3)}_{i,P}
\end{align*}
\]

Here the superscripts \((n)\) and \((\ast)\) denote the values at the old and the new time step, respectively. In this section the superscript \((\ast)\) symbolizes the uncorrected (not divergence–free) velocity field. The superscripts \((1)\), \((2)\) and \((3)\) are the counter of the sub–steps of the low–storage Runge–Kutta method. The above described time integration is called the predictor step.

6.1.4 Predictor–Corrector Scheme

Unfortunately, the velocity field \(\bar{u}^{(*)}_{i,P}\) resulting from the Runge–Kutta scheme (6.19) is not divergence–free. For that reason, the velocity field at the new time step has to be corrected by a predictor–corrector method in order to fulfill the continuity equation. In order to obtain a divergence–free velocity field, the pressure is corrected, i.e., the pressure field is seen as a source term adjusted in order to fulfill the continuity equation (Fröhlich, 2006). The most illustrative way to obtain an equation for the pressure which has to correct the velocity field, is to write the momentum equations in semi–discrete form (Breuer, 2011):

\[
\frac{\bar{u}^{(*)}_{i,P} - \bar{u}^{(n)}_{i,P}}{\Delta t} = \left[ \frac{\partial (u_i u_j)}{\partial x_i} \right]^{(n)}_P + \left( \mu_T \frac{1}{\text{Re}} \left[ \frac{\partial^2 u_j}{\partial x_i \partial x_i} \right]^{(n)}_P - \frac{\partial p^{(*)}_P}{\partial x_j} \right)
\]

(6.20)

Note that the derivation of the equations for the pressure correction is done for simplicity reasons in the physical space. Here \(\bar{u}^{(*)}_{i,P}\) is the uncorrected velocity field which results from the time integration and \(p^{(*)}_P\) is an intermediate pressure field. It can be an estimated pressure or approximated by the pressure from the previous time step \(p^{(n)}_P\). Here the latter is chosen. The above equation can be written in a slightly different way:

\[
\frac{\bar{u}^{(n+1)}_{i,P} - \bar{u}^{(n)}_{i,P}}{\Delta t} = \left[ \frac{\partial (u_i u_j)}{\partial x_i} \right]^{(n)}_P + \left( \mu_T \frac{1}{\text{Re}} \left[ \frac{\partial^2 u_j}{\partial x_i \partial x_i} \right]^{(n)}_P - \frac{\partial p^{(n+1)}_P}{\partial x_j} \right)
\]

(6.21)
\( \overline{u}_{i,P}^{(n+1)} \) is the velocity at the new time step which it is assumed to be divergence free. \( p_P^{(n+1)} \) is the pressure at the new time step which is still unknown. The task is to correct \( \overline{u}_{i,P}^{(s)} \) in order to obtain the velocity field \( \overline{u}_{i,P}^{(n+1)} \) which fulfills the continuity equation. An equation for \( p_P^{(n+1)} \) is obtained by subtracting eq. (6.20) from eq. (6.21). The result reads:

\[
\frac{\overline{u}_{i,P}^{(n+1)} - \overline{u}_{i,P}^{(s)}}{\Delta t} = -\left( \frac{\partial p_P^{(n+1)}}{\partial x_j} - \frac{\partial p_P^{(s)}}{\partial x_j} \right). \tag{6.22}
\]

The still unknown velocity field \( \overline{u}_{i,P}^{(n+1)} \) is eliminated by applying the divergence operator to the above equation. The result is the Poisson equation for the pressure correction \( p_P' \):

\[
\frac{\partial}{\partial x_j} \left[ \frac{\partial p_P'}{\partial x_j} \right] = \frac{1}{\Delta t} \frac{\partial \overline{u}_{i,P}^{(s)}}{\partial x_j} \tag{6.23}
\]

\( p' \) is the pressure correction and is defined as:

\[
p_P' = p_P^{(n+1)} - p_P^{(s)}. \tag{6.24}
\]

Note that the method used to solve eq. (6.23) is described in the following section. For an adequate spatial discretization (e.g., the one achieved on a staggered Cartesian grid) the velocity field which satisfies the continuity equations is achieved in the ideal case after one iteration step (Breuer, 2011). In the discretization used in the code \( \mathcal{L}E\mathcal{S}O\mathcal{C}C \), however, the pressure field \( p_P^{(n+1)} \) obtained by the solution of the Poisson equation is casted in eq. (6.19c) to obtain a new guess of the velocity field \( \overline{u}_{i,P}^{(s)} \). If the new guess of the velocity field satisfies the convergence criterion of the mass conservation equation, the solution is regarded as converged and the velocity field at the new time step is obtained. In order to prove if the solution is converged, the sum of the inflow and outflow mass fluxes over the faces are computed for each control volume. If the maximum mass flux computed in this way is below \( 3 \times 10^{-8} \), the solution is regarded as converged. If the convergence criterion is not fulfilled, the Poisson equation is solved another time to obtain a new pressure field and to correct the fluid velocity.

### 6.1.5 Solution of the Linear System of Equations

In order to obtain a numerical solution of eq. (6.23) the equation has to be transformed into the c–space and discretized. The resulting system of equations is solved by the incomplete LU decomposition of Stone (1968) (also called SIP from strongly–implicit procedure). It is an iterative method ideal for sparse matrices, which usually appear during the solution of CFD problems. The details of the procedure are not explicitly treated here, since it is not in the scope of this thesis. The interested reader is referred to the original paper of Stone (1968) or to standard text books such as Ferziger and Perić (2002) or the lecture notes of Breuer (2011).

### 6.2 Numerical Methods for the Disperse Phase

In this section, the numerical methods to treat the disperse phase are described. In order to compute the forces displacing the particles appearing in equation (4.25a), first the fluid
quantities interpolated to the particle position are required. Then the resulting ordinary
differential equations have to be solved. Afterwards, if the flow is assumed to be four–
way coupled, the collisions have to be accounted for. Following this sequence adopted in
the code, the numerical methods employed in this thesis are presented in the following
subsections.

6.2.1 Interpolation of the Fluid Velocity at the Particle Position

In this thesis two different interpolation schemes to approximate the fluid velocity at the
particle position are analyzed: The trilinear interpolation was used in the early stage of
the present work. This interpolation scheme was found to have a strong filtering effect
on the fluid velocity and therefore, it is not able to reproduce the correct second–order
statistics of tiny particle (see, § 8.1). For this reason this scheme is substituted by the
Taylor series extension proposed by Marchioli et al. (2007a).

6.2.1.1 Trilinear Interpolation

The trilinear interpolation (see also, Breuer et al., 2006) requires the fluid velocity of
the eight cell centers surrounding the particles, i.e., the outcome is a weighted average of
the fluid velocity of eight neighboring cells. The expression reads:

\[
  \mathbf{u}_f \big|_P = \mathbf{u}_f \big|_{i,j,k} \Delta \xi^- \Delta \eta^- \Delta \zeta^- + \mathbf{u}_f \big|_{i+1,j,k} \Delta \xi^+ \Delta \eta^- \Delta \zeta^- + \mathbf{u}_f \big|_{i,j+1,k} \Delta \xi^- \Delta \eta^+ \Delta \zeta^- + \mathbf{u}_f \big|_{i,j,k+1} \Delta \xi^- \Delta \eta^- \Delta \zeta^+ + \\
  \mathbf{u}_f \big|_{i+1,j+1,k} \Delta \xi^+ \Delta \eta^+ \Delta \zeta^- + \mathbf{u}_f \big|_{i+1,j,k+1} \Delta \xi^+ \Delta \eta^- \Delta \zeta^+ + \mathbf{u}_f \big|_{i,j+1,k+1} \Delta \xi^- \Delta \eta^+ \Delta \zeta^+ + \mathbf{u}_f \big|_{i+1,j+1,k+1} \Delta \xi^+ \Delta \eta^+ \Delta \zeta^+.
\]  

(6.25)

Here \( \Delta \xi^+, \Delta \eta^- \) and \( \Delta \zeta^+ \) define the distances of the particle in the c–space from the
node \((i, j, k)\) in \( \xi, \eta, \zeta \) direction, respectively. The quantities with the superscript \( - \) are
defined as follows: \( \Delta \xi^- = 1 - \Delta \xi^+ \), \( \Delta \eta^- = 1 - \Delta \zeta^+ \) and \( \Delta \zeta^- = 1 - \Delta \xi^+ \) (see also, Fig. 33).
Consequently, the trilinear interpolation is done in c–space rather than in p–space. This
is advantageous since the second integration of the ordinary differential equations is also
done in c–space, in order to achieve an efficient tracking method for a huge number of
particles as will be shown below.

![Figure 33: Trilinear interpolation of the fluid velocity at the particle position in c–space extracted from Breuer et al. (2007); for simplicity only shown in two dimensions.](image-url)
6.2.1.2 Taylor Series Expansion

The Taylor series expansion about the cell center next to the particle position proposed by Marchioli et al. (2007a) reads:

\[ u_f |_{P} = u_f |_{N} + \frac{\partial u_f}{\partial x} |_{N} \Delta x + \frac{\partial u_f}{\partial y} |_{N} \Delta y + \frac{\partial u_f}{\partial z} |_{N} \Delta z + O(\Delta x^2, \Delta y^2, \Delta z^2, \Delta x \Delta y, \Delta x \Delta z, \Delta y \Delta z). \]  

(6.26)

Here the index \( P \) denotes the particle position and the index \( N \) denotes the nearest cell center with respect to the particle position. Since the code \( \text{LESOCC} \) works on curvilinear coordinate systems, the above derivatives have to be transformed in a form suitable for such a coordinate system. This is achieved by the following transformation:

\[
\frac{\partial}{\partial x} = \frac{\partial \xi}{\partial x} \frac{\partial}{\partial \xi} |_{N} + \frac{\partial \eta}{\partial x} \frac{\partial}{\partial \eta} |_{N} + \frac{\partial \zeta}{\partial x} \frac{\partial}{\partial \zeta} |_{N},
\]

\[
\frac{\partial}{\partial y} = \frac{\partial \xi}{\partial y} \frac{\partial}{\partial \xi} |_{N} + \frac{\partial \eta}{\partial y} \frac{\partial}{\partial \eta} |_{N} + \frac{\partial \zeta}{\partial y} \frac{\partial}{\partial \zeta} |_{N},
\]

\[
\frac{\partial}{\partial z} = \frac{\partial \xi}{\partial z} \frac{\partial}{\partial \xi} |_{N} + \frac{\partial \eta}{\partial z} \frac{\partial}{\partial \eta} |_{N} + \frac{\partial \zeta}{\partial z} \frac{\partial}{\partial \zeta} |_{N}.
\]

(6.27)

\( \xi, \eta, \zeta \) are the coordinates in the computational space. The application of the above operators to eq. (6.26) results in derivatives of the fluid velocity \( u_f \) with respect to \( \xi, \eta \) and \( \zeta \). These derivatives are approximated by a central difference scheme of second–order accuracy:

\[
\frac{\partial u_f}{\partial \xi} = \frac{1}{2}(u_f |_{i+1,j,k} - u_f |_{i-1,j,k}) + O(\Delta \xi^2)
\]

\[
\frac{\partial u_f}{\partial \eta} = \frac{1}{2}(u_f |_{i,j+1,k} - u_f |_{i,j-1,k}) + O(\Delta \eta^2)
\]

\[
\frac{\partial u_f}{\partial \zeta} = \frac{1}{2}(u_f |_{i,j,k+1} - u_f |_{i,j,k-1}) + O(\Delta \zeta^2).
\]

(6.28)

The resulting scheme is second–order accurate in space and hence consistent with the overall second–order accuracy of the underlying CFD code. In the result chapter (§ 8.1) both interpolation schemes are compared.

6.2.2 Particle Tracking Algorithm

The code \( \text{LESOCC} \) used in this thesis works with a colocated arrangement of the fluid velocities. Due to this reason, all flow quantities required to calculate the fluid forces displacing the particles (velocities and also the gradients of the velocities) are stored at the cell center of the computational cell. Hence, in order to interpolate the fluid quantities at the particle position required to solve eq. (4.25a), the exact determination of the computational cell containing the particles is necessary. In order to determine the position of the particles at the new time step, eq. (4.25a) has to be integrated twice in time. The first integration of eq. (4.25a), which is performed to calculate the particle velocity, is carried out in the physical space (p–space) by a fourth–order Runge–Kutta scheme (see, e.g., Faires and Burden, 1994). For this purpose, eq. (4.25a) can be formally
expressed as follows\(^\text{11}\):

\[
\frac{d\mathbf{u}_p}{dt} = \frac{\mathbf{u}_f - \mathbf{u}_p}{\tau_p/\alpha} + g \left( 1 - \frac{1}{\rho_p} \right) + f_{Lift}(\mathbf{u}_p) .
\]  

(6.29)

\(f_{Lift}(\mathbf{u}_p)\) are the lift forces in eq. (4.25a) which are a function of the particle velocity \(\mathbf{u}_p\). In order to compute the particle velocity \(\mathbf{u}_p^{(n+1)}\) at the new time step \((n+1)\) the following four sub–steps are executed:

\[
k_1 = \Delta t \left[ \frac{\mathbf{u}_f - \mathbf{u}_p^{(n)}}{\tau_p/\alpha} + g \left( 1 - \frac{1}{\rho_p} \right) + f_{Lift}(\mathbf{u}_p^{(n)}) \right] \]  

(6.30a)

\[
k_2 = \Delta t \left[ \frac{\mathbf{u}_f - \left( \mathbf{u}_p^{(n)} + 1/2 k_1 \right)}{\tau_p/\alpha} + g \left( 1 - \frac{1}{\rho_p} \right) + f_{Lift}(\mathbf{u}_p^{(n)}) \right] \]  

(6.30b)

\[
k_3 = \Delta t \left[ \frac{\mathbf{u}_f - \left( \mathbf{u}_p^{(n)} + 1/2 k_2 \right)}{\tau_p/\alpha} + g \left( 1 - \frac{1}{\rho_p} \right) + f_{Lift}(\mathbf{u}_p^{(n)}) \right] \]  

(6.30c)

\[
k_4 = \Delta t \left[ \frac{\mathbf{u}_f - \mathbf{u}_p^{(n)} + k_3}{\tau_p/\alpha} + g \left( 1 - \frac{1}{\rho_p} \right) + f_{Lift}(\mathbf{u}_p^{(n)}) \right] .
\]  

(6.30d)

The final result reads as follows:

\[
\mathbf{u}_p^{(n+1)} = \mathbf{u}_p^{(n)} + \frac{1}{6} \left( k_1 + 2k_2 + 2k_3 + k_4 \right).
\]  

(6.31)

Note that for a Runge–Kutta scheme of the accuracy \(O(\Delta t^4)\) also the lift forces \(f_{Lift}(\mathbf{u}_p)\) should be updated within the four sub–steps performed in eq. (6.30). However, since the lift forces are typically at least one order of magnitude smaller than the drag forces, they are computed only once due to efficiency reasons. For stability reasons of the Runge–Kutta scheme (Antia, 2000), the differential equation (4.25a) is integrated analytically as follows if \((\Delta t\alpha)/\tau_p \geq 2\):

\[
\mathbf{u}_p^{(n+1)} = \mathbf{u}_f + (\mathbf{u}_p^{(n)} - \mathbf{u}_f) \exp \left( -\frac{\alpha \Delta t}{\tau_p} \right) + \frac{\tau_p}{\alpha} \left[ f_{Lift}(\mathbf{u}_p^{(n)}) + g \left( 1 - \frac{1}{\rho_p} \right) \right] \left[ 1 - \exp \left( -\frac{\alpha \Delta t}{\tau_p} \right) \right] .
\]  

(6.32)

In principle, different time step sizes can be applied for the particulate and the continuous phase. However, in order to avoid run–time overheads due to the interpolation of the fluid velocity between two time steps (Breuer et al., 2006), for both phases the same time step size \(\Delta t\) is applied. Furthermore, the interpolation of the fluid velocity between two time steps introduces an additional source of uncertainty in form of interpolation errors. This source of uncertainty is avoided by choosing the same time step size for the particles and the fluid.

The integration of the governing equations lead to the particle velocity \(\mathbf{u}_p\) at each time step. In order to obtain the new location of the particle, the equations have to be integrated once more. The second integration is crucial for the performance of the code. If the second integration is done in the physical space (p–space), the identification of the new computational cell is not trivial since no explicit relation between the coordinates

\(^{11}\text{Note that the gravitational acceleration is defined positive when } g \text{ is pointing in positive direction of the coordinate system.}\)
of the particle and the index of the cell containing the particle is available for a general curvilinear grid (see, Schäfer and Breuer, 2002, and also Fig. 34(a)). Therefore, time consuming search algorithms such as stencil walk, the Newton–Raphson iterative methods or tetrahedral walk are required to determine the cell containing the particle in the new time step (Breuer et al., 2006). In the computational space (c–space) point location is trivial since there exists an explicit relation between the coordinates of the particle in the computational space ($\xi_p$, $\eta_p$, $\zeta_p$) and the cell index $ii_p$ containing it (Schäfer and Breuer, 2002):

$$ii_p = \text{int}(\xi_p) + [\text{int}(\eta_p) - 1] \ast ni + [\text{int}(\zeta_p) - 1] \ast ni \ast nj. \quad (6.33)$$


$n_i$ and $n_j$ are the number of computational nodes in $\xi$– and $\eta$–direction, respectively. Therefore, no time–consuming search algorithms are required if the second integration of eq. (4.25a) is performed in the c–space rather than in the p–space. This leads to CPU time requirements up to an order of magnitude lower than tracking schemes working in the p–space (Schäfer and Breuer, 2002). In order to obtain the position of the particles in the c–space, the velocity in this space is required. Hence, the particle velocity in the p–space obtained by the first integration of eq. (4.25a) has to be transformed to the space where the second integration is executed, i.e., into the c–space. The definition of the particle velocity in c–space:

$$\frac{d\xi_p}{dt} = U_p = \xi_x u_p^T + \xi_y v_p^T + \xi_z w_p^T \quad (6.34)$$

leads to the actual position of the particle in c–space. $\xi_p$ is the coordinate of the particle in the c–space. $\xi_x, \xi_y, \ldots$ denote the precomputed metric coefficient (which are defined at the cell center of the computational cell) trilinearly interpolated at the particle position. After this transformation eq. (6.34) is integrated in time with the same fourth–order Runge–Kutta scheme as used for the determination of the particle velocity in the p–space. The following four sub–steps have to be computed for this purpose:

$$k_1 = \Delta t \ U_p \quad (6.35a)$$
$$k_2 = \Delta t \ (U_p + 1/2 \ k_1) \quad (6.35b)$$
$$k_3 = \Delta t \ (U_p + 1/2 \ k_2) \quad (6.35c)$$
$$k_4 = \Delta t \ (U_p + k_3) \quad (6.35d)$$

Finally, the coordinates $\xi_p$ of the particles in the c–space read:

$$\xi_p^{(n+1)} = \xi_p^{(n)} + \frac{1}{6} \left( k_1 + 2k_2 + 2k_3 + k_4 \right). \quad (6.36)$$

A back–transformation of the c–space particle coordinates to the p–space is not required during the entire algorithm. Solely for visualization purpose such a back–transformation is carried out to enable a representation in physical coordinates ($x_p$, $y_p$, $z_p$) (Breuer et al., 2006).

The temporal evolution of the particle angular velocity is described by the ordinary differential equation (4.25b). Because of its linearity, an analytical solution can be obtained
(see, also Breuer, 2013):

\[
\omega_p^{(n+1)} = \omega_p^{(n)} \exp\left(-\frac{10}{3 \tau_p} \Delta t\right) + \left(\frac{1}{2} \nabla \times \mathbf{u}_f\right) \left[1 - \exp\left(-\frac{10}{3 \tau_p} \Delta t\right)\right].
\] (6.37)

6.2.3 Collision Handling

For a four–way coupled simulation the method how particle–particle collisions are handled is a very critical issue from an efficiency point of view. The collision detection can quickly become the bottleneck of the entire simulation since for a brute–force approach the computational cost scales with the number \(N_p\) of particles squared. Nevertheless, a deterministic collision model is taken into account. The reason why a deterministic detection is preferred over a stochastic model as, e.g., the one described in Sommerfeld (2001), is accuracy. It has no sense to invest a high amount of computational time to adopt accurate but expensive eddy–resolving techniques as the one used in this thesis and after that to settle for a stochastic collision model. As shown by the author in Alletto and Breuer (2014) the collision handling described in the following needs only a few percentage of the total computational time required to advance the particles in time. Therefore, this more accurate methodology does not result in a substantial loss of efficiency compared to stochastic models. In the view of the performance analysis made by Alletto and Breuer (2014) the present collision handling probably is even computational cheaper than a stochastic model when each particle is tracked through the computational domain and the parcel method is not applied. The reason is that for a deterministic collision model the correct collision frequency is computed on the fly whereas a stochastic model as described in Sommerfeld (2001) requires converged particles statistics. Therefore, a stochastic model needs a few iterations to compute converged statistics whereas for a deterministic model one iteration is sufficient.

Note that parts of the algorithm presented here are already published by Breuer and Alletto (2012b). For the derivation of the collision detection algorithm described in the following, only binary collisions are assumed. For this type of collisions the uncoupling
technique developed by Bird (1976) can be applied. For this technique the calculation of the particle trajectories is split into two stages:

1. First, the particles are moved based on the equation of motion without inter–particle interactions.

2. Second, the occurrence of collisions during the first stage is examined for all particles. If a collision is found, the velocities of the colliding particles are replaced by the post–collision ones without changing their position, which is also advantageous for parallelization.

The reason, why the displacements are preferred to be neglected after the collisions, are discussed in detail in Wunsch et al. (2008). Displacing the two participating particles after its collision harbors the inherent risk that an overlap with a third particle is generated. Depending on the instant of time of this event the entire procedure can get disarranged. Especially for dense flows it is therefore advantageous to neglect the displacement during the collisions. Some alteration of the statistical results in non-homogeneous flows has to be expected by this simplification (Wunsch et al., 2008). However, owing to the small time step sizes applied in LES, the error is assumed to be marginal.

Briefly summarized, the collision handling itself is carried out in two steps:

(I) In the first step likely collision partners are identified. Since for small time steps only collisions between neighboring particles are likely, substantial computational savings are achieved by dividing the computational domain into virtual cells (see Fig. 35a). This method, i.e., the restriction of the collision detection on neighboring particles within a virtual cell, is commonly employed in molecular dynamics or smooth particle hydrodynamics (see, e.g., Viccione et al., 2008), for the simulation of granular flows (see, e.g., Hopkins and Louge, 1991) but also for multiphase flows (see, e.g., Wunsch et al., 2008). Choosing the cell size in such a way that the particles per cell are sufficiently low, the cost of checking collisions is reduced from the order $O(N_p^2)$ to $O(N_p)$, which is crucial for large numbers of particles, e.g., $N_p = O(10^7–10^8)$ at high mass loadings. To achieve a nearly optimal cell size, it is dynamically adjusted during the simulation. The detailed explanation how the cell size is adjusted is provided in the following. Furthermore, to avoid overlapping cells or the necessity to take the 26 surrounding cells into account during the first step, the search and collision detection procedure is carried out a second time with cell sizes increased by the factor $17/13$. (see Fig. 35b). The factor is calculated by dividing two prime numbers in order the minimize the risk of two overlapping cell borders.

(II) The second step solely takes the particles in one virtual cell into account. Following a suggestion of Tanaka and Tsuji (1991); Chen et al. (1998a) and Yamamoto et al. (2001) the algorithm relies on the assumption of constant velocity within a time step, which is reasonable for the small time step sizes applied in LES. Based on the assumption of linear displacements during a time step, it is possible to detect the collision of two particles by purely kinematic conditions, i.e.,

(i) the two particles have to approach each other and

(ii) the minimum distance between two particles within a time step has to be less than the sum of their radii.
If a collision is detected, the translational and angular velocities of the colliding particles are changed according to the hard–sphere collision model described in § 5.4.1 or according to the relations derived in § 5.4.2 if agglomeration is considered.

![Virtual grid for the first search](image)

**(a) First Search**

![Virtual grid for the second search](image)

**(b) Second Search**

**Figure 35:** Deterministic collision handling by virtual cells (see, also Breuer, 2013).

After gaining a rough idea about the basic concept of the collision detection algorithm, the single steps are explained in detail:

As already explained, in the first step (I) the particles located in each virtual cell have to be identified (see, Fig. 35(a)). The task is achieved by exploiting the underlining block–structured computational grid. To establish the virtual cells (see, Fig. 35(a)) containing the particles, the computational domain of the size \((n_i, n_j, n_k)\) is split into \((n_{i\text{vc}}, n_{j\text{vc}}, n_{k\text{vc}})\) cells according to

\[
\begin{align*}
n_{i\text{vc}} &= \text{int}(n_i/d^n_c) \\
n_{j\text{vc}} &= \text{int}(n_j/d^n_c) \\
n_{k\text{vc}} &= \text{int}(n_k/d^n_c).
\end{align*}
\]

(6.38)

The factor \(d^n_c\) is adjusted dynamically in order to limit the maximum number of particles contained in a virtual cell:

\[
d^n_c = d^{n-1}_c (N^0_{p,max}/N^{n-1}_{p,max})^{1/3}.
\]

(6.39)

Here \(d^{n-1}_c\) denotes the factor used to adjust the virtual–cell size at the previous time step. \(N^0_{p,max}\) and \(N^{n-1}_{p,max}\) are the maximum number of particles allowed to be contained in a virtual cell and the maximum number of particles found in one of the virtual cells at the previous time step \(n - 1\), respectively. With the aid of the factor \(d^n_c\) defined by eq. (6.39) the virtual–cell size is increased if \(N^{(n-1)}_{p,max} < N^0_{p,max}\) and decreased if \(N^{n-1}_{p,max} > N^0_{p,max}\). The number \(N^0_{p,max}\) is provided by the user. A large number \(N^0_{p,max}\) means that a lot of particles are checked against collision resulting in a drastic increase of the computational
cost. However, it is ensured that almost all occurring collisions are detected. On the other hand, a small number $N_{p,\text{max}}^0$ results in less computational costs but it is possible that not all colliding pairs are found. For the extreme case where $N_{p,\text{max}}^0 = 1$ only one particle is located in a virtual cell and therefore no collision can be detected. For that reason, the user has to find an optimum between computational costs and accuracy. Tests in a turbulent channel flow containing $10^6$ particles were performed to determine the optimum value of $N_{p,\text{max}}^0$. This tests have shown that no substantial difference in the number of collisions were detected and reliable particle statistics can be found for values of $N_{p,\text{max}}^0$ varying from $N_{p,\text{max}}^0 = 10$ to $N_{p,\text{max}}^0 = 100$. Therefore, a value of $N_{p,\text{max}}^0 = 10$ is chosen which ensures an accurate and fast collision handling. Note that even $N_{p,\text{max}}^0 = 10$ seems to be low, for the second collision search performed (see, Fig. 35(b)) the number of particles located in a virtual cell is higher than for the first iteration. The reason is that the virtual cell size is increased for the second iteration.

Based on the particle coordinates in the computational domain ($\xi_p, \eta_p, \zeta_p$) the corresponding index values of the virtual cells can be determined:

$$
i_{vc} = \text{int}(\xi_p/d_c)
$$
$$
j_{vc} = \text{int}(\eta_p/d_c)
$$
$$
k_{vc} = \text{int}(\zeta_p/d_c).
$$

Hence the particle tracking in c–space is also advantageous for the collision algorithm, since the particle coordinates in c–space are naturally available.

Finally, a particle property is defined by assigning each particles the index $ii_{vc}$ of the virtual cell in which it is located according to:

$$
ii_{vc} = i_{vc} + (j_{vc} - 1) \cdot ni_c + (k_{vc} - 1) \cdot n_i_{vc} \cdot n_j_{vc}.
$$

After this short introduction of how the virtual cells are uniquely defined and dynamically adjusted, the subsequent steps of the algorithm employed to identify the particles located in a virtual cell are explained with the help of the example sketched in Figs. 36. Note that for this small example a simplified 1D configuration of the virtual grid is taken. The extension to 3D can be achieved in an analogous way.

In the view of the author this small example is the best way to illustrate the sequence adopted in the algorithm. The following scenario is assumed (see, Fig. 36): The computational domain containing eight particles is divided into five virtual cells. That means that the particles with the indices $i_{\text{particle}} = 2, 3$ and 5 are located in the virtual cell with the index $ii_{vc} = 1$, the particles with $i_{\text{particle}} = 1$ and 4 are located in the virtual cell with the index $ii_{vc} = 2$, the particle with $i_{\text{particle}} = 6$ is located in cell $ii_{vc} = 4$ and the particles with the indices $i_{\text{particle}} = 7$ and 8 are placed in the virtual cell $ii_{vc} = 5$. The virtual cell with the index $ii_{vc} = 3$ is empty. The number of total virtual cells is denoted as $N_{vc}$. Having defined the initial scenario, the following steps are carried out in the algorithm used in the code $\mathcal{LESOCC}$:

1. **Identification of the virtual cells in which the particles are located:**

   The first step is performed in order to identify the virtual cells in which the particles are located. For that purpose an array $\text{ICELLVAL}$ with the length $N_p$ is created. After that, at the $i_{\text{particle}}$–th entry of the array $\text{ICELLVAL}$ the index $ii_{vc}$ of the virtual cell containing the corresponding particle is stored, i.e., $\text{ICELLVAL}(i_{\text{particle}})$
$ii_{vc}$. Since the coordinates of the particles ($\xi_p, \eta_p, \zeta_p$) in the $c$-space are known, the index values of the virtual cell ($i_{vc}, j_{vc}, k_{vc}$) containing the particles with the index $i_{particle}$ can be obtained by eq. (6.40). After that, the index of the virtual cell $ii_{vc}$ is determined by eq. (6.41). In this way it is known in which virtual cell the particles are located without applying any search algorithm. In this example (since...
the particle with \( i_{\text{particle}} = 1 \) is located in the virtual cell with \( ii_{\text{vc}} = 2 \) the first entry of the array \( \text{ICELLVAL} \) is assigned the value \( \text{ICELLVAL}(1) = 2 \). Since the particle with the index \( i_{\text{particle}} = 2 \) is located in the virtual cell with \( ii_{\text{vc}} = 1 \), \( \text{ICELLVAL}(2) = 1 \) is set. For all other values contained in the array \( \text{ICELLVAL}(3: N_p) \) the procedure is analogous.

Note that the next steps are performed in order to create an ordered list of the particles indices \( i_{\text{particle}} \) which have to be checked against collision. For the example sketched in Fig. 36 that means that an array \( \text{ICELLTAB} \) (see the bottom of Fig. 36) is required, where the first three entries contain the indices of the particles \( i_{\text{particle}} = 2, 3 \) and 5 in the virtual cell \( ii_{\text{vc}} = 1 \). The fourth and fifth entry have to contain the indices of the particles \( i_{\text{particle}} = 1 \) and 4 in the second virtual cell, etc. To achieve this goal the following steps are necessary:

(2) **Count the number of particles contained in each virtual cell:**

The second step to achieve an ordered list of particles indices which can be check against collision, is to know how many particles are located in each cell. For that purpose, an array \( \text{ICOUNT} \) with the length \( N_{\text{vc}} \) is created. The array \( \text{ICOUNT} \) is required in order to create the offset table \( \text{IOFFSET} \) (see step (3) described below). Furthermore, it is necessary in order to know that the first three particles whose indices are later on stored in the array \( \text{ICELLTAB} \) (see the bottom of Fig. 36) are potentially colliding particles, etc. The number of particles contained in a virtual cell are stored at the position \( ii_{\text{vc}} \). This task can be achieved by a loop over the array \( \text{ICELLVAL} \): The entry of the array \( \text{ICOUNT} \) at the position \( \text{ICOUNT}(\text{ICELLVAL}(i_{\text{particle}})) \) has to be increased by one each time a particle is found in a virtual cell. Note that since it is not necessary to check cells containing only one particle for collisions, all entries of the array \( \text{ICOUNT} \) equal to one are set to zero. In the example depicted in Fig. 36 it means that \( \text{ICOUNT}(4) \) is set to zero. Since in the virtual cell with \( ii_{\text{vc}} = 1 \) three particles are located, the first entry of \( \text{ICOUNT} \) is equal \( \text{ICOUNT}(1) = 3 \), etc.

(3) **Generation of an offset table**

In the third step of the algorithm an offset table \( \text{IOFFSET} \) with the length \( N_{\text{vc}} \) is created. As explained below, with its help the array \( \text{ICELLTAB} \) containing the sorted indices \( i_{\text{particle}} \) of all particles which have to be checked for collision is easily created. At the \( ii_{\text{vc}} \)-th position of the array \( \text{IOFFSET} \) the sum of all particles contained in the virtual cells with the index 1 to \( ii_{\text{vc}} \) is stored. Since the virtual cell with \( ii_{\text{vc}} = 1 \) contains three particles, the first entry of \( \text{IOFFSET} \) is equal to \( \text{IOFFSET}(1) = 3 \). Since in the second virtual cell two particles are located, the second entry of \( \text{IOFFSET} \) is \( \text{IOFFSET}(2) = 5 \), i.e., the sum of the particle placed in the first two virtual cells. Note that the entries of the array \( \text{IOFFSET} \) associated with cells containing zero or only one particle are set to zero.

(4) **Generation of a sorted array containing the indices \( i_{\text{particle}} \) of the colliding particles:**

After these preliminary operations the final step of the algorithm sorts the indices of the particles which have to be checked for collision (see, Fig. 36). This is achieved by creating the array \( \text{ICELLTAB} \) which has the same number of entries as potentially colliding particles. In the example depicted in Fig. 36 the length of \( \text{ICELLTAB} \)
is seven. This number is determined by the number of particles present in the domain diminished by one, i.e., the number of particles located alone in a virtual cell. In order to generate ICELLTAB, the arrays ICELLVAL and IOFFSET are required. Based on ICELLVAL it is known that the particle with \( i_{\text{particle}} = 1 \) is located in the virtual cell with \( i_{vc} = 2 \), i.e., ICELLVAL(1) = 2. By means of the array IOFFSET it is known that five particles are contained in the first two cells. Therefore, the particle with \( i_{\text{particle}} = 1 \) is stored at the fifth position of the array ICELLTAB. Now the value of the array IOFFSET at the position \( i_{vc} = 2 \) is reduced by one, i.e., it is assigned to the actual value four. In this way, the second particle (i.e., the one with \( i_{\text{particle}} = 4 \)) located in the second virtual cell can be stored at the fourth position of ICELLTAB. The numbers located on the arrows depicted in Fig. 36 between the arrays IOFFSET and ICELLTAB symbolize the actual values of the array IOFFSET. The same procedure is repeated for all other particles in order to fill the array ICELLTAB. Note that the indices of the particles which are alone in a virtual cell are stored at the dummy index zero of the array ICELLTAB. This operation is performed in order to exclude cells where only one particle is located from the collision check procedure.

(5) Check for collisions:
After having sorted the particle indices in the array ICELLTAB, the collision check procedure described in the following can be achieved with the help of the array ICOUNT (see Fig. 36). By means of the array ICOUNT it is known that three particles are contained in the first virtual cell. Therefore, the first three particles stored in the array ICELLTAB are analyzed for collision. After that, since it is known from the array ICOUNT that two particles are located in the second virtual cell, the next two particles are checked, etc.. In this way the cost for the collision handling can be drastically reduced compared to the brute–force method as explained above.

After storing the indices of the potentially colliding particle pairs, in the second step (II) the method suggested by Tanaka and Tsuji (1991), Chen et al. (1998a) and Yamamoto et al. (2001) is applied to identify the colliding particle pairs. They assumed linear displacements of the particles within a time step. Especially for the small time steps used in LES, this assumption of the particle trajectories is a reasonable approximation. In this way the trajectories of crossing particles can be easily calculated. As already mentioned, in order that two particles collide they have to (i) approach each other and (ii) their minimum distance between the particles within a time step has to be less than the sum of their radii. The first condition (i) for collision is expressed by (see Fig. 37):

\[
\mathbf{x}_r \cdot \mathbf{u}_{p,r} = \left( \mathbf{x}_{p,2} - \mathbf{x}_{p,1} \right) \cdot \left( \mathbf{u}_{p,2} - \mathbf{u}_{p,1} \right) < 0.
\]

The above negative scalar product expresses that the relative motion \( \mathbf{u}_{p,r} \) of the two particles points against the relative separation \( \mathbf{x}_r \) of the particles. Otherwise, the particles are not approaching each other and a collision is impossible. \( \mathbf{x}_{p,2} \) and \( \mathbf{x}_{p,1} \) are the positions of the two potentially colliding particles before the collision.

Note that these quantities are different from the position \( \mathbf{x}_{p,2} \) and \( \mathbf{x}_{p,1} \) at the collision time defined in § 5.4.1. \( \mathbf{x}_r \) and \( \mathbf{u}_{p,r} \) are the relative distance and the relative velocity
between the two particles before the collision, respectively. If this condition is fulfilled, the time \( \Delta t_{\text{min}} \) at which the particle distance is a minimum \( x_{r,\text{min}} \) is computed as follows:

\[
\Delta t_{\text{min}} = -\frac{x_r \cdot u_{p,r}}{|u_{p,r}|^2} \quad \text{with} \quad x_{r,\text{min}} = x_r + u_{p,r} \Delta t_{\text{min}}. \tag{6.43}
\]

Requirement (ii) for the occurrence of a collision is checked by the following conditions:

\[
\left( \Delta t_{\text{min}} \leq \Delta t \right) \quad \& \quad |x_{r,\text{min}}| \leq \frac{d_{p,1}}{2} + \frac{d_{p,2}}{2} \quad \lor \quad \left( |x_r| \leq \frac{d_{p,1}}{2} + \frac{d_{p,2}}{2} \right). \tag{6.44}
\]

\( d_{p,1}/2 + d_{p,2}/2 \) is the sum of the radii of the two colliding particles. The first condition means that the time \( \Delta t_{\text{min}} \) computed by eq. (6.43) when the minimum separation occurs has to lie within the time step \( \Delta t \). Furthermore, the minimum separation computed by means of eq. (6.43) has to be less than the sum of the radii \( d_{p,1}/2 + d_{p,2}/2 \). The expression at the right-hand (logical or) means that the relative distance at the beginning of the time step is already less than \( d_{p,1}/2 + d_{p,2}/2 \). That means that the particles have already interpenetrated each other. Also in this case the particles collide. If the above condition is fulfilled, the collision time \( \Delta t_{\text{col}} \) is calculated from the condition that the relative distance at that time has to be equal to \( d_{p,1}/2 + d_{p,2}/2 \):

\[
|x_r - \Delta t_{\text{col}} u_{p,r}|^2 = \left( \frac{d_{p,1}}{2} + \frac{d_{p,2}}{2} \right)^2. \tag{6.45}
\]

The solution of this equation is given by:

\[
\Delta t_{\text{col}} = \Delta t_{\text{min}} \left( 1 - \sqrt{1 - K_1 K_2} \right), \quad K_1 = \frac{|x_r|^2 |u_{p,r}|^2}{(x_r \cdot u_{p,r})^2}, \quad K_2 = 1 - \left( \frac{d_{p,1}}{2} + \frac{d_{p,2}}{2} \right)^2 / |x_r|^2. \tag{6.46}
\]

Note that equation (6.45) has two solutions. The second one, not shown here, belongs to the state, where the particles have already interpenetrated each other and is excluded a-priori. The relative distance \( x_{r,\text{col}} \) at the collision time \( \Delta t_{\text{col}} \) is obtained as follows:

\[
x_{r,\text{col}} = x_r + u_{p,r} \Delta t_{\text{col}}. \tag{6.47}
\]

The collision-normal vector can be calculated by taking the norm of the above expression:

\[
n_c = \frac{x_{r,\text{col}}}{|x_{r,\text{col}}|}. \tag{6.48}
\]

Figure 37: Relative motion of two colliding particles according to Tanaka and Tsuji (1991).
Now the collision model described in § 5.4.1 can be applied to calculate the post–
collision translational and angular velocities of the particles. If agglomeration between
two particles is taken into account, the model described in § 5.4.2 is adopted to calculate
the post–collision state of the particles.

6.3 Determination of the Statistics

The particle statistics are calculated on–the–fly by updating the following series every
time a particle is found in a cell, whose center is located at the point \((x, y, z)\):

\[
\langle \Phi^k_p(x, y, z) \rangle = \Phi^k_p(x, y, z) \frac{1}{N^k_p(x, y, z)} + \left(1 - \frac{1}{N^k_p(x, y, z)}\right) \langle \Phi^{k-1}_p(x, y, z) \rangle.
\] (6.49)

The superscript \(k\) denotes the event number and \(N^k_p(x, y, z)\) are the accumulated number
of particles found in a control volume located at the position \((x, y, z)\). The brackets \(\langle \ldots \rangle\)
denote the mean value of a particle quantity (velocities, velocity fluctuations and particle
diameter). \(\Phi^k_p(x, y, z)\) stands for the instantaneous realization of the statistical quantity
of the particle. Writing eq. (6.49) down for the first few events, it turns out that this
expression leads to a classical arithmetic mean value. This on-the-fly prediction is neces-
sary since otherwise an enormous amount of data would have to be stored, which is fully
impractical. The computed three–dimensional statistics are averaged in the homogeneous
direction during the post processing (if required for the case considered).

The fluid statistics are calculated in a similar way in case of time averagin-
g. In this
case \(N^k_p(x, y, z)\) is substituted by the actual number of averaging time steps \(N_{av}\):

\[
\langle \Phi^N_{av}(x, y, z) \rangle = \Phi^N_{av}(x, y, z) \frac{1}{N_{av}} + \left(1 - \frac{1}{N_{av}}\right) \langle \Phi^{N-1}_{av}(x, y, z) \rangle.
\] (6.50)

If there are homogeneous directions, the instantaneous value of the fluid statistic \(\Phi^N_{av}(x, y, z)\)
is substituted by the averaged value in the respective directions. As for the particle statistics
eq. (6.50) correspond to the arithmetic mean value. The averaging is done on–the–fly
in order to avoid to store a huge amount of data.
7 Description and Numerical Setup of the Test Cases

In order to validate a new model or a new implementation of a code, suitable reference cases are required. This section describes the reference experiments and the numerical setups of the simulations performed to validate the code. Since for simple configurations the identification of error sources is much easier than for complex configurations, the validation process starts with the simplest wall–bounded configuration available, i.e., a plane channel flow. The interpolation scheme to determine the fluid velocity at the particle position and the SGS model for the particles are tested in a turbulent channel flow at Re = 10,935 (§ 7.1). For the validation of the collision handling (§ 7.2) and the wall–roughness model (§ 7.3) the Reynolds number is changed according to the available experiments used for comparison. After having proved the reliability of the method to simulate turbulent particle–laden flows involving particle–particle collisions and rough walls seen by the particles, a downward (§ 7.4) is tackled. The scope is to further gain confidence in the method presented in this thesis. After that, in § 7.5 the same downward pipe flow is used to perform the first evaluations of the agglomeration model valid for inter–particle collisions with friction. The scope of the computations performed in a horizontal pipe (§ 7.6) is threefold: (i) Further validate the deterministic collision treatment and the wall roughness model for the particles against the experimental data of Huber and Sommerfeld (1998) for smooth and rough walls. (ii) Prove the applicability of eddy–resolving methods in horizontal pipe flows with periodic boundary conditions. (iii) Study the influence of the wall roughness and the mass loading on the dynamics of the continuous and solid phase in a horizontal pipe. After that, the flow in complex configurations such as the cold flow in a model combustion chamber (§ 7.7) and in a cyclone separator (§ 7.8) is simulated. The scope is to test the applicability of the method presented in practically relevant devices.

7.1 Channel Flow at Re = 10,935 with Zero Gravity

In order to test the influence of the interpolation scheme (see § 6.2.1) on the statistics of massless tracers, a one–way coupled channel flow at a bulk Reynolds number based on the bulk velocity $U_B^*$ and the channel half–width $\delta_{Ch}^*$ of $\text{Re} = \frac{U_B^* \delta_{Ch}^*}{\nu_f^*} = 10,935$ ($\text{Re}_\tau = 590$) is simulated by LES. $\text{Re}_\tau$ corresponds to the Reynolds number based on the friction velocity. This specific choice of the Reynolds number is motivated by two reasons. The first reason is that, especially to evaluate the SGS model for the particles (the setup is described later on), the Reynolds number should not be too small in order to have a non–negligible influence of the subgrid scales. Furthermore, in order to validate the SGS model a suitable reference case performed by DNS is required. Since no one–way coupled DNS for higher Reynolds numbers than $\text{Re} = 2100$ (see, e.g., Marchioli et al., 2008c) were available when the SGS model for the particles was implemented, the statistics of tiny (massless) particles are compared with the continuous phase data of Kim et al. (1987). This DNS at $\text{Re} = 10,935$ is a well accepted reference case in the literature and is therefore taken to validate the SGS model. The trajectories of the massless tracers are computed by interpolating the fluid velocity at the position of the tracers either by the trilinear interpolation (see § 6.2.1.1) or the Taylor series expansion (see § 6.2.1.2). Afterwards, the velocity of the tracers is set equal to the interpolated fluid velocity since for massless tracers both should by identical. The new position is determined by the Runge–Kutta scheme described in § 6.2.2 (see eq. (6.35) and (6.36)). The scope of these simulations is to compare the statistics of the tracers with the fluid statistics, which should be identical.
for an ideal interpolation scheme.

The second test case performed at \( \text{Re} = 10,935 \) is conducted to elucidate the influence of the subgrid–scale velocity model for the particles (see § 5.2) on the statistics of tiny particles. The density ratio is set to \( \rho_p^* / \rho_f^* = 769 \) and is chosen equal to the density ratio found in one–way coupled DNS available in the literature (see, the collaborative benchmark test of Marchioli et al., 2008c). Unfortunately, the DNS of Marchioli et al. (2008c) is performed at a bulk Reynolds number of \( \text{Re} = 2100 \) for which the influence of the subgrid scales can be assumed to be small. Since the simulation tool improved in this thesis is thought to be applied at much higher Reynolds numbers than \( \text{Re} = 2100 \), the present Reynolds number (\( \text{Re} = 10,935 \)) is chosen to evaluate the model. In order to compare the particle statistics with the DNS of Kim et al. (1987), a small diameter ratio \( d^* / \delta_{rCh}^* = 5.8 \times 10^{-5} \) is chosen. The resulting Stokes number \( \text{St} \) is equal to \( \text{St} = \tau_B^* / \delta_{rCh}^* = \rho_p^* d_p^* u_B^* / (18 \mu_f^* \delta_{rCh}^*) = 1.57 \times 10^{-3} \) and thus very low. As shown in the results (see § 8.1) these tiny particles behave similar to fluid tracers. Therefore, the statistics of these tiny particles can be compared with the flow results of the DNS of Kim et al. (1987). In order to reduce the considerations solely to the influence of the interpolation scheme and the model for the SGS velocity, the gravity is set to zero and only the drag force is considered.

Note that the simulation parameters described in the following are identical for both test cases and therefore mentioned only once. The extension of the computational domain is \( 2 \pi \delta_{rCh}^* \times \pi \delta_{rCh}^* \times 2 \delta_{rCh}^* \) in streamwise, spanwise and wall–normal direction, respectively. Here \( \delta_{rCh}^* \) denotes the channel half–width. Periodic boundary conditions are applied at the stream– and spanwise boundaries and the no–slip condition at the bottom and top wall. In order to evaluate the influence of the resolution on the interpolation scheme and on the model for the subgrid–scale velocity, the results computed on two different grids are compared: a finer grid with \( 64 \times 64 \times 64 \) cells and a coarser grid with \( 32 \times 32 \times 32 \) cells. In wall–normal direction the first cell center is located at \( \Delta y^*/\delta_{rCh}^* = 0.005 \) for both grids. In this direction the grids are stretched according to a geometric series with a stretching factor of \( r = 1.18 \) and \( r = 1.05 \) for the coarse and the fine grid, respectively. This dimensionless wall distance corresponds to \( y^+ = 0.68 \) for the fine grid (\( 64^3 \) cells) and \( y^+ = 0.64 \) for the coarse grid (\( 32^3 \) cells). Since the predicted mean wall shear stress for the coarse grid is smaller than for the fine grid but the grid spacing of the first cell adjacent to the wall of both grids is equal, this results in a smaller value of \( y^+ \) for the coarse grid. In streamwise and spanwise direction an equidistant grid is used. The dimensionless grid spacing in streamwise direction is \( \Delta x^+ \approx 50 \) for the coarse grid and \( \Delta x^+ \approx 26 \) for the fine grid. In spanwise direction the grid spacings are chosen to be equal to \( \Delta z^+ \approx 25 \) for the coarse grid and \( \Delta z^+ \approx 13 \) for the fine grid, respectively. According to Piomelli and Chasnov (1996) these values lie in between the constraints required for a wall–resolved LES, i.e., \( y^+ \leq 2, 50 \leq \Delta x^+ \leq 150 \) and \( 15 \leq \Delta z^+ \leq 40 \). For the subgrid–scale modeling the Smagorinsky model as specified in § 3.2.1 with a constant of \( C_s = 0.065 \) is used. The dimensionless time step size is chosen equal to \( \Delta t = \Delta t^*_B / \delta_{rCh}^* = 0.01 \) for both grids, where \( U_B^* \) represents the bulk velocity. The statistics of both, fluid and particles, are averaged for a dimensionless time of \( \Delta T = \Delta T^*_B / \delta_{rCh}^* = 100 \) and additionally in both homogeneous directions. The averaging is started after ensuring that the fluid and the particles have reached a statistically stationary state. Particles hitting a wall are regarded as deposited. The reason for this choice is that no other implementation of the solid wall boundary condition for the particles was available at the early stage of the work in which
the simulations described in this section were performed. However, by introducing 400,000 particles (or tracers depending on the test case) at the beginning of the simulation it is ensured that during the averaging period a sufficient amount of particles is present in the computational domain to guarantee converged statistics (only a few percent of the particles are deposited during the simulations performed). In order to achieve a constant mass flow over the simulation period, the forcing term described in § 3.3.2 is applied.

7.2 Downward Channel Flow at Re = 11,900 with Smooth Walls

In order to validate the deterministic collision model described in § 5.4.1 and the collision detection algorithm described in § 6.2.3, the experiments performed by Benson et al. (2005) are used as a reference case. They studied the influence of the wall roughness on the continuous and the particulate phase. In the present case solely the data provided for the smooth acrylic wall case are taken into account for comparison. The reason is that the main objective is to validate the deterministic collision handling without considering the effect of the wall roughness. Benson et al. (2005) motivated their studies with the discovery of a layer of particles covering the wooden developing section of the channel originally used by Kulick et al. (1994) to measure the attenuation of turbulence by solid particles. Benson et al. (2005) guessed that the particles sticking at the wall of the channel development section could possibly have had a strong influence on the particle statistics measured in the smooth test section located further downstream. For that reason they concluded that it was not possible to numerically reproduce the often cited experimental research of Kulick et al. (1994) without considering the wall roughness. The Reynolds number based on the bulk velocity $U^*$ and the channel half–width $\delta^*_c$ is Re = 11,900 ($Re_\tau = 644$), the ratio of particle diameter to channel half-width is $d^*_p/\delta^*_c = 0.0075$ ($d^*_p = 150 \, \mu m$, St = $\rho^*_p d^*_p U^*_B / (18 \mu^*_f \delta^*_c) = 74.6$), the ratio of particle to fluid density is $\rho^*_p/\rho^*_f = 2061$ and the mass loading is $\eta = 15\%$. The gravitational acceleration $g^*$ is made dimensionless by $U^*_B$ and $\delta^*_c$ ($g_x^* = g^* \delta^*_c / U^*_B = 2.4 \times 10^{-3}$) and points in the mean flow direction.

The computational domain is $2\pi \delta^*_c \times \pi \delta^*_c \times 2 \delta^*_c$ in streamwise, spanwise and wall–normal direction, respectively. The grid employed has $128 \times 128 \times 128$ cells. In wall–normal direction the first cell center is located at $\Delta y^+ = 0.65$ and it is stretched according to a geometric series with a stretching factor of $r = 1.05$. In streamwise and spanwise direction an equidistantly spaced grid is used with a dimensionless spacing of $\Delta x^+ \approx 64$ and $\Delta z^+ \approx 32$, respectively. According to Piomelli and Chasnov (1996) these values lie within the constraints required for a wall–resolved LES, i.e., $y^+ \leq 2$, $50 \leq \Delta x^+ \leq 150$ and $15 \leq \Delta z^+ \leq 40$. Periodic boundary conditions are applied at the streamwise and spanwise boundaries and the no–slip condition is used at the walls. The wall–normal velocity of the particles hitting a wall is inverted in order to mimic a perfectly elastic smooth–wall collision. That means that the wall–normal restitution coefficient in eq. (4.30) is set to $e_{n,w} = 1$ and no friction during the particle–wall collision is considered. Regarding the particle–particle interaction no friction during an inter–particle collision is considered and the normal restitution coefficient is set to unity, i.e., $e_{n,p} = 1$. For this test case only the gravity, the buoyancy, the drag and the lift force due to liner shear are assumed to be relevant for the particle dynamics. The lift force due to the particle rotation is neglected since the particles neither acquire an angular velocity during the wall impact nor during an inter–particle collision. In order to take the influence of the unresolved scales on the
particle motion into account the model described in § 5.2 is applied. The dimensionless time step is set to \( \Delta t = \Delta t^* U_B^* / \delta_{Ch}^* = 7.0 \times 10^{-3} \). For the subgrid–scale modeling the Smagorinsky model described in § 3.2.1 with a constant of \( C_s = 0.065 \) is used.

The instantaneous flow field and the particle velocities are averaged in both homogeneous directions and additionally in time over a dimensionless time interval of about \( \Delta T = \Delta T^* U_B^* / \delta_{Ch}^* = 980 \) (about 80 flow–through times) in order to reach a statistically steady state. In order to achieve a constant mass flow over the simulation period, the forcing term described in § 3.3.2 is applied. Note that parts of the test case presented in this section were already published in Breuer and Alletto (2012a,b).

### 7.3 Horizontal Channel Flow at Re = 21,292 with Rough Walls

This specific choice of the numerical setup is motivated by the experiments of Kussin and Sommerfeld (2002) and Kussin (2004) who carried out detailed measurements based on phase–Doppler anemometry in a particle–laden horizontal channel flow. This experiment is attractive due to the variety of particle diameters considered and especially because of the detailed quantification of the wall roughness. This makes the experiments of Kussin and Sommerfeld (2002) and Kussin (2004) an excellent test case for the validation of the wall roughness model presented in § 4.3.2. Since the channel is set up horizontally, the gravitational force plays an important role and causes an increase in the concentration of the particles close to the bottom wall. Consequently, besides the wall roughness effect also particle–particle collisions at the investigated high mass loadings (up to \( \eta = 200\% \)) have a dominant influence on the particle and fluid statistics. Because of the aforementioned reason the experiments of Kussin and Sommerfeld (2002) and Kussin (2004) represent an attractive test case to validate both the collision handling and the wall roughness model presented in this thesis. Using a 6000 mm long channel with a height of \( H = 35 \text{ mm} \), it is ensured that the channel flow is fully developed. Three different Reynolds numbers were studied experimentally. In the present study only a value of \( \text{Re} = \delta_{Ch}^* U_B^*/\nu_f^* = 21,292 \) is chosen. It corresponds to a Reynolds number based on the friction velocity \( u_f^* \) of \( \text{Re}_f = \delta_{Ch}^* u_f^*/\nu_f^* = 946 \). \( \delta_{Ch}^* \) denotes the channel half–width and \( U_B^* \) is the bulk velocity. The gravitational acceleration \( g^* \) is made dimensionless by \( U_B^* \) and \( \delta_{Ch}^* \) (\( g_y = g^* \delta_{Ch}^* / U_B^2 = -4.42 \times 10^{-4} \)) and points towards the bottom wall, i.e., in negative \( y \)–direction.

The particles used in the experiments were spherical glass beads (\( \rho_p^* = 2500 \text{ kg/m}^3 \)). Experiments with different nominal diameters ranging from 60 \( \mu \text{m} \) to 1 mm were performed. The size distribution associated with a certain nominal diameter used in the experiments of Kussin and Sommerfeld (2002) and Kussin (2004) were narrow, i.e., they had a small standard deviation. For that reason in the present simulations mono–disperse particles are used. The nominal diameters of \( d_p^* = 60 \mu \text{m}, 100 \mu \text{m} \) and 195 \( \mu \text{m} \) are considered and characterize a small size class and two medium size classes. Note that the flow containing the bigger particles (625 and 1000 \( \mu \text{m} \)) is not simulated. The reason is that big particles violate the point–particle approach. This becomes evident by the observations made in the experiments of Kussin and Sommerfeld (2002) and Kussin (2004) that the 625 and 1000 \( \mu \text{m} \) particles provoke an enhancement of the streamwise fluid fluctuations. This observed increase of the fluid velocity fluctuations is more pronounced for higher mass loadings at a constant particle diameter. Kussin and Sommerfeld (2002) concluded that the wake generated behind the particles at rather high particle Reynolds numbers \( \text{Re}_p \) is responsible for this phenomenon. Therefore, since with the point–particle approach it is not possible to reproduce the effect on the continuous phase due to the vortices gen-
erated behind the particle, particles with a diameter greater than \(d_p^* = 195 \, \mu m\) are not considered in this work. The chosen particle classes correspond to a Stokes numbers of \(St = \frac{\rho_p d_p^2 U_p^*}{18 \mu_p \delta_{Ch}}\) = 28.5, 79.4 and 294.9, respectively, where \(\mu_p^*\) represents the dynamic viscosity of the carrier phase. Exchangeable stainless steel plates allowed to investigate the effect of different degrees of the wall roughness. In Kussin and Sommerfeld (2002) a low (denoted \(R_1\)) and a high degree of roughness (\(R_2\)) were investigated. In Kussin (2004) additionally an even lower (\(R_0\)) and even higher (\(R_3\)) degree of roughness were set to constant values for the cases chosen to evaluate the model: \(\varepsilon_{n,w} = 0.9, \varepsilon_{t,w} = 0.3, \mu_{dy,w} = 0.4\) and \(\rho_{st,w} = 0.5\). The constants \(\varepsilon_{n,w}\) and \(\mu_{dy,w}\) are set in order to lie within the range of values given by the empirical relation used by Lain and Sommerfeld (2008). Joseph et al. (2001) found that the measured normal restitution coefficient \(\varepsilon_{n,w}\) of a particle rebounding at a flat wall depends on the fluid in which the particles are immersed, i.e., different values of \(\varepsilon_{n,w}\) are measured for the same approaching velocity \(|u_p^* \cdot \mathbf{n}|\) if a particle is immersed in a viscous fluid (e.g., water or silicon) or in air. The crucial parameter which influences the values of \(\varepsilon_{n,w}\) is the Stokes number \(St_{vis} = 2 \frac{m_p^* |u_p^* \cdot \mathbf{n}|}{(3\pi \mu_p^* d_p^* \varepsilon_{n,w})} = \frac{d_p^* \rho_p^* |u_p^* \cdot \mathbf{n}|}{\mu_p^*}\). For small values of \(St_{vis}\) the measured normal restitution coefficient is zero and for high values of \(St_{vis}\) the restitution coefficient \(\varepsilon_{n,w}\) approaches the values measured in vacuum. For the smallest particles considered in the present simulations a value of \(St_{vis} = 1056\) is obtained. For this value the restitution coefficients measured by Joseph et al. (2001) and Gondret et al. (2002) for immersed spheres have already approached the one obtained in vacuum. Therefore, no modification of \(\varepsilon_{n,w}\) due to the viscous dissipation as proposed by Joseph et al. (2001) is required here.

Since no experimental result is available for \(\rho_{st,w}\), the constant is set to a slightly higher value than \(\rho_{dy,w}\), which is quite reasonable. \(\varepsilon_{t,w}\) is set to a realistic value already used in other wall–bounded particulate flow simulations, see, e.g., Vreman (2007). Furthermore,
some results will be shown varying the above constants in order to analyze their influence on the particle statistics (§ 8.3.5). For this test case only the gravity, buoyancy, the drag force and the lift force due to the linear shear are considered as relevant forces displacing the particles. The lift force due the particle rotation is not considered since it was not implemented in the code at the stage when the roughness model for the particles was developed. In order to take the influence of the unresolved scales on the particle motion into account the model described in § 5.2 is applied.

The computational domain is $2\pi \delta^*_Ch \times 2\delta^*_Ch \times \pi \delta^*_Ch$ in streamwise, wall–normal and spanwise direction, respectively. The grid employed has $128 \times 150 \times 150$ cells and the dimensionless time step based on $U_B^*$ and $\delta^*_Ch$ is $\Delta t = \Delta t^*U_B^*/\delta^*_Ch = 0.004$. In streamwise and spanwise direction an equidistant grid is used with a dimensionless grid spacing of $\Delta x^+ \approx 80$ and $\Delta z^+ \approx 35$, respectively. According to Piomelli and Chasnov (1996) these values lie within the constraints required for a wall–resolved LES. In wall–normal direction the grid is stretched geometrically with a stretching factor $r = 1.06$ and the first cell center is located at $\Delta y^+ = 0.8$ for the unladen flow. Thus the resolution also satisfies the requirements of Piomelli and Chasnov (1996) for a wall–resolved LES. Periodic boundary conditions are applied in streamwise and spanwise direction. It is noteworthy that for all three roughness values investigated in the present study, the heights of the roughness elements are below $y^+ \leq 5$ (the highest roughness level $R2$ considered corresponds to $k^+ = R^*_z u_1^*/\nu_1 = 0.42$) and thus they are within the viscous sublayer. Consequently, the continuous flow is not directly influenced by the wall roughness and the no–slip condition is applied at the wall. For the subgrid–scale modeling the Smagorinsky model described in § 3.2.1 with a constant of $C_s = 0.065$ is used.

The released particles are uniformly distributing over the entire computational domain at the beginning of the simulation using a fully developed unladen flow as an initial solution for the continuous phase. After the particles approach a statistically stationary state within a dimensionless time interval of $\Delta T = 100 = \Delta T^*U_B^*/\delta^*_Ch$, the particle and fluid statistics are predicted by averaging over a time period of $\Delta T = \Delta T^*U_B^*/\delta^*_Ch = 200$ and additionally in streamwise and spanwise directions. For the description of the procedure employed to calculate the statistics, see § 6.3. In order to achieve a constant mass flow over the simulation period, a forcing term as described in § 3.3.2 is applied. Note that parts of the test case presented in this section were already published by the author in Breuer and Alletto (2012c), Breuer, Alletto, and Langfeldt (2012) and Breuer and Alletto (2013).

### 7.4 Downward Pipe Flow at Re = 2253

The test case presented in this section is chosen to further validate the deterministic collision handling and the wall roughness model for the particles. Especially regarding the particle–wall collisions, the curved pipe walls represent a more complicated geometrical shape than the flat channel walls. The reason is that the wall–normal vector changes its orientation along the wall in circumferential direction. Therefore, the pipe geometry represents the logical successive step in the validation process after the channel geometry. The scope of the validation process is to increase step by step the complexity of the test cases in order to facilitate the identification of possible error sources and to detect space for further improvements.

For that purpose the experiments of Borée and Caraman (2005) are taken as a reference case. They obtained two–component phase–Doppler anemometry measurements of a
dilute poly-disperse two-phase flow at the exit of a long aluminum pipe. Unfortunately, no roughness specification is given for the pipe. The radius is \( R_{\text{pipe}} = 10 \text{ mm} \), the bulk velocity is \( U_B^* = 3.4 \text{ m/s} \), the centerline velocity is \( U_c^* = 4 \text{ m/s} \) and the Reynolds number based on the bulk velocity and the pipe radius is \( \text{Re}_{\text{pipe}} = 2253 \). The gravity points in flow direction \( (g_z = g^* R_{\text{pipe}}^* U_B^2 = 8.49 \times 10^{-3}) \). The initial diameter distribution of the spherical glass beads ranges from \( d_p^* = 37 \mu m \) to \( 116 \mu m \) (see Table 3). The density is \( \rho_p^* = 2470 \text{ kg/m}^3 \) \( \rho_f^* = 2250 \). The values in Table 3 are taken from the discrete number distribution found in Borée and Caraman (2005). For the definition of the number distribution \( q_{0,i}(d_{p,i}^*) \) see § 4.4. The bidispersed particle number distribution shows two peaks at \( d_p^* \approx 60 \mu m \) and \( d_p^* \approx 90 \mu m \). Borée and Caraman (2005) grouped particles with a diameter \( 55 \mu m \leq d_p^* \leq 65 \mu m \) to the 60 \( \mu m \) size class and particles with a diameter of \( 85 \mu m \leq d_p^* \leq 95 \mu m \) to the 90 \( \mu m \) size class. The particle statistics in the experiment are evaluated for these two size classes. Two different mass loadings of \( \eta = 11\% \) and \( 110\% \) are considered in the experiment.

<table>
<thead>
<tr>
<th>( i )</th>
<th>( d_{p,i}^* [\mu m] )</th>
<th>Number distribution ( q_{0,i}(d_{p,i}^*) )</th>
<th>St = ( \frac{\rho_p^* \rho_f^* U_B^<em>}{15 \mu m R_{\text{pipe}}^</em>} )</th>
</tr>
</thead>
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<td></td>
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<tr>
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<td>6</td>
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<td></td>
</tr>
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<td>7</td>
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<td></td>
</tr>
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</tr>
<tr>
<td>10</td>
<td>0.033</td>
<td>36.71</td>
<td></td>
</tr>
</tbody>
</table>

Table 3: Initial distribution of the particle sizes by Borée and Caraman (2005).

In order to compare the simulations with the experiment, the parameters modeling the velocity and angular velocity changes during the wall impact are set to the following values: \( \epsilon_{n,w} = 0.831 \), \( \epsilon_{t,w} = 0.31 \), \( \mu_{dy,w} = 0.125 \) and \( \mu_{st,w} = 0.6 \). The parameters chosen for the hard–sphere collision model are set to \( \epsilon_{n,p} = 0.97 \), \( \epsilon_{t,p} = 0.44 \), \( \mu_{dy,p} = 0.092 \) and \( \mu_{st,p} = 0.94 \). All values except \( \mu_{st,w} \) and \( \mu_{st,p} \) are taken from Foerster et al. (1994). They experimentally determined the values for the normal and tangential restitution coefficient and the dynamic coefficient of friction for both material pairings used in this test case, i.e., glass–glass (particle–particle collisions) and and aluminum–glass (particle–wall collisions). The values of \( \mu_{st,w} \) and \( \mu_{st,p} \) are common values found in textbooks for dry friction of the material pairing glass–aluminum and glass–glass (see, e.g., Serway and Vuille, 2006).

In order to evaluate the roughness model, two equivalent sandgrain roughnesses \( k_s^* = C_{\text{Surface}} R_s^* = 0.0 \mu m \) and \( 15.0 \mu m \) are chosen. Note that the chosen roughness height \( R_s^* = 15 \mu m \) lies in the range given in the literature for aluminum pipes \( k_s^* = 1.5 - 60 \mu m \) (Idelchik, 1986). For this test case the gravity, the buoyancy, the drag force and the lift forces due to the linear shear and the particle rotation are considered. In order to evaluate the simulated particle statistics of the poly-disperse distribution described in Table 3, the particles with the size classes \( i = 3 - 5 \) (see Table 3) are compared with the measurements of the 60 \( \mu m \) size class found in Borée and Caraman (2005) and particles with the classes \( i = 7 - 8 \) are compared with the 90 \( \mu m \) size class of the measurements Borée and Caraman (2005). The statistics of the other size classes are calculated but not shown in the result section since no experimental data are available for these classes. The influence of the unresolved scales on the particle motion is taken into account by the model described in § 5.2.

The computational domain has a dimensionless radius \( R^*/R_{\text{pipe}}^* = 1 \) and an extension
of $L^*/R_{\text{pipe}}^* = 24$ in streamwise direction for the low mass loading case and $L^*/R_{\text{pipe}}^* = 12$ for the high mass loading. The longer computational domain for the low mass loading is chosen to ensure that the two–point correlations reaches values close to zero at the half of the pipe length. An evaluation of the two–point correlations for the high mass loading turned out that an extension of the computational domain in streamwise direction of $L^*/R_{\text{pipe}}^* = 12$ is sufficient.

The computational domain is discretized by an O–type grid with $2 \times 10^6$ cells for the low mass loading and $1 \times 10^6$ for the high mass loading (see Fig. 38). The first cell center is placed at a wall distance $\Delta r^+ = 0.14$ for the unladen flow and thus the no–slip boundary condition is applied. The resolution in streamwise and in circumferential direction was $\Delta z^+ = 19.3$ and $\Delta(R_{\text{pipe}}^* \theta)^+ = 4.05$, respectively. A dimensionless time step size of $\Delta t = \Delta t^* U_B^*/R_{\text{pipe}}^* = 2.8 \times 10^{-3}$ is applied. After allowing the fluid and the particles to achieve a statistically stationary state, the particle and fluid statistics are averaged over a time period of $\Delta T = \Delta T^* U_B^*/R_{\text{pipe}}^* = 800$ and additionally in streamwise and circumferential directions. For the subgrid–scale modeling the Smagorinsky model as specified in § 3.2.1 with a constant of $C_s = 0.065$ is used. The flow is periodic in streamwise direction. In order to achieve a constant mass flow over the simulation period, the forcing term described in § 3.3.2 is applied.

7.5 Downward Pipe Flow at Re = 2253 to Test the Agglomeration Model

7.5.1 Influence of the Particle Diameter $d_p^*$ and the Normal Restitution Coefficient $e_{n,p}$

In order to perform first tests of the agglomeration model described in § 5.4.2.5, the agglomeration rate is studied as a function of the particle diameter $d_p^*$ and of the normal restitution coefficient $e_{n,p}$. For this purpose the mono–disperse turbulent particle–laden downward pipe flow at a bulk Reynolds number of $\text{Re} = 2253$ is simulated. The same grid with a streamwise extension $L^*/R_{\text{pipe}}^* = 12$ as described in § 7.4 is used and all forces

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{grid.png}
\caption{Grid of the pipe in a cross–section normal to the axis (only every second grid line is shown).}
\end{figure}
represented by eq. (4.25) are accounted for. In this first test the particles are assumed to rebound at a specular wall and the two–way coupling is disregarded. The scope of this choice is to reduce the considerations made about the agglomeration criterion solely to the particle diameter $d_p^*$ and the normal restitution coefficient $e_{n,p}$ and the disregard of all other effects. Three different particle diameters are analyzed, i.e., $d_p^* = 1 \mu m$, 5 $\mu m$ and 10 $\mu m$. For all simulations performed the mass loading is set to $\eta = 0.0332\%$. Unfortunately, it is not possible to perform computations at higher mass loadings using such small particles since the limiting parameter is the number of particles present in the computational domain. The mass loading described above results from the choice to limit the number of particles $N_p$ with a diameter of $d_p^* = 1 \mu m$ to $N_p = 10^7$. For the other two diameters the number of particles present in the computational domain are set to $N_p = 8.0 \times 10^4$ and $1.0 \times 10^4$ for the 5 $\mu m$ and 10 $\mu m$ particles, respectively, in order to achieve the same mass loading of $\eta = 0.0332\%$.

If a collision between two particles occurs, the events which satisfy criterion (5.115) are counted. The criterion (5.115) says that if the total (rotational and translational) kinetic energy after the collision calculated by the standard hard–sphere approach is less than the kinetic energy of the agglomerate plus the work required to overcome the van–der–Waals force, agglomeration occurs. The post–collisional state, however, is determined without considering the van–der–Waals forces or agglomeration, i.e., it is determined by the standard hard–sphere collision described in § 5.4.1. For the first evaluation of the agglomeration criterion this measure (“passive mode”) is taken since the objective is to study the number of agglomerations found as a function of the particle diameter $d_p^*$. If after a detection of agglomeration the particles are treated as volume–equivalent or porous spheres, this implies that also the particle diameter $d_p^*$ changes throughout the simulation. Therefore, the post–agglomeration treatment of the particles is completely disregarded in order to keep the diameter of the particles present in the computational domain constant. Three different values for $e_{n,p}$ ($e_{n,p} = 0.4$, 0.6 and 0.8) are evaluated since this constant is expected to have the biggest influence on the agglomeration criterion (5.115). The reason is that the computed van–der–Waals energy is directly affected. The other parameters modeling the post–collisional velocity of the particles are set to the following values: $e_{t,p} = 0.44$, $\mu_{dy,p} = 0.6$ and $\mu_{st,p} = 0.85$. The static $\mu_{st,p}$ and dynamic coefficient of friction $\mu_{dy,p}$ are taken from the review of experimental results published by Byerlee (1978). For the tangential restitution coefficient the same value as used in § 7.4 and 7.6 for glass–glass inter–particle collisions is chosen since no measured values are found. The Hamaker constant is set to $H^* = 3.8 \times 10^{-20}$ J, the particle density to $\rho_p^* = 2710 \text{ kg/m}^3$, the minimal contact distance to $\delta_0^* = 3.36 \times 10^{-10}$ m and the mean yield stress to $\bar{\sigma}^* = 3.0 \times 10^8$ Pa. The constants $H^*$, $\rho_p^*$, $\delta_0^*$ and $\bar{\sigma}^*$ are taken from limestone particles and can be found in Tomas (2007).

At the beginning of the simulation the particles are homogeneously distributed in the computational domain. The statistics are gathered for a dimensional time interval $\Delta T = \Delta T^* U_B^* / R_{pipe}^* = 224$ after the particles had reached a statistically steady state.

### 7.5.2 Influence of Post–collision Treatment without Agglomeration and the Influence of the Modeling of the Agglomerate

The second issue investigated also relies on the test case of the turbulent particle–laden downward flow in a pipe. The Reynolds number and the grid are the same as described above. The purpose of these computations is to study the differences between the different
models for the agglomerate (as a porous sphere or a volume–equivalent sphere) and the influence of the van–der–Waals force on the calculation of the post–collisional velocities of the particles which do not agglomerate. At the beginning one simulation is performed where $10^6$ particles with a diameter of $d_p^* = 1 \mu m$ and a density $\rho_p^* = 2710 \text{ kg/m}^3$ are homogeneously distributed in the computational domain. The resulting mass loading is $\eta = 0.003\%$. This small mass loading is chosen in order to keep the computational costs at a reasonable level. However, since the number of particles present in the computational domain is still high ($N_p = 10^6$), the author is confident that the statistics obtained are meaningful. After this initialization, this simulation is run for a dimensionless time interval of $\Delta T = \Delta T^* U_p^*/R_{\text{pipe}}^* = 56$ (about 4.5 flow–through times) without considering agglomeration in order to make the particle statistics independent of the initial condition. For the subsequent investigations nine different simulations are carried out. All these nine computations are started with the same initial solution obtained from the procedure described above. In one simulation the particles are assumed to rebound at a specular wall (denoted SW) and for the other simulations the wall is treated as rough (denoted RW). For each of these two settings, one case is computed by considering the van–der–Waals forces in the calculation of the post–collisional velocities (denoted w. vdW.). That means that the coefficients $k_{n,p}$, $k_{t,p}$, $k_{\omega,1}$ and $k_{\omega,2}$ are computed according to the procedure explained in § 5.4.2.6. The other cases disregard the influence of the van–der–Waals forces in case that no agglomeration occurs (denoted wo. vdW.). If the van–der–Waals force is disregarded for the case that no agglomeration occurs (the van–der–Waals force is set to zero), $k_{n,p}$ is set to unity (see eq. (5.131)). As described in § 5.4.2.5, for positive values of $k_{n,p}$ all other coefficients used to compute the post–collisional state if no agglomeration occurs are set to unity. Therefore, all coefficients $k_{n,p}$, $k_{t,p}$, $k_{\omega,1}$ and $k_{\omega,2}$ are set equal to unity in this case. From eq. (5.146) it is obvious that for these values the post–collisional state of the particles is solely determined by means of the standard hard–sphere model. Furthermore, for each of the resulting four settings, one simulation is carried out by treating the agglomerate as a porous sphere and one simulation by treating the agglomerate as a volume–equivalent sphere (denoted VES). For the simulations where the agglomerate is treated as a porous sphere, the diameter $d_{ps}$ and the density $\rho_{ps}$ are calculated according to eq. (5.124) and eq. (5.123), respectively. For the simulations where the agglomerate is treated as a volume–equivalent sphere, the diameter $d_{ves}$ is calculated according to eq. (5.95) and the density is kept constant. The ninth simulation is carried out in a smooth wall configuration but frictionless inter–particle collisions are assumed, i.e., the original, strongly simplified agglomeration model described in § 5.4.2.3. is applied. The nine different simulations described above and the abbreviations adopted are summarized in Table 4.

The parameters modeling the particle–wall collision are set to the following values: $e_{n,w} = 0.8$, $e_{t,w} = 0.44$, $\mu_{dy,w} = 0.6$, $\mu_{st,w} = 0.85$ and $k_{s}^* = 15 \mu m$. Since no experimentally determined values for the material pairing limestone–steel (the particles are assumed to be conveyed through a steel pipe) the parameters have to be estimated. For $e_{t,w}$, $\mu_{dy,w}$ and $\mu_{st,w}$ the same values as employed for the inter–particle collision between limestone particles are used. The normal restitution coefficient is set to a slightly lower value than used for the material pairing glass–aluminum (see § 7.4). The roughness height $k_{s}^*$ is chosen in such a way that it clearly influences the particle trajectory after a wall rebound. The Hamaker constant is set to $H^* = 3.8 \times 10^{-20} \text{ J}$, the minimal contact distance to $\delta_0^* = 3.36 \times 10^{-10} \text{ m}$ and the mean yield stress to $\bar{\sigma}^* = 3.0 \times 10^8 \text{ Pa}$. The parameters
Abbreviation | Settings
--- | ---
fricless. coll. | smooth pipe wall, frictionless inter–particle collisions, volume–equivalent sphere
SW w. vdW. | smooth pipe wall, with considering the van–der–Waals forces if no agglomeration occurs, porous sphere
SW wo. vdW. | smooth pipe wall, without considering the van–der–Waals forces if no agglomeration occurs, porous sphere
SW w. vdW. VES | smooth pipe wall, with considering the van–der–Waals forces if no agglomeration occurs, volume–equivalent sphere
SW wo. vdW. VES | smooth pipe wall, without considering the van–der–Waals forces if no agglomeration occurs, volume–equivalent sphere
RW w. vdW. | rough pipe wall, with considering the van–der–Waals forces if no agglomeration occurs, porous sphere
RW wo. vdW. | rough pipe wall, without considering the van–der–Waals forces if no agglomeration occurs, porous sphere
RW w. vdW. VES | rough pipe wall, with considering the van–der–Waals forces if no agglomeration occurs, volume–equivalent sphere
RW wo. vdW. VES | rough pipe wall, without considering the van–der–Waals forces if no agglomeration occurs, volume–equivalent sphere

<table>
<thead>
<tr>
<th>Table 4: Overview of the simulations performed to test the agglomeration model and abbreviations used.</th>
</tr>
</thead>
<tbody>
<tr>
<td>modeling the particle–particle collisions are set to the same values as used for the limestone particles described above: $\epsilon_{n,p} = 0.6$, $\epsilon_{t,p} = 0.44$, $\mu_{dy,p} = 0.6$, $\mu_{st,p} = 0.85$.</td>
</tr>
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</table>

### 7.6 Horizontal Pipe Flow at Re = 58,800

The objective of the test case presented in this section and published in Alletto and Breuer (2013) is threefold: (i) To further validate the deterministic collision treatment and the wall roughness model for the particles against the experimental data of Huber and Sommerfeld (1998) for smooth and rough walls. (ii) To prove the applicability of eddy–resolving methods in horizontal pipe flows with periodic boundary conditions. (iii) To study the influence of the wall roughness and the mass loading on the dynamics of the continuous and solid phase in a horizontal pipe in order to provide supplementary information about particle and fluid quantities not measurable in experiments. In this way phenomena can be explained using the great amount of data available in computational simulations which are impossible to gather experimentally. Furthermore, the development of the interesting secondary flow structures induced by the particles in the pipe cross–section is investigated in detail by means of LES combined with the point–particle approach. The appearance of this flow structure was very recently confirmed by the experiments of Belt et al. (2012).

The reference test case can be found in Huber (1997) and Huber and Sommerfeld (1998) who carried out PDA measurements in horizontal glass and steel pipes with a radius $R_{\text{pipe}} = 40$ mm. Based on the mean gas velocity $(U_B^* = 24$ m/s) of the air at standard ambient conditions a Reynolds number of $\text{Re} = U_B^* R_{\text{pipe}}^{\nu_f} \approx 60,000$ results. The particles were
introduced into the pipe system by a screw feeder. The 5 m long measurement section followed after a flow straightener. The measurements were taken after a development length of about 4.5 m, where the flow is assumed to be fully developed. The particles were spherical glass beads ($\rho_p^* = 2500 \text{ kg/m}^3$) with a size distribution ranging between about 1.5 to 98 $\mu$m and a number mean diameter $d_{p,N}^*$ of about 40 $\mu$m (see eq. (4.63a) for the definition). The size distribution of the 30 classes into which the poly-disperse distribution was grouped, is depicted in Fig. 39. A mass loading of $\eta = 30\%$ was investigated. This setup is used to validate the predictions carried out (see § 8.6.3).

![Figure 39: Particle size distribution of the poly-disperse spherical glass beads investigated by Huber (1997) and Huber and Sommerfeld (1998).](image)

The computational domain has an extension of 12 $R_{pipe}^*$ and is discretized by an O–grid containing $3 \times 10^7$ cells in total and 400 cells in streamwise direction. Since the reference case is assumed to be fully developed, periodic boundary conditions are applied in streamwise direction. In order to achieve a constant mass flow over the simulation period a forcing term as described in § 3.3.2 is applied. For the unladen flow the first cell center is located at $\Delta r^+ = 9.34$ and the resolution in streamwise and in circumferential direction is $\Delta z^+ = 73.48$ and $\Delta (r_{pipe} \theta)^+ = 38.47$, respectively. Thus, the wall model of Schumann (1975) is applied for the continuous flow. For the unladen flow computations with two different subgrid–scale models for the fluid are performed in order to study their influences on the turbulent pipe flow. For the first computation the model of Smagorinsky (1963) is applied with a constant of $C_s = 0.1$. In order to investigate the influence of the subgrid–scale model for the fluid, for the second computation the dynamic model of Germano et al. (1991) is used (see also § 3.2.2). For this simulation the numerator and to denominator of eq. (3.22) are averaged in the homogenous (streamwise) direction in order to calculate $(C_s \Delta)^2$. Since no substantial differences to the results obtained with the Smagorinsky (1963) model are noticeable (see § 8.6.1), the computationally cheaper model of Smagorinsky (1963) is adopted for the following two–phase flow simulations.

Regarding the particles, the following constants modeling the velocity and angular velocity changes during an inter–particle collisions are used: $e_{n,p} = 0.97$, $e_{t,p} = 0.44$, $\mu_{st,p} = 0.94$, $\mu_{dy,p} = 0.092$. The constants $e_{n,p}$, $e_{t,p}$, and $\mu_{p,dy}$ are taken from the measurements by Foerster et al. (1994), who experimentally determined these quantities for two colliding glass beads. The value of $\mu_{st,p}$ is a common value found in textbooks for the dry friction of the material pairing glass–glass (see, e.g., Serway and Vuille, 2006).
For the particle–wall collisions at the smooth glass pipe the same model constants are chosen as for the particle–particle collisions: $\eta_{n,wg} = 0.97$, $\eta_{t,wg} = 0.44$, $\mu_{st,wg} = 0.94$, $\mu_{dy,wg} = 0.092$. Obviously, for an ideally smooth surface the wall–normal vector is not allowed to be randomly inclined which is automatically ensured by the wall model.

For the rough steel pipe the same constants as used in Breuer et al. (2012) to model the particle–wall collisions involving glass beads in a channel confined by rough steel walls are taken: $\eta_{n,ws} = 0.9$, $\eta_{t,ws} = 0.3$, $\mu_{st,ws} = 0.5$, $\mu_{dy,ws} = 0.4$. This choice is motivated as follows: Lain and Sommerfeld (2008) used empirical relations for the constants $\eta_{n,ws}$ and $\mu_{dy,ws}$ as functions of the incident angle. The functional dependence was extracted from measurements performed for spherical glass beads impinging on a steel plate. Since in the present model the influence of the incident angle on the above constants is not taken into account for simplicity reasons, a mean value within the range given in Lain and Sommerfeld (2008) is taken. The aforementioned approach provides a reasonable estimation of the values of $\eta_{n,ws}$ and $\mu_{dy,ws}$ which are commonly assumed to be dependent on the material pairings (in this case steel and glass). Since no experimental results are available for $\mu_{st,ws}$, the constant is set to a slightly higher value than $\mu_{dy,ws}$, which is quite reasonable. Furthermore, $\eta_{t,ws}$ is set to a realistic value already used in wall–bounded particulate flow simulations (see, e.g., Vreman, 2007).

Since no specification about the roughness height $R^*_z$ are found in Huber (1997) or Huber and Sommerfeld (1998) a reasonable value of $R^*_z = 10 \, \mu m$ is assumed. The constant modeling the surface finishing described in § 4.3.2.2 (see, also Breuer et al., 2012) is set to $C_{\text{surface}} = 3$ which leads with the relation $k^*_s = C_{\text{surface}} R^*_z$ to a value for the equivalent sandgrain roughness height $k^*_s = 30 \, \mu m$. This value lies within the range found for new stainless steel tubes (Idelchik, 1986). Moreover, this roughness level corresponds to a $k^+ = k^*_su^*_s/\nu_f^* = 1.84$ and thus is located within the viscous sublayer. Consequently, the continuous flow is not directly influenced by the wall roughness and the application of the wall model of Schumann (1975) which assumes a mean velocity profile obtained in smooth–wall flow configurations is justified. For this test case the gravity, the buoyancy, the drag force and the lift forces due to the liner shear and the particle rotation are considered. In order to account for the influence of the unresolved scales on the particle motion, the model described in § 5.2 is applied.

In addition to the mass loading $\eta = 30\%$ investigated by Huber (1997) and Huber and Sommerfeld (1998) one more mass loading $\eta = 70\%$ for both pipe surfaces is analyzed in detail to allow considerations about the influence of the inter–particle collisions in smooth and rough pipes. The total number of particles $N_p$ present in the computational domain is $N_p = 5.36 \times 10^6$ and $N_p = 1.25 \times 10^7$ for $\eta = 30\%$ and $\eta = 70\%$, respectively. Especially the high number of particles tracked for the high mass loading underlines the efficiency of the procedure presented in this thesis. The same size distribution as depicted in Fig. 39 is used in these predictions.

Furthermore, in order to check whether with the present methodology comparable results to the work of Lain and Sommerfeld (2012) can be obtained, two more simulations are performed. These differ from the previous cases by much larger mono–disperse particles and a higher mass loading. The particle diameter is set to $d^*_p = 134 \, \mu m$ in order that the Stokes number St = $\tau^*_p/\tau_i^* = (\rho_p d^*_p^2/18 \mu_f^*)/(R^*_z(U^*_p))$ is the same as in the work of Lain and Sommerfeld (2012). Furthermore, the same mass loading of $\eta = 100\%$ ($N_p = 9.0 \times 10^5$) as in Lain and Sommerfeld (2012) is used. The constants modeling the velocity and angular velocity changes during the particle–particle and the particle–wall
collisions are chosen to be equal to those used for the steel pipe. Since the roughness used by Lain and Sommerfeld (2012) was solely defined by roughness angles and not by heights, two roughness heights $k_s^* = 30 \ \mu m$ and $150 \ \mu m$ are compared to each other. In this way (together with the rather inertial particles and the high mass loading) it can be analyzed if the momentum transferred from particles hitting a rough surface to the fluid is the origin of the secondary flow as claimed by Lain and Sommerfeld (2012). The results are presented in § 8.6.5 where the present data are compared with available studies in the literature.

In order to compute the fluid statistics, the instantaneous flow quantities are averaged in time for a dimensionless time period of $\Delta T = \Delta T^* U_B^*/R_{pipe} = 2280$ (i.e., about 190 flow–through times) and in streamwise direction. The particle statistics are initialized at the same time step as the fluid statistics and averaged over the same period of time. (For the computation of the statistics, see § 6.3.) Furthermore, before starting the averaging procedure it is carefully checked that the flow and the particles have reached a statistically stationary state. This is achieved by ensuring that the center of mass of the particles do not any more experience any mean displacement in gravitational direction. The dimensionless time step size $\Delta t = \Delta t^* U_B^*/R_{pipe}$ is equal to $\Delta t = 5.0 \times 10^{-3}$, $7.5 \times 10^{-3}$ and $8.0 \times 10^{-3}$ for the $\eta = 30\%$, $70\%$ and $100\%$ simulations, respectively. For increasing mass loading the particles lead to an increase of the attenuation of turbulence, i.e., the fluctuations decrease. For that reason the maximum velocity in the smallest cells decreases and therefore larger time step sizes are allowed by the stability criterion of the Runge–Kutta scheme.

### 7.7 Cold Flow in a Combustion Chamber Model

In order to go a step further in the complexity of the investigated flow configuration, the cold flow without swirl in a combustion chamber model experimentally examined by Borée et al. (2001) is tackled. This kind of test case is chosen because of its practical importance and the variety of complex flow phenomena present in this flow configuration. For this reason it is an excellent test case for the methodology presented in this thesis. Confined bluff–body flows are typical flow configurations relevant for a variety of practical applications involving particle–laden or droplet–laden turbulent flows especially for combustion devices. For example, in pulverized coal combustion primary air and coal particles are injected in the center of the burner and a secondary stream of air is introduced on the periphery. For this kind of configuration a cone–shaped body is located close to the exit of the primary air in order to generate a recirculation region to stabilizes the flame generated by the combustion of the coal particles (Xu et al., 1995; Shi et al., 1997). For non–premixed combustion the same stabilization measure is adopted to prevent that the flame is lifted–off or even extinguished: The fuel jet is injected inside a recirculation region generated by either a bluff–body flow (Schefer et al., 1987; Chen et al., 1990; Schefer et al., 1994; Chen et al., 1998b) or a diverging flow with swirl (Chen et al., 1990). The simulations presented here are the first four-way coupled simulations of the experimental configuration investigated by Borée et al. (2001). Until now only one–way and two–way coupled simulations of this experiment were available in the literature (see Minier et al., 2004; Riber et al., 2009; Fede and Simonin, 2010; Chrigui et al., 2010, and also the comments in the introduction).

For this case two different numerical setups are investigated. The first simulations are performed on a coarse grid in order to analyze the influence of the coupling assumptions
(one-, two- or four-way coupling). This part of the investigation can also be found in Alletto and Breuer (2012), Breuer and Alletto (2012a) and Breuer and Alletto (2012b). Then the grid is refined in order to analyze the grid independence of the solution. Using the fine grid, different inflow conditions are chosen in order to illustrate their influence on the dynamics of the particle–laden flow. In this section the experimental reference case and the numerical setup are divided explicitly into two different subsections in order to facilitate the overview for the reader.

7.7.1 Experimental Reference Case

The configuration investigated by Borée et al. (2001) is depicted in Fig. 40. They obtained detailed particle and fluid data by two-component phase–Doppler anemometer measurements in a configuration typical for combustion devices. The gravitational acceleration acts in the streamwise direction. The particle–laden air flow with a mean velocity $U^*_{jet} = 3.01 \text{ m/s}$ enters the chamber through a circular pipe ($R^*_{pipe} = 10 \text{ mm}$) located on the chamber axis (Fig. 40). The Reynolds number $Re = R^*_{pipe} U^*_{jet} / \nu^*$ based on the pipe radius and the mean (bulk) inflow velocity is $Re = 2006$. Additionally, clean air enters through an annular ring ($R^*_a/R^*_i = 7.5$, $R^*_a/R^*_{pipe} = 15$) with a mean velocity $U^*_e = 5.36 \text{ m/s}$. This specific choice of the inlet velocities and of the geometrical settings leads for the unladen case and the low mass loading case (for the details see below) to the appearance of two recirculation regions inside the combustion chamber. The stagnation points are denoted $S_1$ and $S_2$ and are located on the axis (see Fig. 40). For the high mass loading the momentum transported by the particles results in disappearing stagnation points on the axis.

Because of the existence of complicated flow phenomena and the substantial alteration of the mean flow by the particles, the configuration examined by Borée et al. (2001) represents an ideal test case for the methodology presented in this thesis to treat four–way coupled turbulent flows. Furthermore, the rather simple bounding surfaces allow the generation of a body–fitted curvilinear grid for which the code used in this thesis was developed. A development section upstream of the chamber inlet of $L^*_d = 2 \text{ m}$ ensured a fully developed turbulent pipe flow ($L^*_d/R^*_{pipe} = 200$) but, as pointed out by Borée et al. (2001), the length of the annular ring flow in front of the inlet seems to be too short to ensure a fully developed flow ($L^*_d/(R^*_a - R^*_i) = 54$). The test section had a length of $L^*_t = 1.5 \text{ m}$ ($L^*_t/R^*_{pipe} = 150$), i.e., the end of the test section is located far enough downstream of the inlet to disregard any effect on the recirculation region. The gravity pointed in streamwise direction.

The spherical glass beads injected into the chamber through the pipe flow have a density ratio of $\rho^*_p/\rho^*_f = 2100$ and diameters varying in the range of $d^*_p = 20$ to $100 \mu\text{m}$ subdivided into nine classes. The number distribution of the single classes follows the settings of Borée et al. (2001) detailed in Table 5. For the definition of the number distribution $q_{0,i}(d^*_p)$ and the mass distribution $q_{3,i}(d^*_p)$ see § 4.4. The resulting values in the present case are $d^*_{p,M} = 63 \mu\text{m}$ and $d^*_{p,N} = 50 \mu\text{m}$, respectively. For the definitions of $d^*_{p,N}$ and $d^*_{p,M}$ see eq. (4.63).

According to the estimation of Riber et al. (2009) the distribution covers a Stokes number range of $0.4 \leq St \leq 11$. For this purpose the Stokes number $St = \tau^*_p/\tau^*_f$ is determined as the ratio of the particle relaxation time $\tau^*_p$ and a characteristic time scale of the fluid most energetic eddies $\tau^*_f$. The former is based on the classical Stokes flow assumption, whereas for the latter the length of the most energetic eddies is estimated as a third of the pipe diameter and their velocity as the maximum fluctuating velocity in.

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Two different mass loadings were investigated by Borée et al. (2001). The mass loading was either \( \eta = 22\% \) (denoted by moderate = M) or 110\% (denoted by high = H). It is worth to mention that the present specification of the mass loading is a global parameter defined for the pipe flow in front of the chamber. The particle concentration strongly decreases when the jet enters the combustion chamber. Then, the particulate phase is significantly diluted since the particles are dispersed in a much wider area.

<table>
<thead>
<tr>
<th>( i )</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
<th>9</th>
</tr>
</thead>
<tbody>
<tr>
<td>( d_{p,i}^* ) [( \mu m )]</td>
<td>20</td>
<td>30</td>
<td>40</td>
<td>50</td>
<td>60</td>
<td>70</td>
<td>80</td>
<td>90</td>
<td>100</td>
</tr>
<tr>
<td>Mass distribution ( q_{3,i}(d_{p,i}^*) )</td>
<td>0.004</td>
<td>0.005</td>
<td>0.091</td>
<td>0.224</td>
<td>0.264</td>
<td>0.215</td>
<td>0.107</td>
<td>0.065</td>
<td>0.025</td>
</tr>
<tr>
<td>Number distribution ( q_{0,i}(d_{p,i}^*) )</td>
<td>0.085</td>
<td>0.028</td>
<td>0.234</td>
<td>0.295</td>
<td>0.202</td>
<td>0.103</td>
<td>0.034</td>
<td>0.015</td>
<td>0.004</td>
</tr>
<tr>
<td>Relaxation time ( \tau_p^* ) [ms]</td>
<td>3.1</td>
<td>6.9</td>
<td>12.3</td>
<td>19.2</td>
<td>27.6</td>
<td>37.6</td>
<td>49.1</td>
<td>62.2</td>
<td>76.6</td>
</tr>
<tr>
<td>Stokes number ( \text{St} = \tau_p^<em>/\tau_{f,t}^</em> )</td>
<td>0.4</td>
<td>1.0</td>
<td>1.8</td>
<td>2.7</td>
<td>3.9</td>
<td>5.4</td>
<td>7.9</td>
<td>8.9</td>
<td>11.0</td>
</tr>
</tbody>
</table>

Table 5: Initial distribution of the particle sizes by Borée et al. (2001) \( (\overline{d_{p,M}} = 63 \mu m, \overline{d_{p,N}} = 50 \mu m) \) with estimated Stokes numbers by Riber et al. (2009). For the definition of the number distribution \( q_{0,i}(d_{p,i}^*) \) and the mass distribution \( q_{3,i}(d_{p,i}^*) \) see § 4.4.

### 7.7.2 Numerical Setup

In the following, the two different setups employed to study the cold flow in the combustion chamber model are described. In the first setup a coarse grid is used with the aim to investigate the influence of the one–, two– and four–way coupling assumptions on the particle–laden flow for the moderate and high mass loading. In the second numerical setup a finer grid and improved inlet conditions compared to the first setup are employed with the aim to study the influence of the resolution and the inlet boundary conditions on the flow in the combustion chamber model.
7.7.2.1 Numerical Setup to Study the Influence of the One–way, Two–way and Four–way Coupling

Domain Size and Grid
In order to reduce the required CPU time the length of the computational domain is reduced to $L^*/R_{pipe}^* = 90$ which is still four to five times longer than the expected re-circulation region and thus ensures that the region of interest is not disturbed by the outlet. The chamber is discretized by an O–type grid consisting of 13 blocks and about $1.3 \times 10^7$ cells (140 cells in streamwise direction and 95,625 cells in the cross–section parallel to the axis). The front view of the grid is displayed in Fig. 41(a) (only every third grid line is shown). The grid is stretched towards the walls of the pipe, the walls of the annular ring and the inlet. The first computational nodes are located at $\Delta r^*/R_{pipe}^* = 0.01, 0.029, 0.041$ and 0.015 at the pipe wall, the inner wall of the annular ring, the outer wall of the annular ring and downstream of the inlet, respectively. For the unladen case the first computational node of the pipe flow (see the five inner blocks in Fig. 41(b) which have the same cross–section in the combustion chamber and the pipe flow simulation) corresponds to a wall distance of $\Delta r^+ = 0.14 \left( u^*/U_{jet}^* = 6.67 \times 10^{-2} \right)$. The stretching factor is set in order to be less than 1.1 in the whole computational domain. This value is chosen in order not to reduce too much the accuracy of the discretization (Breuer, 2011). To avoid discontinuities in the derivatives of the body–fitted grid around the central patch located on the axis of the chamber, the first layer of the mesh is smoothed by the commercial tool ICEM-CFD 12.0 (ANSYS, 2009) and then copied in streamwise direction to obtain the three–dimensional geometry. The dimensionless time step chosen is $\Delta t = \Delta t^* \cdot (U_{jet}^*/R_{pipe}^*) = 5 \times 10^{-4}$.

Figure 41: (a): Grid of the combustion chamber, front view. (b): Zoom of the inlet of the inner pipe, front view (In both figures only every third grid line is displayed).

Boundary Conditions and Models for the Fluid
Riber et al. (2009) pointed out the sensitivity of the flow in the combustion chamber to
any changes in the inlet conditions, especially those of the inner pipe. Thus in order to avoid artificially generated boundary conditions, the inflow conditions in the present numerical setup are provided by two additional LES predictions using pipe and annular ring flows with periodic boundary conditions. If the same cross-sectional grid and the same time step size as for the main simulations is also used for these two supplementary simulations, the data extracted at a cross-sectional plane can directly be used as inflow conditions for the main computation (see §3.3.3.1). For all computed cases with the same mass loading, the same inflow data are used to reduce the considerations solely to the chamber flow. For the moderate mass loading case a four-way coupled pipe flow with particles rebouncing at the specular pipe walls is used as inflow data for the continuous and the disperse phase. The statistics obtained for the inflow data are in good agreement with the inflow measurements of Borée et al. (2001). Due to the low Reynolds number a four-way coupled prediction for the high mass loading leads to a relaminarization of the pipe flow. The same effect was observed in the pipe flow DNS computation of Vreman (2007) for the same Reynolds number and mass loading, but using mono-disperse particles with a diameter of $d_p^* = 60 \, \mu m$ which approximately corresponds to the mass-averaged diameter of the experiments of Borée et al. (2001). Therefore, the inflow data for this case are generated by solely taking into account the particle–particle collisions without considering the influence of the particle on the fluid. This simplification yields a reasonable agreement with the particle and fluid inflow statistics measured by Borée et al. (2001).

As described in §7.7.1 the particle–laden air flow enters the chamber through a circular pipe. In the present study the corresponding mean velocity is set to $U_{jet}^* = 3.01 \, m/s$. This value is calculated from the mass flow specified in Borée et al. (2001) dividing it by the cross-sectional area of the pipe rather than from the specified mean inlet velocity. This approach is chosen in order to achieve a good agreement between the measured and simulated mean inlet profiles (see Fig. 83).

For the clean air entering the chamber through an annular ring a slightly different mean velocity ratio of $U_e^*/U_{jet}^* = 1.78$ is chosen compared with the ratio $U_e^*/U_{jet}^* = 1.21$ specified by Borée et al. (2001). Since some discrepancies between the measured profile of the annular flow at the inlet and the volume flux specified in Borée et al. (2001) are noticed, the mean annular velocity $U_e^*$ is calculated by integrating the experimental velocity profile at the inlet leading to the value specified above. This represents an important and critical issue since an extreme sensitivity of the bluff-body flow to the value of the ratio of the momentum flux of the inner jet to the momentum flux of the annular flow is already well known in single-phase situations (see, e.g., Chen et al., 1990) and maybe is intensified in two-phase flows.

At the outflow the convective boundary condition described in §3.3.4 is prescribed to ensure that vortices can leave the integration domain without reflections (Breuer, 2002). Based on the near-wall resolution described above a wall-resolved simulation results and thus the no-slip condition is applied at all walls. For the subgrid-scale modeling the Smagorinsky model as described in §3.2.1 with a constant of $C_s = 0.065$ is used.

As mentioned above, the present numerical setup is used to investigate the influence of the coupling mechanisms on the flow behavior in a cold combustion chamber. For this purpose a one-way, a two-way and a four-way coupled simulation are performed at the moderate mass loading M. This simulations are denoted MH1, M2 and M4, respectively. For the high mass loading H only a two-way coupled (H2) and a four-way coupled (H4) simulations are realized since a one-way coupled simulation would not produce any
different statistics compared to the one–way coupled simulation for the moderate mass loading.

**Models for the Particles and Generation of the Statistics**

All particle classes present in the experiments of Borée et al. (2001) are released into the combustion chamber according to their corresponding number distribution (see Table 5).

At the stage when this simulations were performed, friction between the particles undergoing a collision was not implemented in the code yet. Therefore, regarding the particle–particle interaction for the simulations used to generate the inflow conditions as well as for the four–way coupled chamber flow, friction during an inter–particle collision is not considered and the normal restitution coefficient was set to unity, i.e., \( e_{n,p} = 1 \). Furthermore, at this stage only a specular reflection of the particles was available in the code as wall boundary condition for the particles. Nevertheless, all particles hitting a chamber wall are removed from the domain in order to save computational costs. This simplification is not expected to substantially influence the reliability of the solution because of the very small ratio of the particle diameter to the outer radius of the combustion chamber model. Therefore, the time span between two subsequent wall collisions is large and the particle dynamics are predominantly influenced by turbulence. For this test case only the gravity, the buoyancy and the drag forces are considered. Since the regions of interest are far away from the walls where the steepest fluid velocity gradients occur, the lift force due to the liner shear is neglected. The lift force due the particle rotation is not considered since the particles can neither acquire an angular velocity during a wall collision nor during a particle–particle collision. In order to account for the influence of the unresolved scales on the particle motion, the SGS model described in § 5.2 is applied.

The most relevant flow regions of this test case are the pipe entrance and the shear layer generated by the annular ring flow. In streamwise direction the interesting region ends behind the recirculation region where the flow recovers. Hence, in order to save CPU time, particles hitting the wall or passing the plane normal to \( z^*/R_{\text{pipe}}^* = 45 \) are removed from the domain. This measure is motivated by the fact that the local particle volume fraction is such low that it does not influence any more the fluid. Furthermore, no experimental data are available in this part of the chamber but the particles would partially stay for a very long time in the chamber and thus would waste a lot of CPU time.

The fluid statistics are obtained by averaging the instantaneous flow about 15 flow–through times based on the mean velocity at the outlet and the chamber length \( L_t^* \) in the simulation. Additionally, the data are averaged in circumferential direction. Regarding the particle statistics, for each of the particle classes shown in Table 5 separated statistics are computed by averaging them the same time span as the fluid and also in circumferential direction.

### 7.7.2.2 Numerical Setup to Study the Influence of the Resolution and the Inlet Boundary Conditions

**Domain Size and Grid**

In order to test the influence of the grid size on the simulation of the cold flow in a combustion chamber, two finer grids than the one described in the former section are used. For both fine grids the chamber is discretized by an O–type grid consisting of 264
blocks and about $2.8 \times 10^7$ cells (240 cells in streamwise direction and 116,781 cells in the cross-section normal to the axis). The difference between these two grids is the spatial resolution in axial direction (see Fig. 42(a)). For the first fine grid (denoted FINE 1) an equidistant grid is used for the region $7.5 \leq z^*/R_{pipe}^* \leq 43$. For the second fine grid (denoted FINE 2) the grid is refined towards the midpoint between the two stagnation points present on the axis of the moderate mass loading flow. Figure 42 shows the differences between the coarse grid (denoted COARSE) and the two fine grids. As shown in Fig. 42(b) the grid points in the cross-section (radial direction $r^*$) are redistributed without a substantially increase of the grid resolution (116,781 cells in the cross-section for the fine grids and 95,625 cells for the coarse grid). That means that in order to achieve a finer resolution in the region of the developing shear layer between the recirculation region and the annular flow (see Fig. 40) a coarser grid near the axis is accepted (see Fig. 42(c)). Note that also in a small region close to the position where the annular flow enters the domain the resolution of FINE 1 and FINE 2 is lower compared to COARSE (see Fig. 42(b) at $r^*/R_{pipe}^* \approx 7.5$).

**Figure 42:** (a) Comparison of the grid spacings in axial direction. (b) Comparison of the grid spacings in radial direction. (c) Zoomed view of the grid spacing in radial direction near the axis.
Boundary Conditions and Models for the Fluid

Contrarily to the former section, for this numerical setup only four–way coupled simulations are analyzed. Regarding the generation of the inflow boundary conditions, different methodologies are adopted all based on simulations with of the pipe flow periodic boundary conditions. Concerning the pipe flow used to generate the inflow conditions, for all cases described later on the following constants modeling the translational and angular velocity changes during a particle–particle or a particle–wall collision are used: $e_{n,p} = 0.97$, $e_{t,p} = 0.3$, $\mu_{dy,p} = 0.1$, $\mu_{st,p} = 0.9$, $e_{n,w} = 0.9$, $e_{t,w} = 0.3$, $\mu_{dy,w} = 0.4$, $\mu_{st,w} = 0.5$ and $k_s^* = 10 \mu m$ (rough wall). For the $\eta = 22\%$ mass loading case the agreement between the four–way coupled pipe flow results with periodic boundary conditions assuming rough walls seen by the particles and the measurements of Borée et al. (2001) taken at the inlet section is fairly well. Therefore, the fluid and particle data generated by this pipe flow are extracted at a plane normal to the axis and are used as inflow conditions. For the high mass loading, however, one–way coupled simulations are performed additionally considering the particle–particle collisions. Before using the data generated in this way as inflow conditions, they are manipulated according to the methodology described in § 3.3.3.2 for the continuous phase and according to the procedure described in § 4.3.5 for the disperse phase. The constants $C_x$, $C_y$ and $C_z$ (see eq. (3.33)) used to adjust the fluid velocity fluctuations (the mean profile is taken from the experiment) are set equal to $C_x = 1$, $C_y = 1$ and $C_z = 0.75$. The values for $C_x$ and $C_y$ are motivated by the fact that the wall–normal velocity fluctuations (no circumferential measurements are available) of the one–way coupled simulations agree well with the measurements. Since the streamwise velocity fluctuations of the one–way coupled simulations are slightly higher than the measured quantities, a value of $C_z$ lower than unity is chosen. Regarding the particles, $C_{pz}$ is set to $C_{pz} = 0.75$ (see eq. (4.59)). The choice of these constants is motivated by the same reasons as the choice of the constants used for the fluid.

In order to generate the inflow conditions for the annular flow (without particles), two different methodologies are adopted. In the first approach the inflow data are generated by a simulation with periodic boundary condition. In the following, the simulations where this boundary condition is applied are denoted AF–PER (AF stands for annular flow and PER for periodic). For the second approach the data obtained by the simulation with periodic boundary conditions are manipulated in order to achieve a good agreement between the injected flow field and the measurements taken by Borée et al. (2001) at the inflow. For this purpose, the fluctuations obtained are scaled with the factors $C_x$, $C_y$ and $C_z$ (see eq. (3.33)) and superimposed by the mean measured profile. Since the simulation with periodic boundary conditions predicts slightly lower wall–normal fluctuations (no circumferential data were available) compared with the experiment, the factors $C_x$ and $C_y$ are set equal to $C_x = 1.2$, $C_y = 1.2$. Since the agreement between the simulation and the experiment regarding the streamwise velocity fluctuations is fairly well, $C_z$ is set to unity. In the following, the simulations where this boundary condition is applied are denoted AF–EXP (AF stands for annular flow and EXP for experiment).

Since for the simulations using the FINE grids the minimal cell size is larger than for the COARSE grid (see Fig. 42(c)) a larger dimensionless time step $\Delta t = \Delta t^* \cdot \left( \frac{U_{jet}^*}{R_{pipe}^*} \right) = 1.35 \times 10^{-3}$ can be chosen in order to fulfill the stability requirements of the Runge–Kutta scheme.
Models for the Particles and Generation of the Statistics

Differences compared with the numerical setup of the COARSE case concern not only the grid and the generation of the inflow conditions. Since the simulations described in this section are performed at a later stage of this work, the entire forces displacing the particles given by eq. (4.25) are considered. Furthermore, also the temporal evolution of the particle angular velocity is considered. In order to account for the influence of the unresolved scales on the particle motion, the SGS model described in § 5.2 is applied.

Regarding the particle–particle collision, for the cases considered in this section frictional collisions are assumed. The parameters chosen for the hard–sphere collision model are set to $c_{n,p} = 0.97$, $c_{t,p} = 0.3$, $\mu_{dy,p} = 0.1$ and $\mu_{st,p} = 0.9$. These values are taken from Foerster et al. (1994) for the pairings glass–glass. Since no detailed information about the constitution of the test section of the experiments are available, the chamber walls are assumed to be smooth and the constants modeling the particle translational and angular velocity change at the wall are set equal to $c_{n,w} = 0.97$, $c_{t,w} = 0.3$, $\mu_{dy,w} = 0.1$ and $\mu_{st,w} = 0.9$. These values are taken from Foerster et al. (1994) for the pairings glass–glass.

For this setup the particles are removed from the computational domain only when they pass the boundary of the grid located at $z^*/R_{pip}^* = 90$. The reason is that on the massive parallel machine Cray XE6 (Hermit) where the simulations described here were performed, the ratio of the computational time required by the particle solver to the computational time required by the fluid solver is smaller than on the vector machine NEC–SX9. Therefore, the particle side of the code does not represent a crucial issue from the performance point of view and the particles are allowed to remain for a longer time in the computational domain.

The fluid statistics are obtained by averaging the instantaneous flow about 15 flow–through times based on the mean velocity at the outlet and the chamber length $L^*_t$ in the simulation. Additionally, the data are averaged in circumferential direction. Regarding the particle statistics, for each of the particle classes shown in Table 5 separated statistics are computed by averaging them the same time span as the fluid and also in circumferential direction.
7.8 Cyclone Separator Flow

In cyclone separators (see, e.g., Obermair, 2002; Obermair et al., 2003, 2005) the particle-laden gas flow enters the cyclone body tangentially inducing a highly rotatory flow (see Fig. 43). Centrifugal forces lead to a migration of the large and thus heavy particles towards the cyclone walls, where they are transported downwards and collected in the dust bin located at the bottom of the apparatus. Turbulent fluctuations lead to a mixing of the particles throughout the cyclone body. Hence, the entrainment of the small and thus light particles from the cyclone walls towards the cyclone axis increases with increasing velocity fluctuations (Derksen et al., 2006). In the region near the axis the air flow is pointing upwards and leaves the cyclone through the vortex finder located at the top of the device. Consequently, the objective of a cyclone to separate particles of a broad spectrum of sizes can be fulfilled. As the representative diameter of the separated particles the cut point is used, i.e., the particle size which is removed with 50% efficiency from the air stream. The transport and separation mechanism of the particles in a cyclone separator is accompanied by complex flow structures such as curved streamlines, secondary flows and a precessing vortex core already present in the unladen flow. Hence, this type of flow configuration represents a challenging test case for computational approaches treating turbulent flows. Introducing particles further complicates the description of the flow since the interaction between the particles and the turbulent eddies, the particles and the cyclone walls and the particles themselves have to be accurately modeled. Owing to the complicated flow structures and the various interaction mechanisms involved by the disperse phase, it is mandatory to employ an adequate simulation tool in order to reliably predict the pressure loss and the separation efficiency of the cyclone separator. Furthermore, because of the huge number of particles present in such a device, efficient methods to treat the disperse phase are mandatory. Due to the above mentioned complexity of the flow phenomena and the interaction mechanisms, the turbulent flow in a cyclone separator represents an excellent test case in order to validate the methodology presented in this thesis. Because of the very few LES simulations of the turbulent flow in cyclone separators present in the literature (see Derksen, 2003; Derksen et al., 2006, 2008; de Souza et al., 2012, and also the comments in the introduction), the test case described in the following is used to gain further experience in adopting the methodology presented in this thesis for this complex type of flows.

7.8.1 Experimental Reference Case

The numerical simulation of the flow in a cyclone separator described in the following is based on the two experimental investigations, i.e., the unladen flow experiment of Obermair et al. (2003) and the two-phase flow experiment of Obermair et al. (2005). An extensive description of the measurements published in these two articles and supplementary information can be found in the dissertation of Obermair (2002). Obermair et al. (2003) carried out LDA measurements of the clean flow in five different cyclone geometries. In the geometry denoted A (see Obermair et al., 2003, for the details) the dust bin followed right after the conical part of the cyclone. The geometries denoted B and E were similar to A. The difference is that in B an apex cone was located in the dustbin and in E the apex cone was placed in the conical part of the cyclone. In the configuration C a downcomer tube was placed between the conical part and the dust bin and in D an additional dust bin was placed between the conical part and the downcomer.
tube. Among these various geometries, Obermair et al. (2003) found that the geometry C with a downcomer tube (the straight tube between the conical part and the dust bin shown in Fig. 43) leads to the best separation efficiency. The geometry of the cyclone separator with the downcomer tube is sketched in Fig. 43(a). For this geometry LDA data are available in the $x$–$z$ plane parallel to the cyclone axis (see Fig. 43(b)) starting from approximately the first read line sketched in Fig. 43(a) until almost the bottom of the dust bin. Additionally, Obermair (2002) performed also LDA measurement in nine cross–sections normal to the cyclone axis. The read lines in Fig. 43(a) symbolize the axial positions of the $x$–$y$ planes, where the experimental data are compared with the present unladen simulations (see § 8.8.1).

The mean inlet air velocity at standard conditions ($20 \, ^\circ\text{C}$ and 101.3 kPa) was $U_{in}^* = 12.7 \, \text{m/s}$ resulting in a Reynolds number of $Re = 333,000$ based on the mean inlet air velocity at standard conditions and the diameter of the cyclone body $d_{body}^* = 400 \, \text{mm}$. Unfortunately, no detailed information about the design of the experimental setup upstream of the cyclone inlet are available. The gravity pointed in $x$-direction of the coordinate system displayed in Fig. 43(b), i.e., in the direction of the flow in the inlet section. Due to a better accessibility of the measurement plane, a horizontal configuration of the cyclone was chosen. This choice was motivated by the assumption that the influence of the gravity can be neglected with respect to the centrifugal forces (Obermair, 2002).

![Figure 43: Cyclone geometry: (a) Geometry investigated by Obermair et al. (2005, 2003) (dimensions in mm), (b) Computational domain.](image)

Obermair et al. (2005) carried out PDA measurements of the poly–disperse two–phase flow in a cyclone separator containing limestone particles with a density of $\rho_p^* = 2770 \, \text{kg/m}^3$. In the dissertation of Obermair (2002) in addition to the PDA data published by Ober-
mair et al. (2005) also LDA measurements of the same two-phase flow are available. In contrast to the unladen flow, for the two-phase flow experimental data are only available in the $x-z$ plane of the downcomer tube parallel to the cyclone axis. The blue lines in Fig. 43(a) symbolize the axial positions in the midplane where the experimental data are compared with the present two-phase flow simulations (see § 8.8.2.2). The mass loading was $\eta = 0.065\%$. It is defined as the ratio of the particle mass flow to the fluid mass flow at the inlet. The inlet velocity and the geometry of the cyclone is the same as described in Obermair et al. (2003). The diameters of the particles used by Obermair et al. (2005) ranged between $d_p^* = 0.9 \mu m$ and $30 \mu m$. The cumulative mass distribution of the particles shown in Fig. 44 is obtained by extracting the data from the figures present in Obermair (2002) by the software DIGITIZELT (Bormann, 2006). Obermair (2002) obtained the distribution function by measuring the particle diameter distribution with the laser diffraction sensor HELOS from SYMATEC\(^{12}\). The curve in Fig. 44 denoted HELOS visualizes the cumulative mass distribution $Q_3(d_p^*)$ measured in situ in the inflow section. The curve in Fig. 44 denoted HELOS SUCELL shows the cumulative mass distribution obtained after deagglomerating the particles in an ultrasonic bath containing a dispersant. From these measurements it is obvious that the particles have already agglomerated during their way from the injection position to the cyclone inflow. For that reason the mass distribution obtained with the HELOS method is used for the subsequent simulations in order to reproduce the same conditions at the inlet as in the reference experiment. The statistics obtained by the LDA measurements were achieved by averaging over 2500 bursts. Unfortunately, the averaging time is not specified.

![Figure 44: Cumulative mass distribution $Q_3(d_p^*)$ measured by Obermair (2002) in the inlet section of the cyclone.](image)

### 7.8.2 Numerical Setup

The computational domain employed is depicted in Fig. 43(b). The length of the outlet pipe $L_{out}^*/d_{body}^* = 2$ is chosen to reduce the influence of the zero-gradient outlet boundary.

\(^{12}\)The home page http://www.sympatec.com/, (2013) provides a description of the system.
condition for the flow to a minimum. The application of a convective boundary condition typically used for LES was not possible for the two meshes used since it produces numerical oscillations near the domain outlet. The length of the inlet \( L_{in}/d_{body} = 1.5 \) is specified in order to ensure a sufficiently long distance between the duct inlet and the cyclone inlet. That allows the steady turbulent velocity profile (no fluctuations, for the mean profile see Reichardt, 1951, and § 3.3.3.3 for the details) applied at the inlet boundary of all cases described in the following to destabilize and develop. This measure leads to a realistic time–dependent velocity field at the inlet of the cyclone body. For the details of the generation of the inflow condition, see § 3.3.3.3.

Two different grids are used in order to study the grid independence of the flow in the cyclone separator. The first grid employs \( 4.4 \times 10^6 \) control volumes to discretize the computational domain. For this mesh the maximum wall resolution is \( \Delta r^+ = 122, 255, 110, 50 \) and 247 in the outlet section, the cylindrical part of the cyclone body, the conical part of the cyclone body, the downcomer tube and the dust bin, respectively. \( \Delta r^+ \) is calculated by means of the local wall shear stress of the corresponding unladen flow. In the following, this grid is abbreviated by COARSE. The second grid employs \( 5.6 \times 10^6 \) control volumes to discretize the computational domain. For this grid the maximum wall resolution is \( \Delta r^+ = 45, 256, 48, 22 \) and 247 in the outlet section, the cylindrical part of the cyclone body, the conical part of the cyclone body, the downcomer tube and the dust bin, respectively. In order to determine \( \Delta r^+ \), the local wall shear stress of the corresponding unladen flow determined. In the following, this grid is abbreviated by FINE. The basic difference between the COARSE and the FINE grid is that the resolution at the walls of the cyclone body (conical part and downcomer tube) is refined for FINE with respect to COARSE. Furthermore, the axial resolution in the outlet section and in the dust bin is refined for the FINE grid compared with the COARSE grid. Figures 45(a) and (b) display the \( x–y \) cross–section of the FINE grid in the entrance section (Fig. 45(a)) and in the downcomer tube (Fig. 45(b)). Unfortunately, in the entrance section it was not possible to generate an orthogonal grid with the software ICEM CFD 12.0. In the core region, however, it was possible to smooth the mesh generating a high–quality grid. The \( x–z \) cross–section of the FINE grid at the midplane is displayed in Fig. 45(c).

In order to avoid the resolution of the steep velocity gradients at the walls which is not possible with the grids introduced, the wall model of Werner and Wengle (1993) is used. Note that for the COARSE grid also a simulation applying the wall model of Schumann (1975) was performed. Since similar results as for the model of Werner and Wengle (1993) are achieved, this results adopting the model of Schumann (1975) are not shown for the sake of brevity but can be found in Alletto and Breuer (2014).

The dimensionless time step is \( \Delta t = \Delta t^* U_{in}^* / d_{body}^* = 1.0 \times 10^{-4} \) when the model of Smagorinsky (1963) and \( 1.5 \times 10^{-4} \) when the model of Germano et al. (1991) is applied. Since the simulation adopting the dynamic model of Germano et al. (1991) shows the smallest circumferential velocity among the cases presented here, a larger time step size can be adopted in order to fulfill the stability requirements of the Runge–Kutta scheme.

The particle density is set to \( \rho_p^* = 2770 \text{ kg/m}^3 \) (\( \rho_p^* / \rho_f^* = 2250 \), limestone), i.e., the same material as used in the particle–laden PDA measurements of Obermair et al. (2005). In order to obtain the particle size distribution used in the experiment, the following steps are performed: First the discrete cumulative mass distribution function \( Q_{3,i}(d_{p,i}^*) \) extracted from Obermair (2002) (see also the curve HELOS in Fig. 44) has to be differentiated numerically with respect to the particle diameter \( d_{p,i}^* \) in order to obtain the mass dis-
Figure 45: FINE grid (a): x–y cross–section of the cyclone separator grid at the entrance (b): x–y cross–section at the downcomer tube (c): x–z cross–section at the midplane (In all figures only every third grid line is displayed).

distribution function \( q_{3,i}(d_{p,i}^*) \). Note that the definitions of \( q_{0,i}(d_{p,i}^*) \), \( Q_{0,i}(d_{p,i}^*) \), \( q_{3,i}(d_{p,i}^*) \) and \( Q_{3,i}(d_{p,i}^*) \) can be found in § 4.4. For this purpose a central difference scheme is adopted. For setting up the simulation, however, the number distribution function \( q_{0,i}(d_{p,i}^*) \) (see eq. (4.60a)) is required. The reason is that for the injection of the particles into the computational domain, the number of particles \( N_{p,i} \) belonging to each size class \( i \) is required. Unfortunately, \( q_{0,i}(d_{p,i}^*) \) (see eq. (4.60a)) cannot be calculated directly from \( q_{3,i}(d_{p,i}^*) \) (see eq. (4.60b)) since this requires the a–priori knowledge of all particle numbers \( N_{p,i} \) belonging to the size classes \( i \). For that reason, \( q_{0,i}(d_{p,i}^*) \) has to be determined iteratively from the known distribution \( q_{3,i}(d_{p,i}^*) \). The iterative loop works as follows:

Starting from an initial guess of the number of particles \( N_{p,i}^{(0)} \) belonging to the size class \( i \) an initial guess of the total mass \( m_{pi}^{(0)} \) of the particles belonging to the size class \( i \) can be determined. Hence, also an initial guess of the mass distribution \( q_{3,i}(d_{p,i}^*)^{(0)} \) is obtained (see also eq. (4.60)). After that, the factors \( q_{3,i}(d_{p,i}^*)^{mes}/q_{3,i}(d_{p,i}^*)^{(0)} \) are calculated. Here
\( q_{3,i}(d_{p,i}^{*})^{\text{mes}} \) denotes the size distribution extracted from the measurements. The new number of particles are obtained by multiplying \( N_{p,i}^{(0)} \) with the factors \( q_{3,i}(d_{p,i}^{*})^{\text{mes}} / q_{3,i}(d_{p,i}^{*})^{(0)} \), i.e., \( N_{p,i}^{(1)} = N_{p,i}^{(0)} q_{3,i}(d_{p,i}^{*})^{\text{mes}} / q_{3,i}(d_{p,i}^{*})^{(0)} \). That means, if the initial guess of \( N_{p,i}^{(0)} \) delivers values of the distribution \( q_{3,i}(d_{p,i}^{*})^{(0)} \) larger than the measured one, \( N_{p,i}^{(1)} \) is reduced compared to \( N_{p,i}^{(0)} \) and vice versa. Following this iteration scheme, after a few iterations a converged solution is obtained, i.e., \( N_{i}^{(n)} \approx N_{i}^{(n-1)} \). The result of this procedure is summarized in Table 6 and in Fig. 46 (see also Bennek, 2012). The resulting number mean diameter of the distribution summarized in Table 6 is \( d_{p,N}^{*} = 1.74 \ \mu \text{m} \) (see eq. (4.63a) for the definition). Particles with size classes greater than \( i = 15 \) are not considered since the corresponding numbers are already very low.

<table>
<thead>
<tr>
<th>( i )</th>
<th>( d_{p}^{*} ) [( \mu \text{m} )]</th>
<th>( q_{3,i}(d_{p,i}^{*}) )</th>
<th>( q_{0,i}(d_{p,i}^{*}) )</th>
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<tr>
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<td>6.94 ( \times 10^{-2} )</td>
<td>5.77 ( \times 10^{-4} )</td>
</tr>
</tbody>
</table>

**Table 6:** Distribution of the particle sizes injected into the cyclone.

**Figure 46:** Distribution of the particle sizes injected into the cyclone.

In order to estimate the total number of particles \( N_{p,tot} \) present in the cyclone as a first guess an overall mass loading of \( \eta = 0.065\% \) is assumed according to the experimental
setup. This mass loading yields together with the mean particle diameter of 1.74 \( \mu \text{m} \) a total number of particles contained in the computational domain of \( N_{p,\text{tot}} = 1.47 \times 10^{10} \). In order to limit the total number of particles to an affordable number of \( N_{p,\text{tot}} = 5.0 \times 10^{6} \), 2963 particles are grouped into a parcel. That means that in order to account for the momentum transfer of the particles to the fluid in the two–way coupled simulation, the force exerted by each parcel tracked is multiplied by the factor 2963. The aerodynamic behavior of the parcel, however, is the same as for the single particle. Since the simulations described in this section are performed at the final stage of this work, the entire forces displacing the particles given by eq. (4.25) are considered. Furthermore, also the temporal evolution of the particle angular velocity is considered. In order to account for the influence of the unresolved scales on the particle motion, the SGS model described in § 5.2 is applied.

In § 8.8.1 four different simulations for the unladen flow and three different simulations for the particle–laden flow are discussed. Regarding the unladen flow, a computation on the COARSE grid with the model of Smagorinsky (1963) and a constant of \( C_s = 0.1 \) is performed. The same constant of \( C_s = 0.1 \) is also used for a second computation on the FINE grid in order to study the grid independency of the solution. The other two computations on the FINE grid are performed to study the influence of the subgrid–scale model for the fluid on the unladen flow. For one of these simulations the model of Smagorinsky (1963) with a constant of \( C_s = 0.15 \) is used and for the second simulation the model of Germano et al. (1991) is employed. In order to prevent large spatial fluctuations of the predicted turbulent viscosity \( \mu_T \), the values of \( (C_s \Delta)^2 \) obtained by the low–pass filtering (see eq. (3.23)) is filtered again in space with a filter width of \( \tilde{\Delta} = 2\Delta \).

Regarding the particle–laden flow, the simulation on the FINE grid with \( C_s = 0.15 \) is taken to evaluate the influence of the one–way and two–way coupling assumption on the fluid and the particle statistics. This setup is chosen since the best accordance with the unladen flow data of Obermair et al. (2003) is found. For these two simulations the particles are assumed to specularly rebounce from the wall. A four–way coupled simulation is not possible since it requires that all particles present in the experiment are also tracked in the simulation. At the moment this is not feasible because of the prohibitively large number of particles resulting from this requirement. In addition to the aforementioned two simulations a two–way coupled simulation with particles impinging at rough walls is performed. For this computation the constants modeling the rebouncing at the wall are set to the following values: \( e_{n,w} = 0.9 \), \( e_{t,w} = 0.3 \), \( \mu_{dy,w} = 0.4 \) and \( \mu_{st,w} = 0.5 \). Since no experimental data providing the aforementioned constants for limestone particle impinging a steel wall are found, the same values as for glass particles hitting a steel wall (see § 7.6) are taken. For the wall roughness a value of \( k_s = 45 \mu \text{m} \) is assumed \( (C_{\text{surface}} = 3, \, R = 22.5 \mu \text{m}) \). This value lies within the range of wall roughnesses found for new steel pipes (Idelchik, 1986).

All statistics shown are achieved by averaging the fluid and particles quantities for about a dimensionless time of \( \Delta T = \Delta T^* U_{in}^*/d_{body}^* = 90 \). Unfortunately, it was not possible to achieve a longer averaging time because of the long runtime required (about one month on the massive parallel machine Cray XE6 (Hermit) for the aforementioned averaging time). The particles were introduced into the computational domain only after it is asserted that the flow field has reached a statistically stationary state. Regarding the particles the achievement of a statistically steady–state is not as simple as for the fluid. A statistically steady–state for the particles means that at least the same number of particles have to
be present in the computational domain for a longer time period. When the particles are injected into the cyclone separator they can either leave the domain at the outlet or being collected into the dust bin. Since the dust bin is closed (see Fig. 43), keeping the particles inside this part of the device will result in an accumulation of a huge number of particles. Unfortunately, this is not feasible from the view of the computational costs and furthermore not reasonable to keep tracking the particles inside the dust bin. Therefore, the particles have to be removed from the dust bin by postulating some assumption. Different strategies are adopted in the literature to remove the particles from cyclones with closed dust bins similar to the one considered in this thesis. A common method is to consider the particles as deposited when they enter the dust bin (Shalaby, 2007; Elsayed and Lacor, 2012) or when they are located at a certain distance from the bottom of the dust bin (Derksen et al., 2006). Shalaby (2007) also proposed to remove the particles from the domain after a certain residence time. Unfortunately, adopting a method available in the literature is not possible since the objective of the present simulations is to reproduce the measurements of Obermair et al. (2003) and Obermair et al. (2005). They observed drastic changes between the unladen flow and the particle–laden flow. Since they observed a large number of particles deposited in the dust bin, they attributed these changes to the decelerating effects of the particles located in the dust bin (see also § 8.8.1). Therefore, removing the particles when they enter the dust bin or at a certain position form the bottom seems to be not the right strategy to follow in order to reproduce the reference experiment. Instead the particles are removed when they are hitting the dust bin walls in order to keep them in the dust bin as long as they can possibly influence the fluid motion. With this approach a statistically steady–state is achieved. This is insured by checking that the center of mass of all particles in axial direction does not experience any mean displacement.

7.9 Summary of the Test Cases

Finally, in Table 7 a list of the test cases performed and the objectives pursued with each test case is provided.
<table>
<thead>
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<th>Test case</th>
<th>Objective</th>
<th>Sect.</th>
</tr>
</thead>
<tbody>
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<td>Channel Flow at Re = 10,935 with Zero Gravity</td>
<td>Test the interpolation scheme and the subgrid–scale model for the particles</td>
<td>7.1</td>
</tr>
<tr>
<td>Downward Channel Flow at Re = 11,900 with Smooth Walls</td>
<td>Evaluate the collision handling</td>
<td>7.2</td>
</tr>
<tr>
<td>Horizontal Channel Flow at Re = 21,292 with Rough Walls</td>
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<td>Downward Pipe Flow at Re = 2253</td>
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<td>Downward Pipe Flow at Re = 2253 to Test the Agglomeration Model</td>
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<td>Horizontal Pipe Flow at Re = 58,800</td>
<td>Provide an explanation for the origin of the secondary flow found in particle–laden horizontal pipes and further validate the simulation tool</td>
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Table 7: Overview of the test cases and the objectives pursued.
8 Results

8.1 Channel Flow at \(Re = 10,935\) with Zero Gravity

8.1.1 Influence of the Interpolation Scheme

At first, in Fig. 47 the influence of the interpolation scheme (Fig. 47(a) for the \(32^3\) grid and Fig. 47(b) for the \(64^3\) grid) on the mean streamwise particle velocity is shown. It is evident that the mean fluid velocity also depicted in Fig. 47 shows the typical slight grid dependence of LES predictions of a turbulent channel flow: For decreasing resolution the mean velocity profile becomes flatter (compare Fig. 47(a) with (b)). The flattening of the mean velocity profile can be attributed to the decreased momentum transfer between the wall region and the bulk flow for the coarse grid compared with the fine grid. Furthermore, it is obvious that the interpolation scheme does not influence the first–order moment. For both interpolation schemes studied, the mean tracer velocity matches exactly the mean fluid velocity (see Fig. 47(a) and (b)).

![Figure 47](image.png)

**Figure 47:** Influence of the interpolation scheme on the mean velocity of tracers for two different grid resolutions.

Figure 48 compares the second–order moments of the massless tracers computed on the coarse grid (\(32^3\) cells) with those obtained on the finer grid (\(64^3\) cells). In addition to the statistics obtained by the two different interpolation schemes, the results for the continuous phase and the DNS of Kim et al. (1987) are also visualized. The flow statistics are included in these figures since for an ideal interpolation the statistics of massless tracers should be equal to the fluid statistics. As obvious from Fig. 48 for all three second–order statistics the trilinear interpolation scheme has a pronounced filtering effect on the velocity fluctuations. Contrarily, the method based on Taylor series expansions suggested by Marchioli et al. (2007a) very closely resembles the fluid fluctuations. For the trilinear interpolation the grid dependency on the accuracy of the scheme should be noted: The differences between the flow statistics and the statistics computed by tracking the tracers through the domain are more pronounced for the coarse grid (Figs. 48(a), (c) and (e)) than for the finer grid (Figs. 48(b), (d) and (f)). Regarding the results of the Taylor series expansion, no clear grid dependence can be stated. This implicates that for a coarse grid the errors introduced by interpolating the fluid velocity at the particle position can
be expected to be less pronounced for the Taylor series expansion than for the trilinear interpolation. For the trilinear interpolation the interpolated velocity fluctuations of the particles in all three directions are smaller than the corresponding fluid statistics computed.
at the cell center. On the other hand, the interpolation scheme suggested by Marchioli et al. (2007a) predicts a slight increase of the interpolated streamwise velocity fluctuations of the particles compared to the fluid statistics (see Fig. 48(a) for the coarse grid and Fig. 48(b) for the fine grid). For the spanwise velocity fluctuations (see Fig. 48(e) for the coarse grid and Fig. 48(f) for the fine grid), however, the Taylor series expansion leads to a slight reduction of the peaks compared to the fluid statistics. Regarding the wall–normal velocity fluctuations the Taylor series expansion gives very close agreement between the fluid and tracer statistics computed on the coarse grid (Fig. 48(e)). For the fine grid a slight increase of the fluctuations of the tracers compared to the fluid fluctuations can be observed (Fig. 48(f)). Regarding the comparison of the tracer velocity fluctuations with the DNS data, it is evident that the wall–normal and the spanwise fluctuations are too low. These discrepancies can be explained for LES computations by the circumstance that only the resolved scales are used to compute the velocity fluctuations. In principle, the modeled contribution can be determined and added to the resolved part in order to calculate the total fluctuations. However, at least for the Smagorinsky model applied here, the modeled stresses are not accurately predicted. Thus typically solely the resolved contribution is plotted. For increasing resolution the deviations between DNS and LES data decrease since a broader spectrum is resolved and the amount of modeled scales decreases.

Based on the pronounced discrepancies between the second–order moments of the tracers computed by the trilinear interpolation and the second–order moments of the fluid, in all following simulations performed the interpolation scheme suggested by Marchioli et al. (2007a) is employed to interpolate the fluid velocity at the particle position. As a concluding remark on this issue dedicated to the interpolation scheme, it should be mentioned that the difference between the trilinear interpolation and the Taylor series expansion was also studied as a function of the Stokes number \(St = \frac{\tau_p^* U_B^*}{\delta_{Ch}^*}\) of the particles. The main outcome was that the mean velocity profile of the particles was independent of the interpolation scheme. Furthermore, it was observed that the differences between the second–order moments obtained by the trilinear interpolation and those obtained by the Taylor series expansion decrease with increasing Stokes number, i.e., with increasing particle inertia. The results are, however, not shown here for the sake of brevity.

### 8.1.2 Influence of the SGS Model for the Particles

Figure 49 shows the influence of the SGS model for the particles (Fig. 49(a) 32\(^3\) grid and Fig. 49(b) 64\(^3\) grid) on the mean velocity of the small particles with a Stokes number of \(St = 1.57 \times 10^{-3}\). As shown in the following, for this very low value the particles behave similar to fluid tracers and thus can be compared with the DNS fluid data of Kim et al. (1987). The same observation as made in § 8.1.1 can also be made regarding the subgrid–scale model for the particles: The mean particle velocity computed by applying the SGS model presented in § 5.2 matches perfectly the mean fluid velocity (see Fig. 49(a) and (b)). Furthermore, the same slight grid dependency of the mean velocity is observed as in the former section.

Figure 50 shows the influence of the SGS model for the particles on the second–order moments of the small particles computed on the coarse (32\(^3\) cells) and the fine grid (64\(^3\) cells). As obvious from Figs. 50(a) and (b) the SGS model has a marginal effect on the particle streamwise velocity fluctuations for both, the coarse and the fine grid. It
Figure 49: Influence of the subgrid–scale model on the mean velocity of small particles for the two grid resolutions.
Figure 50: Influence of the subgrid–scale model for the particles on the statistics of small particles, (a)-(b) streamwise velocity fluctuations, (c)-(d) wall–normal velocity fluctuations, (e)-(f) spanwise velocity fluctuations.

is evident that more or less only the peak values of the particle streamwise velocity fluctuations computed with the SGS model are slightly increased compared with the statistics computed without the SGS model. Figure 50(c) and (d) display the velocity
fluctuations in wall–normal direction for the coarse and the fine grid, respectively. It is evident that for both resolutions the statistical moments obtained for tiny particles closely resembles the DNS statistics of Kim et al. (1987). Furthermore, the model reproduces the expected dependence on the resolution: For a coarse grid, where the contribution of the unresolved scales is larger than for a finer grid, the influence of the model is more accentuated. The same observation holds for the spanwise velocity fluctuations (Fig. 50(e) for the coarse grid and Fig. 50(f) for the fine grid). In this case the particle fluctuations obtained with the model for the subgrid–scale velocity are slightly lower than the DNS statistics. As a concluding remark, it should be mentioned that the influence of the SGS for the particles was also studied as a function of the Stokes number $\text{St} = \frac{\tau_p^* U_f^*}{\delta_{Ch}^*}$. The main outcome was that the mean velocity of the particles was not affected by the model and the difference between the statistics computed with and without the model observed in Fig. 50 decreases with increasing Stokes number, i.e., with increasing particle inertia. This results are, however, not shown here for the sake of brevity.

8.2 Downward Channel Flow at Re = 11,900 with Smooth Walls

8.2.1 Influence of the One–way, Two–way and Four–way Coupling

As an introducing remark to this section, note that some of the results presented in the following can also be found in Breuer and Alletto (2012a,b). Contrarily to the previous section the discussion of the results starts with the particle statistics, since the particles are directly affected by the consideration of the inter–particle collisions, whereas the continuous phase is only indirectly influenced. Figure 51(b) shows the mean particle velocity in comparison with the experimental data of Benson et al. (2005). The mean velocities (fluid and particles) and also the normalized particle concentration (Fig. 52(b)) are plotted as a function of the dimensionless wall distance $y^+$ using a logarithmic scale of the axis. For all plots mentioned, $y^+$ is determined with the friction velocity of the unladen flow. The computed four–way coupled case is in very good agreement with the LDA measurements. It is obvious that considering the particle–particle interactions leads to a flatter mean velocity profile which indicates an enhanced momentum transfer between the particles. This is underlined by looking at the particle wall–normal fluctuations (see Fig. 51(f)), where particle–particle collisions lead to an increase of the fluctuations by a factor of about three with respect to the one–way and two–way coupled cases. At a first glance this observation is astonishing since the global mass loading is only $\eta = 15\%$ and the corresponding volume fraction is about $7.3 \times 10^{-5}$. However, similar observations, i.e. a flatter mean particle velocity profile and enhanced particle fluctuations, were made by Yamamoto et al. (2001) in their LES channel flow predictions at a global mass loading of $\eta = 20\%$ corresponding to an even lower volume fraction of $2.7 \times 10^{-5}$. According to the classification of Elghobashi (1994), both cases are dilute two-phase flows, where collisions between particles are rare and consequently a two–way coupling should be sufficient. However, it has to be noted that Elghobashi’s criterion is based on the assumption of a homogeneous spatial distribution of the particles in the fluid to be found in the free flow case or for high-Re flows. In the present wall–bounded low–Re flow, strong local particle concentrations occur in the near–wall region for the one–way and two–way coupled simulations (see Fig. 52(b)). Consequently, the global criterion by Elghobashi (1994) is no longer reasonable and has to be replaced by local considerations. Nevertheless, the influence of the inter-particle collisions on the continuous fluid flow is still marginal, as
will be shown next.

Figure 51(a) shows the predicted mean fluid velocities for the three cases (one–way, two–way and four–way coupling). It can be noticed that they are almost not affected by the presence of the particles. For comparison, the LDA measurements of Benson et al. (2005) are displayed for the unladen flow since no fluid data are available for the case with particles. The streamwise and wall–normal velocity fluctuations of the fluid depicted in Figs. 51(c) and (e) are only insignificantly attenuated by the particles. According to Elghobashi’s classification this is not surprising for this moderate mass loading (volume fraction, respectively). Comparing the fluid data of the one–way and two–way coupled simulations, even the influence of the two–way coupling is negligible. Unfortunately, also for these second–order moments no experimental two–phase data are available. Thus the measured data depicted in Fig. 51(c) correspond to the single–phase flow and are in reasonable agreement with the simulations.

Figure 51(d) shows the particle streamwise velocity fluctuations. For the four–way coupled case the profile is flatter in the channel center than for the corresponding one–way and two–way coupled calculations. This may be explained by the flatter mean particle velocity profile visible in Fig. 51(d): If a particle moves from a region with a smaller mean velocity to a region with a larger mean velocity, the difference between the instantaneous particle velocity and the mean velocity is the smaller the flatter the mean profile is. This holds of course, also for the opposite case.

Finally, the spanwise particle velocity fluctuations and the normalized particle concentration $\langle c^* \rangle / c^*_{pav}$ are displayed in Fig. 52. In the simulations $\langle c^* \rangle / c^*_{pav}$ is calculated by the following relation:

$$\frac{\langle c^* \rangle}{c^*_{pav}} = \frac{1}{2} \pi d_p^3 \rho_p^* \langle N_p \rangle V_{c}^* \frac{V_{tot}^*}{m_{p,tot}^*}. \tag{8.1}$$

$\langle N_p \rangle$ is the averaged number of particles found in the slices parallel to the wall used to compute the statistics and $V_c^*$ is the corresponding volume of the slices. $V_{tot}$ and $m_{p,tot}$ are the total volume of the computational domain and the total particle mass present in the computational domain. As obvious from Fig. 52(a) also the spanwise velocity fluctuations predicted by the four–way coupling are drastically increased compared with the corresponding one–way and two–way coupled simulations by considering the enhanced momentum transfer between the particles caused by the inter–particle collisions. Note that for this statistical moment no experimental data for the particles are available. The effect of the particle–particle collisions on the particle concentration is visualized in Fig. 52(b) and obviously a strong influence close to the wall can be observed. Note that the particle concentration is plotted as a function of the dimensionless wall distance $y^+$ using a logarithmic scale of the axis in order to emphasize the drastic changes in the near–wall region. From Fig. 52(b) it is evident that the one–way and two–way coupled simulations lead to a strong particle accumulation in the near–wall regions provoked by turbophoresis. Turbophoresis is the tendency of particles to migrate in the direction of a decreasing turbulence level (Caporaloni et al., 1975). A simple explanation for this phenomenon can be provided by the following scenario: A particle is placed in a region near the wall, where the wall–normal velocity fluctuations (Fig. 51(e)) still have a positive wall–normal gradient (in the viscous sublayer and the buffer layer). Then the particle is captured by a turbulent fluctuation and is transported slightly towards the wall. In this region the wall–normal fluctuations are lower than in the region further away from the wall. Therefore, the probability that the particle is captured by another turbulent fluctuation
Figure 51: Turbulent particle–laden channel flow: (a) mean streamwise velocity of the fluid, (b) mean streamwise velocity of the particles, (c) streamwise velocity fluctuations of the fluid, (d) streamwise velocity fluctuations of the particles. (e) wall–normal velocity fluctuations of the fluid, (f) wall–normal velocity fluctuations of the particles,
and transported again to the region, where it was placed at the beginning of this small example, is low. This mechanism leads to a migration of the particles towards the wall. A more fundamental explanation of turbophoresis is provided by the DNS of Marchioli and Soldati (2002): They found that the basic mechanism of particle segregation, i.e., high concentration peaks at the wall, is the staggered arrangement of quasi–streamwise vortices. A counter-clockwise rotating vortex located in the buffer layer entrains the particles towards the wall and a clockwise rotating vortex located at the rear end of the first vortex in the viscous layer traps the particles and prevents them to be resuspended towards the outer flow. This mechanism leads to particle accumulations in the low speed streaks (Marchioli and Soldati, 2002). Note that this high particle concentration peaks at the wall are typical for one– and two–way coupled DNS or LES (see, e.g., Kuerten, 2006; Marchioli et al., 2008c; Wang, 2010). The four–way coupled simulation, however, predicts an almost uniform concentration distribution over the channel height. This underlines the drastic effect of the inter–particle collisions on this statistical quantity caused by the momentum transfer between the particles. Due to the effect of the inter–particle collisions the particle trajectories randomize and therefore they are less influenced by the coherent near–wall structures. As a result the mechanism described by Marchioli and Soldati (2002) which leads to a strong particle accumulation in the near–wall region for one– and two–way coupled predictions is inhibited and the concentration close to the wall is reduced for four–way coupled flows (see also Nasr et al., 2009). Unfortunately, for the concentration no experimental data are available for comparison.

Summing up, the deterministic collision treatment described in § 5.4.1 and § 6.2.3 is successfully validated by means of the experiments of Benson et al. (2005), since close agreement is found between the present four–way coupled simulation and the reference case. As a final remark, especially in the view of the drastic concentration changes induced by a four–way coupled simulation compared with a one–way or two–way coupled simulation (see Fig. 52(b)), the accuracy of one–way and two–way coupled LES or DNS in predicting the particle concentration in wall–bounded channel flows should be considered as critical.
8.3 Horizontal Channel Flow at Re = 21,292 with Rough Walls

In the following, the results obtained by adopting the wall roughness model presented in § 4.3.2 in a horizontal turbulent channel flow are presented. Note that a part of the results given here is already published in Breuer, Alletto, and Langfeldt (2012). In order to illustrate that the model gives reasonable agreement with experimental data for a variety of parameter variations, the next sections are organized as follows: First, in § 8.3.1 the behavior of the wall roughness model for the particles is analyzed by increasing the wall roughness and keeping the mass loading $\eta$ constant. Here no fluid data are shown since the influence of the particle dynamics affected by the different asperity heights on the fluid motion is negligible. In § 8.3.2 the evolution of the particle statistics with the number of wall collisions is analyzed in detail. After that, in § 8.3.3 the particle diameter and the wall roughness are set to a constant value and the mass loading $\eta$ is varied. The scope is to study the influence of the mass loading and therewith associated also the influence of the inter–particle collisions on the particle statistics. In § 8.3.4 the particle diameter is varied with a constant wall roughness and a constant mass loading. The objective of this section it to analyze if the model reproduces the correct influence of the wall roughness on particles with different diameters. This is an important issue in practical applications, where the particles usually have a more or less broad size distribution. Next, in § 8.3.5 the most important parameters characterizing the material pairing $e_{n,w}$ and $\mu_{dy,w}$ are varied. The intention is to study their influence on the rebound behavior of the particles. In § 8.3.6 the influence of the two–way coupling on the continuous phase is studied. Finally, in § 8.3.7 the results of the new model are compared with Euler–Lagrange computations available in the literature. For that purpose, the recently published LES computations of Mallouppas and van Wachem (2013) and the RANS simulations of Lain and Sommerfeld (2008) are chosen. Both investigations analyzed the influence of the wall roughness on the particle motion using the same channel flow as described in § 7.3.

8.3.1 Influence of the Wall Roughness

In the following section the behavior of the wall roughness model with increasing asperity heights is presented. The results obtained for the roughnesses R0, R1 and R2 are compared with the experiments of Kussin (2004). Furthermore, the special case of a smooth wall is included. In addition to the first and second–order particle statistics the wall collision frequency $f_{w}$, the particle–particle collision frequency $f_{pp}$, the mean incident angle before the collision $\delta^-$, the mean wall inclination $\alpha_R$ (see Fig. 12 for the definition of the angles $\delta^-$ and $\alpha_R$), the mean particle wall–normal velocity $u_{p-} \cdot n_R$ before the wall collision, the percentage of sliding wall collisions and shadow events, the mean difference of the particle streamwise velocity after a wall collision $\Delta u_{px}$ and the mean pressure gradient in the channel $\frac{d\rho}{dx}$ are evaluated. The scope is to elucidate the basic mechanisms of how the roughness model influences the particle dynamics. The statistics listed in Table 8 are obtained during an averaging period of $N_t = 5000$ time steps. The averaging is started at a dimensionless time of $\Delta T = 300$ (about 47 flow–through times) after releasing the particles in order to ensure the independence of the initial conditions. The frequencies are determined by counting the collision events and dividing it by the averaging time:

\[13\text{Note that the quantities without the superscript } \ast \text{ are dimensionless. The velocities are made dimensionless with the bulk velocity } U_B, \text{ the lengths with the channel half–width } \delta_{Ch}, \text{ the pressure with } \rho_f U_B^2 \text{ and the time with } \delta_{Ch}/U_B.\]
\( f_{cw} = N_{cw}/(N_{i} \Delta t) \) and \( f_{cp} = N_{cp}/(N_{i} \Delta t) \). Here, \( N_{cw} \) and \( N_{cp} \) are the number of particle–wall and particle–particle collisions during the averaging time, respectively. The number of particles present in the computational domain for the case with \( \eta = 30\% \) are 8000.

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**Table 8:** Statistical results of the plane channel flow for the case with \( d_{p}^* = 195 \mu m \), \( \eta = 30\% \), \( \epsilon_{n,w} = 0.9 \), \( \mu_{d,y,w} = 0.4 \): mean collision frequencies \( f_{cw} \) and \( f_{cp} \), mean incident angle \( \bar{\delta} \), mean wall inclination angle \( \bar{\alpha}_{R} \), mean wall–normal velocity \( \bar{u}_{p} \cdot \bar{n}_{R} \) before the wall collision, percentage of sliding collisions and shadow events, mean difference of the streamwise particle velocity \( \bar{\Delta}u_{px} \) after a wall collision and pressure gradient \( d\bar{\rho}/dx \) for different roughness values (dimensionless quantities).

Figure 53(a) shows the mean streamwise particle velocity for mono-disperse particles \( (d_{p}^* = 195 \mu m) \), which agrees very well with the measurements of Kussin (2004). It is clearly evident that the mean particle velocity decreases with increasing roughness. This leads to an additional pressure drop \( d\bar{\rho}/dx \) (see Table 8) since the particles considerably lag behind the continuous flow causing an additional net force directed against the mean flow direction. Two main reasons can be identified for the deceleration of the particles in this study:

(i) The increased collision frequency with the wall \( f_{cw} \) leads to an increased momentum loss. Note that in Table 8 the total collision frequency has more than doubled from the smooth wall case to the roughness R2. The number of collisions at the upper wall is strongly intensified due to the rough wall which yields that more particles are reaching the upper part of the channel. This is in line with the findings of Kussin (2004) who estimated a reduction of the mean free path between two wall collisions from R1 to R2 for the same particle diameter but for a higher and a lower mass loading \( (\eta = 10\% \text{ and } 100\%\) by a factor of two. The present simulations can only report an increment of 29% (averaged over top and bottom wall) for the wall collision frequency \( f_{cw} \) from R1 to R2. Kussin (2004) assumed the mean free path
Figure 53: Variation of the wall roughness: Statistical results of the plane channel flow for the particles $d_p^* = 195 \, \mu m$, $\eta = 30\%$, $\epsilon_{n,w} = 0.9$, $\mu_{dy,w} = 0.4$: (a) mean velocity, (b) streamwise fluctuations, (c) wall–normal fluctuations, (d) spanwise fluctuations, (e) shear stress, (f) normalized particle number concentration.

between two wall collisions to be inversely proportional to the particle fluctuations in wall–normal direction $\langle u_{py}^* u_{py}^* \rangle_{rms}$. Since the measured wall–normal fluctuations are doubled from R1 to R2 (see Fig. 53(c)), he obtained a reduction of the mean free path by a factor of two. In the present simulation the wall–normal fluctuations increase by approximately 31% from R1 to R2. Hence, the increase is similar to the rise of the wall collision frequency $f_{cw}$. Thus the behavior of the prediction is
consistent with the experimental observations, but a difference remains between the simulations and the experiments due to the different increase of the wall–normal velocity fluctuations.

(ii) The mean wall–normal velocity $\overrightarrow{u_p} \cdot \overrightarrow{n_R}$ before the collision is tripled from the smooth wall case to R2. This leads to increased momentum losses during a sliding collision which is the predominant event as visible in Table 8. This is evidenced by looking at the equation describing the particle velocity change in the sliding case (eq. (4.45a)): The difference of the particle velocities parallel to the wall before and after the wall rebound $\Delta \overrightarrow{u_p}_x = \overrightarrow{u_p}^+_x - \overrightarrow{u_p}^-_x$ is proportional to the wall–normal velocity before the collision ($\overrightarrow{u_p} \cdot \overrightarrow{n_R}$). The correlation between the mean wall–normal velocity before the collision $\overrightarrow{u_p} \cdot \overrightarrow{n_R}$ and the streamwise momentum loss is underlined by the mean particle velocity difference in streamwise direction $\Delta u_{px} = u_{px}^+ - u_{px}^-$ before and after the wall impingement illustrated in Table 8. This difference is tripled from the smooth wall to the case R2 similar to the wall–normal velocity.

Figure 53(b) shows the streamwise particle velocity fluctuations. The fluctuations increase with increasing wall roughness. This can be attributed to the following reasons:

(i) The additional momentum loss of the particles hitting the wall: A particle coming from the bulk flow is decelerated when hitting the wall and due to its inertia needs a certain time to adjust to the mean flow. This results in increasing fluctuations throughout the entire channel.

(ii) As visible in the a–priori analysis presented in Fig. 13(b) of § 4.3.3, the possible trajectories of the reflected particles lie within a cone with an apex angle of $3 \sigma$. When increasing the roughness, this cone points more pronounced towards the bulk flow (the emergent angle not shown here increases equal to the incident angle) and the apex angle increases, since $\sigma$ is proportional to the roughness. This leads to a larger spreading and thus dispersion of the particles throughout the channel and hence to increased fluctuations.

Good agreement with the experiments is found for R0 and R2, while the predicted fluctuations are too high for R1. It is noticeable that in the experiments of Kussin (2004) there are substantial changes in all statistical quantities illustrated in Fig. 53 except the streamwise particle velocity fluctuations when the roughness is increased from R0 to R1. This is difficult to explain and maybe a hint for measurement uncertainties.

The simulated particle wall–normal velocity fluctuations illustrated in Fig. 53(c) show an almost linear increase with the wall roughness height. The increased wall–normal fluctuations are correlated with the mean wall–normal velocity $\overrightarrow{u_p} \cdot \overrightarrow{n_R}$ before the collision in the following manner: Animations have shown that the particles describe approximately straight trajectories after bouncing from a wall and due to their inertia (St = 108.33) they are only slightly influenced by the turbulent fluid motion. The mean wall–normal particle velocity $\overrightarrow{u_{py}}$ throughout the channel is almost zero ($O(10^{-3} * U_B^*)$). Combining this observation with the fact that the particles follow straight lines without being strongly influenced by the turbulent flow, it is clear that the wall–normal fluctuations are proportional to the mean wall–normal velocity before the collision: $\overrightarrow{(u_{py} - u_{py})}^2 = u_{py}^2 \approx (\overrightarrow{u_p} \cdot \overrightarrow{n_R})^2$. The raised wall–normal velocities before the collision $\overrightarrow{u_p} \cdot \overrightarrow{n_R}$ are a direct consequence of the increased mean incident angle $\overrightarrow{\delta^c}$. The mechanism leading from a mean incident
angle $\overline{\delta^-} = 1.74^\circ$ in the smooth wall case to $\overline{\delta^-} = 6.64^\circ$ in the R2 case will be discussed in detail in § 8.3.2.

The spanwise particle fluctuations depicted in Fig. 53(d) represent an evidence that the model leads to an increase of the particle fluctuations in all directions as expected from the collision of the particles with the wall surface covered by wall spheres. The particle shear stress shown in Fig. 53(e) additionally underlines the enhanced momentum exchange between the streamwise and wall–normal direction.

It is especially remarkable how the normalized particle concentration $\langle c_p^* \rangle / c_{pav}^*$ (see eq. (8.1) for the computation) shown in Fig. 53(f) is influenced by the roughness: While a smooth channel wall leads to an accumulation of the particles at the bottom wall, the computed concentration for the roughness R2 delivers an almost uniform profile. Furthermore, there are consistent changes in the concentration profiles if the present wall model is applied to the R0 roughness rather than assuming a smooth wall. This is astonishing since for this case the roughness height $R^*_z$ is two orders of magnitude smaller than the particle diameter $d_p^*$. Good agreement with the experiments is observed except in the near–wall region, where the computed profiles show a strong peak at the bottom wall. This discrepancy in the near–wall region, can probably be explained by the observations of Konan et al. (2009). They pointed out that Gaussian distributed wall inclinations with zero mean lead to a non–zero probability of particles hitting the wall with a small incident angle to remain grazing, i.e., to leave the wall with a very small or zero rebound angle. Konan et al. (2009) argued that even if a particle after its first wall collision still moves towards the wall or leaves the wall with a very small deflection angle, it will hit a second wall asperity. This mechanism deflects the particle towards the inner part of the domain. These multiple collisions at the wall lead to a zero probability of the particles to remain grazing. Unfortunately, the wall roughness model presented in this thesis does not account for this effect.

It is also noteworthy that the inter–particle collision frequency $f_{cp}$ rises with increasing roughness (see Table 8), certainly due to the increased relative particle velocities for which the velocity fluctuations are an indicator. The mean incident angle $\overline{\delta^-}$ (see Table 8) augments with increasing $R^*_z$. Together with the increased wall–normal velocity this indicates a stronger migration of the particles from one wall to the other. Surprisingly, there is no evident trend correlating the radius of the wall sphere $R$ with the percentage of the shadow event (Table 8). In this model the shadow effect only occurs when the wall inclination is greater than the incident angle $\delta^-$ (see Fig. 13). From Table 8 it is visible that the mean incident angle $\overline{\delta^-}$ raises with the wall roughness. Hence, although the standard deviation $\sigma$ of the virtual wall increases, the percentage of the shadow events does not significantly increase with the wall roughness.

### 8.3.2 Evolution of the Particle Statistics with the Number of Wall Collisions

In this section it is discussed how it is possible to get a rather large mean incident angle of $\overline{\delta^-} = 6.64^\circ$ for the R2 case, although the mean inclination of the wall $\overline{\alpha_R} = -0.69^\circ$ in the statistically stationary state is rather small. In order to explain this observation the evolution of the mean incident angle $\overline{\delta^-}$ is studied as a function of the number of wall collisions. Furthermore, the mean emergent angle $\overline{\delta^+}$ and the mean wall inclination $\overline{\alpha_R}$ are recorded. Additionally, the mean particle streamwise velocity $\overline{u_{px}}$ and the absolute value of the particle velocity normal to the original wall before ($|u_{py}|^-$) and after the impact ($|u_{py}|^+$) is evaluated. Note that the statistics visualized in Fig. 54 are achieved
by averaging over all particles which have hit the wall the same number of times $N_{cwi}$.
That means that the first points in Fig. 54 is obtained by averaging over all particles which have hit the wall the first time after being released in the computational domain.
The second point in the curves visualized in Fig. 54 are obtained by averaging over all particles which have hit the wall the second time after being released, etc.. All settings regarding the particles, i.e., diameter, density, mass loading and the normal restitution coefficient $e_{n,p}$ for the particle–particle collisions, and of the wall roughness model, i.e., $e_{n,w}$, $e_{t,w}$, $\mu_{dy,w}$, $\mu_{st,w}$ and the diameter of the wall spheres are borrowed from the R2 case described in § 8.3.1. The particles are distributed homogeneously in the entire channel and the velocity is set according to give the particles an initial trajectory with $\delta^- = 2^\circ$ and a velocity magnitude of unity. The flat trajectory is chosen to approximately match the mean incident angle $\delta^-$ of the smooth wall case (see Table 8). The initial angular velocity is set to zero. In order to save computational time, a frozen flow field of the four–way coupled R2 case is used to account for the mild influence of the continuous phase on the particles, i.e., only the particles are advanced in time keeping the flow field unchanged. This case is taken to illustrate the mechanism responsible for the observation that particles with a rather flat initial trajectory rebounding at rough walls get rather steep incident angles when they reach the statistically stationary state. Note that the same effects as will be shown below for R2 could be observed in the R0 case but less pronounced (not shown for the sake of brevity). To better understand the transitional mechanisms, the first two wall collisions are explained in detail.

![Figure 54](image-url)

**Figure 54:** Evolution with the number of wall collisions: (a) incident angle $\delta^-$, emergent angle $\delta^+$, mean wall inclination $\alpha^*_{R1} = -2 \alpha_R$, (b) mean particle streamwise velocity and mean absolute value of the wall–normal velocity before the collision $|u_{px}|$, $|u_{py}|$ and after the collision $|u_{px}^+|$, $|u_{py}^+|$.

1. **Collision:** As shown in Fig. 54(a) particles hitting the wall for the first time have a mean incident angle of $\delta^- = 2^\circ$. Due to the rather flat trajectories and the shadow effect predicted by the model under these circumstances a mean inclination of the wall of $\alpha_{R1} = -1.62^\circ$ results (Note that in Fig 54(a) $\alpha^*_{R1} = -2 \alpha_R$ is depicted for clarity). The emergent angle raises to approximately $\delta^+ \approx \delta^- - 2 \alpha_{R1} \approx 5^\circ$ after the first wall collision. The particle mean velocity in y-direction $|u_{py}|$ increases by almost the same amount as the streamwise velocity $|u_{px}|$ decreases, i.e., during the wall collision the momentum is distributed from the streamwise direction to the wall–normal direction due to the shadow effect.
2. Collision: The second time the particles hit a wall the mean incident angle is similar to the emergent angle at the first wall collision \( \delta_2 \approx \delta_1 \). Since the incident angle at the second wall collision is greater than at the first wall collision \( \delta_2 > \delta_1 \), the mean inclination angle decreases, i.e., \( \alpha_{R1}^\ast < \alpha_{R2}^\ast \) (see Fig. 14 in § 4.3.3 for comparison). The difference of the mean particle streamwise velocity before and after the collision increases at the second wall collision \( \Delta u_{px2} > \Delta u_{px1} \) with respect to the first collision. The reason is that the increased wall-normal velocity yields larger friction forces for the dominant sliding case. The velocity in y-direction further increases but the difference over the collision \( \Delta u_{py2} = |u_{py2}^\ast| - |u_{py2}| \) is not as pronounced as for the first wall collision because of the smaller mean inclination \( \alpha_{R2}^\ast \).

**Statistically steady state:** The steady state is reached after approximately six wall collisions. The mean incident angle \( \delta^- \) reaches the maximum. Hence, also the velocity normal to the original wall and the velocity difference in streamwise direction \( \Delta u_{pz} \) tend towards their maxima. The wall inclination \( \alpha_R^\ast \) converges to its minimum. Unexpectedly, the difference \( \Delta u_{py} \) is still positive at the steady state (\( |u_{py2}^\ast| > |u_{py2}| \)) in spite of a restitution coefficient \( e_{n,w} = 0.9 \) which according to eq. (4.29) denotes the ratio \( -(u_p \cdot n_R)/(u_p \cdot n_R) \). This is a proof that due to the shadow effect some momentum is transferred from the streamwise direction to the direction normal to the original wall. Note that all values displayed in Fig. 54 are in good agreement with the values obtained by the R2 simulation in § 8.3.1 when the steady state is reached (see Table 8). Summarizing the statistically steady state motion of the particles yields the following steps:

1. The particles reach the wall and lose momentum in streamwise direction due to the frictional collision. The emergent angle \( \delta^- \) raises due to the deceleration in streamwise direction and the negative mean inclination angle of the wall due to the shadow effect. The velocity normal to the original wall remains nearly constant owing to two competing mechanisms: The reduction of the wall-normal velocity by the inelastic collision \( (e_{n,w} < 1) \) and the increase by the turned normal vector due to the shadow effect.

2. After the rebound the particles are accelerated by the mean flow when crossing the channel from one wall to the other. However, since the particle relaxation time is larger than the time between two collisions, the velocity increase is only about \( U_B^\ast/10 \) as obvious in Fig. 54(b).

3. The particle reaches the opposite wall and step (1) is repeated.

### 8.3.3 Influence of the Mass Loading \( \eta \)

In this section the influence of the mass loading and the associated influence of the inter-particle collision frequency on the particle and fluid statistics are analyzed. The R2 roughness is chosen and particle diameter is set to \( d_p^* = 100 \, \mu m \). For this setup three different mass loadings, i.e., \( \eta = 10\%, \, 50\% \) and 100% are compared with the experiments of Kussin and Sommerfeld (2002) and Kussin (2004).

Figure 55 shows the results obtained for the R2 channel configuration. As depicted in Fig. 55(a) the increase of the mass loading leads to slightly flatter mean particle ve-
locity profiles indicating an increased momentum transfer between the particles due to the particle–particle collisions. The enhanced momentum transfer between the particles is additionally confirmed by the homogenization of the normalized particle concentration (see Fig. 55(d)). An overall good agreement with the experiments is found for the mean particle velocity and for the normalized particle concentration. The particle streamwise velocity fluctuations (see Fig. 55(b)) are also in good accordance with the experiments for $\eta = 10\%$ and slightly overpredicted for $\eta = 50\%$. However, the drop of the particle streamwise velocity fluctuations with increasing mass loading is very well captured. Kussin and Sommerfeld (2002) connected the damping of the particle fluctuations with the energy dissipation associated with the inelastic inter–particle collisions. Interestingly, the same effect can be predicted by the present simulation although a normal restitution coefficient for the particle–particle collisions of $e_{n,p} = 0.97$ seems to be too close to unity to justify a massive energy dissipation. As shown in Fig. 55(c) the wall–normal fluctuations increase with increasing mass loading in the bottom part of the channel and remains unchanged in the top part. This quantity is slightly underpredicted by the present model.

![Figure 55: Variation of $\eta$: Statistical results of the plane channel flow for the particles $d_p^* = 100$ µm, $e_{n,w} = 0.9$, $\mu_{dy,w} = 0.4$, roughness R2: (a) mean velocity, (b) streamwise fluctuations, (c) wall–normal fluctuations, (d) normalized particle number concentration.](image-url)
8.3.4 Influence of the Particle Diameter $d_p$

Figure 56 depicts the particle statistics obtained for the R2 channel configuration by varying the particle diameter $d_p$ and therewith the Stokes number between 18.8 and 100.4. The mass loading is set to $\eta = 10\%$ for the particles with a diameter of $d_p = 100 \mu m$ and $195 \mu m$. For the $60 \mu m$ particles a mass loading of $\eta = 12\%$ is considered, since no measurement were available for $\eta = 10\%$.

The influence of inertia is clearly visible considering the mean particle velocity (see Fig. 56(a)): Even though the $60 \mu m$ particles are much stronger influenced by the roughness structures in the near-wall region (the mean wall inclination is $\bar{\alpha}_R = -4.32^\circ$ for the $60 \mu m$ particles compared to a mean wall inclination of $\bar{\alpha}_R = -0.69^\circ$ for the $195 \mu m$ particles) they adjust much quicker to the fluid flow leading to a higher mean velocity compared to the $195 \mu m$ particles (see also Sommerfeld et al., 2008). Good agreement with the experiments of Kussin (2004) is found for all cases. Figure 56(b) shows the particle streamwise velocity fluctuations which also reasonably agree with the experiments of Kussin (2004). By increasing the particle diameter, a visible increase in the fluctuations is seen which underlines that the dynamics of bigger particles is much more wall–collision dominated than for smaller particles. Although the smaller particles are stronger influenced by the wall roughness in the vicinity of the wall (Note the peak of the streamwise velocity fluctuations near the walls for the $60 \mu m$ particles), due to their smaller inertia ($St = 18.8$) they adjust quicker to the continuous phase leading to a decay of the particle streamwise fluctuations towards the channel center, where the streamwise fluid velocity fluctuations (Fig 59(b)) are much lower than the particle fluctuations. On the other hand, the $195 \mu m$ particles feel less the wall roughness, but they keep in memory the wall impact over a longer period than the smaller particles due to their inertia (Note that the streamwise velocity fluctuations of the $195 \mu m$ particles are almost constant throughout the channel).

The wall–normal velocity fluctuations (Fig. 56(c)) computed for the small $60 \mu m$ particles are in close agreement with the experiments, whereas for the larger particles the fluctuations are underpredicted. Similar to the wall–normal velocity fluctuations, no specific trend can be observed for the normalized particle concentration (Fig. 56(d)). For the smallest particles, a local maximum of the concentration is detected in the bottom half of the channel which is hard to explain.

8.3.5 Influence of the Model Parameters $\mu_{dy,w}$ and $e_{n,w}$

In this section we briefly discuss the influence of the model parameters $\mu_{dy,w}$ and $e_{n,w}$ keeping $\mu_{st,w} = 0.5$, $e_{t,w} = 0.3$ and the roughness height $R_0$ unchanged. As shown in Table 8 sliding collisions were the predominant events for the particles $d_p = 195 \mu m$ and the aforementioned parameters are the determining model constants describing the velocity change during a sliding collision (see eq. (4.45a)).

Figure 57 shows the statistical results obtained by varying the dynamic friction coefficient $\mu_{dy,w}$ between the values $\mu_{dy,w} = 0.2$, 0.4 and 0.5. As expected there are only substantial changes in the mean particle velocity (Fig. 57(a)) and in the streamwise particle velocity fluctuations (Fig. 57(b)) since the dynamic friction coefficient $\mu_{dy,w}$ solely influences the particle motion parallel to the wall (eq.(4.45a)). Since the momentum loss at the wall increases with $\mu_{dy,w}$, the mean particle velocity decreases. The streamwise velocity fluctuations increase with raising $\mu_{dy,w}$. This additionally underlines one of the
mechanism illustrated in § 8.3.1 responsible for the increased streamwise fluctuations at rough walls: A particle coming from the bulk flow is decelerated at the wall. After the rebound a certain velocity difference exists compared to the mean velocity leading to increased fluctuations throughout the channel. Therefore, an increased dynamic friction coefficient $\mu_{d_{y,w}}$ yields an increased momentum loss in streamwise direction and hence increased velocity fluctuations in the same direction. Contrarily, the velocity fluctuations in wall–normal direction (Fig. 57(c)) and the normalized particle concentration (Fig. 57(d)) are nearly unchanged.

Figure 58 shows the statistical results obtained by varying the normal restitution coefficient $\epsilon_{n,w}$ between the values $\epsilon_{n,w} = 0.8$, 0.9 and 1.0. As visible modifying this parameter leads to changes in all statistics presented. This becomes evident by considering eq. (4.45a) where the normal restitution coefficient influences the post–collision velocity component in wall–normal as well as in parallel direction. The mean velocity shown in Fig. 58(a) decreases with increasing normal restitution coefficient $\epsilon_{n,w}$ due to the enhanced frictional momentum loss in streamwise direction during the sliding wall impact. The enhanced momentum loss at the wall is also responsible for the increased streamwise velocity fluctuations (see Fig. 58(b)) based on the same mechanism already explained above. Increasing $\epsilon_{n,w}$ leads to an enhanced resuspension of the particles underlined by
the increased wall–normal fluctuations (see Fig. 58(c)) and the homogenization of the particle concentration (see Fig. 58(d)). The resuspension is especially pronounced for a restitution coefficient of $e_{n,w} = 1$. In this case the magnitude of the wall–normal velocity is kept unchanged during the collision. Additionally, this case manifests the biggest momentum loss parallel to the wall (see eq. (4.45a)). Both conditions together lead to an increased emergent angle $\delta^+$ and hence to an increased resuspension.

### 8.3.6 Influence on the Continuous Flow

Figure 59 shows the fluid statistics compared with the experiments of Kussin and Sommerfeld (2002) and the data of Hoyas and Jiménez (2008) who carried out DNS computations for a Reynolds number based on the friction velocity $u_\tau$ of $Re_\tau = 934$. Only the R2 case with the 100 $\mu$m particles is considered since no substantial deviation to the flow statistics of the R1 case could be found. This indicates the minor importance of the particle dynamics influenced by the roughness on the fluid flow for particles with the present diameter. From Fig. 59(a) it is obvious that the mean fluid velocity profiles remain almost unchanged by the presence of the particles with the exception of the channel center and the region near the bottom wall for $\eta = 50\%$. At the channel center the flow is slightly
decelerated where the velocity difference between the fluid and the particles leads to a net force pointing against the direction of the continuous flow and hence denoting a deceleration of the fluid. Contrarily, near the bottom wall, where the particles are faster than the carrier phase, the force exerted by the particles points in streamwise direction and hence leads to an acceleration of the fluid.

Figure 59(b) shows the fluid velocity fluctuations in streamwise direction which are attenuated by the particles throughout the channel. All predicted velocity fluctuations are lower than the experimental data. This is not surprising since the unladen velocity fluctuations are already too low which is inherent to LES computations because only the resolved scales are used to compute the velocity fluctuations and the SGS contribution is not taken into account. This becomes evident when comparing the unladen LES with the DNS of Hoyas and Jiménez (2008) in Fig. 59(b): The DNS of Hoyas and Jiménez (2008) who computed the velocity fluctuations using the full turbulent spectrum is in good agreement with the unladen measurements of Kussin and Sommerfeld (2002). The computed streamwise velocity fluctuations by the present LES, which only partly resolves the turbulent spectrum, are therefore lower than the reference data. The trends observed for different mass loadings $\eta$, however, are in good agreement with the experiments with the exception of the channel center, where the prediction of the turbulence attenuation

Figure 58: Variation of $e_{n,w}$: Statistical results of the plane channel flow for the particles $d_{p}^* = 195 \, \mu m$, $\eta = 30\%$, $\mu_{dy,w} = 0.4$, roughness R0: (a) mean velocity, (b) streamwise fluctuations, (c) wall-normal fluctuations, (d) normalized particle number concentration.
is too high. The deviations found between the experiment and the simulation should not influence the particle statistics owing to two reasons: (i) The considered particles have a relatively high Stokes number and are hence marginally influenced by the turbulent flow and (ii) the particle dynamics are prevalently dominated by the wall and inter–particle collisions.

Figure 59(c) shows the fluid velocity fluctuations in wall–normal direction. For the unladen flow this quantity is higher in the near–wall region and lower in the channel center compared with the experimental data. For the particle–laden flow the attenuation is somewhat higher than reported by Kussin and Sommerfeld (2002) for the case with a mass loading of $\eta = 10\%$ (Note that no measurements where available for a mass loading of $\eta = 50\%$ and thus no considerations are made). The same observation has been made by Lain et al. (2002) in their RANS simulations for particles with the same diameter and the same roughness. Lain et al. (2002) attributed the discrepancies between their simulations and the experiments to problems in accurately measuring the wall–normal velocity component of the continuous phase. Comparing the measured wall–normal fluctuations of Kussin and Sommerfeld (2002) with the DNS of Hoyas and Jiménez (2008) (Fig. 59(c)) additionally underlines the assumption of a problem in the measurements: While the measured streamwise velocity fluctuations are in good agreement with the DNS of Hoyas and Jiménez (2008), the measured wall–normal velocity fluctuations for the unladen case
are lower than the DNS. This is a contradiction since the velocity fluctuations obtained by the experiment or the DNS should be similar in shape and magnitude since both consider the full turbulent spectrum. On the other hand, the LES statistics of the unladen case are observed to be only slightly lower than the DNS data as expected for the resolved part of the spectrum.

8.3.7 Comparison with the Literature

As the final point in this part of the thesis dedicated to the turbulent flow in a horizontal channel, the results obtained with the roughness model described above are compared with the LES of Mallouppas and van Wachem (2013) and the RANS prediction of Lain and Sommerfeld (2008). Both studies compared their simulations with the experimental data of Kussin (2004) for the 195 µm particles at a mass loading \( \eta = 100\% \) hitting the R2 roughness.

Lain and Sommerfeld (2008) treated the continuous phase in the RANS framework using a Reynolds stress model. The flow was assumed as two-dimensional. The influence of the wall roughness is accounted for by the model of Sommerfeld and Huber (1999) which Sommerfeld and Huber (1999) assumed a Gaussian distributed wall inclination with a standard deviation of \( \sigma = 5.1^\circ \). That means that the wall is assumed to have an irregular shape where the inclination of the wall obeys a Gaussian distribution. Furthermore, in the wall roughness model applied by Lain and Sommerfeld (2008) the normal restitution coefficient \( e_{n,w} \) and the dynamic coefficient of friction \( \mu_{dy,w} \) are taken as empirically determined functions of the incident angle of the particles.

Mallouppas and van Wachem (2013) evaluated the influence of the wall roughness on the motion of the particles treated as hard and as soft spheres. For the hard–sphere model they used the wall roughness model developed by Sommerfeld (1992). In the roughness model of Sommerfeld (1992) the wall is assumed to have a sinusoidal shape (in contrast to the model of Sommerfeld and Huber, 1999, which assumed an irregular shape of the wall):

\[
y^* = A^*_r \sin \left( \frac{2\pi}{L^*_r} x^* + \omega \right) .
\]  

\( y^* \) denotes the height of the wall roughness, \( x^* \) the coordinate along the wall, \( A^*_r \) the amplitude and \( L^*_r \) the periodic length of the wall roughness, respectively. \( A^*_r \) and \( L^*_r \) are determined empirically and are set equal to the following relations: \( A^*_r/d^*_p = 1/40 \) and \( L^*_r/d^*_p = 10 \). \( \omega \) stands for an uniformly distributed random number in the range \([0 - 2\pi]\). The shadow effect is considered by recomputing the random number \( \omega \), if the particle hits a wall region which is negatively inclined with respect to the incoming trajectory. Unfortunately, Mallouppas and van Wachem (2013) do not mention explicitly the constants determining the state after the wall collision of the hard–sphere model. Sommerfeld (1992), however, used the following values: \( \mu_{dy,w} = 0.3 \), \( \mu_{st,w} = 0.4 \), \( e_{t,w} = 0 \). For the normal restitution coefficient \( e_{n,w} \) he used an empirically determined functions of the incident angle of the particles. For the soft–sphere model Mallouppas and van Wachem (2013) employed the wall roughness model proposed by Konan et al. (2009). The latter refined the model proposed by Sommerfeld and Huber (1999) by taking into account the influence of a grazing wall collision: Konan et al. (2009) recomputed the randomly inclined wall–normal vector for incident angles which lead to a non–zero probability of the particles to remain grazing, i.e., leave the wall with a very small emergent angle. Note that all
statistics of Mallouppas and van Wachem (2013) shown here are computed by applying the SGS model of Smagorinsky (1963) and the wall damping of Van Driest (1956). The reason is that Mallouppas and van Wachem (2013) questioned the correctness of the dynamic model of Germano et al. (1991) for a four-way coupled flow. Unfortunately, Mallouppas and van Wachem (2013) did not specify the value of the Smagorinsky constant they used. Similar to the present LES Mallouppas and van Wachem (2013) applied an additional source term in the LES equations in order to keep the mass flow rate constant (forcing term).

Figure 60(a) compares the mean particles velocity obtained by the model presented in this thesis with the results obtained by Mallouppas and van Wachem (2013) adopting a hard-sphere (MvW-hard–sphere) and a soft-sphere (MvW-soft–sphere) model for the particles. The data of Lain and Sommerfeld (2008) are marked by (LS–RANS). It is evident that the results of all models are in good agreement with the experiments of Kussin (2004). That means that the momentum loss of the particles hitting rough walls is reliably reproduced by the different wall models compared.

![Figure 60](image)

**Figure 60:** Comparison of the present particle statistics with the LES of Mallouppas and van Wachem (2013) where the particles are treated as hard spheres (MvW-hard–sphere) and soft spheres (MvW-soft–sphere) and the RANS of Lain and Sommerfeld (2008) (LS–RANS) for \( \eta = 100\% \), \( d_p^* = 195 \, \mu m \) and the roughness R2: (a) mean velocity, (b) streamwise fluctuations, (c) wall-normal fluctuations (d) normalized particle number concentration.

Figure 60(b) shows the particle velocity fluctuations in streamwise direction. For this statistical quantity the model presented here and the simulations performed by Lain and
Sommerfeld (2008) exhibit a very good agreement with the reference experiment. The results of the predictions by Mallouppas and van Wachem (2013) for \( \langle u_{\text{px}}' \rangle_{\text{rms}}/U_B^* \) are, however, lower than the experimental data of Kussin (2004) for both, the hard– and the soft–sphere model. The fluctuations predicted by the soft–sphere model are higher than the one predicted by the hard–sphere model. Unfortunately, Mallouppas and van Wachem (2013) adopted for the hard–sphere and the soft–sphere model two different wall roughness treatments. Therefore, it is difficult to trace back the differences found in Fig. 60(b) to either the collision or the wall modeling.

Figure 60(c) displays the particle wall–normal velocity fluctuations. It is obvious that the simulation of Lain and Sommerfeld (2008) shows very close agreement with the experiments of Kussin (2004). The fluctuations predicted by the simulations of Mallouppas and van Wachem (2013) and the present simulations are lower than the reference case. A possible explanation for these discrepancies is that Lain and Sommerfeld (2008) treated the flow as two–dimensional, whereas the other cases visualized in Fig. 60(c) consider the flow as three–dimensional. The three–dimensional geometry allows particles approaching the wall to be redirected also in spanwise direction after the impact, whereas for a two–dimensional geometry this is not possible. The guess that there is a substantial difference when the roughness is treated as two– or three–dimensional is further supported by comparing the results of Lain and Sommerfeld (2008) with the soft–sphere results of Mallouppas and van Wachem (2013) (see Fig. 60(b)–60(d)). As already mentioned, for the case where the particles are treated as soft spheres, Mallouppas and van Wachem (2013) employed a similar version of the wall roughness model by Sommerfeld and Huber (1999). Note that Lain and Sommerfeld (2008) adopted the original form of the model by Sommerfeld and Huber (1999). Since Lain and Sommerfeld (2008) and Mallouppas and van Wachem (2013) adopted similar wall roughness models, they should obtain similar particle statistics. This is, however, not the case. Therefore, a possible explanation for the differences between the two studies is that the model of Sommerfeld and Huber (1999) (and also the enhanced version of Konan et al., 2009) gives different results for two– and three–dimensional flows. Unfortunately, the reason why the 2–D simulations achieve better results than the 3–D simulation is still not clear. Probably, performing two different simulations in a 3–D channel where for one calculation the particles are allowed to change their trajectory in spanwise direction and for the other not, could shed some light on this issue.

Figure 60(d) depicts the normalized particle concentration. Also for this quantity the computations performed by Lain and Sommerfeld (2008) achieve the best accordance with the experiments. The other three simulations show a very similar concentration profile: The predicted particle concentration at the bottom wall is slightly higher than the experimental data of Kussin (2004), whereas at the top part it shows the opposite trend with respect to the reference. Note that the present computation shows a strong increase of the concentration near the bottom wall. The LES of Mallouppas and van Wachem (2013) does not show this peak at the wall. This can possibly be explained by disregarding the grazing collisions in the present simulations.

Figure 61 compares the unladen fluid statistics with the statistics achieved by the four–way coupling. Here only the LES of Mallouppas and van Wachem (2013) (denoted as MvW–unladen for the unladen and MvW–two–phase for the laden flow) and the present LES are shown. The results of Lain and Sommerfeld (2008) are not depicted in order to keep the figures clear. However, a similar dependency of the flow from the coupling
assumptions can be observed in both, the RANS of Lain and Sommerfeld (2008) and the LES results shown in Fig. 61. Therefore, no excessive information loss results in omitting the RANS of Lain and Sommerfeld (2008). Note that in the LES of Mallouppas and van Wachem (2013) only marginal differences between the four–way coupled fluid statistics computed by either the hard–sphere or the soft–sphere simulations can be asserted. Therefore, only the fluid quantities computed by Mallouppas and van Wachem (2013) for the case where the particles are treated as hard spheres are shown.

![Graph](image)

**Figure 61:** Comparison of the fluid statistics with the LES of Mallouppas and van Wachem (2013) for $\eta = 100\%$, $d_p^* = 195 \mu m$ and R2: (a) mean velocity, (b) streamwise fluctuations, (c) wall–normal fluctuations.

Figure 61(a) shows the mean fluid velocity. It is evident that both LES computations are in good agreement with the experiments of Kussin (2004). A slightly higher center–line velocity for the unladen flow computed by Mallouppas and van Wachem (2013) compared with the present LES can be observed. In the LES of Mallouppas and van Wachem (2013), however, the influence of the particles on the mean fluid flow is more pronounced than in the present LES. This conclusion can be drawn from the observation that the mean fluid velocity in the center region is stronger reduced by the influence of the particles in the LES of Mallouppas and van Wachem (2013) than in the present simulations.

From Fig. 61(b) it is clear that very close agreement between both LES computations shown (unladen and laden case) can be observed for the fluid streamwise velocity fluctuations. Compared with the experiment, however, this quantity is underpredicted.
Remarkable is that both LES show the same level of turbulent attenuation. Note that the magnitude of the attenuation of the turbulent fluctuations is similar to the experiment (see also Fig. 61(c)). This indicates that the particle–source–in–cell method accurately captures the influence of the disperse phase on the continuous phase for the particle diameter considered here.

Figure 61(c) shows the fluid velocity fluctuations in wall–normal direction. It is evident that for both LES this statistical moment is reduced by a similar magnitude compared with the reference experiment if the four–way coupling is considered. The wall–normal velocity fluctuations computed by Mallouppas and van Wachem (2013) are slightly reduced compared with the present simulation. These discrepancies are difficult to explain. A cautious guess is that the Smagorinsky constant, which unfortunately is not explicitly specified in Mallouppas and van Wachem (2013), differs from the Smagorinsky constant $C_s = 0.065$ adopted by the present LES.

### 8.3.8 Summary of the Wall Roughness Model

Wall roughness considerably alters the rebound behavior of particles. Thus for Euler–Lagrange predictions of particle–laden wall–bounded flows the wall collision model has to mimic the roughness effect. Since in practice typically only minimal information is available to characterize the rough surface (e.g., mean roughness), a sandgrain roughness model is developed for the particular phase following the basic idea of Nikuradse (1933) and Schlichting (1936) for the fluid flow. The wall is covered by a densely packed layer of mono–disperse spheres modeling sandgrain. The radius of the spheres is related to a given roughness parameter ($R_q^*$ or $R_z^*$) requiring only one additional parameter ($C_{\text{surface}} \approx 3$ to 5) depending on the surface finishing also borrowed from the continuous phase (Schlichting, 1936; Hama, 1954; Zagarola and Smits, 1998; Shockling et al., 2006). Purely based on geometric and kinematic considerations an easy to use model is derived and evaluated in detail based on a–priori and a–posteriori investigations in the context of LES predictions of turbulent plane channel flow. The model is found to possess the following features:

- The range of possible wall inclination angles $\alpha_R$ strongly depends on the ratio $r_p/R$ with the correct limits for $r_p/R \to \infty$ and $r_p/R \leq 1$. For cases without the shadow effect the resulting inclination angles $\alpha_R$ are Gaussian distributed with the standard deviation $\sigma$ determined by the geometry, i.e., $r_p/R$.

- The model accounts for the shadow effect. Depending on the impact angle $\delta^-$ the resulting PDFs of the wall inclination angle $\alpha_R$ are truncated for $\alpha_R > \delta^-$ and is therefore asymmetric around $\alpha_R = 0$. Consequently, the mean normal vector is turned towards the incoming particle trajectories. Although the mean inclination is found to be minor, it is demonstrated that after a few wall collisions with increased emergent angles it has a dramatic effect on the entire statistics of the particles.

- In accordance with measurements the momentum loss in streamwise direction is strongly augmented with increasing wall roughness. That leads to particles which considerably lag behind the continuous flow. Two main reasons are identified. Due to the shadow effect a redistribution of streamwise momentum carried by the particles towards the wall–normal direction takes place which furthermore boosts the total wall collision frequency and the wall–normal particle fluctuations. Additionally,
the impact of the particles at the wall is stronger leading to increased momentum loss due to the predominant sliding motion.

- In close agreement with experiments and other simulations the present wall model yields a homogenization of the particle concentration with increasing wall roughness.

- A variation of the dynamic friction coefficient \( \mu_{dy,w} \) solely influences the velocity statistics in streamwise direction, whereas the normal restitution coefficient \( e_{n,w} \) has an impact on all statistics.

- Inter-particle collisions at higher mass loadings lead to slightly flatter mean velocity profiles, lower streamwise fluctuations, increased wall-normal fluctuations, and a homogenized particle concentration profile.

- In agreement with measurements the conveying velocity of the particles is reduced when particles with increasing diameter \( d_p \) rebound at surfaces having the same roughness height \( R_z^* \).

- The model is generally applicable in 3-D arbitrary curvilinear domains and in the context of DNS, LES, RANS and all hybrid variants.

- Comparisons of the present computations with the LES simulations of Mallouppas and van Wachem (2013) and the 2-D RANS of Lain and Sommerfeld (2008) showed that similar results are obtained. Regarding the particle statistics the 2-D RANS of Lain and Sommerfeld (2008) show slightly better agreement with the reference experiments than the LES computations (higher particle velocity fluctuations in wall-normal direction and a more uniform concentration profile). The level of attenuation of the turbulence fluctuations is comparable for the three studies compared.

8.4 Downward Pipe Flow at Re = 2253

In the following the results of the methodology presented in this thesis is applied to a turbulent pipe flow and the outcome is discussed in detail. Note that parts of the results shown in the following can be also found in the articles Breuer and Alletto (2012c) and Breuer and Alletto (2013). The objective of this section is twofold: (i) Since the curved pipe walls represent a slightly more complicated geometry than the flat channel wall, this test case represents the logical subsequent evaluation step of the wall roughness model for the particles. (ii) The poly-disperse particle size distribution considered in this test case allows to study the influence of the momentum exchange between different size classes induced by the particle-particle collisions. The discussion of the results is sub-divided into three section. The reason is that it is tried to distinguish in the discussion of the results (when ever possible) the influence of the wall roughness (§ 8.4.1) and the inter-particle collisions (§ 8.4.2) on the particle statistics. The influence of the particles on the continuous phase is analyzed in a separate section (§ 8.4.3).

8.4.1 Influence of the Wall Roughness on a Poly-disperse Pipe Flow

Figure 62 shows the the mean particle velocity (Figs. 62(a)–(b)) and the particle concentration (Figs. 62(c)–(d)) applying the roughness model described in § 4.3.2.2 for the
two mass loading. The predicted results are compared with the experiments of Borée and Caraman (2005). In the subsequent figures the color black is used to mark the $d_p^* = 60 \mu m$ particles and the color red is used for $d_p^* = 90 \mu m$ particles. The line type (dotted for $k_s^* = 0 \mu m$ and solid for $k_s^* = 15 \mu m$) is used to symbolize the height of the wall asperities. The experimental results of Borée and Caraman (2005) are visualized by points. Note that for Figs. 62(a)–(d) only one legend is displayed since the presentation of the data does not change throughout the figures. The same holds for Figs. 63(a)–(d) and Fig. 64(a)–(b).

Figures 62(a) and (b) show the mean streamwise particle velocity ($d_p^* = 60$ and 90 $\mu m$) for the low and the high mass loading, respectively. Note that all displayed velocities are normalized by the centerline velocity of the unladen flow $U^*_c$. From Figs. 62(a) and (b) it is evident that adopting the wall roughness model leads to a reduction of the mean particle velocity in the pipe center and a slight increase in the near-wall region. The reduction of the mean particle velocity with increasing wall roughness is in line with the observations made for the horizontal channel (see Fig. 53(a)). The reason for the decrease of the mean velocity of the disperse phase is two-fold. First, due to the shadow effect the streamwise momentum is redistributed towards the wall-normal direction. An additional analysis yields that 31% and 23% of the events at the wall are shadow events for the low and the high mass loading, respectively. Since for the low mass loading the wall–normal velocity fluctuations (Fig. 63(c)) are lower than for the high mass loading (Fig. 63(d)), the mean incident angle $\delta^\eta$ is smaller for $\eta = 11\%$ than for $\eta = 110\%$. Therefore, the dependency of the shadow events from the mass loading mentioned above, is consistent with the a–priori analysis of the model made in § 4.3.3 (see Fig. 14) where it is shown that for small incident angles more shadow events occur than for large incident angles. Note that for the $k_s^* = 0 \mu m$ case no shadow event occurs. The second reason is identified in the increased root–mean squared wall–normal velocity fluctuations $\langle u_{pr}^* \rangle_{rms}$ of the particles with increasing wall roughness (see Fig. 63(c)–(d)). For a zero mean wall–normal velocity as found in fully developed vertical pipe flows, the mean wall–normal velocity $u_p \cdot n_R$ before the wall collision is proportional to $\langle u_{pr}^* \rangle_{rms}$. Since the majority of the particle–wall collisions are sliding collisions (about 95% for $k_s^* = 15 \mu m$ and 99% for $k_s^* = 0 \mu m$), the momentum loss at the wall is proportional to the mean wall–normal particle velocity before the wall collision $u_p \cdot n_R$ (see also eq. (4.45a)). Hence, since the wall–normal velocity fluctuations for the case $k_s^* = 15 \mu m$ are higher than for the case $k_s^* = 0 \mu m$, also the momentum loss of the particles during a wall collision is higher for the former.

The next conclusion which can be drawn from Fig. 62(a) and 62(b) is that the 90 $\mu m$ particles are stronger influenced by the wall roughness than the 60 $\mu m$ particles. Also this observation is in line with the horizontal channel flow simulations (see Fig. 56(a)). This phenomenon can be traced back to the effect of inertia on the particles: Even though the 60 $\mu m$ particles are stronger influenced by the wall roughness than the 90 $\mu m$ particles (the standard deviation $\sigma$ defined in eq. (4.50) of the random wall–normal vector $n_R$ is higher for the smaller particles), they adjust quicker to the fluid flow (see also Sommerfeld, 2000). Therefore, the bigger particles keep in memory the wall collision for a longer time than the small particles. This leads to a stronger reduction of the mean particle velocity of the 90 $\mu m$ particles compared with the 60 $\mu m$ particles.

Remarkably is the effect of the wall roughness on the particle concentration. From Figs. 62(c)–(d) it is evident that the particle concentration is significantly increased in the pipe center and reduced in the vicinity of the wall. The concentration of both displayed particle
classes is normalized by the average concentration \( c_{pav} = m_{p,tot}/V_{tot} \) of the disperse phase. \( V_{tot} \) and \( m_{p,tot} \) are the total volume of the computational domain and the total particle mass present in the computational domain. The accumulation of the particles in the pipe center can be explained in the following manner: Due to the shadow effect the model leads to a redistribution of the streamwise momentum towards the wall–normal direction. For the pipe flow the wall–normal vector points towards the pipe center (concave mirror effect) and hence the component of the particle trajectory in this direction is increased after rebouncing at a rough wall. This effect leads to a stronger accumulation of the particles in the pipe center region. Note that Lain and Sommerfeld (2012) denominate the described phenomenon as the focusing effect.

Figure 63 compares the particle streamwise and wall–normal velocity fluctuations with the experiments of Borée and Caraman (2005). It is obvious that the application of the wall roughness model leads to an improvement of the second–order statistics of the particles (Figs. 63(a)–(d)). For increasing wall roughness the streamwise particle velocity fluctuations computed for the low mass loading \( \eta = 11\% \) (Fig. 63(a)) are increased in the pipe center and in the near–wall region and remain nearly unchanged elsewhere. Remarkably is that both, simulation and experiment, show a local maximum of the steamwise
velocity fluctuations in the pipe center for the 90 µm particles.

Figure 63: Variation of the wall roughness: Statistical results of the poly-disperse pipe flow; (a)–(b) particle streamwise velocity fluctuations; (c)–(d) particle wall–normal velocity fluctuations. Experiments performed by Borée and Caraman (2005).

Figures 63(c)–(d) show the particle wall–normal velocity fluctuations for the low and the high mass loading, respectively. Remarkable is the strong enhancement of the wall–normal particle velocity fluctuations for both mass loadings and particle classes evaluated. This indicates that by means of the wall roughness the particles achieve a steeper trajectory due to their deflection towards the pipe center. Comparing the wall–normal velocity fluctuations of the low mass loading (Fig. 63(a)) with the corresponding fluctuations for the high mass loading (Fig. 63(b)), it is obvious that for the smooth wall only a small difference is noticeable between the different mass loadings. On the other hand, if the wall roughness model is adopted, a distinctive increase of the wall–normal particle velocity fluctuations with increasing mass loading can be observed. Unfortunately, for η = 110% there still remain major differences in shape and magnitude of this component of the particle fluctuations with respect to the experiments. However, for the assessment of these results it has to be kept in mind that the roughness of the pipe wall is solely estimated since it is not provided by the experimenters.

Finally, Fig. 64 shows the particle shear stress for both mass loadings analyzed in comparison with the measurements of Borée and Caraman (2005). It is evident that applying
the wall roughness model yields an increase of this statistical moment. An analogous
dependency of this quantity from the asperity height is found in the horizontal channel
flow (see Fig. 53(e)). This indicates that particles hitting rough asperities provide better
mixing properties than particles hitting smooth walls. In contrast to the other statistical
quantities shown, the particle shear stress does not show a pronounced dependency on
the mass loading. However, no contradiction arises from this observation. This can be
deduced by comparing the particle fluctuations in streamwise (Figs. 63(a)–(b)) and in
wall–normal direction (Figs. 63(c)–(d)). For the low mass loading the particle stream-
wise velocity fluctuations are higher than for the high mass loading. On the other hand,
the particle velocity fluctuations in wall–normal direction are higher for the
$\eta = 110\%$ case than for the $\eta = 11\%$ case. Therefore, the inverse behavior of $\langle u_{pz}^\prime \rangle_{rms}/U_C^*$ and
$\langle u_{pr}^\prime \rangle_{rms}/U_C^*$ with increasing $\eta$ balance each other. This causes an almost constant shear
stress for both mass loadings.

![Graph](image)

**Figure 64:** Variation of the wall roughness: particle shear stress of the poly–disperse pipe flow.
Experiments performed by Borée and Caraman (2005).

### 8.4.2 Influence of the the Inter–particle Collisions on a Poly–disperse Pipe Flow

An evidence of the role of the inter–particle collisions is provided by comparing the mean
particle velocity for the low (Fig. 62(a)) and the high mass–loading (Fig. 62(b)). It is
obvious the reduction of the mean velocity of the disperse phase at constant wall roughness
is more pronounced for the high mass loading than for the low mass loading. Note
that a similar observation can be made for the horizontal channel (see Fig. 55(a)). This
clearly indicates the role of the particle–particle collisions in redistributing the momentum
throughout the pipe cross–section. For the low mass loading where the inter–particle
collisions play a minor role, the particles which loose their momentum at the wall do not
reach the pipe center (see the high concentration peaks at the wall for $\eta = 11\%$ in Fig.
62(c)). For the high mass loading, however, the particles hitting the wall are efficiently
redistributed towards the pipe center (see the reduced concentration peaks at the wall for
$\eta = 110\%$ in Fig. 62(d)). Therefore, low–momentum particles can reach also the pipe
center. This leads to a reduction of the mean particle velocity in this region.

The influence of the particle–particles collisions reflects also on the computation of
second–order moments of the particles (see Fig. 63). For the low mass loading the stream-
wise velocity fluctuations of the 90 µm particles are higher in the pipe center than the velocity fluctuations of the 60 µm particles (see Fig. 63(a)). The same holds also for the wall–normal velocity fluctuations (see Fig. 63(c)) but only for the rough wall. Especially for the \( k_s^* = 15 \) µm case, the differences of \( \langle u_{pz}' \rangle \text{rms} / U_C^* \) between the classes observed for the low mass mass loading \( \eta = 11\% \) vanish for the high mass loading case (compare Fig. 63(a) with (b)). The same observation but much less pronounced holds also for the wall–normal fluctuations in the case where the particles hit a rough wall (compare Fig. 63(c) with (d)). Borée and Caraman (2005) attributed this observation to the increased inter–class collisions and hence to an increased momentum exchange between the size classes.

8.4.3 Influence on the Continuous Phase

Figure 65 compares the present fluid statistics with the fluid flow DNS data of Vreman (2007). Unfortunately, Borée and Caraman (2005) did not measured the two–phase fluid statistics. Therefore, for the low mass loading (Fig. 65(c) and (c)) only the unladen fluid statistics of Borée and Caraman (2005) are included for comparison. For the low mass loading Vreman (2007) presented only simulations with mono–disperse 60 µm particles and therefore the particle size distribution of the DNS differs substantially from the poly–disperse distribution considered here (see Table 3). Thus, only the unladen flow results are taken for comparison. For the high mass loading \( \eta = 110\% \), Vreman (2007) carried out simulations with 90 µm mono–disperse particles. The influence on the carrier phase are not expected to differ substantially from the poly–disperse scenario, since 87% of the particle mass belongs to the 90 µm size class (Borée and Caraman, 2005). Therefore, the data can be compared with the present simulations.

For the high mass loading the increased particle concentration at the pipe center (Fig. 62(d)) induced by the wall roughness obviously influences also the mean streamwise fluid velocity (Fig. 62(b)) as a consequence of the four–way coupling. The observation of the local minimum of the streamwise fluid velocity at the pipe center in case of a rough wall seen by the particles (green line in Fig. 62(b)) can be explained as follows: Particles hitting the wall loose momentum during the wall collision. The shadow effect leads to a redistribution of the streamwise momentum towards the wall–normal direction and hence to a further reduction of the streamwise particle velocity. The shadow effect also causes these decelerated particles to be deflected towards the pipe center and hence to an accumulation in this region. Note that for \( \eta = 110\% \) the concentration of the 90 µm particles, which are responsible for 87% of the mass (Borée and Caraman, 2005), has a clear maximum at the pipe center. This accumulation of particles with velocities lower than the fluid velocity in the pipe center results in a maximum of the force exerted by the particles against the streamwise flow direction. This leads to a deceleration of the continuous phase in this region. Note that the DNS of Vreman (2007) shows the same minimum of the mean fluid velocity at the pipe center. Unfortunately, Borée and Caraman (2005) did not provide data for the continuous phase in order to confirm this observation.

The fluid streamwise velocity fluctuations (Figs. 63(c) and (d)) evidence the drastic effect of the particles on the continuous phase with increasing mass loading: For \( \eta = 11\% \) the fluid velocity fluctuations are still in close agreement with the unladen DNS data of Vreman (2007). For \( \eta = 110\% \) on the other hand the streamwise fluid velocity fluctuations almost completely vanish due to the influence of the particles. Note that the same observation was made by Vreman (2007). Unfortunately, the reasons for the drastic
reduction of the turbulent fluid motion are still unknown. Recently, however, two–way coupled (Bijlard et al., 2010) and four–way coupled (Dritselis and Vlachos, 2008, 2011a) turbulent channel flow DNS predictions indicate that the particles inhibit the quasi–streamwise vortices responsible for the momentum transfer between the viscous sublayer and the buffer layer. This leads to a reduction of the turbulence production. No detailed research study is available which investigated the effect of the particles on the coherent structures of a turbulent pipe flow, but similar mechanisms have to be expected. An analysis of the unsteady flow shows that for the high mass loading the streaks typically present in the buffer layer of an unladen pipe flow completely disappear. Contrarily, for the low mass loading no substantial difference to the unladen flow can be found. This observation indicates that the momentum transfer between the viscous sublayer and the buffer layer caused by the quasi–streamwise vortices is strongly inhibited by the particles for \( \eta = 110\% \).
8.4.4 Summary of the Results

Summing up, reasonable agreement between the four-way coupled LES applying the recently developed wall roughness model and the experiments of Borée and Caraman (2005) is found. The accordance is acceptable concerning all statistical moments presented by the experimental study. This is true for both classes of the poly-disperse distribution analyzed.

In view of the results obtained in this section, the following dependency of the particles statistics from the wall roughness and the mass loading can be observed:

- The wall roughness leads to a reduction of the mean particle velocity with increasing roughness height. As expected, this effect is more pronounced for the high mass loading than for the low mass loading.

- An enhancement of the particle wall-normal fluctuations can be found indicating steeper particle trajectories and an additional momentum transfer between the streamwise and the wall-normal direction.

- Both effects described above are more pronounced for larger particles than for smaller particles since large particles keep memory of the wall impact for a longer period of time than small particles.

- If applied in a pipe flow the new wall roughness model causes an accumulation of the particles in the pipe center. In case of the four-way coupled prediction this leads to an increase of the forces exerted by the particles on the continuous flow and hence to a reduction of the mean fluid flow in this region.

- An improvement of the particle statistics for both mass loadings analyzed can be achieved by applying the sandgrain roughness model presented in this thesis.

8.5 Downward Pipe Flow at Re = 2253 to Test the Agglomeration Model

In the following two sections the agglomeration model derived in § 5.4.2 is briefly analyzed. The focus is set on the agglomeration model valid for the general case of a collision with friction. The model valid for the special case of a frictionless collision is only briefly discussed in § 8.5.2 since it was already evaluated in Jürgens (2012). First, in § 8.5.1 the influence of the particle diameter $d_p^*$ and the normal restitution coefficient $e_{n,p}$ on the agglomeration rate is discussed. Second, in § 8.5.2 the influence of the van–der–Waals force on the treatment of the particles which do not agglomerate and the influence of the model used for the agglomerate (as a porous sphere or as a volume-equivalent sphere) is analyzed.

8.5.1 Influence of the Particle Diameter $d_p^*$ and the Normal Restitution Coefficient $e_{n,p}$

Table 9 displays the dependency of the agglomeration rate $\beta$ as a function of the particle diameter $d_p^*$ and the normal restitution coefficient $e_{n,p}$. The agglomeration rate $\beta$ is calculated as the ratio of the number of collisions $N_{agg}$ which satisfy criterion (5.115) to the total number of collisions found at all $N_{col}$, i.e., $\beta = N_{agg}/N_{col}$. Furthermore, the
number of collisions and the number of collisions with satisfy criterion (5.115) are also added in Table 9. It is evident that the agglomeration rate $\beta$ decreases with increasing diameter of the particles. This result confirms the a–priori analysis made in § 5.4.2.8. Furthermore, it can be seen from Table 9 that the number of collisions $N_{\text{coll}}$ (therefore also the number of agglomerations $N_{\text{agg}}$) drastically decrease from the 1 $\mu$m particles to the 5 $\mu$m particles. This observation is in line with the dependence of the collision frequency $f^*_c$ from the particle diameter $d^*_p$ and the number of particles $N_p$ present in the computational domain predicted by stochastic analyses (see, e.g., Sommerfeld, 2000; Wang et al., 2000; Borée and Caraman, 2005, and references therein):

$$f^*_c = \frac{N_{\text{coll}}}{\Delta T^*} \sim \frac{1}{V_{\text{al}}^*} N_p^2 d_p^{*2} \langle |u_{\text{pr}}^*| \rangle. \quad (8.3)$$

$\langle |u_{\text{pr}}^*| \rangle$ is the average relative velocity between two particles and $V_{\text{al}}^*$ the total volume of the computational space. For the following analysis it is assumed that the average relative velocity $\langle |u_{\text{pr,1}\mu m}^*| \rangle$ of the 1 $\mu$m particles is roughly the same as the average relative velocity $\langle |u_{\text{pr,5}\mu m}^*| \rangle$ of the 5 $\mu$m particles. This assumption is plausible since both particle classes possess a small diameter and therefore the dynamics of the particles are predominantly influenced by the turbulent fluid motion. Using this assumption the ratios of the collision frequency $f^*_{c,1\mu m}$ of the 1 $\mu$m particles to the collision frequency $f^*_{c,5\mu m}$ of the 5 $\mu$m particles can be estimated:

$$\frac{f^*_{c,1\mu m}}{f^*_{c,5\mu m}} = \frac{N_{p,1\mu m}^2 (1\mu m)^2}{N_{p,5\mu m}^2 (5\mu m)^2} = 625. \quad (8.4)$$

The above ratio expresses that for a given mass loading the collision frequency $f^*_c$ rises with decreasing particle diameter $d^*_p$. The explanation of this dependency is quite simple: The probability of two objects (in our case particles) moving in a domain to collid, is proportional to the surface of both objects. Since for a given mass loading the total surface of the particles increases with decreasing particle diameter, also the collision frequency increases with decreasing $d^*_p$. $N_{p,1\mu m} = 10^7$ and $N_{p,5\mu m} = 8 \times 10^4$ are the number of 1 $\mu$m particles and the number of 5 $\mu$m particles present in the computational domain, respectively. The above estimated value is similar to the simulated ratios $f^*_{c,1\mu m}/f^*_{c,5\mu m} = 436, 646$ and 668 found for a normal restitution coefficient of $e_{n,p} = 0.4, 0.6$ and 0.8, respectively. Therefore, the results of the simulations are in line with the estimation given by the stochastic analysis. Regarding the ratio of the collision frequency $f^*_{c,5\mu m}$ of the 5 $\mu$m to the collision frequency $f^*_{c,10\mu m}$ of the 10 $\mu$m particles, no clear trend can be observed. A possible explanation is that the decreased total surface of the 10 $\mu$m particles with respect to the 5 $\mu$m particles is balanced by the increased mean relative velocity of the 10 $\mu$m particles with respect to the 5 $\mu$m particles.

A further conclusion which can be drawn from Tab. 9 is that the agglomeration rate $\beta$ decreases with increasing normal restitution coefficient $e_{n,p}$ for the 1 $\mu$m and the 5 $\mu$m particles. Since for increasing $e_{n,p}$ the plastic deformation of the particles also decreases, the computed van–der–Waals energy appearing in eq. (5.115) decreases. Therefore, also the number of collisions which satisfy criterion (5.115) diminishes. For the 10 $\mu$m particles, however, $\beta$ shows a maximum for $e_{n,p} = 0.6$. Unfortunately, this behavior is difficult to explain. However, since the collisions and the agglomerations found are low, the statistics are maybe not completely converged.
Table 9: Agglomeration rate $\beta = N_{agg}/N_{col}$ as a function of the particle diameter $d_p^*$ and the normal restitution coefficient.

<table>
<thead>
<tr>
<th>$e_{n,p}$</th>
<th>1 $\mu$m</th>
<th>5 $\mu$m</th>
<th>10 $\mu$m</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.4</td>
<td>$\beta = \frac{6.47 \times 10^4}{1.13 \times 10^5} = 5.58 \times 10^{-1}$</td>
<td>$\beta = \frac{45}{259} = 1.61 \times 10^{-1}$</td>
<td>$\beta = \frac{21}{1660} = 1.11 \times 10^{-2}$</td>
</tr>
<tr>
<td>0.6</td>
<td>$\beta = \frac{4.46 \times 10^4}{1.06 \times 10^5} = 4.04 \times 10^{-1}$</td>
<td>$\beta = \frac{20}{164} = 1.13 \times 10^{-1}$</td>
<td>$\beta = \frac{27}{579} = 5.00 \times 10^{-2}$</td>
</tr>
<tr>
<td>0.8</td>
<td>$\beta = \frac{2.43 \times 10^4}{1.05 \times 10^5} = 2.10 \times 10^{-1}$</td>
<td>$\beta = \frac{7}{157} = 4.63 \times 10^{-2}$</td>
<td>$\beta = \frac{24}{637} = 3.18 \times 10^{-2}$</td>
</tr>
</tbody>
</table>

8.5.2 Influence of Post–collision Treatment without Agglomeration and the Influence of the Modeling of the Agglomerate

The results presented in the following concerns the second test case described in § 7.5 performed to evaluate the agglomeration model. In contrast to the results described above, for this case the particles are allowed to agglomerate. In order to provide a first overview of the influence of the consideration of the van–der–Waals forces if no agglomeration occurs and the influence of the model for the agglomerate (a porous sphere or a volume–equivalent sphere) different statistical quantities are summarized in Table 10. $N_{col}$ denotes the number of collisions and $N_{agg}$ the number of agglomerations found during the dimensionless averaging period of $\Delta T = 560$ (about 46 flow–through times). $\beta = N_{agg}/N_{col}$ represents the agglomeration rate, $i_{agg}$ the total number of agglomerates present in the computational domain, $d_{\text{min}}^*$ the diameter of the smallest particles and $d_{\text{max}}^*$ the diameter of the biggest particles (agglomerates) located in the pipe. $\rho_{\text{min}}^*$ and $\rho_{\text{max}}^*$ are the minimum and maximum density of the particles (agglomerates). Note that only the rough wall simulations are shown since during the whole simulation time no particles touched the wall and therefore no difference between the rough and smooth wall case can be observed.

As obvious from Table 10 the modeling of the agglomerate has a remarkable effect on the statistics displayed. Especially drastic is the effect on maximum diameter $d_{\text{max}}^*$ and the minimum $\rho_{\text{min}}^*$ and maximum density $\rho_{\text{max}}^*$ of the particles present in the computational domain. It is evident that if the agglomerate is treated as a volume–equivalent sphere, no density variations occur. If it is treated as a porous sphere, large variations in the density can be observed. The agglomerates with the lowest densities for the cases RW w. vdW. and RW wo. vdW. are two orders of magnitude lower than the density of the single limestone particles. The agglomerates with the highest densities for the cases RW w. vdW. and RW wo. vdW., on the other hand, are about twice the density of the particles initially distributed in the computational domain.

The reason for the occurrence of such low densities if the the porous sphere model is applied, can be detected from the a–priori analysis in § 5.4.2.8: If the angular velocity of the agglomerate is aligned with either the tangential vector $t_{agg}$ or the vector $z_{agg}$ (the axis around which the two spheres stuck together has the greatest moment of inertia), the porous sphere has to possess a large diameter in order to guarantee that the rotational energy is preserved. This results in a decrease of the homogeneously distributed density of the porous sphere $\rho_{ps}$ compared with the density of the two particles involved in the generation of the agglomerate. The reason for the decreasing density is that additionally mass conservation is required (see § 5.4.2.8 for the details).
Table 10: Summary of the differences between the treatment of the particles if no agglomeration occurs and the treatment of the agglomerate. For the abbreviations, see Table 4.

The occurrence of a density of the porous sphere greater than the initial particle density $\rho_p^* = 2710 \text{ kg/m}^3$ can be explained by analyzing eq. (5.124) and (5.123) for a simple configuration. Let us assume that the agglomerate which is formed after a collision consists of two particles with the same diameter and the same density, i.e., $d_{p,1} = d_{p,2} = d_p$ and $\rho_{p,1} = \rho_{p,2} = \rho_p$. Furthermore, the angular velocity of the agglomerate should have only a component in the collision–normal direction, i.e., $\omega_{ag,ntz} = [\omega_{ag,n} 0 0]$. For the configuration explained above, only the first entry of the inertial tensor of the agglomerate (see also eq. (5.103)) has a contribution to the expression used to calculate the diameter of the porous sphere (see eq. (5.124)). For this small example analyzed here, the diameter of the porous sphere results as follows:

$$I_{ag,nn} = 0.1 \, m_{p,1} d_{p,1}^2 + 0.1 \, m_{p,2} d_{p,2}^2$$

(8.5)

of the inertial tensor of the agglomerate (see also eq. (5.103)) has a contribution to the expression used to calculate the diameter of the porous sphere (see eq. (5.124)). For this small example analyzed here, the diameter of the porous sphere results as follows:

$$d_{ps} = \left( \frac{60}{2 \pi \rho_p d_p^3} I_{ag,nn}^2 \omega_{ag,n}^2 \right)^{1/2} = \left( \frac{60}{2 \pi \rho_p d_p^3} 0.2 \pi \rho_p \frac{d_p^3}{6} d_p^2 \right)^{1/2} = d_p.$$  

(8.6)

Therefore, for the configuration where the angular velocity of the agglomerate has only a component in collision–normal direction and both particles involved in the agglomeration process have the same diameter, i.e., the diameter of the porous sphere is equal to the diameter of the original particles involved and the above equation reduces to $d_{ps} = d_p$.

The density of the porous sphere can then be calculated by inserting the above expression into the mass conservation eq. (5.123):

$$\rho_{ps} = \frac{2}{d_p^3} = 2 \rho_p.$$  

(8.7)

It is obvious that the density of the porous sphere is doubled with respect to the density of the two particles involved in the agglomeration. This unphysical result follows from the three requirements requested by the simplification of the agglomerate by a porous sphere, i.e., the angular momentum, the energy and mass conservation.

Regarding the different maximum diameters of the particles present in the computational domain (see Table 10) there are big differences between the cases RW w. vdW. and RW wo. vdW. on the one hand and the cases RW w. vdW. VES and RW wo. vdW. VES on the other hand. If the agglomerates are treated as a porous sphere, the maximum diameter is roughly one order of magnitude higher than for the simulations where the
agglomerates are modeled as volume–equivalent spheres. The reason for this large spread in the diameters for the porous sphere cases is the same as for the occurrence of the large density variations explained above.

A further difference between the two models used to treat the agglomerate concerns the number of collisions $N_{\text{coll}}$ found and the number of agglomeration $N_{\text{agg}}$ occurred. Assuming the agglomerate as a porous sphere generates about 30% more inter–particle collisions than assuming the agglomerate as a volume–equivalent sphere. Since the diameters resulting from the porous sphere model are larger than the diameters resulting from the volume–equivalent sphere model, the generated agglomerates are more likely to collide with the neighboring particles or agglomerates. However, the number of agglomerates $i_{\text{agg}}$ present in the pipe differs only about 10% between the different treatments of the two particles after the agglomeration. The reason is that the agglomeration rate $\beta$ is smaller for the porous sphere model. The cause is probably that, as shown in the a–priori analysis in § 5.4.2.8 and in the results shown of the last section, the probability of two particles to agglomerate decrease for increasing diameter. Since the porous sphere model results in agglomerates of larger diameters than the volume–equivalent sphere model, the larger particles are more likely to collide with neighboring particles but the probability to agglomerate is lower.

Comparing the simulations where the inter–particle collisions are assumed to be frictionless (fricless. coll. in Table 10) with the cases where the collisions are assumed to be frictional (RW w. vdW. VES and RW wo. vdW. VES in Table 10) it is evident that for the former a slightly lower number $N_{\text{coll}}$ of collisions is found. Since for the frictionless collisions the particle velocity is changed only in collision–normal direction, it seems to be reasonable to assume that the relative velocity with respect to the neighboring particles is lower compared with the frictional collision where the particle velocity is changed also in the direction of $u_{\text{pr}}$. Therefore, the probability of particles which undergo a frictionless collision to impact on neighboring particles is lower compared with particles which undergo a collision with friction. As expected, for the friction less case, the agglomeration rate $\beta$ is the highest among the cases investigated since the particles do not acquire an angular velocity over the collision process and therefore the probability to agglomerate is the highest.

Regarding the consideration of the van–der–Waals forces in the calculation of the post–collisional particle trajectories for the case where no agglomeration occurs, only small differences can be found. The computations where the van–der–Waals forces are taken into account, show for both treatments of the agglomerate (porous sphere or volume–equivalent sphere) a smaller agglomeration rate compared with the computations without considering the van–der–Waals forces. Regarding the number of collisions no clear trend can be observed. Unfortunately, no explication for this observation can be given.

For the next evaluation step, Table 11 show the number of agglomerates $i_{\text{agg},j}$ consisting of a given number $j$ of particles. Therefore, $i_{\text{agg},1}$ stands for the number of single particles (which have never agglomerated), $i_{\text{agg},2}$ for the agglomerates consisting of two particles, etc. Note that because of the large number of primary particles this representation of the results is chosen instead of a bar diagram for a better visualization of the number of agglomerates consisting of several particles. From Table 11 it is evident that most particles present in the domain are not agglomerated. Furthermore, the number of agglomerates $i_{\text{agg},j}$ decreases with increasing number $j$ of particles forming the agglomerate. This is reasonable for two reasons: (i) Since there are much more single particles the agglomer-
ates consisting of two particles, it is much more probable that two single particles collide forming an agglomerate consisting of two particles than that a \( i_{\text{agg},2} \) agglomerate collides with a single particles forming and \( i_{\text{agg},3} \) agglomerate. (ii) Since the agglomeration criterion predicts a smaller probability of agglomeration for bigger particles, agglomerates consisting of more particles are less prone to agglomerate.

A further conclusion which can be drawn from Table 11 is that there are some differences in the distribution of \( i_{\text{agg},j} \) between the different modeling strategies adapted to simplify the geometry of the agglomerate. If the agglomerate is treated as a porous sphere, there are more higher order agglomerates (consisting of more than eight particles) than for the case where the agglomerate is modeled as a volume-equivalent sphere. Since, as demonstrated in the a-priori analysis in §5.4.2.8, the porous sphere model produces agglomerates with a larger diameter than the volume-equivalent sphere model, for the former it is more probable to collide with a neighboring particle than for the latter and forming agglomerates consisting of more than two particles.

<table>
<thead>
<tr>
<th>( i_{\text{agg},1} )</th>
<th>RW w. vDW</th>
<th>RW wo. vDW</th>
<th>RW w. VES</th>
<th>RW wo. vDW. VES</th>
<th>fricless. coll.</th>
</tr>
</thead>
<tbody>
<tr>
<td>994,551</td>
<td>991,823</td>
<td>992,241</td>
<td>995,081</td>
<td>992,283</td>
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<tr>
<td>1759</td>
<td>1691</td>
<td>1954</td>
<td>1954</td>
<td>1952</td>
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<td>415</td>
<td>402</td>
<td>450</td>
<td>449</td>
<td>444</td>
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<td>37</td>
<td>18</td>
<td>19</td>
<td>16</td>
<td></td>
</tr>
</tbody>
</table>

Table 11: Number of agglomerates consisting of a given number \( j \) of particles. For the abbreviations, see Table 4.

Figure 66 shows the particle diameter size distributions for the cases RW w. vDW. VES (Fig. 66(a)), fricless. coll. (Fig. 66(b)) and RW w. vDW. (Fig. 66(c)). Since the consideration of the van–der–Waals forces in the collisions which do not lead to agglomeration has only a marginal influence on the statistics shown here, this case is not considered for the sake of brevity. Note that the single particles are not considered in the generation of the plot shown in Fig. 66 in order keep the plots clear. In order to obtain the histograms depicted in Fig. 66, the interval between the minimum diameter \( d_{\text{min}}^* \) and the maximum diameter \( d_{\text{max}}^* \) found for each of the single cases displayed, is divided into nine equally sized diameter intervals. For each of this nine diameter classes a representative diameter \( d_{p,i}^* \) is defined consisting in the average of each diameter intervals considered. After that, all agglomerates are counted which belong to one of this 9 intervals. The height of the bars represent the number of particles \( N_{p,i} \) belonging to the diameter size class \( j \). It is evident that for all cases considered the number of particles \( N_{p,i} \) decrease for increasing representative diameter \( d_{p,i}^* \) of the classes. The reason of this observation are the same as
the one for the decrease of the number of agglomerates $i_{agg,j}$ consisting of a given number $j$ of particles with increasing $j$ explained above. Note, however, that the diameter size intervals in the RW w. vdW. are larger because of the larger spread between $d_{min}^*$ and $d_{max}^*$ (see Table 10). Furthermore, only small differences between the simulation assuming frictionless collisions (Fig. 66(b)) and the simulation assuming collisions with friction (Fig. 66(a)) can be found. This further confirms the small differences observed between this to cases already shown in Table 11.

Figure 66: Particle diameter size distributions considering different modelings of the agglomerate and of the inter–particle collisions. For the abbreviations, see Table 4.

Figure 67 shows the temporal evolution of the averaged diameter $\langle d_p^* \rangle$ and the averaged density $\langle \rho_p^* \rangle$ of all particles including the agglomerates present in the computational domain. In accordance with the results summarized in Table 10, the averaged diameter of the cases where the agglomerates are treated as a porous sphere grows faster in time than for the cases where the agglomerates are treated as volume–equivalent sphere (see Fig. 67(a)). As already discussed in the a–priori analysis in § 5.4.2.8 and also above, for most orientations of the angular velocity of the agglomerate $\omega_{ag,ntz}$ with respect to the three main axes of the inertial tensor of the agglomerate $I_{ag,ntz}$ the porous sphere model results in a larger diameter compared with volume–equivalent sphere model. Consider-
ing the mass conservation, the temporal evolution of the density $\langle \rho_p^* \rangle(t)$ has to behave inversely proportional to the diameter $\langle d_p^* \rangle(t)$ which is visible in Fig. 67(b).

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig67}
\caption{Time evolution of (a) the averaged diameter $\langle d_p^* \rangle$; (b) the averaged density $\langle \rho_p^* \rangle$. For the abbreviations, see Table 4.}
\end{figure}

### 8.5.3 Summary and Conclusions

In this section the agglomeration model of § 5.4.2 was briefly discussed. In the view of the results obtained, the following conclusions can be drawn:

- In accordance with the a–priori analysis in § 5.4.2.8 the agglomeration rate $\beta$ decreases with increasing particle diameter. Except for the 10 $\mu$m particles $\beta$ also decreases with increasing normal restitution coefficient $e_{n,p}$.

- A reasonable distribution of the number $i^\text{agg,j}$ of agglomerates consisting of $j$ particles is found. That means that for all cases discussed $i^\text{agg,j}$ decreases with increasing $j$. In the view of this result, the author is confident that the agglomeration criterion (5.115) delivers reasonable results.

- If the agglomerates are treated as porous spheres, large diameter and density variations occur from the particles present in the computational domain. If the agglomerates are modeled as volume equivalent spheres, more realistic diameter distributions can be observed. However, the energy conservation is not ensured.

- In the view of the large diameter and density variations observed for the porous sphere model maybe another geometrical configuration of the agglomerate (e.g., as a hollow sphere\textsuperscript{14}) should be used to fulfill the conservation of mass, energy, translational and rotational momentum.

- No substantial differences could be found between the cases considering the van–der–Waals forces or not for the calculation of the post–collisional states of the particles if no agglomeration occurs.

\textsuperscript{14}Using a hollow sphere for the post–agglomeration treating of the particles, however, results in a non–linear equation for the outer and inner diameter of the hollow sphere. Unfortunately, the author was not able to obtain an analytical solution for this equation. See Appendix C for a short discussion.
8.6 Horizontal Pipe Flow at Re = 58,800

In this section the results obtained for a turbulent horizontal pipe flow are shown. Note that parts of the results shown here were already published in Alletto and Breuer (2013).

The section is organized as follows: First in § 8.6.1 the unladen flow is validated against DNS and experimental data. After that, in § 8.6.2 the criterion to determine the statistically steady state is shown and in § 8.6.3 the poly–disperse simulation is validated with the experimental data of Huber (1997) and Huber and Sommerfeld (1998). Finally, the cause for the generation of secondary flow structures in the pipe cross–section is analyzed in detail in § 8.6.4.

8.6.1 Unladen Flow

In Euler–Lagrange computations it is indispensable to first correctly describe the continuous flow in order to allow trustworthy considerations about the two–phase flow. Therefore, in this section the computed unladen LES statistics are compared with the DNS data by Wu and Moin (2008) and Boersma (2013) and the experiments by Zagarola and Smits (1998). In order to verify the influence of the subgrid–scale model, two computations are carried out for the unladen LES. One employed the subgrid–scale model of Smagorinsky (1963) (see § 3.2.1) and the second the dynamic subgrid–scale model of Germano et al. (1991) (see § 3.2.2). A direct comparison with the experiments of Huber (1997) or Huber and Sommerfeld (1998) is not possible, since no continuous flow data (neither for the unladen nor for the particle–laden case) are available. The DNS of Wu and Moin (2008) was performed at a lower Reynolds number of Re = 22,000 based on the bulk velocity and the pipe radius. The governing equations were discretized by means of a finite–volume approach. The computational domain was 15 pipe radii long and discretized by about $6.3 \times 10^8$ cells. The DNS of Boersma (2013) was performed at a Reynolds number of Re = 38,000 based on the bulk velocity and the pipe radius. He used a pseudo–spectral (FFT based) method in circumferential and axial direction. In radial direction Boersma (2013) employed a 6th–order staggered compact finite–difference method. The computational domain was 36 pipe radii long and discretized by about $7.26 \times 10^9$ cells. Zagarola and Smits (1998) solely measured the mean fluid velocity by means of a Pitot probe at different Reynolds numbers. For the current comparison the measurements at Re = 49,000 based on the bulk velocity and the pipe radius were chosen since they are closest to the present Reynolds number of Re = 58,800.

Figure 68(a) shows the computed mean streamwise velocity scaled by the bulk velocity. Obviously, very good agreement is found between both LES results and the measurements performed by Zagarola and Smits (1998) at a slightly lower but still comparable Reynolds number. The centerline velocity computed by Wu and Moin (2008) and Boersma (2013) is higher than the present LES data as expected for a considerably lower Reynolds number than the present LES. Regarding the two LES simulations, hardly noticeable differences between the two simulations with different subgrid–scale models can be observed.

Figures 68(b)–(d) show the streamwise and wall–normal fluctuations (root–mean squared) and the Reynolds shear stress, respectively. Unfortunately, for these quantities no experimental data are available. The second–order statistics are scaled with the friction velocity $u^*\tau$ predicted by the corresponding simulations. The scope is to compare them with both DNS data, which are performed at different Reynolds numbers compared with the present LES simulations. Since the unladen fluid velocity fluctuations are expected to scale ap-
proximately with the friction velocity $\overline{u^*_r}$, i.e., $\langle u'_r \rangle / \overline{u^*_r} \approx \text{const.}$ (see Hoyas and Jiménez, 2006) this approach is best practice in the literature. The values of $\overline{u^*_r} / U_B^*$ are equal to $4.19 \times 10^{-2}$ for both LES simulations. Since only very small differences between the two LES simulations are found in the Reynolds shear stress (see Fig. 68(d)) this finding is consistent with the results shown in this section. Regarding the two DNS data $u^*_r / U_B^*$ is equal to $5.19 \times 10^{-2}$ and $4.84 \times 10^{-2}$ for the simulations of Wu and Moin (2008) and Boersma (2013), respectively. For the aforementioned scaling the streamwise velocity fluctuations predicted by both LES are slightly lower than the DNS data, while the wall–normal fluctuations are slightly higher than the reference case. Besides the differences in the Reynolds number the deviations observed may be partially attributed to the application of wall functions in the LES. Nevertheless, for the Reynolds shear stress (Fig. 68(d)) excellent agreement is found. Regarding the two LES predictions, only small differences between the computations performed with the two subgrid–scale models for the fluid can be found. Since the computational domain is discretized by $3 \times 10^7$ cells and the wall region is not resolved, this leads to a very fine resolution in the bulk region. Therefore, the influence of the subgrid scales is still small, explaining the small differences observed between the results of the model of Smagorinsky (1963) and the model of Germano et al.
Summing up, both LES data of the unladen flow computed either with the model of Smagorinsky (1963) or the dynamic model of Germano et al. (1991) satisfactorily agree with the reference cases of Zagarola and Smits (1998), Wu and Moin (2008) and Boersma (2013). Therefore, reasonable preconditions are established in order to allow reliable computations if solid particles are added to the flow configuration. Regarding the two LES predictions no substantial differences are noticeable between the application of the model of Smagorinsky (1963) or the dynamic model of Germano et al. (1991). For this reason, the computationally cheaper model, i.e., the model of Smagorinsky (1963), is applied in the following.

8.6.2 Establishment of the Statistically Stationary State

Since simulations with periodic boundary conditions can only reproduce statistically steady flows, a suitable condition has to be derived to ensure that this is actually the case. For unladen flows an integral quantity such as the wall shear stress can be monitored to check if the flow is fully developed. For the present particle–laden horizontal pipe flow another quantity is chosen. In a horizontal pipe configuration, particles, which are initially uniformly distributed in the computational domain, start to settle towards the bottom part of the pipe due to the influence of gravity. For a smooth glass pipe the downward movement of the particles is balanced by the resuspension induced due to the inter–particle collisions. For the rough steel pipe the resuspension of the particles is further enhanced by the wall roughness. For a fully developed flow these mechanisms balance the gravitational settling leading to a mild oscillation of the center of mass of the particles around its mean value. Therefore, the center of mass of the particles is monitored in order to determine when the two–phase flow has reached a statistically steady state.

The history of the vertical position $y_{cm}^*/R_{pipe}^*$ of the center of mass of the particles during the simulation is displayed in Fig. 69. It shows the vertical position $y_{cm}^*/R_{pipe}^*$ of the center of mass for the mass loadings $\eta = 30\%$ and $70\%$ and the glass and steel pipe. Note that the pipe center is located at $y_{cm}^*/R_{pipe}^* = 0$.

Figure 69: Time evolution of the position $y_{cm}^*/R_{pipe}^*$ of center the of mass of the particles in vertical direction, (a) initialisation phase; (b) averaging phase.

Figure 69(a) shows the evolution of the vertical position $y_{cm}^*/R_{pipe}^*$ of the center of mass of the particles from the beginning of the injection of the particles. $T_{start}$ denotes the
time when the particles are introduced into the computational domain. For all simulations except the $\eta = 70\%$ steel pipe, the particles are homogeneously distributed over the pipe cross-section at the beginning of the two-phase flow simulation resulting in a starting position of the center of mass located at $y^*_cm/R^*_{pipe} = 0$. For the $\eta = 70\%$ steel pipe a solution of the same mass loading taken from the glass pipe is used to initialize the particle–laden simulation. For the three simulations for which the particles are homogeneously distributed at the injection time $T_{start}$ ($\eta = 30\%$ glass and steel and $\eta = 70\%$ glass), it is evident that the particles start to settle towards the bottom of the pipe due to the influence of gravity. The center of mass reaches a statistically steady state when the effect of the particle–particle collisions and the effect of the wall roughness counterbalance the influence of the gravity. The evolution of $y^*_cm/R^*_{pipe}$ for the $\eta = 70\%$ steel pipe flow remarks the influence of the wall roughness on the particles motions. For this case the particles initially located at the bottom part of the pipe are resuspended by the wall roughness leading to a mean position of the center of mass at about $y^*_cm/R^*_{pipe} = 0.05$.

Figure 69(b) shows the evaluation of the vertical position $y^*_cm/R^*_{pipe}$ of the center of mass of the particles during the averaging period $\Delta T = 2280$. $T_{aver}$ denotes the time when the averaging procedure is initiated. For the steel pipe $T_{aver} - T_{start}$ is equal to 157 and 515 for the $\eta = 30\%$ and $70\%$ case, respectively. For the glass pipe $T_{aver} - T_{start}$ is equal to 980 and 2280 for the $\eta = 30\%$ and $70\%$ case, respectively. This figure further underlines the two mechanisms which counteract the gravitational settling, i.e., the particle–particle collisions and the wall roughness. For the glass pipes the mean position of the center of mass is located closer to the bottom wall than for the steel pipes. The increased influence of the inter–particle collisions with increasing mass loading $\eta$ is reflected by the averaged position $\langle y^*_cm/R^*_{pipe} \rangle$ of the center of mass of the particles: For the same wall material $\langle y^*_cm/R^*_{pipe} \rangle$ is located closer to the center for $\eta = 70\%$ than for $\eta = 30\%$. For the glass pipe long vertical oscillations of the vertical position with low frequencies of the center of mass of the particles can be observed. The amplitude of the oscillation is higher for the $\eta = 70\%$ glass pipe than for $\eta = 30\%$ glass pipe and reaches values of about 3% of the pipe radius for the former. Unfortunately, no explanation for this phenomenon can be provided. However, the influence of the periodic boundary conditions can be excluded since the period length of the oscillations are much longer than the flow–through time of the particles in streamwise direction.

8.6.3 Comparison of the Two–phase Flow with the Experimental Reference Case

In this section the simulated particle statistics are compared with the available experimental data of Huber (1997) and Huber and Sommerfeld (1998) who measured the mean particle velocity, the particle streamwise velocity fluctuations, the mean particle diameter and the particle streamwise mass flux in the pipe midplane parallel to the axis of gravity (Fig. 70). The objective is to show that the results obtained by the Euler–Lagrange code agree well with the experiments and hence the author is confident about the reliability of the simulations performed at the present ($\eta = 30\%$) and the higher mass loadings $\eta = 70\%$ to be analyzed later.

Figure 70(a) depicts the simulated mean particle velocity for the glass and the steel pipe compared with the experiments. Obviously, good agreement is found for both cases. Furthermore, it is evident that the wall roughness of the steel pipe leads to a reduction of the influence of the gravitational settling. In case of the glass pipe the mean particle
velocity profile shows a strong asymmetry between the lower and upper half of the cross-section. The reason is that particles settling under the influence of gravity lost momentum during the wall impact and combined with the high particle concentration in this region (Fig. 70(d)) also slowed down the carrier phase via the two-way coupling. The mutual interaction between the particles and the fluid thus leads to an asymmetric mean particle velocity profile. The continuous phase exhibits a very similar mean velocity profile but is not depicted here since no experimental data are available and the objective of this section is to validate the simulation against the experiment.

In case of the steel pipe due to the shadow effect the roughness leads to a redistribution of the particle streamwise momentum towards the wall–normal direction and additionally to a slight increase of the inter-particle collisions. Both effects (shadow effect and inter-particles collisions) are responsible for a resuspension of the particles and hence to a reduction of the particle concentration at the bottom wall (Fig. 70(d)). This again causes a reduction of the force exerted by the particles on the fluid against the mean flow direction in the bottom part of the tube compared with the smooth pipe and hence via the mutual interaction between the particles and the fluid to a higher mean particle velocity near the bottom wall.

Figure 70(b) shows the simulated particle streamwise velocity fluctuations compared with the experimental data. In case of the smooth glass pipe the shape of the distribution
of the particle fluctuations agrees well with the experiment but the magnitude is lower. The reason is probably that already the predicted fluid streamwise velocity fluctuations are slightly too weak (see Fig. 68(b)). Since the majority of the particles inside the domain were rather small, they are expected to be strongly influenced by the continuous flow and hence it seems plausible that also the streamwise particle fluctuations are lower than the reference case. In case of the steel pipe the simulated streamwise particle velocity fluctuations are increased with respect to the glass pipe. The experimental data for the steel pipe, however, show a reduction of the fluctuations compared to the smooth pipe data at the bottom half of the pipe, while the fluctuations remained unchanged at the top part of the pipe. Unfortunately, no explanation is found yet for the differences between the result of the experiment and the simulation. Since the wall roughness is expected to increase the particle velocity fluctuations (Kussin and Sommerfeld, 2002; Sommerfeld, 2003; Sommerfeld and Kussin, 2003; Benson et al., 2005; Vreman, 2007; Breuer et al., 2012) the trend observed in the simulated results seems to be reasonable. The experimental data of Huber and Sommerfeld (1998), however, showed an inverse trend which is at least astonishing.

Figure 70(c) depicts the simulated mean particle diameter (in this case $\Phi_p$ is substituted in eq. (6.49) by $d_p^*$) compared with the experiments of Huber (1997) and Huber and Sommerfeld (1998). It is obvious that a close agreement is found between simulation and experiment for this quantity. In case of the smooth glass pipe it is evident that gravity caused a segregation of the particles (see also Huber and Sommerfeld, 1998): While bigger particles settled down faster under the influence of gravity, the smaller particles were more efficiently dispersed by the turbulent eddies and remained suspended throughout the pipe cross-section. This causes an increase of the mean particle diameter from top to bottom. In case of the rough wall the mean particle diameter profile shows a weak minimum at a position slightly above the pipe center and increases towards both, bottom and top wall.

A possible explanation for this behavior arises from the evaluation of the velocity component of the particle trajectory in wall–normal direction $|\mathbf{u}_p \cdot \mathbf{n}|/|\mathbf{u}_p|$ before and after a wall collision (Fig. 71). The minus sign – in the legend of Fig. 71 denotes the quantities before the wall collision and the plus sign + denotes the quantities after the wall impact. $\mathbf{n}$ is the wall–normal vector of the smooth wall, i.e., the wall–normal vector before its random inclination by the wall model for the particles (see Breuer et al., 2012). Separate statistics of a 45° sector of the bottom and top half of the pipe circumference are calculated in order to account for a possible influence of the gravitational acceleration and the secondary flow on the impact trajectory. The statistics are averaged over a dimensionless time period of $\Delta T = \Delta T^* U_{\text{B}}^*/R_{\text{pipe}}^* = 100$. From Fig. 71 it is evident that particles with a smaller diameter $d_p^*$ acquire a greater wall–normal component (the component towards the pipe center) after a wall impact than the bigger particles. The reason for this behavior is that the predicted mean inclination of the wall seen by the particles against the incoming trajectory increases for increasing ratio of $R_{\text{z}}^*/d_p^*$ at constant incident angle (see also the a–priori analysis in Breuer et al., 2012). Hence, the redistribution of the streamwise momentum towards the wall–normal direction predicted by the roughness model is more pronounced for the smaller than for the bigger particles at constant $R_{\text{z}}^*$ and constant incident angle. The stronger deflection of the small particles towards the pipe center leads to a stronger accumulation of smaller particles near the pipe center and hence to the minimum of the mean particle diameter observed in Fig. 70(c). The nearly constant wall–normal component of the particle velocity until $d_p^* \approx 30 \mu m$ arises from the limitation of the stan-
The standard deviation of the random wall inclination to \( \sigma = 30^{\circ} \) for \( d_p^* \leq k_s^* \) (Breuer et al., 2012). The standard deviation \( \sigma \) in Breuer et al. (2012) is calculated by
\[
\sigma = \arcsin\left(\frac{k_s^*/(k_s^* + d_p^*)}{2}\right)
\]
Since the angles computed by a Gaussian distribution lay approximately within the range \( \pm 3\sigma \), the standard deviation has to be limited to \( \sigma \leq \arcsin(1/2) \leq 30^{\circ} \) in order to avoid unrealistic values of the wall inclination larger than 90\(^{\circ}\) (a vertical wall). The limiting ratio \( k_s^*/(k_s^* + d_p^*) = 1/2 \) is reached for \( d_p^* = k_s^* = 30 \mu m \).

The difference between the bottom and the top wall of the wall–normal component of the particle velocity before the wall impact is hard to explain because of the difficulties to separate the effects influencing this quantity, i.e., the gravity, the cross–sectional secondary flow, the inter–particle collisions and the turbulent dispersion. However, even for the bigger particles the shadow effect still has an important influence on the rebound behavior of the particles at the rough wall. As visible in Fig. 71 the difference between the wall–normal component of the particle trajectory before \( (|\mathbf{u}_p \cdot \mathbf{n}|/|\mathbf{u}_p|)^- \) and after the wall impact \( (|\mathbf{u}_p \cdot \mathbf{n}|/|\mathbf{u}_p|)^+ \) is still high for the particles with the biggest diameter.

Figure 70(d) shows the mean particle mass flux in streamwise direction at the midplane parallel to the axis of gravity. In the simulations the mass flux is calculated by the following relation
\[
\langle \dot{m}_p^* \rangle = \frac{1}{6 \pi \rho_p^* (\langle N_p \rangle) (d_p^*)^3 / V_{av}^* A_{av}^*} \langle u_{pz}^* \rangle^3 A_{av}^*.
\]
\( \langle N_p \rangle \) is the time–averaged number of particles found in a cell used to compute the statistics at the midplane, \( V_{av}^* \) and \( A_{av}^* \) are the volume and the projection of the surface in streamwise direction of the cell used to compute the particle statistics, respectively. The mean particle mass flux is normalized by its integral over the midplane \( \dot{m}_{pav}^* \). It is evident that the wall roughness has a drastic effect on this particle statistic. For the smooth wall the particle mass flux near the bottom wall is very high due to the influence of the gravity. For the steel pipe, however, the particles streamwise momentum is redistributed towards the wall–normal direction due to the shadow effect (see Sommerfeld (2000); Breuer et al. (2012) and also Fig. 71). Hence, after a wall impact the particles acquire a steeper trajectory towards the pipe center since in a pipe the wall–normal vector points towards the pipe center. Consequently, the particles tend to accumulate in this region. This effect is called focusing effect (see Lain and Sommerfeld, 2012). Also for the mean particle mass flux good agreement is found between the simulation and the experiment for both cases.

![Figure 71: Evaluation of the particle trajectories $|\mathbf{u}_p \cdot \mathbf{n}|/|\mathbf{u}_p|$ before (-) and after (+) the collision at the rough wall as a function of the particle diameter.](image-url)
8.6.4 Analysis of the Secondary Flow Structure

According to Belt et al. (2012) and others secondary flows in straight pipes can be divided into two different categories depending on the driving mechanisms: (i) secondary flows of first and (ii) second kind. Secondary flows of first kind are driven by external forcing such as pressure gradients, buoyancy forces or potentially by moving particles or fixed particles with non-linear drag (Belt et al., 2012). On the other hand, secondary flows of second kind are driven by the anisotropy of the Reynolds stress tensor in the pipe cross-section and hence, by turbulence itself (Speziale, 1982; Belt et al., 2012). Based on these considerations there are two different ways how particles can induce a secondary flow in the pipe cross-section: They can either directly drive the secondary flow by the forces exerted on the fluid or indirectly due to the inhomogeneous distribution of the particles over the cross-section. Such an inhomogeneous distribution of the particles leads to a inhomogeneous attenuation of turbulence and hence to an anisotropy of the Reynolds stress tensor which is originally identified by Speziale (1982) as the driving mechanism of secondary flows of second kind.

Hence, the objective of this section is to identify if the particles are directly or indirectly responsible for the development of the secondary flow. Furthermore, the variation of the secondary flow for different combinations of the mass loading and the wall roughness are discussed.

8.6.4.1 Qualitative Analysis

Projected Streamlines
Figure 72 shows the projected streamlines of the averaged flow field in the pipe cross-section for the four cases investigated for the poly-disperse particles. The colormap displays the fluid velocity component against the gravitational acceleration. For the lowest mass loading $\eta = 30\%$ (Fig. 72(a) and (b) depict the glass and steel pipe, respectively) and for the intermediate mass loading $\eta = 70\%$ (Fig. 72(c) and (d)) the structure of the secondary flow is similar, i.e., two rotating cells developed. The fluid flows upstream along the symmetry line. Then it deflects to the left and right in order to circulate downstream along both side walls building a closed vortex. Note that in the experiments of Belt et al. (2012) a similar flow structure was found for the fixed particles. Differences between the glass and the steel pipe arise in the intensity of the secondary flow and the position of the maximum upward and downward movement of the flow. The intensity of the secondary flow in the glass pipe (Fig. 72(a) and (c)) is in the order of 2% of the bulk velocity and thus approximately doubled compared with the steel pipe (Fig. 72(b) and (d)).

The position of the maximum upward and downward movement of the flow is located in the bottom part of the cross-section for the glass pipe (Fig. 72(a) and (c)) and slightly below the pipe center in the case of the steel pipe (Fig. 72(b) and (d)). Note that for the low and intermediate mass loading (Fig. 72(a)–(d)) the maximum upward velocity is located at the same vertical position as the maximum downward velocity. Furthermore, the location of the maxima is slightly shifted upwards for both, the glass and steel pipe, if the mass loading is increased from $\eta = 30\%$ to 70%.

Forces of the Particles on the Fluid
As already mentioned the objective of this section is to identify, whether the mechanism leading to the secondary flow observed in the pipe cross-section is of first or second
kind. To exclude that the particles push the continuous flow and hence, that the driving mechanism is of first kind, the direction and the magnitude of the force \( \mathbf{F}_{pf} \) exerted by the particles on the fluid plays a decisive role. \( \mathbf{F}_{pf} \) is the force predicted by the particle–source–in–cell method mentioned in §5.3. Since \( \mathbf{F}_{pf} \) is time–dependent it requires temporal and spatial (spanwise) averaging for a reasonable analysis leading to \( \langle \mathbf{F}_{pf} \rangle \). Since the author had the inspiration to perform the analysis presented in this section when the statistics were almost converged and the restart of the averaging was not possible due the long averaging time (order of one month to obtain converged statistics), a reasonable estimation has to be obtained from the available statistics. For this purpose the drag force is predicted based on the averaged fluid and particle velocities. Owing to non–linearity the formulation is not exact. However, since the direction of the driving force is of main interest, this is not a critical issue. Figure 73 displays the result of this analysis for \( \eta = 30\% \) and 70\%. The colormap depicts the magnitude of \( \langle \mathbf{F}_{pf} \rangle \) and the lines with arrows show the direction of \( \langle \mathbf{F}_{pf} \rangle \). Additionally, Figs. 73(e) (glass pipe) and (f) (steel pipe) show the vector plots of the difference between the mean particle and the mean fluid
velocity components in the cross-section \( \langle u_p \rangle - \langle u_f \rangle \). The scope is to get a clear picture of the direction of the force exerted by the particle on the fluid. Regarding the arrow plot only the case \( \eta = 70\% \) is shown for the sake of brevity. However, the main finding, i.e., that the particles are driven by the secondary flow and not the other way round, remains the same for all other cases analyzed here. Note that the vectors have the same length for a better overview. As obvious from the direction of the force fields in Fig. 73(a)–(d) the particles have to be pushed upwards by the continuous phase near the midplane of the cross-section. This is also evident from the vector plots displayed in Figs. 73(e)–(f): Although both, continuous and disperse phase, move upwards near the midplane (see Figs. 72(a)–(d) for the direction of the fluid, the particle contour plot is not shown for the sake of brevity) the particles are slower than the fluid and hence have to be carried. Thus, the particle exert a force against the flow direction in this region. On the other hand, near the wall both, fluid and particles, move downward but as for the midplane the particles lag behind the continuous phase. Hence, they exerted a force against the mean flow direction also in the region near the pipe walls. Obviously, the magnitude of \( \langle F_{pf} \rangle \) for the lower mass loading (Figs. 73(a)–(b)) is lower than for the higher mass loading (Figs. 73(c)–(d)). When comparing the magnitude of \( \langle F_{pf} \rangle \) computed for the glass pipes (Figs. 73(a) and (c)) with the same quantity computed for the steel pipes (Figs. 73(b) and (d)) at constant mass loading, it is noticeable that \( |\langle F_{pf} \rangle| \) is higher for the glass pipe than for the steel pipes. Furthermore, the maximum of the force exerted by the particles on the fluid is located at the bottom half of the pipe cross-section for the glass pipe and near the center for the steel pipe. This observations (the magnitude and the location of maximum of \(|\langle F_{pf} \rangle|\)) can be explained by looking at the particle concentration (Fig. 75). Since the force exerted by the particle on the fluid is proportional to the particle concentration, the position of the maxima of both quantities should be correlated. Furthermore, the magnitude of \(|\langle F_{pf} \rangle|\) at constant mass loading is higher for the case where the local particle concentration is higher. i.e., for the glass pipe. Based on the entire analysis it is obvious that in the major part of the cross-section the particles tend to decelerate the fluid. Therefore, it can be concluded that the secondary flow observed in this work is not of the first kind.

Anisotropy of the Reynolds Stress Tensor

Stated that the driving mechanism of the secondary flow is the anisotropy of the Reynolds stress tensor, the difference in the magnitude between the glass and the steel pipe of the cross-sectional flow can be explained by analyzing the circumferential Reynolds stress \( \langle u'_{f\theta} u'_{f\theta} \rangle / U_B^2 \) depicted in Figs. 74(a) and (c) for the glass and in Figs. 74(b) and (d) for the steel pipe. For the interpretation of the results the finding of Belt et al. (2012) is recalled which associates the direction of the secondary flow near the pipe wall to the negative gradient of the Reynolds stress tensor, i.e., the negative gradient of \( \langle u'_{f\theta} u'_{f\theta} \rangle / U_B^2 \). The same conclusion can be drawn from the LES of van’t Westende et al. (2007) and the DNS published in the dissertation of Belt (2007) of a horizontal pipe flow with increasing wall roughness from the top to the bottom. In this case the circumferential Reynolds stress had a larger magnitude in the lower than in the upper part of the pipe. Also for this configuration two secondary flow cells developed where the direction of the secondary flow near the wall agreed with the negative gradient of \( \langle u'_{f\theta} u'_{f\theta} \rangle / U_B^2 \), i.e., the fluid was transported from the bottom to the top and thus rotated in the opposite direction compared to the present case. As obvious from Figs. 74(a) and (c) in case of the glass pipe.