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Novel Experimental Techniques for Granular Flow

Kay Buist
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PROEFSCHRIFT

ter verkrijging van de graad van doctor aan de Technische Universiteit Eindhoven, op gezag van de rector magnificus, prof.dr.ir. F.P.T. Baaijens, voor een commissie aangewezen door het College voor Promoties, in het openbaar te verdedigen op donderdag 20 oktober 2016 om 16:00 uur

door

Kay Arnout Buist

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Het onderzoek of ontwerp dat in dit proefschrift wordt beschreven is uitgevoerd in overeenstemming met de TU/e gedragscode wetenschapsbeoefening.
Summary

Novel Experimental Techniques for Granular Flow

Gas-solid contactors are widely used in industry for many chemical and physical processes as; polymerization, cracking, gasification, coating and drying. With the emerging improvements in computational power, numerical techniques and strategies are being developed to cover the challenges across the different length scales. In this work novel non-invasive measuring techniques have been developed to help validate these models.

Magnetic Particle Tracking (MPT) is a particle tracking technique that, other than conventional particle tracking techniques, is inherently safe and an order of magnitude less expensive. MPT tracks a single magnet through sensing the magnetic field strength at a number of sensors and reconstruction of the magnetic field of the magnet. From minimization of the difference of the sensor data and the reconstructed field the most probable position and orientation can be determined.

MPT has been compared to a well established non-invasive monitoring technique; Particle Image Velocimetry (PIV) and a good quantitative agreement was obtained. Rotational motion of granular material in a pseudo 2D fluidized bed modelled with a Discrete Particle Model (DPM) was validated, by comparison with MPT. Because MPT can determine the orientation of a tracer particle it is uniquely suited to study the behaviour of granular systems with non-spherical particles. The hydrodynamic and orientational behaviour of equal volume and density spheres and rods was compared using MPT as well as a newly developed Digital Image Analysis (DIA) technique.

A Constant Temperature Anemometer (CTA) was reconfigured to act as a heat transfer probe. In combination with semi-structured arrays of particles the heat transfer effects of arrays with varying porosity and Reynolds numbers could be studied. Data obtained from Direct Numerical Simulations (DNS) show a remarkable agreement of the heat transfer data obtained from the
reconfigured CTA experiments.

Finally a hybrid collision integration scheme for Discrete Element Model (DEM) was developed that combines the approaches of the well-known hard and soft sphere methods. It was shown that for a typical CFD-DEM simulation the amount of binary contacts is dominant, which allows the use of analytical solutions or a hard sphere approach. The remaining Multi-Body Contacts (MBC) is still substantial and have to be solved with a soft-sphere method. The combination of the two allow the use of a time step in the order of the collision duration. The speedup gained is about a factor 7 to 8.
Samenvatting

Nieuwe Experimentele Technieken voor Granulaire Stroming

Gas-vast contactapparatuur wordt veel gebruikt in de industrie voor chemische en fysische processen zoals; polymerisatie, kraken, vergassen, coatings en drogen. Door continue verbetering van de rekenkracht van computers worden betere modellen en modelleerstrategieën ontwikkeld die de uitdagingen van deze systemen over de verschillende lengteschalen beschrijven. In dit werk worden nieuwe niet-invasieve meettechnieken ontwikkeld die deze modellen helpen te valideren.

Magnetic particle tracking (MPT) is een particle tracking techniek die anders dan conventionele particle tracking technieken intrinsiek veilig en een orde grootte goedkoper zijn. MPT volgt een enkele magneet door het meten van de magneetveldsterkte bij een aantal sensoren en reconstructie van het magneetveld van de magneet. Minimalisering van het verschil van de sensor-data en de reconstructie van het magneetveld levert de meest waarschijnlijke positie en oriëntatie van het deeltje.

De resultaten van de MPT zijn vergeleken met een andere bewezen niet-invasieve meettechniek: Particle Image Velocimetry (PIV) en vertonen een goede kwantitatieve overeenkomst. Rotatie van granulair materiaal in een pseudo 2D gefluïdiseerd bed is gemodelleerd met een Discrete Paricle model (DPM) en gevalideerd door vergelijking met MPT. Omdat MPT de oriëntatie van een deeltje kan bepalen is het bij uitstek geschikt om het gedrag van niet-sferische deeltjes te bestuderen. Het hydrodynamische en oriëntatie gedrag van bollen en staafjes van gelijke volume en dichtheid is vergeleken met MPT alsmede met een nieuw ontwikkkelde Digital Image Analysis (DIA) techniek.

Een Constant Temperature Anemometer (CTA) is geconfigureerd om dienst te doen als warmte-overdrachtsonde. De warmteoverdracht kon hiermee bepaald worden voor semigestuctureerde arrays van deeltjes met verschillende porositeiten en bij verschillende Reynolds getallen. Simulaties
met Direct Numerical Simulations (DNS) vertoonden een opmerkelijk goede overeenkomst met de warmte overdrachts data van de geherconfigureerde CTA experimenten.

Als laatste is een hybride botsings-integratie schema ontwikkeld voor Discrete Element Model (DEM) welke de voordelen van de welbekende harde en zachte bollen methoden combineert. In een typische CFD-DEM simulatie zijn de binaire contacten dominant, waardoor het gebruik van analytische oplossingen of de harde bollen methode mogelijk is. Het restant aan botsingen met meerdere deeltjes tegelijkertijd wordt opgelost met de klassieke zachte-bollen methode. De combinatie van de twee technieken maakt het mogelijk om een tijdstap te nemen in de ordegrootte van de botsingsduur. De snelheidswinst van de simulaties is daarmee een factor 7 tot 8.
Contents

Summary v
Samenvatting vii
Nomenclature xiii

1 Introduction 1
   1.1 Granular flows ............................................ 1
   1.2 Multiscale modelling ........................................ 2
   1.3 Non-invasive measurements techniques ....................... 3
      1.3.1 Whole field techniques ............................... 3
      1.3.2 Particle tracking techniques ........................... 4
   1.4 Outline ..................................................... 4

2 Improved Magnetic Particle Tracking method 7
   2.1 Introduction .................................................. 7
   2.2 Experimental setup .......................................... 9
   2.3 Principle .................................................... 12
      2.3.1 Non-linear optimization ............................... 14
      2.3.2 Filtering and Sampling ................................ 15
      2.3.3 Particle image velocimetry ........................... 16
      2.3.4 Digital image analysis .................................. 16
   2.4 Validation ................................................... 17
      2.4.1 Effect of magnetic moment ............................. 17
      2.4.2 Effect of distance ....................................... 19
      2.4.3 Pendulum motion ......................................... 21
   2.5 Comparison PIV-DIA and MPT ................................. 22
   2.6 Conclusions .................................................. 26
3 Particle rotation in a pseudo 2D fluidized bed

3.1 Introduction ........................................... 29
3.2 Methods ............................................... 31
  3.2.1 Magnetic particle tracking ......................... 31
  3.2.2 Discrete particle modelling ....................... 33
  3.2.3 Hydrodynamic torque ............................ 34
  3.2.4 Rolling friction .................................. 36
3.3 Experimental setup .................................... 37
3.4 Results ............................................... 41
  3.4.1 High superficial velocity $u_0 = 3.5\text{m/s}$ ... 42
  3.4.2 Low superficial velocity $u_0 = 2.5\text{m/s}$ .... 46
3.5 Conclusions ......................................... 47

4 Experimental Techniques for Non-Spherical Particles

4.1 Introduction ........................................... 49
4.2 Setup ............................................... 51
4.3 MPT .................................................. 53
  4.3.1 Results .......................................... 53
4.4 DIA .................................................. 58
  4.4.1 Segregation .................................... 60
  4.4.2 Orientation .................................... 63
4.5 Conclusions ......................................... 65

5 Heat transfer study using Constant Temperature Anemometry

5.1 Introduction ........................................... 67
5.2 Methods ............................................... 70
  5.2.1 Constant Temperature Anemometry (CTA) .......... 70
  5.2.2 Direct Numerical Simulations ..................... 72
5.3 Setup ............................................... 74
5.4 Results ............................................... 75
  5.4.1 Single particle .................................. 76
  5.4.2 Inline array .................................... 79
  5.4.3 Semi-structured arrays .......................... 82
5.5 Conclusion ........................................... 85
6 Hybrid collision integration scheme

6.1 Introduction ................................................. 87
6.2 Classical collision schemes ................................. 89
  6.2.1 Hard sphere scheme .................................... 89
  6.2.2 Soft sphere scheme ....................................... 90
6.3 Hybrid collision integration scheme ......................... 92
  6.3.1 Binary collisions ......................................... 93
  6.3.2 Multibody collisions ..................................... 95
  6.3.3 Overview .................................................. 95
6.4 Results ....................................................... 100
  6.4.1 Speed up & scalability ................................... 100
  6.4.2 Varying restitution coefficient .......................... 101
  6.4.3 Number of contact partners ............................. 102
  6.4.4 Relaxing the classical scheme ......................... 103
6.5 Conclusions ................................................. 104

7 Conclusion and outlook ......................................... 111

Bibliography .................................................. 115

List of publications ........................................... 125

Curriculum Vitae .............................................. 127

Acknowledgements ............................................... 129
Nomenclature

Variables

\( A \) fitting parameter \([-]\)
\( \text{surface area } [m^2] \)
\( B \) fitting parameter \([-]\)
\( \text{collision constant } [1/kg] \)
\( C \) drag coefficient \([-]\)
\( C_p \) heat capacity \([J/Kg \cdot K]\)
\( \vec{F} \) force \([N]\)
\( \vec{H} \) magnetic field \([A/m]\)
\( I \) moment of inertia \([kg \cdot m^2]\)
\( J \) impuls \([kg \cdot m/s]\)
\( L \) length \([m]\)
\( M \) Magnification \([pixels/m]\)
\( \text{mixing index } [-]\)
\( N \) number off \([-]\)
\( O \) occupancy \([-]\)
\( P \) probability function \([-]\)
\( \text{pressure } [N/m^2] \)
\( Q \) quality function \([-]\)
\( \text{heat loss } [W] \)
\( R \) resistance \([\Omega]\)
\( S \) standard deviation \([-]\)
\( St \) sensor signal \([A/m]\)
\( \tilde{S}_p \) source term \([N/m^3]\)
\( \vec{T} \) torque \([N/m]\)
\( T \) temperature \([K]\)
\( V \) volume \([m^3]\)
voltage \([V]\)
c \(\text{integration constant \([-]}\)
d \(\text{diameter \([m]\]}\)
\(\vec{e}\) \(\text{unit vector \([-]}\)
e \(\text{restitution coefficient \([-]}\)
f \(\text{momentum source term \([N/m^3]\]}\)
f \(\text{frequency \([1/s]\]}\)
\(\text{fraction \([-]}\)
h \(\text{heat transfer coefficient \([W/m^2 \cdot K]\]}\)
\(\text{height \([m]\]}\)
k \(\text{spring stiffness \([N/m]\]}\)
\(\text{thermal conductivity \([W/m \cdot K]\]}\)
l \(\text{magnification \([\text{pixel/cm}]\]}\)
m \(\text{mass \([kg]\]}\)
\(\vec{n}\) \(\text{normal \([-]}\)
p \(\text{position \([m]\]}\)
\(\text{pixel \([-]}\)
q \(\text{volumetric heat source \([W/m^3]\]}\)
\(\vec{r}\) \(\text{distance vector \([m]\]}\)
r \(\text{radius \([m]\]}\)
\(\text{reflection count \([-]}\)
s \(\text{pixel displacement \[\]}\)
t \(\text{time \([s]\]}\)
\(\text{tangent \([-]}\)
\(\ddot{u}\) \(\text{velocity \([m/s]\]}\)
\(\dot{v}\) \(\text{velocity \([m/s]\]}\)
\(\ddot{x}\) \(\text{position \([m]\]}\)

\textbf{Greek letters}

\(\beta\) \(\text{drag coefficient \([-]}\)
\(\text{tangential restitution coefficient \([-]}\)
\(\Omega\) \(\text{relative tangential velocity \([m/s]\]}\)
\(\alpha\) \(\text{temperature correction \[%/K\]}\)
\(\alpha_f\) \(\text{thermal diffusivity \([m^2/s]\]}\)
δ overlap [m]
ε porosity [-]
emissivity [-]
ζ damping ratio [-]
η damping coefficient [kg/s]
θ inclination angle [°]
μ magnetic moment [A/m²]
viscosity [Pa s]
friction factor [-]
ρ density [kg/m³]
σ standard deviation [-]
Stefan Boltzmann constant [5.67E-8 W/m² K⁴]
τ stress [N/m²]
φ azimuthal angle [°]
ω solids volume fraction [-]
rotational velocity [rot/s]
frequency [1/s]

Subscripts and superscripts

D, B balance point
a, b particles a and b
amb ambient
c cable
cell
coll collision
circ circles
d dampened
eff effective
ex excess
f fluid
i, j counter
l lead
last duration of a lasting collision
m measured
\begin{itemize}
\item max \quad \text{maximum}
\item mf \quad \text{minimum fluidization}
\item n \quad \text{normal}
\item p \quad \text{particle}
\item ps \quad \text{particle-sensor}
\item s \quad \text{solid support}
\item t \quad \text{theoretical tangential}
\item top \quad \text{top}
\item x, y, z \quad \text{direction}
\item 0 \quad \text{old timestep}
\item 1, 2, 3 \quad \text{resistance leg}
\item 20 \quad \text{at 20 C}
\end{itemize}

\section*{Abbreviations}

\begin{itemize}
\item CTA \quad \text{Constant Temperature Anemometer}
\item DEM \quad \text{Discrete Element Model}
\item DIA \quad \text{Digital Image Analysis}
\item DNS \quad \text{Direct Numerical Simulation}
\item DPM \quad \text{Discrete Particle Model}
\item IB \quad \text{Immersed Boundary}
\item LM \quad \text{Levenberg Marquardt}
\item MPT \quad \text{Magnetic Particle Tracking}
\item MRI \quad \text{Magnetic Resonance Imaging}
\item PEPT \quad \text{Positron Emission Particle Tracking}
\item PIV \quad \text{Particle Image Velocimetry}
\item RPT \quad \text{Radioactive Particle Tracking}
\item SQP \quad \text{Sequential Quadratic Programming}
\end{itemize}

\section*{Dimensionless numbers}

\begin{itemize}
\item \text{Nu} \quad \text{Nusselt number, } \frac{h_d}{\kappa}
\item \text{Pr} \quad \text{Prandtl number, } \frac{c_p \mu}{k}
\end{itemize}
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ra</td>
<td>Rayleigh number</td>
<td>$\frac{g \beta d^3 (T_s - T_\infty)}{\nu \alpha}$</td>
</tr>
<tr>
<td>Re</td>
<td>Reynolds number</td>
<td>$\frac{\rho v d}{\mu}$</td>
</tr>
</tbody>
</table>
This PhD project has been part of the ERC advanced grant, contract no. 247298 (Multiscale Flows), which has been awarded to prof. J.A.M. Kuipers. The topic of this grand was Multiscale modelling of mass and heat transfer in dense gas-solid flows. The project involves modelling of gas-solid flows at three different levels across the relevant length-scales as well as one-to-one comparison of these models with data obtained from non-intrusive measurement techniques. This PhD project was specified to develop novel experimental techniques for granular flow and was strengthened with funding from the 3TU Centre of Excellence: multi-scale phenomena. As such both the development of the techniques as well as simulation results obtained at the various levels are discussed.

1.1 Granular flows

Granular flows are encountered in industry in many processes, for instance; granulation, coating, drying, gasification and polymerization as well as transportation. Also in nature quite a number of phenomena occur that can be classified as granular flow; sand dune formation, river deposits and avalanches. All these processes involve particle-particle interactions and often also gas-solid or liquid-solid interactions. As such understanding and modelling of these processes is very complex involving exchange of momentum, heat and mass from granule to granule or from the solid phase to the liquid/gas phase. The combination of these transport phenomena and the coupling of the separate phases is often not straightforward and changes with the type of model used. The flow properties and overall process behaviour is handled at a very large scale while the relevant physics often occurs at the particle or even sub-particle level. This difference in length scales has resulted in the use of a multiscale modelling approach.
1.2 Multiscale modelling

Figure 1.1 gives an overview of the available models and techniques that are part of the multiscale modelling approach (Van der Hoef et al., 2008). At the smallest scale, Direct Numerical Simulations (DNS) are used to model granular flow without closures. The use of a Eulerian grid that is much smaller than the particles and by enforcing the no-slip and fixed temperature conditions, closures can be derived for the higher scales. This type of model allows for a small number of particles to be simulated such that the effects of clustering, packing density and velocity can be conveniently studied. Different shapes of particles are also possible in which case mutual alignment can be studied. Typically 1-1000 particles are used.

The Discrete Particle Model (DPM) is a technique that uses a combined Eulerian-Lagrangian approach. The particles are represented individually and the fluid is modelled on a Eulerian grid that is typically 3-5 times larger than
the particles. Because of this closures are needed for the momentum, heat and mass transfer. Also for the solids interactions a model is needed to account for energy dissipation due to collisions. In DPM the collisions can be handled individually using either a hard sphere or a soft sphere collision model. The update of the particles motion is done using Newton's equations of motion. For a soft sphere model, which is most often used for its speed, especially in dense granular flow, typically a time step of one tenth the collision duration is needed. DPM currently allows for typically $O(10^6)$ particles.

To allow for simulation of even larger systems the energy dissipation due to collisions has to occur on a larger scale than one particle. As such ensembles of particles are simulated as one whole; stochastic models, or the solids are handled with a separate set of Navier-Stokes equations. The solids are simulated as an interpenetrating fluid and the collisions are handled using the Kinetic Theory of Granular Flow (KTGF). On top of the exchange of transport phenomena between the phases, additional closures are needed for the kinetic energy dissipation.

1.3 Non-invasive measurements techniques

For each of these models it is of paramount importance to conduct proper validation. As such a range of experimental techniques have been developed. Especially the non-invasive measurement techniques are important as they do not hinder the granular flow in any manner (Chaouki et al., 1997). An overview of some of the most important techniques is outlined here. Most of these techniques can be classified as either a particle tracking technique or as a whole field/tomographic technique.

1.3.1 Whole field techniques

Experimental techniques that can produce quasi-instantaneous data for the entire flow field, or at least one plane of the flow field are very powerful techniques. Particle Image Velocimetry (PIV) is probably the most well-known and most used of these techniques. PIV uses a high speed camera to obtain information on optically accessible systems; pseudo 2D. Cross-correlation of two subsequent images allows for analysis of particle velocities and position within a 2D plane. Many hydrodynamic studies have so far been performed with PIV.
for granular flow problems; fluidized and spouted beds. Currently extensions to include mass- and heat transfer using Infrared (IR) Imaging show large potential in studying both the hydrodynamics and heat/mass transfer at the same time. Also extensions to endoscopic PIV have allowed the study of granular flow under high-temperature and high-pressure systems.

Other well-known techniques involve Electrical Capacitance Tomography (ECT) and X-ray tomography as well as MRI. These techniques have allowed the study of 3D geometrical structures in granular flow and as such focus more on the bubble-solids dynamics instead of the particle behaviour.

1.3.2 Particle tracking techniques

Particle tracking techniques focus on the study of a single particle. To get sufficient data for flow characterization often at least 1 hour measurements are needed. Most of these techniques can be used for 3D systems and give full 3D information as well, instead of 1 plane. Both Positron Emission Particle Tracking (PEPT) and (Computer Aided) Radioactive Particle Tracking (CARPT) use nuclear decay of an isotope to study the movement of a particle. Particle Tracking Velocimetry (PTV) like PIV is an optical technique that can capture the movement of individual particles. More exotic techniques involve the tracking of a microwave heated particle with Infrared (IR).

In general these techniques are very powerful, but unfortunately often quite expensive and subject to (severe) safety measures; MRI, X-Ray and radioactive techniques.

In this work we will discuss a new technique that is inherently save and a lot more cost-effective to study particle behaviour, both translation and rotation: Magnetic Particle Tracking (MPT). Second we will show a new technique to study particle-fluid heat transfer, re-configured Constant Temperature Anemometer (CTA) to study heat transfer in granular systems.

1.4 Outline

In this work two novel experimental techniques are discussed; Magnetic Particle Tracking (MPT) and a reconfigured Constant Temperature Anemometer (CTA) for the use of heat transfer experiments. Some key results are presented that so far have been very difficult to obtain with other techniques.
The outline of this thesis is as follows: first the MPT technique will be introduced, showing an improvement on previous results and stretching the limits and capabilities of this technique in chapter 2. In chapter 3 MPT is used in comparison to results from DPM simulations to study the rotational behaviour of spherical particles in a pseudo 2D fluidized bed. In chapter 4 the behaviour of rods and spheres in a 3D cylindrical fluidized bed is studied using MPT. A new Digital Image Analysis (DIA) technique is introduced to study the segregation of a system of rods and spheres of equal size and density, that is capable of determining the orientation as well. Chapter 5 introduces the reconfigured CTA probe and the results on heat transfer of differing packing fractions and superficial velocities. These results are successfully compared with DNS simulations using an Immersed Boundary (IB) method. Finally in chapter 6 a new collisions integration scheme for the DPM is discussed revealing an order of magnitude speed increase with respect to a classical soft sphere collision model.
Chapter 2

Improved Magnetic Particle Tracking method

2.1 Introduction

Gas solid fluidization is an important industrial multiphase operation for various chemical and physical processes in the industry, including gasification, combustion, catalytic cracking, gas phase polymerization, drying and coating. Favourable characteristics include excellent solids mixing, good contacting between gas and solids and excellent heat transfer characteristics. Because these multiphase flows are highly complex, they have been subject to many studies, both experimentally and computationally. Recent advances in computational power and modelling have allowed detailed studies of solids motion, gas-solid interactions and process performance. This consequently asks for more and/or better experimental methods for validation. The outcome of these studies should eventually lead to improvements in operation and design.

Most of the experimental techniques used in dense granular flows rely on non-invasive monitoring techniques. Among these, particle tracking techniques have shown great potential in characterization of dense granular flows: mixers, fluidized- and spouted beds. Positron Emission Particle Tracking (PEPT) (Parker et al., 2008), Radioactive Particle Tracking (RPT), computer aided radioactive particle tracking (CARPT) (Degaleesan et al., 2002) and Particle Tracking Velocimetry (PTV) are the most well known (Chaouki et al., 1997). Recently a new and promising technique was introduced; Magnetic Particle Tracking (MPT). MPT is a technique that has been used in the medical field to study the motility tract and targeted drug delivery (Richert et al., 2009) and originates from the work of Richert et al. (2007). Typically

This chapter is based on Kay A. Buist, A.C. van der Gaag, N.G. Deen, J.A.M. Kuipers., Improved magnetic particle tracking technique in dense gas fluidized beds, AIChE Journal, 60(9) (2014), pp: 3133-3142.
Table 2.1: qualitative comparison of particle tracking techniques

<table>
<thead>
<tr>
<th>Property</th>
<th>PTV</th>
<th>CARPT/RPT/PEPT</th>
<th>MPT</th>
</tr>
</thead>
<tbody>
<tr>
<td>Costs</td>
<td>++</td>
<td>−−</td>
<td>++</td>
</tr>
<tr>
<td>Safety measures</td>
<td>+</td>
<td>−−</td>
<td>+</td>
</tr>
<tr>
<td>Spatial resolution</td>
<td>+</td>
<td>−</td>
<td>−</td>
</tr>
<tr>
<td>Geometry &amp; size setup</td>
<td>−</td>
<td>++</td>
<td>+</td>
</tr>
</tbody>
</table>

This technique uses a small magnetic source, usually a magnetic dipole, the magnetic signal of which can be detected by a series of sensors. Based on these signals a reconstruction of the magnetic field can be made and thus the position and orientation of the magnet can be determined via an appropriate algorithm.

One of the main advantages of the MPT over other particle tracking techniques is its relatively low cost and the ease of use with respect to PEPT or RPT and its compatibility with 3D systems with respect to PTV. In PEPT and RPT the sensors and the use, preparation and handling of radioactive tracer material introduces high cost and special safety issues. In MPT the use of tri-axis Anisotropic Magneto Resistive (AMR) sensors and neodymium magnets reduces the costs by at least a factor 10 and has no safety issues. MPT, however, is restricted by the use of rather large magnetic markers, a topic which will be addressed in this work. The magnetic field strength sensed at the sensor does not only depend on the strength of the magnet and the distance to the sensors, but also on the relative orientation of the magnet to the sensor. This allows to also study rotational motion, which might be especially interesting for non-spherical particles. Table 2.1 summarizes the advantages and disadvantages of several particle tracking techniques.

The use of MPT in dense granular flow has first been proposed by Mohs et al. (2009) in a spout fluidized bed. They were able to follow a rather large magnetic marker at 62.5 Hz. Halow et al. (2012) studied segregation effects in fluidized beds using just four Hall effect sensors. Finally Neuwirth et al. (2013) have used MPT to enable comparison of measured particle motion in a rotor granulator with simulated results obtained from Discrete Element Model (DEM). An increase of the measurement rate to 200 Hz in their study revealed an increase in accuracy. Furthermore, Idakiev and Mörl (2013) have recently used MPT to study particle trajectories and solids translation motion.
in a prismatic spouted bed and a fluidized bed.

For MPT to compete as a technique for particle tracking in granular flow, the limits of the technique have to be established and expanded. Also a first comparison with established techniques for granular flow is currently lacking. Hu et al. (2010) have studied the effects of multiple non-linear optimization algorithms build for speed mostly. In this work we will present a new algorithm which is able to determine the position and orientation more accurately and more precise. The new MPT technique will be tested using a set of comprehensive tests and will finally be compared with a well-established technique; Particle Image Velocimetry combined with Digital Image Analysis (de Jong et al., 2012; Van Buijtenen et al., 2011) (PIV-DIA).

The organization of this chapter is as follows. In section 2.2, the experimental setup will be described whereas in section 2.3 the principle of the two experimental techniques will be discussed. In section 2.4, the new MPT analysis technique will be tested and finally in section 2.5, the results of the MPT and PIV-DIA techniques will be compared.

### 2.2 Experimental setup

For the MPT technique two sensor arrays are used. A pseudo 2D configuration to measure the particle motion for a pseudo 2D fluidized bed setup which is suitable to enable comparison with PIV-DIA. A 3D setup is used to test the limits of the experimental technique.

The 2D setup is presented in figure 2.1 and an overview of all settings and properties is given in table 2.2. The MPT sensor setup consists of an array of 6x4 tri-axis AMR-sensors, giving in total 72 signals. Setup and control are courtesy of Matesy GmbH, the setup is capable of measuring at 1000 Hz. The 2D sensor array is mounted to the frame of the pseudo 2D bed. A minimum distance of 0.02 m between the sensors and the domain of interest was maintained.

The pseudo 2D fluidized bed setup has dimensions of 0.3 x 0.015 x 1.0 m (W x D x H). The depth is chosen to be small enough to exhibit 2D behaviour and large enough to avoid bridging effects. The bottom is covered by a porous distributor plate of 3 mm thickness and an average pore size of 10 μm. All other parts of the setup are made of aluminium and non-magnetic stainless
<table>
<thead>
<tr>
<th><strong>Table 2.2: Settings and Parameters</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Fluidized Bed</strong></td>
</tr>
<tr>
<td>Width</td>
</tr>
<tr>
<td>Height</td>
</tr>
<tr>
<td>Depth</td>
</tr>
<tr>
<td>Porous plate</td>
</tr>
<tr>
<td>Average pore size</td>
</tr>
<tr>
<td>Mass flow controller (max capacity)</td>
</tr>
<tr>
<td>Material front plate</td>
</tr>
<tr>
<td>Other materials</td>
</tr>
<tr>
<td><strong>High speed camera</strong></td>
</tr>
<tr>
<td>Effective resolution</td>
</tr>
<tr>
<td>Exposure time</td>
</tr>
<tr>
<td>Inter-frame time</td>
</tr>
<tr>
<td>Interogation size (multipass)</td>
</tr>
<tr>
<td><strong>MPT sensor array</strong></td>
</tr>
<tr>
<td>Sensor type</td>
</tr>
<tr>
<td>Amount</td>
</tr>
<tr>
<td>Frequency</td>
</tr>
<tr>
<td>dimensions</td>
</tr>
<tr>
<td><strong>Particles</strong></td>
</tr>
<tr>
<td>Bed material size</td>
</tr>
<tr>
<td>Density</td>
</tr>
<tr>
<td>Minimum fluidization velocity</td>
</tr>
<tr>
<td>Magnetic marker size</td>
</tr>
<tr>
<td>Density</td>
</tr>
<tr>
<td>Magnetic moment</td>
</tr>
<tr>
<td>Minimum fluidization velocity</td>
</tr>
</tbody>
</table>
steel parts. The flow rate is controlled with a mass flow controller with a maximum capacity of 1200 l/min. The front plate is made of glass for visual access.

To be able to compare the MPT with the PIV-DIA technique the bed is illuminated using 4 LED-arrays for homogeneous illumination. Images are recorded using a LaVision HSG4M high speed camera with an image resolution of 2048 x 2048 pixels and images are captured at 200 Hz. Analysis of the images is done in Davis 8.1.7 and Matlab.

The 3D sensor array consists of 4 rings of 6 triaxis AMR sensors with a total height of 0.45 m and a distance of 0.26 m between opposing sensors. Figure 2.2 is a photo of the 3D sensor array, clearly depicting the 4 rings. Each ring contains 6 boxes with 3 sensors each, to a total of 72 sensors for the
whole array. All the triaxis sensors are connected to a control box which reads the data and sends it to a lab computer. Before each experiment the offset of the sensors is determined, by measuring the field of an empty domain. After offset determination a magnetic marker can be added to the domain and the change in magnetic field can be measured.

2.3 Principle

The principle of the MPT measurement technique relies on tracking of a single magnetic marker. Evaluation of the quasi-static magnetic field results in a position estimate. This is an inverse problem with five degrees of freedom, three for position and two for orientation, (see figure 2.3). When the magnetic moment of the marker is unknown this can act as a sixth degree of freedom. The magnetic field is measured by several sensors that are positioned in a known configuration. The theoretical signals are calculated using the derivation of a magnetic field of a magnetic dipole at sufficient distance from the dipole:

$$\hat{H}(\vec{e}_p, \vec{r}_{ps}) = \frac{1}{4\pi} \left( -\frac{\mu_m \vec{e}_p}{|\vec{r}_{ps}|^3} + \frac{3\mu_m (\vec{e}_p \cdot \vec{r}_{ps}) \vec{r}_{ps}}{|\vec{r}_{ps}|^5} \right)$$  \hspace{1cm} (2.1)
With $\vec{r}_{ps} = \vec{r}_p - \vec{r}_s$, $\mu_m$ the magnetic moment of the marker, $\vec{e}_p$ the orientation unit vector of the magnet, calculated via a transformation of the angles; $\phi$ and $\theta$ from the spherical to the Cartesian coordinate system.

By multiplication of this magnetic field with the orientation of the sensor, the signal strength can be estimated:

$$S_t = \vec{H}(\vec{e}_p, \vec{r}_{ps}) \cdot \vec{e}_s$$  \hspace{1cm} (2.2)

To determine the position and orientation, the theoretical signal strengths ($S_t$) given by equation 2.2 are compared to the actual signals given by the 72 sensors ($S_m$). The difference between the two fields is minimized using a quality function:

$$Q = \sum_{i=1}^{72} \frac{((S_{m,i} - \langle S_m \rangle) - (S_{t,i} - \langle S_t \rangle))^2}{\Delta S_{m,i}^2}$$  \hspace{1cm} (2.3)

The quality function 2.3 is corrected for deviations in each individual sen-
sor given by a min/max deviation \( \frac{1}{\Delta S_{m,i}^2} \), this ensures that less accurate sensors, have less influence on the quality function. Secondly, the quality function is corrected for stray fields using a gradiometer \( \langle S \rangle \).

### 2.3.1 Non-linear optimization

Hu et al. (2010) have studied several optimization algorithms among which a linear function for the initial guess and several non-linear optimization methods to determine the optimum. They found the Levenberg-Marquardt (LM) algorithm to be both fast and accurate. For research purposes the algorithm does not need to be fast and hence different optimization algorithms can be investigated. The effectiveness of the optimization algorithm can be improved by providing as much information from the experiment as possible. Besides the 72 sensor signals this also includes the bounds for the possible marker positions. Some non-linear optimization methods allow such constraints to the solution. In this work, the strength of the Sequential Quadratic Programming (SQP) (Nocedal and Wright, 2006) algorithm will be shown. For the pseudo 2D setup the following constraints have been set, slightly outside the physical domain to allow for error margins:

\[
-0.2 \leq x \leq 0.2 \tag{2.4}
\]
\[
-0.3 \leq y \leq 0.3
\]
\[
0.01 \leq z \leq 0.07
\]

For the 3D setup the following constraints have been set:

\[
\sqrt{x^2 + y^2} \leq 0.13 \tag{2.5}
\]
\[
0.3 \leq z \leq 0.3
\]

In the LM-algorithm the solution of equation 2.1 is done by solving for the positions \( x, y, z \) and the angles \( \varphi, \theta \). Because \( \varphi \) is periodic, estimates across this periodic boundary, 180 to -180, are difficult to solve and result in erroneous solutions. The SQP algorithm allows for the addition of an extra degree of freedom by changing to the orientation unit vector and adding a
non-linear constraint for the norm of the vector:

\[ |\bar{e}_p| = 1 \]

\[ -1 \leq e_x \leq 1 \]
\[ -1 \leq e_y \leq 1 \]
\[ -1 \leq e_z \leq 1 \]

These three degrees of freedom are tied by one extra function, in effect reducing the total number of degrees of freedom back to five.

### 2.3.2 Filtering and Sampling

In particle tracking techniques the sensor signals are often filtered to suppress high noise levels. Among those, wavelet filters are often used for their capability to handle sharp transitions in the signal (Degaleesan et al., 2002). Depending on the size of the magnet the signal on the sensors can be quite noisy and smart ways of filtering have to be used. The Levenberg-Marquardt method uses an averaging filter, which in principle reduces the measuring frequency from 1000 Hz to 50 or 200 Hz. We found that the use of a wavelet filter allows for smoother signal data and increases the accuracy of the optimization method. The wavelet toolbox of Matlab is used to separate noise from the signal.

### Initialization

Gradient-search methods like the LM and SQP algorithms, need an initial estimate to converge to a local minimum of the target function 2.3. At the beginning of the analysis the algorithm is initialized using a multistart method, a functionality in Matlab. This multistart method uses multiple starting positions to find the global minimum. For any consecutive time step, the previous time step is used as an initial estimate. However, if the algorithm is unable to converge or the quality function is too high, the algorithm is set to reinitialize. Principally, if the algorithm finds its minimum on the boundary/constraint of the setup, this solution must be seen as erroneous and the algorithm is also set to reinitialize. Any final solution at the physical constraints is seen as an outlier.
2.3.3 Particle image velocimetry

The results of the MPT will be compared to results of an established technique; combined Particle Image Velocimetry (PIV) and Digital Image Analysis (DIA) (Van Buijtenen et al., 2011; de Jong et al., 2012). PIV is a non-intrusive optical technique that provides the displacement of particles between two consecutive images of a high-speed camera. For analysis the images are split in interrogation areas, where a cross-correlation function is used to determine the most likely displacement. In this study, interrogation areas of 64x64 pixels are used with 50% overlap. The instantaneous particle velocity is determined from the particle displacement, with $M$ the image magnification in pixels/m:

$$\bar{v}_p(x, t) = \frac{s_p(x, t)}{M \Delta t}$$ (2.7)

Outliers were removed using a median filter. PIV does not account for differences in dense and dilute areas, which would result in averaged particle velocities biased towards dilute areas where high velocities generally occur. To correct for this, Digital Image Analysis (DIA) is used. DIA is able to determine the local solids fraction of a cell.

2.3.4 Digital image analysis

The digital image analysis technique used in this work is based on the algorithm of Van Buijtenen et al. (2011) and de Jong et al. (2012). Given the
intensity of the interrogation area, a 2D or apparent particle volume fraction is obtained for each interrogation area. Afterwards a correction for 2D to 3D particle volume fraction is used, following equation 2.8

\[ \varepsilon_{p,3D} = \min \left( 0.6, \frac{A \varepsilon_{p,2D}}{1 - \frac{1}{B} \varepsilon_{p,2D}} \right) \]  

(2.8)

An example of the conversion of an original image to a 3D solids volume fraction is given in figure 2.4. Combining the information of the DIA with that of PIV results in a weighted average velocity following equation 2.9

\[ \langle \bar{v}_p \rangle_{i,j} = \frac{\sum_{i,j} \bar{v}_p(x,t) \varepsilon_{p,3D}}{\sum_{i,j} \varepsilon_{p,3D}} \]  

(2.9)

This weighted velocity is comparable to the velocity obtained with MPT as it is no longer biased by differences in solids volume fraction.

2.4 Validation

2.4.1 Effect of magnetic moment

To study the effect of the magnetic moment on the performance of the MPT technique, magnets with different sizes and thus magnetic moments where
Table 2.3: Properties of magnetic markers

<table>
<thead>
<tr>
<th>No.</th>
<th>Magnet shape</th>
<th>Magnet diameter mm</th>
<th>Particle diameter mm</th>
<th>Particle density kg/m³</th>
<th>Magnetic moment Am²</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>sphere</td>
<td>2</td>
<td>3</td>
<td>3300</td>
<td>0.003</td>
</tr>
<tr>
<td>2</td>
<td>sphere</td>
<td>3</td>
<td>3.5</td>
<td>4950</td>
<td>0.013</td>
</tr>
<tr>
<td>3</td>
<td>sphere</td>
<td>3.5</td>
<td>4.8</td>
<td>2900</td>
<td>0.021</td>
</tr>
<tr>
<td>4</td>
<td>sphere</td>
<td>4</td>
<td>4</td>
<td>7400</td>
<td>0.03</td>
</tr>
<tr>
<td>5</td>
<td>cylinder</td>
<td>2</td>
<td>10.2</td>
<td>1500</td>
<td>0.05</td>
</tr>
<tr>
<td>6</td>
<td>cylinder</td>
<td>2</td>
<td>12</td>
<td>1550</td>
<td>0.18</td>
</tr>
</tbody>
</table>

positioned in the centre of the 3D sensor array on top of a platform in between the second and third ring. A schematic representation is given in Figure 2.5. The properties of the different markers used in this study are given in Table 2.3. Using the SQP and LM algorithms the spread in data points was determined by looking at the standard deviation of the data positions in x- and y-direction, by sampling the data at 50 Hz. The results are shown in Figure 2.6, depicting the error of the analysis as a function of the magnetic moment for the two different non-linear optimization schemes.

Figure 2.6 shows a first order dependency of the magnetic field with the magnetic moment, which was expected. It can also be seen that for this most extreme case (largest distance from the sensors), for low magnetic moments near 0.01 Am², the error rapidly increases to 10 mm, which would be unsuited for actual experiments in fluidized beds.

To better display the power of the SQP analysis, the scatter of the 0.013 Am² marker (no. 2) is shown in Figure 2.7 for the LM and SQP Algorithms, using the data sampled at 200 Hz. The LM method is less accurate and can reach ±∞, which happens three times. Furthermore 1 % of all LM data falls outside of the physical bounds of the setup. The SQP method is able to contain all position calculations within physical bounds and is a factor two more accurate, which is possible by addition of constraints to the optimization function and using smart filtering. In general the SQP method is better suited to determine the position of a stationary marker.
2.4.2 Effect of distance

Similar experiments were performed for two of the markers (no. 4 and 6) with magnetic moments of 0.03 Am$^2$ and 0.18 Am$^2$, to study the effect of the relative distance of the magnets with respect to the sensors. The markers were positioned with increasing distance from one of the sensors as depicted in Figure 2.5. The results are shown in Figure 2.8. The results for the largest marker are acceptable as only a small decrease in accuracy was found with increasing the relative distance. However, for the smaller marker the error in the analysis of the position increases rapidly to 2.5 mm, when the marker is positioned towards the centre of the setup. This clearly indicates the importance of a proper design of the sensor array combined with a proper choice of marker with respect to the domain of interest.

Furthermore, no radical effects of the orientation were found in the 3D setup; the results follow a similar trend as the particle position. An endurance test for the system was performed and no decrease in performance or signal drift was found for two hours.
Figure 2.7: Scatter of x,y-positions for LM and SQP algorithms at 200 Hz sampling (top), where the red circle indicates the radial position of the sensors, and histograms of the found locations with respect to the centre of the setup (bottom).
2.4.3 Pendulum motion

To study the performance of the MPT as a particle tracking technique, movement of the magnet was induced. In a second test case a magnetic marker was suspended from a thin wire and given a swing. The resultant pendulum motion was compared with a dampened harmonic oscillator function, for the sideways motion (x):

\[ x = e^{-\gamma t} a \cos(\omega t - \alpha) \]  \hspace{1cm} (2.10)

The two smallest markers, i.e. with the smallest magnetic moment: \( \mu = 0.013 \) and \( \mu = 0.003 \text{ Am}^2 \), have been used in combination with the 2D sensor array. Note that the pseudo 2D setup and sensor array allow for a short distance between the markers and the sensor array, giving good signal quality, even with small magnetic moments.

The sideways motion of the magnetic marker with \( \mu = 0.013 \text{ Am}^2 \) is shown in Figure 2.9. A very well behaved dampened harmonic motion can be observed and it can be seen that the fit with equation 2.10 is very good. The marker with \( \mu = 0.003 \text{ Am}^2 \) is shown in Figure 2.10. For comparison results from both the LM and the SQP algorithms are shown. The LM algorithm has difficulties to properly locate the marker and sometimes shows some strange
Figure 2.9: Results of the pendulum swing with a marker with a magnetic moment of 0.013 Am$^2$, using SQP analysis. Fitted with a dampened harmonic oscillator, equation (3.10), with R$^2$=99.7 %.

peaks at the end of the swing, which is near to the edge of the 2D sensor array. The inability of the LM algorithm can be attributed to the lack of constraints. By adding these constraints via the SQP algorithm the optimization converges to the correct point. This can clearly be seen in Figure 2.10, where for the SQP algorithm a smooth profile can be seen. The fit is not as good as for the marker with magnetic moment $\mu = 0.013$ Am$^2$, but still a remarkable fit with the motion of a dampened harmonic oscillator is found.

2.5 Comparison PIV-DIA and MPT

As a true performance test the MPT was compared to PIV-DIA, a well-established measurement technique. A magnetic marker was fluidized in a pseudo 2D fluidized bed for 1 hour for the MPT and a mere 25 seconds for the PIV-DIA. This results in an average of 5000 data points per interrogation area for PIV-DIA and 230 for MPT. The properties of the magnetic marker and the bed material are given in Table 2.3. A magnetic marker with $\mu = 0.0125$ Am$^2$ was chosen as from the pendulum swing we already found that this marker was easy to follow. The minimum fluidization velocity of the bed material is 1.7 m/s, determined with standard pressure drop analysis. The estimated minimum fluidization velocity of the magnetic marker is 1.82 m/s using the Beetstra correlation Beetstra et al. (2007). To avoid segregation of the magnetic marker, background velocities $u_{bg}$ of 2.5 and 3.5 m/s have been used.
Figure 2.10: Results of the pendulum swing with a marker with a magnetic moment of 0.003 Am$^2$, using LM analysis; top, and SQP analysis bottom, fitted with a dampened harmonic oscillator, equation (3.10), with R$^2$=98.5%.

The time-averaged velocity fields of the fluidized beds obtained with the two techniques are shown in figure 2.11, fluidized with a background velocity of 2.5 m/s. High particle velocities can be found in the centre of the bed, where the bubbles predominately rise. The particle velocities in the annulus are very low. A larger part of the flow seems to come from the right side of the bed, which can be attributed to maldistribution of the distributor plate. Still the typical circulation patterns are clearly obtained. Overall the results of the MPT and PIV-DIA compare very well.

Figure 2.12 and 2.13 show the vertical velocity components obtained from the two techniques at three different heights in the pseudo 2D bed. These results reveal very good agreement between the two techniques. At low velocities some deviations for the MPT can be seen which can be attributed to the larger error margins, which can be expected from the magnetic marker position determination and the lower number of data points per interrogation area.
The large velocities in the centre of the bed compare very well however, especially for the experiment with a background velocity of 3.5 m/s.

The solids volume fractions were obtained from MPT and DIA as well using equations 2.8 and 2.9 respectively. Figure 2.14 shows the time-averaged solids fraction in the fluidized bed. The dense packing in the annulus can be clearly seen, also the slight maldistribution of the distributor plate shows again with both techniques. The DIA technique is however much more smooth which is due to the larger amount of data available for averaging. The MPT technique has fewer data points which is reflected in this contour plot.

Figure 2.15 shows the direct comparison of the solids volume fractions of all interrogation areas. In this parity plot the lack of data points for the MPT shows more clearly. Especially in the dense zone the MPT sometimes has a lower solids volume fraction, the general trend however is quite clear and shows a reasonable agreement between MPT and DIA based results. The results of the MPT in general compares very well to PIV-DIA qualitatively. Quantitatively the particle velocities compare very well, a quantitative de-
Figure 2.12: Comparison of averaged particle velocity for PIV and MPT in vertical direction at three cross-sections of the bed. \( u_{bg} = 2.5 \) m/s.

Figure 2.13: Comparison of averaged particle velocity for PIV and MPT in vertical direction at three cross-sections of the bed. \( u_{bg} = 3.5 \) m/s.
Figure 2.14: Contour plots of the solids volume fraction in the pseudo 2D fluidized bed, left; PIV-DIA, right; MPT, $u_{bg} = 2.5 \text{ m/s}$.

scription of the solids fraction with MPT is currently not able to match with DIA. Possibly with longer measurement time, yielding more data points per interrogation area, this might be countered.

2.6 Conclusions

The newly developed analysis tool for the Magnetic Particle Tracking technique (MPT) using Sequential Quadratic Programming (SQP) and wavelet filtering has been presented and extensively tested. It was shown that the strength of the MPT depends heavily on the magnetic moment ($\mu$) of the marker and the relative distance to the sensor array. Furthermore the newly developed method for data analysis, SQP in combination with wavelet filtering shows a great improvement on the results, owing largely to the addition of physical constraints to the non-linear optimization function.

The results of the Magnetic Particle Tracking technique (MPT) have been compared for a pseudo 2D fluidized bed with a well-established non-invasive measuring technique for granular flow: particle image velocimetry (PIV) and digital image analysis (DIA). The results compare well, showing the strength of the MPT for measuring granular flow behaviour.
Figure 2.15: Parity plot of the solids fractions obtained with MPT and DIA. $u_{bg} = 2.5$ m/s

In the next chapter results on the rotational behavior of spheres are presented and compared to results from a Discrete Particle Model.
Chapter 3

Particle rotation in a pseudo 2D fluidized bed

3.1 Introduction

In many industries fluid-solid interactions are of great importance, for instance in drying, granulation or pelletization, combustion and food processing. Often the solids phase is non-ideal and composed of non-spherical particles. This makes accurate prediction of the solids motion using CFD modelling difficult. Particularly the effect of the relative orientation of the particle to the flow direction on the drag and lift is difficult to assess. Secondly, lack of experimental data on the orientation and rotational behaviour makes validation difficult if not impossible. In this paper we will discuss, for ideal spherical particles, the rotational behaviour and orientation in a pseudo 2D fluidized bed based on experimental data obtained with a Magnetic Particle Tracking (MPT) technique. We will also compare the results with data obtained from a Discrete Particle Model (DPM).

Attempts at studying the rotational behaviour of solids in granular flow have been made with moderate success. Using Particle Tracking Velocimetry (PTV) Wu et al. (2009) have been able to study rotation of 500 µm particles in a circulating fluidized bed. Phillips et al. (2014) have used Laser Doppler Anemometry (LDA) to study the rotation of 150 µm oil particles. However these techniques are restricted to use in systems with optical access. Yang et al. (2008b) have used a multi Positron Emission Particle Tracking (multi-PEPT) technique to study the motion of 12 mm cubes in a rotating can. By embedding three markers in the cube the relative orientation could be

This chapter is based on Kay A. Buist, T.W. van Erdewijk, N.G. Deen, J.A.M. Kuipers., Determination and comparison of rotational velocity in a pseudo 2-D fluidized bed using magnetic particle tracking and discrete particle modeling, AIChE Journal, 61(10) (2015), pp: 3198-3207.
determined. The technique is based on correlating the trajectories of the back-to-back gamma rays. By removing the trajectories of the strongest tracer the position of the second and third tracer could be determined. Unfortunately, the minimum relative distance between the tracers is limited to 5 mm. Yang et al. (2008b) have been able to determine translational and rotational motion of 12 mm cubes at 40 Hz with 6 mm standard deviation errors, with translation and rotational velocities up to 0.5 m/s and 50 rpm.

Magnetic Particle Tracking (MPT) on the other hand is by its nature capable of determining the orientation with no need to modify the tracer particles either by adding markers or applying a pattern on the particle surface. The position and orientation of the magnet induces a distinct magnetic field (Buist et al. (2014)). This allows the use of tracer particles in the order of a few millimetres in size. Neuwirth et al. (2013) have shown the capability of determining the translational and rotational velocity of 6 mm spheres in a rotor granulator. In their study they compared the results with a Discrete Element Method, and found a good comparison for the spread in rotational velocities in the rotor granulator.

In the DPM the particle translation and rotation are described by Newton’s second law of motion. So far, mostly the translation was studied, as this is the dominant factor in describing the particle dynamics. Questions have arisen whether rotation has any influence at all (Jajcevic et al., 2013). Van Buijtenen et al. (2011) found that the near wall translational velocity predicted by the DPM does not match well with experiments for the case of a spout-fluidized bed. They thought this was a problem related to the friction and increased the particle-wall friction for the whole system. Goniva et al. (2012) opt for a different explanation and implemented a model to describe rotational friction. Both studies reveal that changing either one of the parameters increases the accuracy in the translation of the DPM for a pseudo 2D setup. However, the most noticeable effect should be in the rotational behaviour which was not directly studied, due to lack of experimental data. With the addition of information on the rotation of particles in granular flows it is possible to look at the completeness of the DPM and more specifically on the role of the different frictional forces.

This chapter is organized as follows. In the methods section we will discuss the MPT technique and the DPM. In the section experimental setup we will
discuss the pseudo 2D fluidized bed, the sensor array and the Helmholtz coil. Thereafter, the results will be presented and conclusions will be summarized.

3.2 Methods

3.2.1 Magnetic particle tracking

![Figure 3.1: Schematic representation of the principle behind magnetic particle tracking.]

The principle of the MPT technique has been thoroughly discussed in chapter 2. We will give a short summary here. A schematic representation of the technique is given in figure 3.1. A magnetic tracer particle is added to the fluidized bed. This magnetic tracer particle will induce a quasi-static magnetic field at the sensor given by equation 3.1:

\[
\vec{H}(\vec{e}_p, \vec{r}_{ps}) = \frac{1}{4\pi} \left( -\frac{\mu_m \vec{e}_p}{|\vec{r}_{ps}|^3} + \frac{3\mu_m (\vec{e}_p \cdot \vec{r}_{ps}) \vec{r}_{ps}}{|\vec{r}_{ps}|^5} \right) \tag{3.1}
\]

Where \( \vec{r}_{ps} = \vec{r}_p - \vec{r}_s \) is the relative distance of the tracer particle to the sensor, \( \mu_m \) is the magnetic moment of the tracer particle, and \( \vec{e}_p \) is the orientation...
unit vector of the magnet, calculated via a transformation of the angles; $\phi$ and $\theta$ from the spherical to the Cartesian coordinate system. Equation 3.1 gives the magnetic field. However, to obtain an estimate of the sensor output $S_t$ the magnetic field $\vec{H}$ has to be multiplied with the orientation of the sensor $(\vec{e}_s)$ in this field:

$$S_t = \vec{H}(\vec{e}_p, \vec{r}_{ps}) \cdot \vec{e}_s$$ \hspace{1cm} (3.2)

Evaluation of this field at the sensor positions will result in an estimate of the position and orientation. By comparing the result of the theoretical magnetic field strength at the sensor with the measured value, the most probable position and orientation can be determined. This is an inverse problem with 5 degrees of freedom that can be solved by minimizing the following quantity:

$$Q = \sum_{i=1}^{72} \frac{((S_{m,i} - \langle S_m \rangle) - (S_{t,i} - \langle S_t \rangle))^2}{\Delta S_{m,i}^2} \hspace{1cm} (3.3)$$

The quality function (3.3) is corrected for the standard deviation in each individual sensor signal $(\frac{1}{\Delta S_{m,i}^2})$, this ensures that less accurate sensors have less influence on the quality function. Second, the quality function is corrected for stray fields using a gradiometer $(\langle S \rangle)$. Equation 3.3 is a function that is bounded between zero and infinity. To increase the accuracy and simplicity of the minimization function, we applied a function that calculates the probability of finding a tracer particle at position $x, y, z$ with orientation $\phi, \theta$ from the mean value of a sensor and the standard deviation of the sensor data, following:

$$P = \frac{\sum_{i=1}^{72} \text{erf} \left( \frac{S_{m,i} - S_{t,i}}{\sigma_{S_{m,i}}} \right)}{N} \hspace{1cm} (3.4)$$

Equation 3.4 signifies the average of all the probabilities of finding $S_{t,i}$ given $S_{m,i}$ and $\sigma_{S_{m,i}}$. The main advantage of equation 3.4 over equation 3.3 is that determining the probability allows for a minimization function bound between 0 and 1 instead of 0 and infinity and directly relates the quality of the determined position and orientation in terms of the standard deviation or noise in the signal.

Using sequential quadratic programming (SQP) as the minimization algorithm, the most likely position and orientation of the tracer particle can be
determined. With the SQP method constraints to the solution can be set. For the pseudo 2D setup the following constraints have been set, slightly outside the physical domain to allow for error margins:

\[
0 - \Delta x \leq \frac{x}{W} \leq 1 + \Delta x \\
0 - \Delta y \leq \frac{y}{D} \leq 1 + \Delta y \\
0 - \Delta z \leq \frac{z}{H} \leq 1 + \Delta z
\] (3.5)

For the orientation, formal constraints can be set for the unit vector. By adding a constraint for the norm of the vector the total degrees of freedom remain five \((x,y,z,\phi,\theta)\).

\[
|\bar{e}_p| = 1 \\
-1 \leq e_x \leq 1 \\
-1 \leq e_y \leq 1 \\
-1 \leq e_z \leq 1
\] (3.6)

### 3.2.2 Discrete particle modelling

In the discrete particle model the gas phase is described by the volume-averaged Navier-Stokes equations (Deen et al., 2007):

\[
\frac{\partial}{\partial t} (\varepsilon_f \rho_f) + \nabla \cdot (\varepsilon_f \rho_f \bar{u}) = 0
\] (3.7)

\[
\frac{\partial}{\partial t} (\varepsilon_f \rho_f \bar{u}) + \nabla \cdot (\varepsilon_f \rho_f \bar{u} \bar{u}) = -\varepsilon_f \nabla P - \nabla \cdot (\varepsilon_f \bar{f} \bar{f}) + \bar{S}_p + \varepsilon_f \rho_f \bar{g}
\] (3.8)

With \(S_p\) a source term for the momentum exchange between particles and the gas:

\[
S_p = \sum \frac{\beta V_p}{1 - \varepsilon_f} (\bar{v}_p - \bar{u}) \delta(\bar{r} - \bar{r}_p)
\] (3.9)
The drag coefficient, $\beta$, is calculated using the Ergun (1952) and Wen and Yu (1966) equations:

$$F = \frac{\beta d_p^2}{\mu} = 150 \frac{(1 - \varepsilon_f)^2}{\varepsilon_f} + 1.75 (1 - \varepsilon_f) \text{Re}_p$$

$$F = \frac{\beta d_p^2}{\mu} = \frac{3}{4} C_D \text{Re}_p (1 - \varepsilon_f) \varepsilon_f^{-2.65},$$

$$C_D = \max \left( \frac{24}{\text{Re}_p} \left( 1 + 0.15 \text{Re}_p^{0.687} \right), 0.44 \right)$$

$$\text{Re}_p = \frac{\varepsilon_f \rho_f |\bar{u} - \bar{v}_p| d_p}{\mu_f}$$

(3.10)

The particle phase is described using Newton’s equations:

$$m_p \frac{d^2 \bar{r}_p}{dt^2} = -V_p \nabla p + \frac{\beta V}{1 - \varepsilon_f} (\bar{u} - \bar{v}_p) + m_p \ddot{g} + \sum F_{ab}$$

(3.11)

$$I_p \frac{d^2 \bar{\theta}_p}{dt^2} = \bar{T}_p + \bar{T}_h$$

(3.12)

The forces in equations 3.11 and 3.12 represent the far field pressure force, the drag force, the gravity force and the contact forces. $\bar{r}_p$ is the particle position, $\bar{\theta}_p$ is the orientation $I_p$ is the inertia, $\bar{T}_p$ the torque due to collisions and $\bar{T}_h$ the hydrodynamic torque. The particle contact model is adopted from Cundall and Strack (1979):

$$\bar{F}_{ab,n} = -k_n \delta_n \bar{n}_{ab} - \eta_n \bar{v}_{ab,n}$$

(3.13)

$$\bar{F}_{ab,t} = \min \left( -k_t \delta_t \bar{t}_{ab} - \eta_t \bar{v}_{ab,t}, -\mu_f \bar{F}_{ab,n} \bar{t}_{ab} \right)$$

(3.14)

$$\bar{T}_p = R_a \bar{n}_{ab} \bar{F}_{ab,t}$$

(3.15)

The normal and tangential spring stiffness for each of the particle sizes are chosen such that under the given conditions the maximum particle overlap is always less than 1% of the particle diameter, for a maximum relative velocity of 1 m/s. For a more complete overview the authors refer to Deen et al. (2007).

Table 3.1 gives an overview of the parameters used in the simulations.

### 3.2.3 Hydrodynamic torque

The discrete particle model described in the previous section does not contain a coupling between the rotation of the particle and the fluid phase. In literature this coupling has consistently been neglected as it is expected to have
Table 3.1: Overview of simulation parameters.

<table>
<thead>
<tr>
<th>System properties</th>
<th>Particle properties</th>
</tr>
</thead>
<tbody>
<tr>
<td>Width 0.3 m</td>
<td>d_p 3.0 mm</td>
</tr>
<tr>
<td>Depth 0.015 m</td>
<td>ρ_f 1.2 kg/m³</td>
</tr>
<tr>
<td>Height 1.0 m</td>
<td>μ_f 1.8 · 10^{-5} kg/ms</td>
</tr>
<tr>
<td>N_x 30</td>
<td>ρ_p 2600 kg/m³</td>
</tr>
<tr>
<td>N_y 2</td>
<td>k_n 12000</td>
</tr>
<tr>
<td>N_z 100</td>
<td>k_t 2800</td>
</tr>
<tr>
<td></td>
<td>e_n 0.97</td>
</tr>
<tr>
<td></td>
<td>e_t 0.33</td>
</tr>
<tr>
<td></td>
<td>μ_f,r,p-p 0.10</td>
</tr>
<tr>
<td></td>
<td>μ_f,r,p-w 0.30</td>
</tr>
<tr>
<td></td>
<td>μ_f,r 0.125</td>
</tr>
</tbody>
</table>

For the determination of the translation of particles following the force balance of equation 3.11, there is a similar coupling between the fluid and the particle rotation. So far, in the DPM this was neglected and rightfully so, as the magnitude of this force, especially for gasses, seems small. However, when taking into account the effect the dense packing has on the drag force, the magnitude of this hydrodynamical torque may become large enough to have an influence on the rotational behaviour. Dennis et al. (1980) gave a correlation for the hydrodynamic torque for a single sphere in a flow in the dilute limit, following the work of Sawatzki (1970):

\[ T_h = C_r \frac{1}{2} \rho_f r^5 \mid \bar{\Omega} \mid \bar{\Omega} \tag{3.16} \]

\[ C_r = \frac{32}{\text{Re}_r}(1 + 0.2\text{Re}_r) \tag{3.17} \]

With \( \text{Re}_r \):

\[ \text{Re}_r = \frac{\varepsilon_f \rho_f |\bar{\Omega}| d_p^2}{\mu_f} \tag{3.18} \]

With \( \bar{\Omega} = \frac{1}{2} \nabla \times \bar{u} - \bar{\omega} \) and \( \varepsilon_f = 1 \). One can notice the great similarity with the Schiller and Naumann (1935) equation. By adding a Richardson and Zaki (1954) correction, we can account for the presence of neighboring particles and hence change equation 3.16 such that it is applicable for different
solid fractions $\varepsilon_f \neq 1$ and thus for use in fluidized beds:

$$\bar{T}_h = \varepsilon^{-2.65} \frac{32}{\text{Re}_r}(1 + 0.2\text{Re}_r)0.5\rho_f r^5 |\bar{\Omega}| \bar{\Omega}$$ (3.19)

The Richardson and Zaki (1954) correction is a necessary ad hoc assumption and the proper way of testing its validity would be the use of Direct Numerical Simulations, which is beyond the scope of this work. Simulations have been run with and without the hydrodynamic torque. The profiles and values of the rotational velocity did not change significantly. The magnitude of the collisional and hydrodynamic torque differed by 3 to 4 orders. Even though the hydrodynamic torque is a constant force and the collisional torque acts periodically, it is not enough to dampen the collisional behaviour. Note that for non-spherical particles the effect of hydrodynamic torque might become important, because the effect of hydrodynamic torque increases by two orders of magnitude Zastawny et al. (2012). For non-spherical particles and or small particles the Magnus and Safmann forces also have to be taken into account. A similar approach as in equations 3.16 to 3.19 can be used to apply these lift forces. A parametric study using for instance DNS can be used to check the validity of applying a Richardson and Zaki correction.

### 3.2.4 Rolling friction

In studying the behaviour of particles in a spout-fluidized bed, which is very similar to our system, Goniva et al. (2012) incorporated a rolling friction model:

$$\bar{\bar{T}}_{p,r} = R_{p,\mu}k_{p,n}\Delta x_p \bar{\bar{\omega}}_{p,rel} r_p |\bar{\omega}_{p,rel}| r_p$$ (3.20)

The authors mention that adding a rolling friction model like equation 3.20 with a friction parameter of 0.125 gave the best results in describing the translational velocity near the wall. In the model described above a similar rolling frictional model was incorporated:

$$\bar{T}_{p,r} = \mu_{fr} \Gamma_n |\bar{\dot{t}}_n|$$ (3.21)

In essence adding a rolling friction model like equations 3.20 or 3.21 means lowering the frictional limit allowing for less rotation. As both the particle-particle and particle-wall friction parameter are already 0.1, addition of a
rolling friction of the same order of magnitude would cancel rotation totally we decided to not use the rolling friction model. The addition of a rolling friction thus has the same effect as lowering the friction coefficient. the friction coefficient is thus a lump sum of different frictional effects limiting the rotational behavior of particles.

3.3 Experimental setup

For this study a pseudo 2D fluidized bed setup was used, the same as in chapter 2. This setup is also very suitable to compare with the Discrete Particle Model because of its limited size.

Figure 3.2: Magnetic Particle Tracking sensor array and pseudo 2D fluidized bed setup.

In figure 3.2 a picture of the pseudo 2D fluidized bed is shown. The
Table 3.2: Settings and parameters of the experimental setup

<table>
<thead>
<tr>
<th>Fluidized Bed</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Width</td>
<td>0.3 m</td>
</tr>
<tr>
<td>Height</td>
<td>1.0 m</td>
</tr>
<tr>
<td>Depth</td>
<td>0.015 m</td>
</tr>
<tr>
<td>Porous plate</td>
<td>3 mm thick</td>
</tr>
<tr>
<td>Average pore size</td>
<td>10 (\mu m)</td>
</tr>
<tr>
<td>Mass flow controller</td>
<td>1200 l/min</td>
</tr>
<tr>
<td>Material front plate</td>
<td>glass</td>
</tr>
<tr>
<td>Other materials</td>
<td>aluminium &amp; stainless steel (non-magnetic)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>MPT sensor array</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Sensor type</td>
<td>tri-axis AMR</td>
</tr>
<tr>
<td>Amount</td>
<td>3 * 24</td>
</tr>
<tr>
<td>Frequency</td>
<td>1000 Hz</td>
</tr>
<tr>
<td>dimensions</td>
<td>0.35, 0.65 m (width, height)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Particles</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Bed material size</td>
<td>3.0 mm</td>
</tr>
<tr>
<td>Density</td>
<td>2526 kg/m(^3)</td>
</tr>
<tr>
<td>Minimum fluidization velocity</td>
<td>1.55 m/s</td>
</tr>
<tr>
<td>Magnetic marker size</td>
<td>4.7 mm</td>
</tr>
<tr>
<td>Density</td>
<td>2100 kg/m(^3)</td>
</tr>
<tr>
<td>Magnetic moment</td>
<td>0.0125 Am(^2)</td>
</tr>
<tr>
<td>Minimum fluidization velocity</td>
<td>1.7 m/s</td>
</tr>
</tbody>
</table>

dimensions of the bed are 0.30 by 0.015 by 1.0 m (width, depth, height). The bottom of the bed consists of a distribution chamber topped with a porous distributor plate with a pore size of 10 \(\mu m\). All parts of the setup are made of aluminium or non-magnetic stainless steel. The sensor array, consisting of 6 rows of 4 tri-axis AMR-sensors, is placed directly in front of the setup. Setup and control are courtesy of Matesy GmbH. This leads to a total of 72 sensors capable of operating at 1 kHz. Width and height of the sensor array is 0.35 by 0.65 m. An overview of all settings and properties is given in table 3.2.

As a first test the error in the orientation as a function of the magnetic moment and the distance between the tracer particle and the nearest sensor is studied. Two magnets with magnetic moment 0.031 and 0.181 Am\(^2\) were placed at fixed positions from the radius of the 3D sensor array. Second five magnets with differing size and magnetic moment were placed in the centre
of the sensor array. The error in the determination of the errors is shown in figure 3.3. It can be seen that the error increases linearly with decreasing magnet strength while the error increases linearly with increasing relative distance, as can be expected based on equation 3.1. Except for the magnet with a magnetic moment of 0.181, the error seems constant which is probably due to the large strength of the magnet. Similar results have also been found for the translational behaviour in 2.

![Figure 3.3: Effect of relative distance(left) and magnetic moment(right) on the error in the determination of the angles.](image)

As a second test the particle is fluidized and the distribution in orientation angle is studied. Figure 3.4 shows both the ideal and actual spread of the azimuthal and inclination angles. The ideal shape is governed by a uniform distribution for the azimuthal angle and $\sin \theta$ for the inclination angle. From figure 3.4 it can be seen that there is a deviation between the ideal and actual orientation distributions. There is a slight preferred angle of $\phi = -60^\circ$ and $\theta = 140^\circ$, which relative to the sensor and setup orientation appeared to be an alignment with the earth’s magnetic field; pointing North and downwards. In other words: the magnetic marker acts as a compass, which could have been expected. This is unwanted especially when in a later stage non-spherical particles will be studied, where preferred angles due to its shape are studied. To cancel the effect of the earth’s magnetic field on the particle orientation a Helmholtz coil was installed.

The Helmholtz coil is a set of two square rings of 2 meter in diameter, 1 m in height apart. A schematic picture is provided in figure 3.5.
has to be set opposite to the earth’s magnetic field and the current through the coil has to be set such that the strength of the field equals the earth’s magnetic field, following Biot-Savart’s law. The two fields will oppose each other, cancelling each other out. This will allow the tracer particle to orientate freely. The size of the magnetic free zone follows from the Biot-Savart law leading to 0.5 m in diameter and height.

The experiment in the previous section was repeated to see whether the influence of the earth’s magnetic field was cancelled and the Helmholtz coil was operating properly.

Figure 3.4: Histogram of the angle distributions with the Helmholtz coil off (a) and on (b)

Figure 3.5: Schematic of a Helmholtz coil, depicting the current loop, with current coming out from the surface at the dots and entering the surface at the crosses. The field lines run from left to right.

Figure 3.4 shows the results of the angle distributions of a fluidization
experiment with and without an operational Helmholtz coil. When the earth’s magnetic field is cancelled by the Helmholtz coil the distribution of the angles shows a nice close-to-ideal behaviour. There is some remaining noise that is related to the limited number of data points.

3.4 Results

To make a proper comparison between the results from the Magnetic Particle Tracking and the Discrete Particle Model three phenomena are checked: i) the occupancy to show that the particles have the same distribution inside the pseudo 2D system, ii) the translation via a quantitative comparison of the vertical velocity component at different cross-sections of the bed and iii) a qualitative and quantitative comparison of the rotational velocity of the magnetic marker and a representative tracer particle in the DPM. The experiments have been performed with a superficial velocity of 3.5 m/s and 2.5 m/s at a sampling rate of 50 Hz.

The relevant parameters of the experiment and simulation are given in tables 3.1 and 3.2. Because the magnetic tracer particle has different properties than the bulk material, 600 tracers are added to the DPM simulation. These tracers have the same size and mass as the magnetic tracer and a moment of inertia that is defined as:

\[ I = \int_{r_1}^{r_2} 2\frac{r^2}{3} dm = \frac{8}{3} \int_{r_1}^{r_2} \pi \rho r^4 dr \]  

(3.22)

For the computation of \( I \) it is important to account for the composite nature of the tracer particle with a dense core (\( r < r_1, \rho_c = 7600 \text{kg/m}^3 \)) and a less dense shell (\( r_1 < r < r_2, \rho_s = 250 \text{kg/m}^3 \)).

\[ I = \frac{8}{15} \pi \left( \rho_c r_1^5 + \rho_s \left( r_2^5 - r_1^5 \right) \right) \]  

(3.23)

Secondly because the particles are quite large, we found a difference in bed expansion, especially at lower superficial velocities. We found that the reason for this is a mismatch of the minimum fluidization velocity between experiments and simulations. In the experiments the minimum fluidization velocity is 1.55 m/s, however with the given drag law (Ergun/Wen&Yu), the minimum fluidization velocity in the simulations is 1.45 m/s. To correct for this we choose to keep the excess gas velocity (\( u_{ex} = u_0 - u_{mf} \)) the same for
both the experiments and the simulations. In the simulations therefore we used $u_0 = 2.35 \text{ m/s}$ and $u_0 = 3.28 \text{ m/s}$ for the background velocity, relating to 2.5 and 3.5 m/s in the experiments.

The occupancy is a measure for how often a tracer particle passes a particular position, following:

$$O(i, j) = \frac{N_{\text{gridcells}}}{N_{\text{meas}}} \sum_1^{N_{\text{meas}}} \delta \quad \forall \delta = \begin{vmatrix} 1 & p \in (i, j) \\ 0 & p \ni (i, j) \end{vmatrix}$$

(3.24)

Figure 3.6: Mean bed solids fraction of the magnet(left) in the MPT and tracer particles(right) in the DPM, $u_0 = 3.5 \text{ m/s}$.

A value of 1 for the occupancy signifies the particle has passed that position as often as might be expected based on the average value. Occupancy values higher than 1 signify the particle has a tendency to stay at that particular position more than average. From the occupancy the solids fraction can be calculated (Wildman et al., 2000):

$$\varepsilon_s = \min \left( \frac{\frac{1}{6}\pi d_p^3 N_p}{V_{i,j}} \frac{O_{i,j}}{N_{\text{gridcells}}}, 0.6 \right)$$

(3.25)

3.4.1 High superficial velocity $u_0 = 3.5 \text{ m/s}$

Figure 3.6 shows the comparison of the solids fractions obtained from the MPT by using equation 3.25 and from the DPM. Figure 3.6 shows dense
zones near the wall and a diluted area in the center where the bubbles pass. The qualitative comparison between the DPM and the MPT is very good. Similar bed expansion and solids fraction profiles can be seen. This shows that the hydrodynamic behaviour is captured correctly by the model. Some differences in the shape of the dense zone are observed which might be related to the jump in the Ergun/Wen&Yu model at a porosity of 0.8.

For a contact in the sliding limit the particle rotation is dominated by the normal force. A quantitative comparison of the particle translation velocity is necessary to ensure a proper comparison of the rotational velocity. Figure 3.7 shows the vertical component of the (translational) velocity at three different cross sections inside the fluidized bed. Even though the MPT is slightly more noisy the two profiles are very similar, especially in the central region where the velocities are captured very well by the DPM. In the dense wall region there is a deviation between the experiments and the model, which was also noticed by Van Buijtenen et al. (2011) for a spouted bed. To correct for these effects Goniva et al. (2012) added a rolling friction parameter ranging from 0 to 0.125 and found 0.125 to be the most appropriate based on the differences of translation velocity near the wall. In the simulation discussed in this paper the rolling friction was set to 0 and the friction coefficient to 0.1. For the left, right and bottom walls the friction parameter was set to a value of 0.3, because these are made of aluminium and stainless steel. The front and back plates are made of glass, which have a similar friction parameter as the bed material. An increase of the friction parameters led to a linear increase in the rotational velocity, indicating that the particle wall dynamics and the friction dominate the system. Instead the differences in the vertical velocity component near the wall can be explained by the limited depth of the system as compared to the particle diameter. Because the particle diameter is only five times smaller than the depth of the pseudo 2D system difficulties in determining local porosity, drag and particle bridging might effect the hydrodynamic behaviour. This might also explain the mismatch of the minimum fluidization velocity between the experiment and the simulation.

Now that the translational velocity is captured correctly the rotational velocity can be checked. Figure 3.8 shows a contour plot of the rotational velocity obtained from the Magnetic Particle Tracking and the tracer particle in the Discrete Particle Model. The bed material in the model cannot be used
Figure 3.7: Comparison of the mean vertical velocity component [m/s] of the magnetic tracer particle and DPM bed material at different heights, \( u_0 = 3.5 \text{m/s} \).

Figure 3.8: Contour plot of the mean rotational velocities[rot/s], for the magnetic particle tracking(left), and the discrete particle model tracer particles(right).
for the rotational velocity because the inertial mass of the bed material does not match the tracer particle, which unfortunately is unavoidable. In both cases an hourglass shaped profile can be seen which is expected. The MPT results show some noise that is related to the limited number of data points. For the MPT the results were obtained of tracking one magnet for one hour, relating to 600 tracers in the DPM for 60 s in simulation time. In total about 200,000 datapoints were obtained. The spread in the rotational velocity is quite large and is related to the limited number of samples per grid cell, say \( N \approx 200 \). According to theory, an error of 0.7 rot/s is expected, following:

\[
\sigma_m = \frac{\sigma}{N} \tag{3.26}
\]

The agreement with the DPM is remarkably good and to the best of the authors’ knowledge never shown before. The magnitude and overall profile of the rotational velocity both match very well. Again, near the wall and bottom region slight deviations can be seen, which can most probably be attributed to the mismatch of the translational velocity.

Figure 3.9: Mean rotational velocity [rot/s] comparison of magnetic tracer particle and DPM bed material at different heights, \( u_0 = 3.5 \text{ m/s} \).

Figure 3.9 shows the rotational velocity at three different cross-sections in the fluidized bed with increments of 10 cm from the distributor plate. The magnitude of the rotational velocity matches very well and also the overall
profile matches quite well. Near the wall region at a height of 0.3 m a slightly higher rotational velocity is found for the DPM, which can be directly related to the higher downwards translational velocity which is found in the DPM as can clearly be seen in figure 3.7. The error bar in Figure 3.9 indicates the error in the measured rotational velocity, based on equation 3.26.

### 3.4.2 Low superficial velocity $u_0 = 2.5m/s$

![Figure 3.10: Mean vertical velocity component [m/s] comparison of magnetic tracer particle and DPM bed material at different heights, $u_0 = 2.5m/s.$](image)

The experiments in a pseudo 2D fluidized bed setup were repeated at a lower superficial velocity of 2.5 m/s. Figures 3.10 and 3.11 show the vertical velocity (m/s) and rotational velocity (rot/s) at three different cross-sections in the fluidized bed. Both the rotational and translation velocities are lower in comparison to figures 3.7 and 3.9, respectively. This is expected because of the lower superficial velocity. The rotational velocity again matches fairly well. However, because the overall velocities are lower in comparison to figure 3.9 the noise becomes more apparent. This can most clearly be seen at the lower section of the setup at 0.1 m.
3.5 Conclusions

For the first time, the particle rotational velocity in a gas fluidized bed was measured using a Magnetic Particle Tracking method. It was shown that the error in the orientation of a magnetic marker has a linear dependency on the relative distance between the marker and the sensors and an inverse linear dependency on the magnetic strength. The magnetic particle acts as a compass to the earth’s magnetic field even under fluidization conditions. This was compensated using a Helmholtz coil the operation of which was shown to be successful. An extensive comparison of the MPT technique with the DPM was made, showing a very good comparison. Both the solids fraction profile and particle translation velocity showed a very good comparison.

Finally, because the rotational velocity is measured as well, all aspects of the particle motion are now captured. This makes it possible to study the force balance on the particle in more detail; showing the particle rotation is dominated by the sliding regime. The use of a particle-wall friction parameter is key in getting the correct behaviour. Only the bottom and side wall friction parameters deviate from the particle-particle friction parameter. The friction coefficient used to describe particle-wall friction for the front and back wall is
the same as that used for particle-particle friction, because both involve glass-
glass contacts. Rolling friction has been switched off in these simulations.

Addition of hydrodynamic torque, using an ad-hoc Richardson and Zaki
(1954) correction on the torque on a single sphere, has no noticeable effect for
spherical particles. However a substantial effect is expected for non-spherical
particles. Magnetic Particle Tracking would be the ideal technique to quantify
this effect.

In the next chapter results from the MPT will be presented for a cylindrical
fluidized bed with spheres and rods of equal volume and density. A second
experimental technique will be introduced that is capable of studying the
orientation of rods with Digital Image Analysis (DIA).
4.1 Introduction

The various uses of fluidized beds in chemical and process industries have resulted in a vast amount of research and literature to understand the transport phenomena. In industrial applications fluidized beds are generally very large. For practical reasons though, research has long been restricted to small lab scale experimental studies. These studies often are restricted to pseudo 2D systems for visual access, probes, that disturb local flow phenomena and expensive 3D particle tracking or tomographic techniques.

Since the 1990’s, however, the use of computer simulations have extended the capabilities of research beyond the lab scale. The Discrete Particle Model (DPM) has been a model of interest as the complete particle dynamics can be captured in detail, as such the amount of research has grown explosively, as exemplified by the review articles of Zhu et al. (2007) and Deen et al. (2007) So far most of the research focused on spherical particles, for which the interaction forces are relatively well defined, i.e. drag and contact forces.

Since roughly a decade the focus has slowly shifted to study non-spherical particles. Especially the amount of papers on Discrete Element Modelling (DEM) has grown exponentially Lu et al. (2015). The collision detection of arbitrary shape and size poses a big challenge. Because of this difficulty most of the research has focused on granular flow only, without gas or liquid interactions. When introducing a fluid, particle-fluid interactions as drag and the different lift forces have to be incorporated (Zastawny et al., 2012), which strongly depend on the relative orientation, local packing structure and mutual alignment.

Experimental validation of these models is important to help in understanding the key parameters for the developed models. The amount of tech-
niques that are capable of measuring rotation or orientation of particles however is limited. A multi Positron Emission Particle Tracking (multi-PEPT) method was used to study the rotation of 12 mm cube particles (Yang et al., 2008b). Zhang and Zhong et al. Zhang et al. (2013); Zhong et al. (2010) have used a combination of Infrared imaging and a microwave heater to study a single cylindrical tracer in a fluidized bed. Particle Tracking Velocimetry (PTV) is quite often used to study the rotation and orientation of particles (Wu et al., 2009; Cai et al., 2012; Zitoun et al., 2001). Vollmari et al. Vollmari et al. (2015a,b) have conducted a quite elaborate study on non-spherical particles, studying the pressure drop and orientation of different shapes of particles.

A novel Magnetic Particle Tracking (MPT) technique was developed as a safer and less expensive particle tracking technique, introduced in chapter 2. MPT tracks a single magnetic particle that acts as a dipole, which has a position and the induced magnetic field an orientation. MPT therefore is capable of studying both the translation as well as the orientation of the tracer particle. It has already been used to study granular flow in a rotating drum (Neuwirth et al., 2013), a fluid dynamically downscaled fluidized bed (Sette et al., 2015), spouted beds (Mohs et al., 2009) and pseudo 2D fluidized beds (Buist et al., 2014). In Buist et al. (2015) we have already shown and compared the rotation behavior of spheres in a pseudo 2D fluidized bed, for MPT and DPM (chapter 3). In this study we will show the strength of the MPT to study orientation and rotation of non-spherical particles in a cylindrical fluidized bed.

These techniques so far were only used to study the orientation of particles. The mutual alignment of particles is however to our knowledge not yet addressed. The particle tracking techniques are not capable of this because they track only one particle. Digital Image Analysis (DIA) is capable of studying the orientation of multiple cylinders in a pseudo 2D fluidized bed. Only the cylinders in plane with the wall can be determined, which is demonstrated on a segregating bed of spheres and cylinders of equal mass and volume.

Segregation of mixtures of particles occurs quite often and has been studied quite extensively for mixtures of spherical particles of different size or density, Rao et al. (2011) has given a recent classification of particle segregation based on particle size and density ratios. Mostly segregation occurs due to a difference in the ratio of drag force over the gravity force. Segrega-
tion of particles of different shape also occurs but is generally believed to be much less prominent (Nienow et al., 1978). Particle clustering and entanglement of non-spherical particles make it far more difficult to study. This work will focus on segregation dynamics (Olaofe et al., 2013) of particle mixtures based on shape differences. The rate of mixing for mixtures of spheres and non-spherical particles was numerically studied by Oschmann et al. (2014).

The outline of this work is as follows, first the setup and particles are discussed. Second the results of the MPT are shown, the interested reader is referred to chapters 2 and 3 for a full explanation of the technique. Next the DIA technique for the determination of the de-mixing of a mixture of spheres and rods is discussed and results shown. Second the technique for the orientation determination is explained and some results shown for the distribution of the inclination orientation in a fluidized bed at 1.8 times $u_{mf}$ for different fractions of rods.

4.2 Setup

<table>
<thead>
<tr>
<th>name</th>
<th>Dimensions [mm]</th>
<th>material</th>
<th>aspect ratio [L/D]</th>
<th>sphericity</th>
<th>$u_{mf}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sphere</td>
<td>3.0</td>
<td>304</td>
<td>1</td>
<td>1</td>
<td>2.8</td>
</tr>
<tr>
<td>Small rods</td>
<td>2.0x4.5</td>
<td>303</td>
<td>2.25</td>
<td>0.818</td>
<td>2.47</td>
</tr>
<tr>
<td>Intermediate rods</td>
<td>1.6x7.0</td>
<td>316</td>
<td>4.5</td>
<td>0.719</td>
<td>2.36</td>
</tr>
<tr>
<td>Long rods</td>
<td>1.2x12</td>
<td>316</td>
<td>10</td>
<td>0.579</td>
<td>2.55</td>
</tr>
</tbody>
</table>

The particles that have been used in this work are all of the same volume and density and equivalent to 3 mm diameter spheres. Three different aspect ratio rods have been used of which the longest two have been made by cutting stainless steel 316 welding rods to the correct length. All particles have gone into a tumbler to ground of the sharp edges from the cuts. The smallest aspect ratio rods were turned from 303 stainless steel. The spheres are stainless steel 304 grinding balls. Because the spheres and smallest aspect ratio rods can be magnetizable, they are annealed to get rid of any remaining magnetic activity. The properties of particles are given in table 4.1. Figure 4.1 shows a picture of the spheres and the long aspect ratio rods after annealing.
magnets used in the MPT are Neodymium N50 and have a magnetic moment of 0.014 Am.

Table 4.2: Camera settings

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Setting</th>
</tr>
</thead>
<tbody>
<tr>
<td>Focal distance</td>
<td>2 m</td>
</tr>
<tr>
<td>Diaphragm setting</td>
<td>2.8</td>
</tr>
<tr>
<td>Shutter time</td>
<td>1002 µs</td>
</tr>
</tbody>
</table>

A schematic of the setup for the segregation experiments is given in figure 52.
4.2. It is 100 mm in width 15 mm in depth and 500 mm in height. A JAI AT-2000 GE 3CCD camera is used with a resolution of 1600 by 1200. To get rid of motion blur, a relatively short shutter time and large diaphragm setting is used. Two 250 W LED arrays illuminate the setup.

<table>
<thead>
<tr>
<th>Table 4.3: Properties of the 3D fluidized bed</th>
</tr>
</thead>
<tbody>
<tr>
<td>Internal diameter</td>
</tr>
<tr>
<td>Height</td>
</tr>
<tr>
<td>Scaffold</td>
</tr>
<tr>
<td>Tube</td>
</tr>
<tr>
<td>Distributor plate</td>
</tr>
<tr>
<td>Material</td>
</tr>
<tr>
<td>Thickness</td>
</tr>
<tr>
<td>Pore size</td>
</tr>
<tr>
<td>Open area</td>
</tr>
<tr>
<td>Mass flow controller</td>
</tr>
<tr>
<td>Type</td>
</tr>
<tr>
<td>Max flow rate</td>
</tr>
<tr>
<td>Max superficial velocity</td>
</tr>
</tbody>
</table>

The cylindrical fluidized bed is shown in figure 4.3 and the main properties are given in table 3. The cylindrical fluidized bed is a 174 mm internal diameter Perspex tube. The distributor plate is a drilled brass plate with an open structure of 20 %. The distributor is made of aluminium. All parts are made to be non-magnetizeable. The sensor array is a MagTrack system by Matesy with 72 sensors working at a 1000 Hz.

4.3 MPT

4.3.1 Results

For the results of the MPT the spheres and the intermediate rods are used, pure long aspect ratio rods would not fluidize. Because of high entanglement of the rods only local channels and spouts are formed while the rest of the bed stays stationary. Five different settings for the gas velocity were chosen with increments of 0.5 m/s above $u_{mf}$. A initial bed packing with an aspect ratio H/D of 0.75 is used; roughly 0.13 m height.

Figure 4.4 and figure 4.5 show the vertical velocity component distributions in r,z of the two types of particles at 1 and 2.5 m/s above $u_{mf}$. The circulation
Figure 4.3: Overview of the 3D fluidized setup including the sensor array and Helmholtz coil.
patterns for the rods in figure 4.4 are inverted. At 1 m/s above \( u_{mf} \) the rods move upwards near the wall and downwards near the centre of the fluidized bed, while at 2.5 m/s above \( u_{mf} \) the rods move upwards near the centre of the bed and downwards near the wall. At 2.5 m/s above \( u_{mf} \) a double circulation pattern can be found.

For the spheres (figure 4.5 we see an upward velocity near the centre and a downward velocity near the wall at both 1.0 m/s and 2.5 m/s above \( u_{mf} \). The absolute velocities for the circulation patterns are higher and the double circulation pattern at 2.5 m/s is less pronounced.

Figure 4.6 shows the axially averaged radial profiles of the vertical velocity component. The profiles of the rods are very close to zero. At low velocities above \( u_{mf} \) an inverted profile is seen with upward flow near the wall and downward flow near the centre. At higher velocities a transition to the 'normal' circulation pattern is found, however because of a strong double circulation pattern the absolute magnitude of the averaged velocities is small. For spheres a strong pattern is only seen for 1.5 m/s above \( u_{mf} \) and higher, possibly related to the point of transitioning between a 'normal' and inverted flow profile.

The distribution in angles of the spheres is very similar to the ideal profile for a sphere, which is half cosine, and not shown here. The distribution for the rods is far more interesting however. Figure 4.7 shows the averaged inclination angle at different locations in the bed at an excess velocity of 1 m/s. The angles are distributed from -90 to +90 degrees corresponding to upright positions. 0 degrees corresponds to a horizontal position, the absolute is taken. An averaged alignment for a half cosine distribution is above 32 degrees.

Near the bottom particles have an averaged angle closer to 0 indicating a horizontal position, i.e. aligned with the bottom. Near the walls the averaged angle is large than 32 indicating a preference for a vertical alignment, and thus an alignment with the wall. In the centre the averaged angle is somewhere in between but also smaller than 32, so a slight preference for a horizontal alignment. Averaged along the height the preferred alignment with the wall and the preferred angle of the bulk and bottom is shown even more clearly. The red line indicates the expected averaged angle for a random distribution (behavior of spheres).
Figure 4.4: Azimuthally averaged distribution of the vertical velocity component in \( r,z \) for the intermediate rods in a cylindrical fluidized bed at 1 m/s and 2.5 m/s above \( u_{mf} \), respectively.
Figure 4.5: Azimuthally averaged distribution of the vertical velocity component in r,z for the spheres in a cylindrical fluidized bed at 1 m/s and 2.5 m/s above $u_{mf}$ respectively.
The histogram of the inclination angle for the different excess gas velocities is given in Figure 4.8 and shows another interesting phenomenon. At low excess gas velocities the rods show a preference to lie flat while at higher gas velocities the rods show a preference for an upright position. It might be that at lower gas velocities the larger part of the bed is mostly at rest or gently fluidizing with most of the rods lying flat. At higher velocities the bed behaves more erratic and the particles want to align with the direction of the flow.

4.4 DIA

Digital Image Analysis (DIA) is a visual technique that has been used quite often to study granular flow. In combination with Particle Image Velocimetry (PIV) it is a very powerful technique (de Jong et al., 2012). DIA has also been used to study segregation and mixing, Goldschmidt et al. (2003), Olaofe et al. (2013). The technique presented here has many similarities with the later. A 3CCD camera is used and thus the images contain color.
Figure 4.7: Local averaged inclination angle across $\theta, r$ (left) and averaged along the azimuth across $r$ (right) at $u_{ex} 1 \text{ m/s}$. 
Figure 4.8: Distribution of the inclination angle for the intermediate rods at different excess gas velocities. The red lines indicate the ideal distribution for a sphere.

4.4.1 Segregation

Method

The method used in this work involves several image processing steps to quantify segregation (Figure 4.9). The original image is first cropped to get rid of the walls and the bottom of the fluidized bed (a). The background is subtracted based on a color difference (b). Because the spheres were untreated they have two reflection spots which are easily detected because of their intensity (c). Edge detection of the reflections spots allow a matlab function called imfindcircles to detect and count the circle s (d). The images are divided into square grids and the occupancy is determined based on the number of pixels associated with particles (e):

\[
O = \frac{\sum_i \sum_j p_{i,j}}{N}
\]  

(4.1)
The reflection count is a function accounting for the occupancy of the cell, and scaled to the size of the system, figure 4.9 (f):

\[ r = \frac{n_{\text{circ}}}{O \frac{WH}{n_c} t^2} \]  

(4.2)

The reflection count has units $1/cm^2$. The theoretical maximum number of reflections per grid cell is given as:

\[ r_{\text{max}} = \frac{4}{\sqrt{3}d^2} \]  

(4.3)

With $d$ as 0.3 cm this amounts to about 25.7 per $cm^2$. For simplicity the reflection count is normalized to its maximum value:

\[ |r| = \frac{r}{r_{\text{max}}} \]  

(4.4)
Figure 4.10: Calibration of the normalized reflection count to the fraction of rods in the system (left). Parity plot of the predicted fraction on the obtained calibration curve (right).

The number of reflections scales with the fraction of spheres, but not linearly. This effect was also found for segregation of spheres of different sizes (Olaofe et al., 2013). To account for this the normalized reflection count is calibrated to the actual fraction of spheres $f$. Known fractions of spheres were added to the fluidized bed and an analysis of the reflection counts was done. Figure 4.10 shows the results of $1-f$ (the fraction of rods), as a function of the normalized reflection count. Figure 4.10 shows the parity plot of the known fraction and the predicted fraction by the calibration given by:

$$1 - f = 1.411|r|^3 - 0.389|r|$$  \hspace{1cm} (4.5)

The results shows that the actual prediction is quite reasonable.

Results

To quantify the demixing of the system the Lacey (Lacey 1954) mixing index was used:

$$M = \frac{S_i^2 - S_0^2}{S_R^2 - S_0^2}$$  \hspace{1cm} (4.6)

With the variance of a cell $i$ ($S_i$), variance of a fully segregated bed ($S_0$) and variance of a fully mixed bed ($S_R$) defined as:

$$S_i = \frac{1}{n_c - 1} \sum_{i=1}^{n_i} \sum_{j=1}^{n_j} (f_{i,j} - |f|^2)$$  \hspace{1cm} (4.7)
Figure 4.11: Mixing index as a function of time for several superficial gas velocities.

\[ S_0 = |f| (1 - |f|) \]  
\[ S_R = \frac{|f| (1 - |f|)}{|n|} \]

With \(|n|\) the average number of particles in a cell.

Figure 4.11 shows the evolution of the mixing index over time as a function of the gas velocity for a system with 15 % of rods. It can be seen that demixing occurs in a very small regime. From visual observations we found that demixing occurs by local clustering of rods. As these particles cluster, they act as one large immobile lump of particles, that is bypassed by the gas. This leads to local defluidization. For this to happen the bed must be mobile enough for the rods to move around but not too mobile that remixing occurs due to bubbles. Only the two systems with a \(u_{mf}\) of 1.3 and 1.4 demix.

### 4.4.2 Orientation

**Method**

Figure 4.12 shows the different steps in the determination of the orientation of all the particles. First a canny edge detection algorithm by Matlab is used to determine all edges. The edge detection finds both the edges and reflections of the spheres as well as the edges of the rods. Every edge that is small (diameter of the sphere) can be removed leaving only the cylinders 4.12 (b).
A line detection methodology is used to determine all lines in the image, based on a Hough transform. This method works best for lines with a size similar to the image size. Therefore the image is split in a number of sections. Figure 4.12 (c) shows the results of the first pass of the lines detection method. Only lines with a minimum size of $> 0.5$ of the cylinder length are allowed to prevent any artefacts and double counting of cylinders. Rods that align and are close to each other often are not detected or sometimes just one of rods is detected. Also particles crossing the grid lines are sometimes missed. Therefore a mask of all detected lines is made (d) are removed (e) and another pass of the lines detection method is performed on a different grid (f) to ensure most rods are detected. In total roughly 85-90 % of the cylinders that are
visible are detected.

Only the inclination angles can be determined of the rods that are in plane with the camera view. Also all effects found are heavily affected by the walls in the system, because the rods can almost span the depth of the system.

Results

To see the effect of fraction of rods on the distribution of the inclination angles three mixtures of different fractions of rods were added; 5 %, 15 %, 30 % (figure 4.13) and fluidized at 1.8 times \( u_{mf} \). A preferred upright orientation of the rods was found for all fractions of rod. The rods near the wall seemed to have highest tendency to align in an upright position, which is as was expected, especially for this pseudo 2D fluidized bed where particle-wall interactions dominate.

The amount of preference for the vertical position seemed to drop with an increase in the fraction of rods in the system. For higher fractions of rods the flow direction becomes more chaotic and less structured. Because the particle orientation is also partially determined by the flow direction, a more randomized distribution is found in systems with more rods.

4.5 Conclusions

Both the Magnetic Particle Tracking (MPT) and the Digital Image Analysis (DIA) technique can give very promising results to study non-spherical granular flow. MPT has full 3D capability and can show both the important angles associated with a tracer particle. The distribution of the angles for
spheres follow the predicted values nicely. The rods show a distinctly different behavior for the inclination angle. Also a weak reversed flow pattern was found for the rods.

DIA has shown to be capable to determine the inclination angle of the rods that are in plane with the camera. The distribution of angles shows a similar difference in inclination angle as the MPT although heavily influenced by wall effects. More importantly the distribution in angles is highly dependent on the flow behavior of the system as well as the fraction of rods in the system. Segregation of particles purely on shape differences in a pseudo 2D fluidized bed is possible and follows a repeatable trend. Studying the mutual alignment and local orientation of rods is the next step. All in all there is enough fuel for future research and both Magnetic Particle Tracking as well as Digital Image Analysis have an important role to play.
Chapter 5

Heat transfer study using Constant Temperature Anemometry

5.1 Introduction

In order to improve the design and control of gas-solid contactors, like packed and fluidized beds, detailed understanding of hydrodynamics, mass and heat transfer is needed. Many studies have been performed to obtain empirical correlations for fluid-particle mass and heat transfer, Gunn (1978). Most of these experimental studies have been performed over a very specific range of operating conditions. Often effects of wall channelling and or axial dispersion have been neglected Wakao and Kagei (1982), leading to a large scatter in the obtained fluid-particle heat transfer rates as seen in figure 5.1 in terms of the Nusselt number.

Several empirical correlations have been proposed for the different situations involving non-isothermal gas-particle flows; single particle in unbounded flow, particles in a packed bed or fluidized beds. The following correlations have been used for reference purposes in this work:

The Ranz-Marshall (Ranz and Marshall, 1952) correlation describes the fluid-particle heat transfer of a single particle in unbounded flow:

\[ Nu = 2 + 0.6Re^{0.5}Pr^{0.33} \]
\[ 1 < Re < 10^4, 0.6 < Pr < 380 \]  

(5.1)

The Ranz (Ranz, 1952) equation is an adjustment to the above equation
Figure 5.1: The dependence of the Nusselt group upon Reynolds number according to several investigators, Gunn (1978).

that describes the fluid-particle heat transfer in a packed bed:

\[ Nu = 2 + 1.8 Re^{0.5} Pr^{0.33} \]

\[ 1 < Re < 10^4, 0.6 < Pr < 380 \]  \hspace{1cm} (5.2)

Finally the Gunn correlation accounts for differences in solids fraction ranging from a densely packed bed to a single unbounded particle over a wide range of Reynolds numbers:

\[ Nu = (7 - 10\varepsilon + 5\varepsilon^2)(1 + 0.7 Re^{0.2} Pr^{0.33}) + (1.33 - 2.4\varepsilon + 1.2\varepsilon^2) Re^{0.7} Pr^{1/3} \]

\[ 1 < Re < 10^3, 0.6 < Pr < 380, 0.35 < \varepsilon < 1 \]  \hspace{1cm} (5.3)

On the other hand Direct Numerical Simulations (DNS) have been used to obtain more insight into the complex fluid-particle heat transfer phenomena in dense gas-particle flows. In these systems the heat transfer is strongly
dependent on the fluid flow patterns and the structural features. These simulations allow for modelling of the actual packing geometry and consequently allow to directly relate fluid-particle heat transfer to structural features and fluid flow. It is very difficult to properly validate the DNS, because most information is restricted to limiting and extreme cases. Direct comparison of Nusselt numbers under varying solids fractions and a full range of flow regimes has up till now not been possible, mostly because of the need of a well-defined driving force (Rexwinkel et al., 1997), as well as the need for a well-defined solids volume fraction.

DNS is limited by the domain size that can be treated in reasonable computation times. Therefore DNS is often used in a multi-scale modelling approach (Van der Hoef et al., 2008), where the results of the DNS are used to derive closure laws required in more coarse grained techniques such as Discrete Particle Modelling (DPM) and Two Fluid Modelling (TFM). The latter two techniques allow the study of larger systems.

Most studies addressing validation of DNS data are based on comparison with analytical solutions in limiting cases or comparison with results from empirical correlations. An experimental approach that allows to control the solids structure and the thermal driving force is therefore needed. Preferably such a technique is capable of changing or controlling the solids fraction in a precise manner. For instance Happel and Epstein (1954) made an abacus like structure to study pressure drop of structures with varying solids fraction. Mankad et al. (1997) used a similar structure to study heat transfer, using a 1.5 cm hollow copper sphere with a resistor to heat the sphere, using a constant power input for the sphere. Yang et al. (2012) used a similar technique to study the heat transfer of structured packed beds of particles where particles are stringed in a BCC and FCC structure where the temperature of a couple of particles is measured with an embedded thermocouple. Experiments in fluidized beds can also be performed by addition of a hot freely moving particle to the flow, (Parmar and Hayhurst, 2002; Hayhurst and Parmar, 2002). Changes in magnetic properties due to temperature changes have also been used to study heat transfer in fluidized beds, (Turton et al., 1989).

In this chapter a similar technique as Mankad et al. (1997) will be used. However, in our work an existing piece of equipment is used, i.e. a spherical Constant Temperature Anemometer (CTA) probe. An anemometer is nor-
mally used to study the fluid velocity, by calibrating the heat loss of a probe inserted in a flowing fluid, following Kings law (King, 1914). However, instead of coupling the voltage of the Wheatstone bridge to the fluid velocity it is also possible to convert it to a heat loss of the probe. This form of heat loss is called Joule heating and can almost entirely be attributed to the convective heat loss of the probe.

The outline of this chapter is as follows: First the methods are described, starting with the Constant Temperature Anemometer, then the Immersed Boundary method to perform DNS is shortly described. Second the experimental setup is described. In the Results section three different types of experiments are reported: the heat transfer of a single particle in unbounded flow is used as a benchmark, following the work of Ranz and Marshall (1952). Furthermore, the effect of shielding/enhancement in fluid-particle heat transfer for an inline array of three particles as well as the effect of inter-particle distance is studied, and finally the effect of solids volume fraction and fluid velocity (particle Reynolds number) is studied for stationary arrays of particles over a wide range of solids volume fractions and particle Reynolds numbers.

5.2 Methods

5.2.1 Constant Temperature Anemometry (CTA)

Constant Temperature Anemometry (CTA) finds its origin in the work of King (1914). A thin wire or film is placed in a flow and kept at a constant temperature while the required power is measured. The temperature of the probe is related to the resistance of the probe where the resistance is maintained by adjusting the voltage over the probe, which depends on the fluid velocity. The voltage of the probe is calibrated to the fluid velocity. CTA-probes are used as a means to measure the fluid velocity, and because of its fast response they are often used to study turbulent flows. The working principle of CTA is based on the relation between the fluid velocity and the heat loss of the probe due to convection. The power loss of the probe is directly related to the convective heat loss of the probe because of Joule heating. In this work we use an omni-directional probe by Dantec that consists of a 3.2 mm sphere. Figure 5.2 shows the probe tip, Dantec type 55R49. The probe
Figure 5.2: CTA-probe (left) and Wheatstone bridge (right), with $R_p$ the probe resistance.

consists of one resistance out of four legs of a Wheatstone bridge, see figure 5.2.

$R_p$ resembles the probe resistance whereas $R_3$ is a resistance that can be set, the ratio between these two is the same as the ratio between resistances 1 and 2. The probe resistance $R_p$ follows from the overhead temperature of the probe, as given by King (1914):

$$R_p = R_{20} + \alpha_{20} R_{20} (T_p - T_{amb})$$

(5.4)

When the two parallel resistor legs are balanced, no voltage will be measured in the bridge. This is achieved by adjusting the resistance $R_3$ at the exact same ratio as the top resistances $R_1$ over $R_2$, so the voltage at point D (equation 5.5) will equal that of B (equation 5.6):

$$V_D = \frac{R_p}{R_1 + R_2}$$

(5.5)

$$V_B = \frac{R_3}{R_2 + R_3}$$

(5.6)

$R_3$ follows by taking the ratio of the two top resistances and the sum of all the resistances in the probe-leg, i.e. the resistance of the cables, leads and support are taken into account:

$$R_3 = \frac{R_1}{R_2} (R_p + R_l + R_s + R_c)$$

(5.7)
Table 5.1: Settings and parameters of probe resistances.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>$R_1$</td>
<td>20</td>
<td>Ω</td>
</tr>
<tr>
<td>$R_{20}$</td>
<td>18.44</td>
<td>Ω</td>
</tr>
<tr>
<td>$R_l$</td>
<td>0.50</td>
<td>Ω</td>
</tr>
<tr>
<td>$R_s$</td>
<td>0.49</td>
<td>Ω</td>
</tr>
<tr>
<td>$R_c$</td>
<td>0.20</td>
<td>Ω</td>
</tr>
<tr>
<td>$V_{top}$</td>
<td>0.05-5</td>
<td>V</td>
</tr>
<tr>
<td>$\alpha_{20}$</td>
<td>0.49</td>
<td>%/K</td>
</tr>
<tr>
<td>$T_p$</td>
<td>333</td>
<td>K</td>
</tr>
<tr>
<td>$T_{amb}$</td>
<td>293</td>
<td>K</td>
</tr>
<tr>
<td>$R_p$</td>
<td>22.05</td>
<td>Ω</td>
</tr>
<tr>
<td>$R_3$</td>
<td>464.9</td>
<td>Ω</td>
</tr>
</tbody>
</table>

Table 5.1 shows the relevant parameters for the probe and the set resistances. The voltage over the probe is a measure for the total heat loss of the probe:

\[ V_p = V_{top} \left( \frac{R_p}{R_1 + R_x + R_l + R_s + R_c} \right) \]  \hspace{1cm} (5.8)

The heat loss is then defined as:

\[ Q_p = \frac{V_p^2}{R_p} \]  \hspace{1cm} (5.9)

from which the Nusselt number can be obtained as follows:

\[ Nu = \frac{Q_p d_p}{A_p (T_p - T_f) k_f} \]  \hspace{1cm} (5.10)

### 5.2.2 Direct Numerical Simulations

For the Direct Numerical Simulations (DNS) an Immersed Boundary method is used as illustrated in figure 5.3. The computational domain is divided into control volumes using a structured uniform mesh whereas the spherical particles are represented by Lagrangian marker points evenly distributed among the surface of the sphere.

The fluid dynamics and heat transport are described by the conservation equations for mass, momentum and thermal energy:

\[ \nabla \cdot \vec{u} = 0 \]  \hspace{1cm} (5.11)
\[ \rho_f \frac{\partial \bar{u}}{\partial t} + \rho_f \bar{u} \cdot \nabla \bar{u} = -\nabla P + \mu_f \nabla^2 \bar{u} + \bar{f} \]  
(5.12)

\[ \frac{\partial T_f}{\partial t} + \bar{u} \cdot \nabla T_f = \alpha_f \nabla^2 T_f + \frac{q}{\rho C_p} \]  
(5.13)

where \( f \) and \( q \) represent the momentum and heat source terms. These terms are used to enforce the no-slip boundary condition for the flow and the Dirichlet boundary condition for the temperature respectively. The numerical method utilizes a staggered computational grid. For more details the interested reader is referred to the work of Tavassoli et al. (2013). The particles are stationary and possess a uniform temperature. One active particle is given an elevated temperature of 60 °C. The fluid heats up due to transfer of heat from this active particle and thus all downstream particles can heat up. To account for heating of the passive particles the heat balance for these particles is solved to obtain the new \((n+1)\) particle temperature from the known old \(n\) particle temperature according to:

\[ T_{p,i}^{n+1} = T_{p,i}^n + \frac{Q_i \times \Delta t}{(\rho C_p)_i} \]  
(5.14)
Table 5.2: Simulation parameters.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$dt$</td>
<td>$5 \times 10^{-6}$ s</td>
</tr>
<tr>
<td>$\mu$</td>
<td>$1.8 \times 10^{-5}$ kg/m.s</td>
</tr>
<tr>
<td>$\rho$</td>
<td>1.2 kg/m$^3$</td>
</tr>
<tr>
<td>$C_p$</td>
<td>1005 J/kg.K</td>
</tr>
<tr>
<td>$d_p$</td>
<td>0.0032 m</td>
</tr>
<tr>
<td>$k$</td>
<td>0.0257 W/m.K</td>
</tr>
<tr>
<td>$\alpha$</td>
<td>$2.13 \times 10^{-5}$ m$^2$/s</td>
</tr>
<tr>
<td>$T_p$</td>
<td>333 K</td>
</tr>
<tr>
<td>$T_f$</td>
<td>293 K</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$d_p/d_x$</th>
<th>Single</th>
<th>Inline</th>
<th>Array</th>
</tr>
</thead>
<tbody>
<tr>
<td>$N_p$</td>
<td>1</td>
<td>3</td>
<td>125</td>
</tr>
<tr>
<td>$N_x$</td>
<td>100</td>
<td>100</td>
<td>200-400</td>
</tr>
<tr>
<td>$N_y$</td>
<td>100</td>
<td>100</td>
<td>200-400</td>
</tr>
<tr>
<td>$N_z$</td>
<td>260</td>
<td>390</td>
<td>200-400</td>
</tr>
</tbody>
</table>

Boundary conditions include free-slip or periodic boundaries on the laterally confining walls.

where $Q_i$ is the computed heat flux of particle $i$:

$$Q_i = -\int_{S_{p,i}} (k_f \nabla T_f \cdot \vec{n}) dS$$

In experiments all passive particles are copper beads with $Bi \ll 1$ and thus equation 5.14 is valid. Other boundary and initial conditions include a prescribed velocity and temperature at the inlet, zero gradient conditions at the outlet and either free-slip or periodic boundaries on the laterally confining walls. Other fluid properties and domain characteristics are given in table 5.2.

### 5.3 Setup

The setup consists of two sections. The bottom section consists of a mass-flow controller with a capacity of 400 l/min and a distribution chamber, with a monolithic membrane to allow for uniform gas distribution. The top section consists of a square channel with holes drilled in two opposite sidewalls, to allow for the abacus-like structure of the arrays. The top section is interchangeable to allow for mounting different top sections and thus studying systems at different solids volume fractions. A thermocouple is attached to
the top section to measure the ambient temperature $T_{amb}$. A pressure sensor is mounted to the side (Dwyer MagneSense with a range of 0 to 1250 Pa).

The sizes of the top sections are given in table 5.3. The height of the top section is 0.1 m. The 1 mm holes are organized in a matrix of 11 rows of 9 holes. Strings of 0.12 mm are strung through the holes and hold 3.2 mm copper beads in place (supplied by BeadFX). The beads have an inner diameter of 0.9 mm. Each row is offset by half a particle diameter, such that the beads can be strung in a body-centred cubic (BBC) arrangement. The particle arrangements have been strung by eye and can have a small deviation from an ideal BCC arrangement.

5.4 Results

In total three different systems are studied with both the CTA probe and the DNS simulations. The first system is the heat transfer of a single particle in unbounded flow, which is described by the Ranz-Marshall equation. The second test consists of an inline array of three particles, which allows the
Table 5.3: Top sections.

<table>
<thead>
<tr>
<th>type</th>
<th>size</th>
<th>number of particles per string</th>
<th>porosity</th>
</tr>
</thead>
<tbody>
<tr>
<td>1a</td>
<td>32 mm</td>
<td>10</td>
<td>0.5</td>
</tr>
<tr>
<td>1b</td>
<td>32 mm</td>
<td>8</td>
<td>0.6</td>
</tr>
<tr>
<td>1c</td>
<td>32 mm</td>
<td>6</td>
<td>0.7</td>
</tr>
<tr>
<td>2</td>
<td>40 mm</td>
<td>7</td>
<td>0.8</td>
</tr>
<tr>
<td>3</td>
<td>50 mm</td>
<td>6</td>
<td>0.9</td>
</tr>
</tbody>
</table>

study of shielding and the effect of inter-particle distance on the fluid particle heat transfer. The third and final system consists of semi-structured arrays of particles with varying porosity, most closely resembling the conditions for which the Gunn correlation was established. The experiments are performed in the relevant range of Reynolds numbers, i.e. $0 < Re \leq 1500$. In the simulations the range of Reynolds numbers is restricted to $20 < Re \leq 400$, because of computational limitations. In the semi-structured arrays the range of Reynolds numbers is sometimes smaller due to either the need to avoid fluidization or due to limitations of the probe.

5.4.1 Single particle

![Figure 5.5: Nusselt number as a function of Reynolds number for a single particle in unbounded flow.](image)

Fluid-particle heat transfer for a single particle in unbounded flow is a
fairly well-defined system and follows the well known Ranz-Marshall equation. In the experiments the CTA-probe is put inside an empty top section. The inflow is varied so that the particle Reynolds number is varied between 0 and 1500 (Re=1500 is the maximum capacity of the probe). All experiments are averaged over time to eliminate periodic changes. For the simulations a particle is placed inside a box of 5 by 5 by 15 times the particle size. The particle is placed at \(3 \times d_p\) from the inflow boundary. A free-slip boundary condition is used for the sides of the domain. A grid dependency study was done to check whether the simulations are grid independent. It was found that at 20 grid cells per particle diameter these simulations are nearly grid independent, with a typical deviation of 2 \%.

The results are shown in figure 5.5. It can be seen that the experiments are in very close agreement with the Ranz-Marshall equation. The deviation is about \(\pm 5\%\), except for the lower Reynolds regime, where other heat transfer mechanisms play a role. In general the simulations follow a similar trend and possess deviations of \(\pm 20\%\). Extrapolation of the results, however, would lead to extensive deviations with experiments and the Ranz-Marshall equation. Possibly the transient behaviour of the wake, as visible in figure 5.6, leads to an unsteady solution in the DNS results for higher Reynolds number flows.

![Figure 5.6: Nusselt number as a function of Reynolds number for an inline array of spheres with interparticle distance of \(2 \times d_p\).](image)

Figure 5.6 shows the temperature fields around the single particle for different Reynolds numbers. It can be seen that the wake is axi-symmetric and stable until \(Re = 200\) and shows slight instability from \(Re = 300\), when the
toroidal vortex breaks and a vortex street is formed, see Johnson and Patel (1999).

![Figure 5.7: Heat transfer mechanisms at Stokes flow regime.](image)

The deviations of the experimental results from the Ranz-Marshall at small Reynolds numbers can be explained by the existence of other important modes of heat transfer; free convection, radiation, conduction from probe to support and convection/conduction of exposed wire in between the probe and the support. These mechanisms have been schematically represented in figure 5.7.

Table 5.4 sums the approximate contributions of these mechanisms. Summation of all heat transfer mechanisms leads to a total of 109% of the found experimental value at $Re = 0$.

It is also possible to express the combined effect of forced and free convection in terms of the Nusselt number following the work of Yamanaka et al. (1976):

\[
Nu = 2 + \left[ \left( \frac{126Re + 57Re^{3/2}Pr^{1/3}}{1 + 52Re^{1/2} + 100Re} \right)^{3/2} + (0.44Gr^{1/4}Pr^{1/4})^{3/2} \right]^{2/3}
\]

\[1 < Re < 900, 7 < Pr < 2.4 \times 10^4, 5.7 \times 10^{-3} < Gr < 10^7\]

(5.16)

Figure 5.8 shows the ratio of the obtained Nusselt numbers from combined convection (equation 5.16) over the Ranz-Marshall equation and the experiments in figure 5.5. It can be clearly seen that forced convection makes up
over 95 % of the heat transfer when \( Re > 400 \). It can also be seen that our experiments match to within 2-3 % with the work of Yamanaka et al. (1976) except at \( Re=0 \), which can be attributed to radiation and conduction to the probe support, respectively.

![Figure 5.8: Ratio of Nusselt numbers from the combined convection (Eq 5.16) and Ranz-Marshall (RM, in red) and experiments respectively (in black).](image)

Table 5.4: Influence of various heat transfer mechanisms at \( Re=0 \).

<table>
<thead>
<tr>
<th>Mechanism</th>
<th>Approximation</th>
<th>% of total</th>
</tr>
</thead>
<tbody>
<tr>
<td>total</td>
<td>( Nu = 4.3 )</td>
<td></td>
</tr>
<tr>
<td>conduction of Sphere</td>
<td>( Nu = 2 )</td>
<td>46.6 %</td>
</tr>
<tr>
<td>Radiation</td>
<td>( Q = \epsilon \sigma \Delta T^4 A_p )</td>
<td>12.1 %</td>
</tr>
<tr>
<td>Free convection</td>
<td>( Nu = \frac{0.587 R \alpha^{0.25}}{(1+0.469 r_p T_{amb}^{0.5})^{3/5}} )</td>
<td>36 %</td>
</tr>
<tr>
<td>Wire conduction</td>
<td>( Q = 2 \pi r_w^2 k_w \frac{T - T_{amb}}{L_w} )</td>
<td>12.3 %</td>
</tr>
<tr>
<td>Wire convection</td>
<td>( Q = 4 \pi r_w L_w h_w (T - T_{amb}) )</td>
<td>2.2 %</td>
</tr>
</tbody>
</table>

5.4.2 Inline array

The next system studied concerns an inline array of three particles. This system is used to study the effect of shielding and inter-particle distance on the fluid-particle heat transfer. The system resembles the system in the study of Tavassoli et al. (2013). The difference between these two systems is that here only one active particle is used (i.e. the CTA probe). The other two particles
are initially cold but can heat up because of heated fluid passing the particle. In the simulations this is incorporated using equation 5.14. In simulations only an inter-particle distance of $2 \times d_p$ is used. In the experiments the effect of inter-particle distance is varied to study both the effect of shielding and the inter-particle distance.

Figure 5.10: Left: Measured Nusselt number of the $2^{nd}$ particle in an inline array of 3 spheres as a function of the Reynolds number for different inter-particle distances. Right: Measured Nusselt number normalized by the Nusselt number from the Ranz-Marshall experiment for different Reynolds numbers and inter-particle distances.
The setup is schematically represented in figure 5.9. The first particle is situated at $3 \times d_p$ from the inflow boundary. The active particle is placed in the second position and in experiments the particle-particle distance is varied between 2 to $6 \times d_p$. In the simulations both the side walls are placed at $2.5 \times d_p$ from the centre of the particles and in the wake a domain size of $10 \times d_p$ is available. For $Re > 400$ the side walls are placed at $3.5 \times d_p$, because otherwise the transient behaviour of the wake there would introduce confinement effects. The simulations have been performed with 20 grid cells per diameter, except the simulation at $Re = 600$, which is performed with 30 grid cells per diameter to resolve the thinner boundary layers around the particles.

Figure 5.10 shows the experimental results for the inline array of three spheres with varying inter-particle distances. The results clearly show an increased Nusselt number over the full Reynolds range up to $Re = 1400$. This enhancement effect is largest when the spheres are close to each other and diminishes with increasing inter-sphere distance. From an inter-particle distance larger than $6 \times d_p$ no enhancement was found, just as reported by Reddy et al. (2013). The right figure shows the relative increase in Nusselt number from the inline array with respect to the results of a single particle in unbounded flow (the Ranz-Marshall experiment). From figure 5.10 it can be seen that the obtained Nusselt numbers follow a different trend for $Re < 400$ than for cases with $Re > 400$. This might be explained due to the contributions of other heat-transfer mechanisms, mainly free convection, which still has a substantial effect up to $Re=400$, see also figure 5.8.

Figure 5.11 shows the results of an inline array of three spheres with an inter-particle distance of $2 \times d_p$. The experiments show an enhancement of the Nusselt number with respect to the Ranz-Marshall equation. The simulations however clearly show a shielding effect for the lower Reynolds regime, $Re < 400$, and an enhancement for $Re > 400$. This shielding effect was expected because of the sphere in front of the active sphere, which was also reported by Tavassoli et al. (2013). The enhancement seems to appear at Reynolds numbers exceeding 400. From simulations it can be seen that the enhancement is accompanied with an onset of a transient wake following the first sphere. This transition is also shown in figure 5.12. Up to $Re = 300$ the space between the first and second sphere is slowly heating. From $Re = 400$, however, the
fluid between the two spheres is constantly refreshed because of the transient wake behaviour. In experiments the onset of a transient wake might appear earlier, either by effects of free convection or possibly also because of the inherent flow instabilities from the mass-flow controller or the distributor.

5.4.3 Semi-structured arrays

In the last case discussed in this chapter, experiments have been performed to study the effects of solids volume fraction and Reynolds number on the fluid-particle heat transfer. The Gunn correlation, see equation 5.3, is used as a reference. The top sections as described in table 5.2 are used. The solids
Figure 5.13: Nusselt number as a function of the particle Reynolds number for several different porosities and a parity plot of the results from experiments and simulations.
volume fraction ranges from 0 to 0.5 with increments of 0.1 and Reynolds numbers ranging from 0 to 800. At a solids volume fraction of 0.1 the Reynolds number is limited to 500, because of the capacity of the mass flow controller. Five rows in the top section are strung with beads, except for the third row where space is reserved to position the probe.

The simulations have been performed with very similar structures. All particles are placed in a BCC packing. All simulations are first performed at a grid resolution of 20 to initialize the flow field. After some time the simulation data is interpolated to provide initial conditions for simulations at a finer grid of 40 grids per diameter. Only five rows and five planes of particles are used, giving a total of 125 particles. The simulations have in- and outflow conditions as explained before. However, in this case periodic boundary conditions were applied in the lateral directions. Only the centre particle has an elevated temperature of 60 °C, all other particles are allowed to heat up by the surrounding fluid.

Figure 5.14: Parity plot of the Nusselt number obtained from experiments and the Gunn-correlation.

Figure 5.13 shows the results of both the simulations and the experiments in comparison to the Gunn correlation. It can be seen that in general the agreement between the simulation results and the experimental data is quite good. There is quite a large difference for the experiments and simulations
for a solids volume fraction of 0.5. It might be that for the simulations the grid resolution becomes a problem at higher solids loadings, resulting in an underestimation of the heat transfer. For the experiments the probe support starts to interfere in the local solids distribution at higher packing fractions. The parity plot of the simulations and experiments shows, however, that most of the results fall within a 20 % error margin. At a lower Reynolds number there is also a relatively large deviation due to combined heat transfer effects, as discussed in the section on a single particle in unbounded flow.

Figure 5.14 shows a parity plot of the Nusselt numbers obtained with experiments in comparison to the Gunn correlation. Again it can be seen that most experiments fall well within 20 % error margins. This shows that the use of CTA-probes in combination with a semi-structured setup is very well suited for studying heat transfer of different packings, thus covering the full range of the Gunn-correlation. The simulations using a IB/DNS method are in very close agreement with the experiments and hence also with the Gunn correlation. This is unlike the work of Tavassoli et al. (2013), where a structural underestimation of the Gunn correlation was found. There are of course very distinct differences in the system under study. In the work of Tavassoli et al. (2013) a fully active and random packing is used, which necessitates the use of averaging the temperature in the driving force and over all particles. On the other hand, in this work a single active particle in structured arrays is used, with a very clear driving force and local structure. This might well be related to the differences found in use of the different forms of the driving force in calculating the Nusselt number as studied in the book of Bird et al. (2007).

5.5 Conclusion

A Constant Temperature Anemometer (CTA) was successfully reconfigured to act as a heat-transfer probe in gas-particle flow systems. In combination with an abacus-like semi-structured bed the effects of Reynolds number and solids packing fraction on the Nusselt number was successfully studied. First CTA measurements were performed on a single particle in unbounded flow and compared to the well known Ranz-Marshall equation as well as Direct Numerical Simulations using an Immersed Boundary method. Second, the CTA
technique was used to study the effects of particle shielding and inter-particle distance, showing that the technique is best equipped to study inline arrays of spheres beyond Re=400 where the onset of a transient wake drives the enhancement of the Nusselt number with respect to a single sphere. Third, experimental and numerical results for different solids fractions show a remarkable good comparison to the Gunn correlation, this unlike results from fully active arrays of particles in DNS, that show a distinct underestimation with respect to Gunn. Further study into the proper use of the heat transfer closure law might be studied using a DNS of a small fluidized bed as in the work of Deen et al. (2012) Also the use of coupled Particle Image Velocimetry and infrared imaging as by Patil et al. (2015) might give more insight into the use of closure laws in fluidized bed systems.
Chapter 6

Hybrid collision integration scheme

6.1 Introduction

Since the introduction of the Distinct Element Model (DEM) by Cundall and Strack (1979) for perfect spheres the field of granular flow modelling has expanded dramatically. The model by Cundall and Strack (1979) has since been extended for solid-fluid interactions, CFD-DEM (Xu and Yu, 1997), non-spherical particles (Pourrin et al., 2005; Lu et al., 2015) and other external forces as van der Waals forces (Marshall, 2009), capillary forces (Mikami et al., 1998), electrostatics (Korevaar et al., 2014) and lift forces (Zastawny et al., 2012). For an overview of the relevant inter-particle and particle-fluid forces see Zhu et al. (2007).

Applications of these models in granular flow are widespread; fluidized beds (Van Buijtenen et al., 2011), rotating drums (Gonzalez Briones et al., 2015; Yang et al., 2008a) and tumbling mills, chute flow (Shirsath et al., 2014), sedimentation and hoppers (Cleary and Sawley, 2002). A comprehensive overview of the many applications of discrete particle modelling can be found in the work of Zhu et al. (2008). The foundation of these models is however the contact model which can be split into a hard sphere model as discussed by Hoomans et al. (1996) and a soft sphere model by Tsuji et al. (1993). Regarding the soft sphere models we can also make a distinction between different force models, most of which are based on variations of the spring-dashpot model.

In the hard-sphere approach, collisions are binary and instantaneous. The model can only handle particle-pair interactions and collisions involving mul-

This chapter is based on Kay A. Buist, L.J.H. Seelen, N.G. Deen, J.T. Padding, J.A.M. Kuipers., On an efficient hybrid soft and hard sphere collision integration scheme for DEM, Chemical Engineering Science, 153 (2016) pp: 363-373
tiple particles are not considered. In simulations the collisions are handled in chronological order. Meaning the simulation time scales with the collision frequency; it is an event-driven technique. As such the hard-sphere model is much more efficient in dilute systems.

For higher density or highly dissipative systems a soft-sphere method is to be preferred. In a soft-sphere method Newton’s equations of motion are integrated and a contact force model is introduced to account for particle-particle interaction based on the deformation or overlap of contacting particles. Because particle overlap is allowed, overlapping of particles with multiple partners is also allowed. The time step for a soft-sphere method depends on the chosen number of steps during a contact, which scales with the chosen spring stiffness of the system; therefore it is a time-driven simulation.

The strength of the hard-sphere model lies in the fact that each collision can be handled instantaneously instead of in a number of steps. The strength however of the soft-sphere method lies in the relaxation of the spring stiffness, which allows taking a larger time step. The most time-consuming step for these simulations is always the determination and updating of the collision partners.

Upon analysis of CFD-DEM simulations of dense gas-particle flows, we found that the number of collision partners in a typical soft-sphere simulation is limited. An example of this is given in figure 6.1, from a simulation of a pseudo-2D fluidized bed, which was validated with two experimental techniques in chapter 3. It can be seen that over 90% of the contacts involve two particles. This means that most collisions are binary, just as in a hard sphere model. The rest of the particles have predominantly two other collision partners and on occasion three or more.

To benefit from the efficiency of the hard sphere model and the robustness of the soft sphere model in this work a hybrid collision integration scheme is introduced. This scheme combines elements of a soft-sphere and a hard-sphere method: All binary contacts will have a collision duration but are handled only once. All Multi-Body Contacts (MBC) are handled with a classical soft-sphere methodology. As such this scheme is still time-driven but with a 10 times larger time step compared to the classical soft-sphere method. This chapter is organized as follows: First a short overview is given of the classical contact schemes, second the hybrid scheme is discussed in more detail followed
6.2 Classical collision schemes

The two most used collision integration schemes for discrete particle models are the so-called softsphere and hard sphere models. Both schemes will be shortly discussed here. A comprehensive overview is given in table 6.1. A more extensive explanation of both schemes can be found in Deen et al. (2007).

6.2.1 Hard sphere scheme

The hard sphere collision integration scheme assumes each collision is instantaneous and binary. The collisions are solved in order of occurrence, as such the hard sphere method is an event-driven model. An efficient method to keep track of the sequence of collisions is needed and for very dense systems with a high collision frequency the hard sphere scheme is less efficient than the soft sphere scheme. In this work the hard sphere model is not used but rather shortly discussed as a reference, because we mostly discuss a relatively dense system and because the hybrid model has the most resemblance to a soft-sphere method.
Table 6.1: Short overview of classical collisions schemes; soft sphere and hard sphere methodology.

<table>
<thead>
<tr>
<th>Soft sphere</th>
<th>Hard sphere</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="chart1.png" alt="Diagram" /></td>
<td><img src="chart2.png" alt="Diagram" /></td>
</tr>
</tbody>
</table>

Linear spring dashpot
\[ \bar{F}_n = -k_n \delta_n \bar{n}_{ab} - \eta_n \bar{v}_{ab,n} \]
\[ \bar{F}_t = -k_t \delta_t \bar{t}_{ab} - \eta_t \bar{v}_{ab,t} \]

or in case of sliding (\( \bar{F}_t > \mu |\bar{F}_n| \)):
\[ \bar{F}_t = -\mu |\bar{F}_n| \bar{t}_{ab} \]

Impulse vector
\[ m(\bar{v} - \bar{v}_0) = \bar{J} \]
\[ \bar{J} = J_n \bar{n}_{ab} + J_t \bar{t}_{ab} \]

\[ J_n = -(1 + \epsilon) \frac{\bar{v}_{ab} \cdot \bar{n}_{ab}}{B_2} \]
\[ J_t = -(1 + \beta) \frac{\bar{v}_{ab} \cdot \bar{t}_{ab}}{B_1}, -\mu J_n \]

Time scale of collision
\[ t_{coll} = \frac{\pi}{\omega_d} \]
Collisions instantaneous
\[ t_{coll} = 0 \]

Time step
\[ \Delta t = \frac{t_{coll}}{10} \]

6.2.2 Soft sphere scheme

The soft sphere model is often based on the linear spring-dashpot model with a frictional slider. The force of the collision scales with the overlap of the particles and is used to update the translational and rotational velocities as follows:

\[ \bar{v} = \bar{v}_0 + (\bar{F}_n + \bar{F}_t) \frac{\Delta t}{m} \quad (6.1) \]
\[ \bar{\omega} = \bar{\omega}_0 + \bar{T} \frac{\Delta t}{I} \quad (6.2) \]

Time is discretized with a time step which typically amounts to \( \sim 10 \) times smaller the duration of a collision. The duration of the collision is associated
with the ratio of the spring stiffness and the mass of the particle and the damping ratio ($\zeta$) as follows:

$$t_{\text{coll}} = \frac{\pi}{\omega_d} = \frac{\pi}{\sqrt{\frac{k_n}{m_{\text{eff}}} \left(\sqrt{1 - \zeta^2}\right)}}$$  \hspace{1cm} (6.3)

where $\omega_d$ is the dampened frequency defined as:

$$\omega_d = \sqrt{\frac{k_n}{m_{\text{eff}}} \left(\sqrt{1 - \zeta^2}\right)}$$

where $\zeta$ is the damping ratio defined as:

$$-\ln(e) \sqrt{\pi^2 + \ln(e)^2}$$

For a full derivation of these properties the interested reader is referred to Appendix A. Here $t_{\text{coll}}$ is independent of the impact velocity $\bar{v}_{ab}$ only for the linear spring dashpot model, for non-linear models the duration of a collision is dependent on the impact velocity (Antypov and Elliott, 2011).

The spring stiffness is based on particle material properties and usually quite high, leading to small time steps. For the soft sphere integration scheme the spring stiffness is chosen such that the maximum overlap $\delta_{\text{max}}$ is $\sim 1\%$ of the particle radius: It is possible to show that $k_n$ follows from:

$$k_n = \frac{v_{ab} m_{\text{eff}} \pi}{\delta_{\text{max}}^2} e \sqrt{\frac{2\ln(e)}{\sqrt{\pi^2 + \ln(e)^2}}} \cos^{-1}\left(\frac{-\ln(e)}{\sqrt{\pi^2 + \ln(e)^2}}\right)$$  \hspace{1cm} (6.4)

Figure 6.2 shows the dependence of the spring stiffness on the ratio of the chosen maximum overlap ($\delta_{\text{max}}$) and the impact velocity. Also the damping on the spring stiffness as a function of the restitution coefficient is shown, which is near linear. In Appendix B a full derivation is given. The tangential spring stiffness is given as:

$$k_t = k_n \frac{2}{\pi} \left(\frac{\pi^2 + \ln(e)^2}{\pi^2 + \ln(\beta)^2}\right)$$  \hspace{1cm} (6.5)

With respect to reality the spring stiffness is thus relaxed. Because overlap is allowed, collisions involving more than two particles is thus possible; Multi-Body Contacts (MBC). In figure 6.1 it is shown that for a typical DPM
Figure 6.2: The spring stiffness as a function of the ratio of the maximum overlap and the impact velocity for the two bounds $e = 0$ and $e = 1$ (left), and the damping (exponential part of equation 6.4) on the spring stiffness as a function of the restitution coefficient (right).

simulation the number of MBC's is limited to a few percent of the total number of collision. Because the main part is binary, we suggest a hybrid collision scheme that can handle the binary collisions instantaneously, whereas the MBC's are treated with a classical soft sphere scheme.

6.3 Hybrid collision integration scheme

The first researchers using a time-driven hard sphere approach are Helland et al. (2002). In their work however each collision is still quasi-instantaneous. The first to couple a hard sphere and a soft sphere approach was Gui et al. (2016) in 2016. An extended version of the hard particle model for square particles in 2D was proposed coupled to a soft sphere methodology. In their work however the time step used is still considerably smaller than the duration of a collision. The use of a hard sphere methodology however allows for an accurate description of collisions while maintaining an approximately 10 times larger time step with respect to a classical visco-elastic methodology for non-spherical particles.

The hybrid collision integration scheme that is presented here assumes that most collisions are binary and have a fixed well-defined duration, based on the linear spring dashpot model. The binary collisions are solved using a modified hard sphere methodology. All collisions involving more than two
collision partners are solved using a classical soft sphere methodology. A short schematic overview is given in table 6.2.

The chosen time step is exactly the duration of a collision, generally ten times larger than for a classical soft sphere model. As such only one full collision can be solved per particle per time step. The collision detection has to be done once every time step. For reference the classic soft sphere methodology would need the collision detection ten times per collision duration. With the collision detection being the most time consuming step in a simulation, the simulation time is expected to be roughly and at best ten times lower.

In the next few sections we will discuss in a bit more detail binary collisions and multibody collisions. Finally an overview of the model is given that shows the main extra steps that need to be taken into account.

### 6.3.1 Binary collisions

For the new model, we first assumed particles are of equal size and mass possessing no tangential component ($\mu = 0$ and $v_{t,0} = 0$). For a binary collision it follows that:

$$\bar{v}_n = \bar{v}_{n,0} - \frac{1 + e}{2} \bar{v}_{ab,n}$$  \hfill (6.6)

with $\bar{v}_{ab}$ defined as the relative velocity at the point of contact:

$$\bar{v}_{ab} = \bar{v}_a - \bar{v}_b + r (\bar{\omega}_a + \bar{\omega}_b) \times \bar{n}_{ab}$$  \hfill (6.7)

which consists of a normal and a tangential component:

$$\bar{v}_{ab,n} = \bar{v}_{ab} \cdot \bar{n}_{ab}$$  \hfill (6.8)

$$\bar{v}_{ab,t} = \bar{v}_{ab} - \bar{v}_{ab,n}$$  \hfill (6.9)

$$\bar{n}_{ab} = \frac{\bar{x}_b - \bar{x}_a}{|\bar{x}_b - \bar{x}_a|}$$  \hfill (6.10)

$$\bar{t}_{ab} = \frac{\bar{v}_{ab,t}}{|\bar{v}_{ab,t}|}$$  \hfill (6.11)

Finally the position is defined as:

$$\bar{x} = \bar{x}_0 - \bar{v}_{n,0} t_{last} + \frac{\bar{v}_a + \bar{v}_b}{2} \Delta t + \bar{v} t_{last}$$  \hfill (6.12)
Table 6.2: Short overview of the hybrid collisions schemes.

<table>
<thead>
<tr>
<th>Hybrid model</th>
<th>Binary</th>
<th>Multibody</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$\vec{v}<em>{n,a} = \vec{v}</em>{n,a,0} - \frac{1+e}{2} \vec{v}_{ab,n}$</td>
<td>$\vec{F}<em>n = -k_n \delta_n \vec{r}</em>{ab} - \eta_n \vec{v}_{ab,n}$</td>
</tr>
<tr>
<td></td>
<td>$\vec{x}<em>a = \vec{x}</em>{a,0} + \frac{\vec{v}_a + \vec{v}<em>b}{2} \Delta t + (\vec{v}<em>a - \vec{v}</em>{n,a,0}) t</em>{last}$</td>
<td>$\vec{F}<em>t = -k_t \delta_t \vec{r}</em>{ab} - \eta_t \vec{v}_{ab,t}$</td>
</tr>
<tr>
<td></td>
<td>$t_{last} = \frac{(\vec{r}<em>{ab} \cdot \vec{v}</em>{ab} + \sqrt{(\vec{r}<em>{ab} \cdot \vec{v}</em>{ab})^2 - (</td>
<td>\vec{r}_{ab}</td>
</tr>
<tr>
<td></td>
<td>$t_{coll} = \frac{\pi}{\omega_d}$</td>
<td>$\vec{F}_t = -\mu</td>
</tr>
<tr>
<td></td>
<td>$\Delta t = t_{coll}$</td>
<td>Time step dilation (MBC)</td>
</tr>
<tr>
<td></td>
<td>$\Delta t = \frac{t_{coll}}{10}$</td>
<td></td>
</tr>
</tbody>
</table>

The new position is the sum of respectively the old position, the displacement until collision based on the old velocity, a centre of mass displacement during collision and a displacement after the collision till the end of the time step.

Here, $\vec{x}_0$ and $\vec{v}_0$ are the position and velocity at the time step before collision and $\vec{x}$ and $\vec{v}$ the position and velocity at the time step after the collision. $t_{last}$ is the time between the moment of first contact until the end of the time step. These are given by:

$$\vec{r}_{ab} = \vec{x}_a - \vec{x}_b$$

$$\vec{v}_{ab} = \vec{v}_a - \vec{v}_b$$
\[ t_{last} = \frac{\left( \bar{r}_{ab} \cdot \bar{v}_{ab} + \sqrt{\left( \bar{r}_{ab} \cdot \bar{v}_{ab} \right)^2 - \left( |\bar{r}_{ab}| - (R_a + R_b) \right)^2 |\bar{v}_{ab}|} \right)}{|\bar{v}_{ab}|} \] (6.13)

If the tangential component is added an extension on the normal and tangential velocity is needed also a frictional limit has to be defined, for a full derivation see also Appendix C.

### 6.3.2 Multibody collisions

Multibody contacts cannot be treated analytically. Of course the position and velocity can be easily determined and follows a very similar equation as those for binary collisions. However the time of collision cannot easily be determined. The typical solution of a multibody contact involves:

\[ x_i(t) = \sum_{i=1}^{n} e^{-\zeta \omega_n t} \left( d_{1,i} \cos (\omega_d i t) + d_{2,i} \sin (\omega_d i t) \right) \] (6.14)

where \( n \) is the number of contacts. It is possible to solve this for a number (> 1) of simultaneous contacts, but each (> 2) possible simultaneous contact situation would have a unique solution. Even though it is possible to determine trajectory and the change of velocity of the MBC it is not possible to determine the duration of the collision analytically as the sum of sinusoids with differing frequencies and amplitudes cannot be easily simplified. As such it is not possible to determine the outcome of a MBC in this particular way.

Keeping the above in mind it is simpler to use the classical soft sphere treatment and divide the contact time into a number of steps only for the particles in an MBC.

### 6.3.3 Overview

To give a more clear overview of the hybrid integrations scheme, we go through the several phases of a time step, see also Figure 6.3. In the classical soft sphere scheme, first a collision detection scheme is used, and once all possible collision pairs are found the forces associated with the collisions are calculated. The last step is to sum all the forces of a particular particle and update the velocity and position of the particles. This process is then repeated.

The hybrid scheme follows a reversed order, we have to start the explanation with the collision detection however. The collision detection is done at
the end of the collision, to determine the particles that are in collision mode, but because the time step is the same as the duration of a collision, the collision will finish in the next step. In a new time step, first all particle positions and velocities are updated for all particles. Part of this update is the update of all collision partners that have been determined during the last time step, because their collisions end in this time step. After these updates, collision detection is performed for all particles. In the final step we have to check if collision partners, from the collision detection, contain particles that in the previous time step already had been in collision mode. These collisions
might overlap and have to be solved separately, which is discussed later.

Figure 6.4: Schematic of possible collisions. Each block signifies one time step, each number signifies a particle, the colored lines represent the start and completion of the collision. In green a binary collision, in blue a typical multibody collision, in red and orange two binary collisions possibly overlapping.

An overview of all possible types of collisions is given in figure 6.4. In this figure the numbers relate to a particle and the black lines to the different time steps. The colored lines signify the duration of the collision. In the first time step we notice through collision detection that particles 1 and 2 are undergoing a binary collision, they however keep their respective artificial position and velocities. We solve for the collision in the second time step because the collision should be finished by then.

Particles 3, 4 and 5 are found to be in contact in the third time step. Because this is a multibody collision, the time step is split in ten sub steps.
and the collision is solved following the classical soft sphere methodology.

After the collision detection is performed, all particles in contact are referenced against the particles in collision in the previous time step. The particles that are in contact in both time frames are special cases and have to be solved separately and have three possible outcomes. For instance in figure 6.4 particles 6 and 7 are found to be in contact in the first time step and are solved in the second time step, however in this time step we find particles 7 and 8 to be in contact. Thus particle 7 is found to be in a collision both in time steps 1 and 2. Now the two collisions can be completely separate or adjoining, and when adjoining could last till the second or the third time step. These three situations are depicted in table 6.3.

In the first case the two collisions are non-overlapping and completely separate, meaning nothing is wrong and the collision between particles 7 & 8 can commence in the next time step as usual. The second and third cases are when the two collisions are overlapping, with one lasting until the second time step and one lasting past the second time step. These have to be solved using a soft-sphere method i.e. as an MBC. For the second case the collision has to be solved in the third time step using a soft-sphere method as well but now taking information from the second time step instead of two time steps back as usual. In that case particles 7 & 8 get a special tag signifying the need for special treatment.

To distinguish between these situations the \( t_{last} \) (equation 6.13) of both of the collisions has to be determined. The sum of the \( t_{last} \) of the new collision and \( \Delta t - t'_{last} \) of the old collision makes the distinction between the first and the last two cases. \( \Delta t - t'_{last} \) is the amount of time the collision between particles 6 & 7 is taking place in the time step from \( 1\Delta t \) to \( 2\Delta t \) and if the sum of this with the collision duration from particle 7 & 8 is smaller than \( \Delta t \) the two collisions are separate. If the sum is larger than \( \Delta t \) the two collisions are overlapping. All particles in the last two situations have to be checked for new collision partners or remaining overlap. In the case of new collision partners, the collisions have to be solved again. In the case of remaining overlap they get a special tag and in the case of no remaining collision partners nothing has to be done in the next time step.
Table 6.3: Overview of the three different situations in case of possible overlapping collisions with \( t_{last} \) the duration of the collision of particles 7 & 8 at \( 2\Delta t \) defined by equation 6.13 and \( t'_{last} \) the duration of the contact between 6 & 7 at \( 1\Delta t \)

<table>
<thead>
<tr>
<th>case</th>
<th>schematic</th>
<th>( t_{last} + (\Delta t - t'_{last}) )</th>
<th>solve</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td><img src="image1" alt="Diagram" /></td>
<td>( &lt; \Delta t )</td>
<td>N=2</td>
</tr>
<tr>
<td>2</td>
<td><img src="image2" alt="Diagram" /></td>
<td>( &gt; \Delta t )</td>
<td>MBC</td>
</tr>
<tr>
<td>3</td>
<td><img src="image3" alt="Diagram" /></td>
<td>( &gt; \Delta t )</td>
<td>MBC</td>
</tr>
</tbody>
</table>
### 6.4 Results

Table 6.4: Parameter values used for the simulations.

<table>
<thead>
<tr>
<th>parameter</th>
<th>value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\phi_s$</td>
<td>0.4-0.5</td>
</tr>
<tr>
<td>$N_p$</td>
<td>$10^3 - 10^6$</td>
</tr>
<tr>
<td>$d_p$</td>
<td>0.003 m</td>
</tr>
<tr>
<td>$\rho$</td>
<td>2500 kg/m$^3$</td>
</tr>
<tr>
<td>$k_n$</td>
<td>20000 N/m</td>
</tr>
<tr>
<td>$e$</td>
<td>0.7-1.0</td>
</tr>
<tr>
<td>$\beta$</td>
<td>1</td>
</tr>
<tr>
<td>$\mu$</td>
<td>0</td>
</tr>
<tr>
<td>$&lt;v_n&gt;$</td>
<td>0 m/s</td>
</tr>
<tr>
<td>$v_t$</td>
<td>0 m/s</td>
</tr>
<tr>
<td>$v_{max}$</td>
<td>$\pm0.025-0.15$ m/s</td>
</tr>
</tbody>
</table>

In this section the first results of the new integration scheme will be shown. First, tests are carried out for a bounding box problem. This problem consists of a square box randomly filled with particles. The particles have zero mean velocity and are given a velocity drawn from a Gaussian distribution. The maximum velocity, solids fraction and the box size can be varied to scale the problem. The properties of the simulation are given in table 6.4 and are inspired by simulations of a fluidized bed (see figure 6.1).

#### 6.4.1 Speed up & scalability

The first test involves a bounding box containing 4000 particles with a solids volume fraction of 40%. The particles are allowed to freely bounce in the box for 0.1 s of real time. Simulations were conducted using both the new collision integration scheme as well as the classical soft sphere scheme. This resulted in on average 50 collisions per particle and 0.4 multibody collisions per particle. In this test the particles have ideal collision properties. This implies that the total energy in the system should remain constant. The normalized total kinetic energy of the particles is shown in figure 6.5. The total energy is normalized to the energy given at $t=0$.

The classical soft sphere method shows regular dips in the energy-level associated with energy being stored in the springs as a consequence of the collisions. The hybrid model has a largely static energy profile as most col-
Collisions are binary. Both models are capable of maintaining proper energy conservation, as expected. The difference is, however, that the hybrid model is about eight times faster.

![Normalized energy levels per time step for a bounding box problem with e=1](image)

Figure 6.5: Normalized energy levels per time step for a bounding box problem with e=1. In black the classical soft-sphere method is given, in green the new hybrid model.

To test for the scalability of the hybrid model and the robustness of the gained speed up, the size of the bounding box is gradually increased to $10^6$ particles. The relative speed up for these systems is shown in figure 6.6. It can be seen that an average speed up of a factor 8 is possible with the new hybrid collision integration scheme. This speed up can be attributed to the lower number of collision detection evaluations that are necessary. The maximum possible speed-up factor 10 is not reached because of the overhead associated with the check for overlapping collisions as discussed in the previous section and table 6.3.

### 6.4.2 Varying restitution coefficient

To check if the two models work for a varying restitution coefficient the simulations were run with e=0.7, 0.8, 0.9 & 0.97 and a solids volume fraction of 50%. The time duration was about 0.05 s real time, allowing for 75% of the total energy to dissipate. The result is presented in figure 6.7. It can be seen that the first few time steps no energy is lost, because the particles are initialized on a lattice and collisions take place. With lowering the restitu-
tion coefficient the energy drops faster, as can be expected. The agreement between the two schemes is very good.

Figure 6.6: Speed up as a function of the number of particles (N).

Figure 6.7: Normalized energy loss over time for varying restitution coefficient for the classical and the hybrid model.

6.4.3 Number of contact partners

For the new hybrid model to be competitive with the classical soft sphere model, it has to be capable of dealing with systems with similar solids fractions and granular temperatures. It is the combination of these two parameters that determines the amount of multibody collisions. For this reason a simulation was run with a solids fraction of 50% and a maximum velocity of 0.15 m/s. The results are shown in figure 6.8. The left figure shows the normalized
energy of the system for the two schemes, the figure on the right shows the probability of the number of contact partners, with 2 being binary and every higher number signifying extra particles participating in the collision. It can be seen that the two models show the same trend, now with more energy stored in the springs for the classic model. The amount of multibody collisions add up to about 5% of all collisions which matches the result of figure 6.1. The hybrid model is thus able to match the density and energy of systems in which typically a soft sphere model is used.

![Normalized Energy loss over time](image)

Figure 6.8: Normalized Energy loss over time for the two schemes (left), collision order probability (right), for a bounding box problem with $\varepsilon = 0.5$, $e = 0.9$, $\mu = 0$.

## 6.4.4 Relaxing the classical scheme

In the classical scheme it is also possible to scale the duration of a collision by scaling the spring stiffness. By reducing the spring stiffness by a factor 100 the duration of a collision is multiplied by a factor ten, i.e. the same as for our hybrid model. This will reduce computation time but will also increase the overlap for contacts. To see if this affects the energy balance of the system, the results of such scaling of the spring stiffness is done for the same simulation as before, figure 6.8. Figure 6.9 shows the result for the classical scheme with a scaled spring stiffness in comparison to the classical and the hybrid schemes. The number of contact partners is also shown for the scaled model. The first thing that can be seen is that the scaled scheme has a very sudden and large drop in energy associated with a lot of particles.
going into collision at the same time, often with multiple collision partners. Binary collisions only make up for 65% of all collisions. The rate of energy loss is also much slower than for the classical and the hybrid schemes. This underestimation of the dissipation rate is entirely attributable to the number of multibody contacts and was also found for pure multibody contacts in Pournin et al. (2001). The relative speed up of the scaled model is only in the order of 2.5. The poor performance of this scaled classic model in terms of both the energy conservation and the speed up of the model shows the power and need of a hybrid model all the more.

Figure 6.9: Normalized Energy loss over time for the classic scheme with a scaled spring stiffness (blue), for a bounding box problem with $\varepsilon = 0.5$, $e = 0.9$, $\mu = 0$.

6.5 Conclusions

A novel hybrid collisions integration scheme based on the classical soft-sphere and hard-sphere schemes is presented. Most of the prevailing collisions for a typical dense gas-particle flow problem were shown to be binary which can be accurately handled in a single time step. All Multi-Body Contacts are handled using a classical soft-sphere methodology. The time step of this new scheme was taken to be exactly the duration of a collision based on the linear spring-dashpot force model.

This novel scheme benefits from a reduction in the number of time steps by skipping the numerical integration for all binary collisions and the reduction in the number of collision detection steps. As such, a typical speed-up factor
8 was found for this new scheme, while retaining energy and momentum conservation. Even more so, because for the larger part of the system no energy is stored in the springs of the contact model, the instantaneous velocities of the particles represent the true velocity of the energy state of the system.

The results from this scheme were scalable for the number of particles within the system and showed very good comparison for varying restitution coefficients. The novel scheme is capable of simulating reasonably dense systems with sufficient energy to resemble an actual granular flow problem.

It was also found that relaxing the spring stiffness of the classical scheme to match the time step of the hybrid scheme resulted in an energy dissipation rate that differs distinctly from the classical and novel scheme. Moreover because of the number of collision partners for each particle the simulation was only 2.5 times faster with a 10 times larger time step. As such there is a trade off between not over-relaxing the spring stiffness and not using a too small time step to be able to handle a sufficient amount of particles. With the novel scheme, simulations can either be faster and/or bigger.

The work discussed here serves as a base of principle for a novel hybrid collision integration scheme. For future work we expect to extend the model to include rotation, solid-fluid coupling, non-spherical particles and applications within granular flow problems.

Appendix A

This appendix serves as a precursor to appendices B and C. This appendix gives the full derivation for the linear ordinary homogeneous second order differential equation related to the linear spring-dashpot model:

\[ m_{\text{eff}} \ddot{x} + \eta \dot{x} + kx = 0 \]  \hspace{1cm} (6.15)

This expression signifies the relation between the acceleration, the velocity and position. Now we will define a few new parameters, the natural frequency:

\[ \omega_n = \sqrt{\frac{k}{m_{\text{eff}}}} \]  \hspace{1cm} (6.16)

the damping ratio:

\[ \zeta = \frac{\eta}{2m_{\text{eff}} \omega_n} \]  \hspace{1cm} (6.17)
and the dampened frequency:

\[ \omega_d = \omega_n \sqrt{1 - \zeta^2} \]  

(6.18)

With these parameters equation 6.15 can be rewritten as:

\[ \frac{1}{2} \ddot{x} + \zeta \omega_n \dot{x} + \frac{1}{2} \omega_n^2 x = 0 \]  

(6.19)

This ODE has a solution of the form of \( x = e^{st} \). Upon substitution of \( x = e^{st} \) into equation 6.19 and division by \( e^{st} \) we obtain the characteristic polynomial in terms of parameter \( s \):

\[ \frac{1}{2} s^2 + \zeta \omega_n s + \frac{1}{2} \omega_n^2 = 0 \]  

(6.20)

with roots of the characteristic equation given by:

\[ -\zeta \omega_n \pm \sqrt{\zeta^2 \omega_n^2 - \omega_n^2} = \left( -\zeta \pm \sqrt{\zeta^2 - 1} \right) \omega_n \]  

(6.21)

If \( \zeta < 1 \) than we have an under damped system and a general solution of the form:

\[ x(t) = c_1 e^{-\zeta + \sqrt{\zeta^2 - 1} \omega_n t} + c_2 e^{-\zeta - \sqrt{\zeta^2 - 1} \omega_n t} \]  

(6.22)

which can be rewritten with the use of Euler’s formula as:

\[ x(t) = e^{-\zeta \omega_n t} \left( d_1 \cos (\omega_d t) + d_2 \sin (\omega_d t) \right) \]  

(6.23)

Now we need to define the initial conditions to solve for the two integration conditions \( d_1 \) and \( d_2 \). At \( t = 0 \) we have:

\[ x(t = 0) = x_0 \]
\[ v(t = 0) = v_0 \]

Combination with equation 6.22 gives:

\[ x(0) = e^{-\zeta \omega_n 0} \left( d_1 \cos (\omega_d 0) + d_2 \sin (\omega_d 0) \right) \]  

(6.24)

\[ x(0) = e^{-\zeta \omega_n 0} \left( d_1 \cos (\omega_d 0) + d_2 \sin (\omega_d 0) \right) \]  

(6.25)

\[ x(0) = d_1 \]  

(6.26)

\[ x(t) = e^{-\zeta \omega_n t} \left( x_0 \cos (\omega_d t) + d_2 \sin (\omega_d t) \right) \]  

(6.26)
Differentiation of this function leads to:

\[ \dot{x}(t) = e^{-\zeta \omega_n t} (x_0 \omega_d \sin (\omega_d t) + d_2 \omega_d \cos (\omega_d t) - \zeta \omega_n [x_0 \cos (\omega_d t) + d_2 \sin (\omega_d t)]) \]

\[ \dot{x}(0) = v_0 = (d_2 \omega_d + \zeta \omega_n x_0) \cos (\omega_d t) + (x_0 \omega_d + \zeta \omega_n d_2) \sin (\omega_d t) \]

\[ d_2 = \frac{v_0 + \zeta \omega_n x_0}{\omega_d} \]

and:

\[ x(t) = e^{-\zeta \omega_n t} \left( x_0 \cos (\omega_d t) + \frac{v_0 + \zeta \omega_n x_0}{\omega_d} \sin (\omega_d t) \right) \]

(6.28)

To continue our derivation we will first assume \( x_0 = 0 \). For two colliding spheres this is correct, since we will always solve for the full collision:

\[ x(t) = v_0 e^{-\zeta \omega_n t} \left( \frac{1}{\omega_d} \sin (\omega_d t) \right) \]

(6.29)

\[ \dot{x}(t) = v_0 e^{-\zeta \omega_n t} \left( \cos (\omega_d t) + \frac{\zeta \omega_n}{\omega_d} \sin (\omega_d t) \right) \]

(6.30)

From equation 6.29 it is easy to see that the duration of a collision is given by \( \frac{\pi}{\omega_d} \).

**Appendix B**

The maximum overlap is given when the relative velocity is zero:

\[ \dot{x}(t) = v_0 e^{-\zeta \omega_n t} \left( \cos (\omega_d t) - \zeta \omega_n \frac{\sin (\omega_d t)}{\omega_d} \right) = 0 \]

(6.31)

\[ A \cos (bx) + B \sin (bx) = \sqrt{A^2 + B^2} \cos \left( bx - \tan^{-1} \left( \frac{B}{A} \right) \right) \]

(i)

Using identity (i) we can simplify equation 6.31 to:

\[ \left( \cos (\omega_d t) - \zeta \omega_n \frac{\sin (\omega_d t)}{\omega_d} \right) \sqrt{1 - \left( \frac{\zeta \omega_n}{\omega_d} \right)^2} \cos \left( \omega_d t - \tan^{-1} \left( \frac{\zeta \omega_n}{\omega_d} \right) \right) = 0 \]

(6.32)

Taking only the time dependent part:

\[ \cos \left( \omega_d t - \tan^{-1} \left( \frac{\zeta \omega_n}{\omega_d} \right) \right) = 0 \]
Upon rearranging we get:

\[ \omega_d t - \tan^{-1} \left( \frac{\zeta \omega_n}{\omega_d} \right) = \frac{\pi}{2} \]

Solving for \( t \) and using several trigonometric identities we obtain:

\[ \frac{\pi}{2} - \tan^{-1} (x) = \cot^{-1} (x) = \cos^{-1} \left( \frac{x}{\sqrt{1 + x^2}} \right) \]  

(ii)

\[ t = \frac{\frac{\pi}{2} - \tan^{-1} \left( \frac{\zeta \omega_n}{\omega_d} \right)}{\omega_d} = \frac{\cos^{-1} \left( \frac{\zeta \omega_n}{\omega_d} \sqrt{1 + \left( \frac{\zeta \omega_n}{\omega_d} \right)^2} \right)}{\omega_d} \]  

(6.33)

\[ t = \frac{\cos^{-1} \left( \frac{\zeta \omega_n}{\omega_d} \sqrt{(\zeta \omega_n)^2 + \omega_d^2} \right)}{\omega_d} = \frac{\cos^{-1} \left( \frac{\zeta \omega_n}{\omega_d} \sqrt{(\zeta \omega_n)^2 + (1 - \zeta^2) \omega_n^2} \right)}{\omega_d} = \frac{\cos^{-1} (\zeta)}{\omega_d} \]  

(6.34)

If we substitute this into the equation for the relative distance (overlap) we obtain:

\[ x_{\text{max}} = v_0 e^{-\zeta \omega_n \cos^{-1} (\zeta) \omega_d} \left( 1 - \frac{\omega_d}{\omega_n} \sin \left( \omega_d \cos^{-1} \left( \frac{\zeta}{\omega_d} \right) \right) \right) \]  

(6.35)

\[ \sin \left( \cos^{-1} (x) \right) = \sqrt{1 - x^2} \]  

(iii)

Using identity (iii) and the definitions of \( \omega_d \) and \( \omega_n \) to simplify equation 6.35:

\[ x_{\text{max}} = \frac{v_0 e^{-\zeta \omega_n \cos^{-1} (\zeta) \omega_d}}{\omega_d} \sqrt{1 - \zeta^2} = \frac{v_0}{\omega_n} e^{-\zeta \omega_n \cos^{-1} (\zeta) \omega_d} \]  

(6.36)

\[ x_{\text{max}} = \frac{v_0}{\sqrt{m_{\text{eff}} k_n m}} e^{-\frac{\zeta}{\sqrt{1 - \zeta^2}} \omega_d} \]  

(6.37)

We could thus determine the spring stiffness by solving the above equation for \( k_n \) to obtain:

\[ k_n = \frac{v_0^2 m_{\text{eff}}}{x_{\text{max}}^2} e^{-\frac{2\zeta}{\sqrt{1 - \zeta^2}} \omega_d} \]  

(6.38)

The damping factor \( \zeta \) might to be thought to depend on \( k \) via both the damping coefficient \( \eta \) and the natural frequency \( \omega_n \). However the spring stiffness factors out:

\[ \zeta = \frac{\eta}{2m_{\text{eff}} \omega_n} = \frac{2 \ln(e) \sqrt{k_n m_{\text{eff}}}}{\pi^2 + \ln(e)^2} = \frac{-\ln(e)}{2m_{\text{eff}} \sqrt{\frac{k_n}{m}}} \]  

108
which gives:

\[
k_n = \frac{v_0^2 m_{\text{eff}}}{x_{\text{max}}^2} e \sqrt{\frac{2\ln(e)}{\sqrt{\pi^2 + \ln(e)^2}}} e^{\cos^{-1}\left(\frac{-\ln(e)}{\sqrt{\pi^2 + \ln(e)^2}}\right)}
\]

(6.39)

This expression indicates that the spring stiffness depends on the maximum overlap the maximum relative velocity and the effective mass of the collision pair. This is then corrected for damping with the exponential part of the function. The nice thing is that when restitution is 1 the exponential part is equal to 1, giving:

\[
k_n = \frac{v_0^2 m_{\text{eff}}}{x_{\text{max}}^2}
\]

(6.40)

**Appendix C**

Derivation of the update of the tangential velocity and the friction limit following the hard sphere approach is as follows:

\[
m_a (\bar{v}_a - \bar{v}_{a,0}) = \bar{J}
\]

(6.41)

\[
I_a (\bar{\omega}_a - \bar{\omega}_{a,0}) = -(R_a \bar{n}_{ab}) \times \bar{J}
\]

(6.42)

with J given as:

\[
\bar{J} = J_n \bar{n}_{ab} + J_t \bar{t}_{ab}
\]

(6.43)

\[
J_n = -(1 + \epsilon) \frac{\bar{v}_{ab,0} \cdot \bar{n}_{ab}}{B_2}
\]

(6.44)

\[
J_t = -(1 + \beta) \frac{\bar{v}_{ab,0} \cdot \bar{t}_{ab}}{B_1}
\]

(6.45)

or for the sliding limit if:

\[
\mu < \frac{(1 + \beta) |\bar{v}_{ab,0} \cdot \bar{t}_{ab}|}{|J_n|B_1}
\]

(6.46)

\[
J_t = -\mu J_n
\]

(6.47)

with \(B_1\) and \(B_2\) defined as:

\[
B_2 = \frac{1}{m_a} + \frac{1}{m_b}
\]

(6.48)
\[
B_1 = \frac{7}{2} \left( \frac{1}{m_a} + \frac{1}{m_b} \right) \quad (6.49)
\]

still assuming spheres of equal mass we now have for the normal velocity:

\[
m (\ddot{v}_a - \ddot{v}_{a,0}) = -(1 + e) \frac{\dot{v}_{ab,0,n}}{B_2} - (1 + \beta) \frac{\dot{v}_{ab,0,t}}{B_1} \quad (6.50)
\]

rearranging and discarding the mass leaves:

\[
\ddot{v}_a = \ddot{v}_{a,0} - (1 + e) \frac{\dot{v}_{ab,0,n}}{2} - (1 + \beta) \frac{\dot{v}_{ab,0,t}}{7} \quad (6.51)
\]

To obtain the normal and tangential component we can now simply project it onto the normal and tangent:

\[
\ddot{v}_{a,n} = \ddot{v}_{a,0,n} - (1 + e) \frac{\dot{v}_{ab,0,n}}{2} \quad (6.52)
\]

\[
\ddot{v}_{a,t} = \ddot{v}_{a,0,t} - (1 + \beta) \frac{\dot{v}_{ab,0,t}}{7} \quad (6.53)
\]

The sliding limit can be rewritten in terms of the initial ratio of the projection of the relative velocity in the normal and tangential directions, or also the impact angle:

\[
\mu < \frac{(1 + \beta) |(\ddot{v}_{ab} \cdot \ddot{t}_{ab})|}{(1 + e) |(\ddot{v}_{ab} \cdot \ddot{n}_{ab})| |B_1| |B_2|} \quad (6.54)
\]

\[
\mu < \frac{(1 + \beta) |(\ddot{v}_{ab} \cdot \ddot{t}_{ab})|}{(1 + e) |(\ddot{v}_{ab} \cdot \ddot{n}_{ab})| |B_1|} \quad (6.55)
\]

\[
\mu < \frac{(1 + \beta) |(\ddot{v}_{ab} \cdot \ddot{t}_{ab})|}{(1 + e) |(\ddot{v}_{ab} \cdot \ddot{n}_{ab})| |B_1|} \quad (6.55)
\]

In which case:

\[
\ddot{v}_{a,t} = \ddot{v}_{a,0,t} + \mu (1 + e) \frac{(\ddot{v}_{ab,0} \cdot \ddot{n}_{ab}) \ddot{t}_{ab}}{2} \quad (6.55)
\]
Conclusion and outlook

Because many different topics have been discussed in this work, ranging from particle tracking to heat transfer to novel collision integration schemes, reflection on the current work and outlook for ways forward is needed.

A novel particle tracking technique was developed: Magnetic Particle Tracking (MPT). MPT tracks a single magnetic particle through reconstruction of the magnetic field. This results in information on the particle position as well as the orientation. MPT was compared to both an established non-invasive monitoring technique; Particle Image Velocimetry (PIV) as well as a Discrete Particle Model (DPM) for a pseudo 2D fluidized bed. It was shown that the results match qualitatively pretty well. The results however are limited to relatively large and heavy particles; 3 mm steel spheres. This is mainly due to the fact that size and density of the magnet has to be matched for the bulk material. 3 mm magnetic markers are currently the smallest possible magnets as the magnetic moment of this size of magnet is just enough to generate a magnetic field that is visible for the AMR sensors. To increase the performance of the MPT sensor array, noise reduction is needed. A new sensor array; MagTrack 2.0 is under development that handles digital signals only and has a noise reduction of a factor 5. See figure 7.1 for a first test of the position error as a function of the magnetic moment for the new system (related to figure 2.6 in chapter 2). Indeed the MagTrack 2 system is roughly half an order of magnitude more accurate.

This will allow for either smaller or lower density magnets, such as injection moulded rubber magnets. The strength of the current magnets of type N52 are the strongest possible magnets at this moment, with a $BH_{\text{max}}$ of 52 MGOe. For the foreseeable future greater strengths than 64 MGOe are not envisioned, although a theoretical maximum of 144 MGOe is given for some other compounds. Unfortunately the actual signal on the AMR sensors scales with the magnetic moment of the actual magnet which scales with the volume...
Figure 7.1: Error dependency of the magnetic markers with varying magnetic moment for the two different MagTrack systems using the SQP method.

of the magnet and thus the diameter to the power three. A reduction in magnet diameter by a factor two would need an increase in magnet strength or an increase of S/R by a factor eight. Understandably, such an increase would have to be sought in the hardware design, rather than magnet strength. In this sense MPT can never compete with other particle tracking techniques such as PEPT and RPT, which have reported particle sizes in the order of 100 micron and smaller. Therefore the strength of this technique must be sought in its reduced cost and inherent safety. As well as its straightforward information on the particle orientation and thus rotation, as described in chapters 3 and 4.

Chapter 4 has shown some first results on the hydrodynamic and orientational behaviour of non-spherical particles using MPT and Digital Image Analysis (DIA). These results mainly serve as a proof of concept of the techniques, but many aspects remain unexplored. Currently with MPT only the results of the rods with an aspect ratio of 4.5 have been shown. It would be interesting to see what the effect of the aspect ratio would be on the dynamic behaviour and orientation distribution. Only the inclination angle has been shown, but the azimuthal angle was not shown. It would also be interesting to think on ways to determine the third Euler angle, since the rotation about the axis connecting the poles cannot be determined. For the DIA technique
it would be interesting to determine the mutual alignment using for instance a nematic order parameter. The segregation of other aspect ratio rods might also be very interesting as well as the rate of mixing. Ultimately these techniques can be used to help validate models on non-spherical particles that are currently under development.

Heat transfer of semi-structured arrays of spheres has been studied with a reconfigured Constant Temperature Anemometer (CTA) and Direct Numerical Simulation (DNS). The results compared well for this single active sphere in a semi structured array of passive spheres, but have shown some differences with results from DNS of heat transfer of random configurations of fully active spheres. This still has to be studied further. Only results of mono-dispersed spheres have been shown, extension to bi- or polydispersity and non-sphericity as well as results from pressure drop, to study drag can be very interesting. Preliminary results were obtained of bidisperse packed mixtures, but the results have yet to be extended and further analyzed, see also figure 7.2. First results indicate that with increasing fraction of larger spheres the Nusselt number of the smaller sphere drops. A simple correction on the heat transfer based on the findings of Beetstra et al. (2007) for the effective porosity might not be so straightforward, due to the nature of the Gunn correlation.

Finally a hybrid collision integration scheme was presented that combines the benefits of the hard sphere scheme for binary collisions and the soft sphere scheme for multi-body collisions. The time step is chosen the same as the duration of a collision given by the soft sphere scheme and as such is almost an order of magnitude faster as a classical soft sphere scheme. Over-relaxation of the soft-sphere scheme to use a similar time step was shown to result in a wrong rate of energy dissipation. The method presented here was only used on a model system and to enable the use in typical granular flow models the method has to be extended to account for external forces; gravity and drag being the first. For gas-solid systems the relative differences in external forces might be neglected for the duration for the collision. For gas-liquid and liquid-solid systems this can of course not be the case. The benefit of a constant and equal external force for both particles is the conservation of the time-scale of a collision. Currently the time step of the hybrid DEM is limited to the exact duration of a collision. No study was done to see if an arbitrary time step
Figure 7.2: Nusselt number as a function of Reynolds number for varying volume fractions of 3 and 4 mm spheres in packed beds, obtained from reconfigure CTA experiments, with a 3 mm probe. Legend indicates, left: volume fraction of 3 mm, and right: volume fraction of 4 mm.

around $t_{coll}$ is possible. This would in turn allow for size differences for the particles, without the need to scale the spring stiffness, also this might allow extending the time step beyond $t_{coll}$. The tangential component, rotation and friction was implemented but not used for the current system. Also parallelization of the method is needed to compete with current commercial DEM models.


116


King, L. V. (1914). On the convection of heat from small cylinders in a stream of fluid: determination of the convection constants of small platinum wires with applications to hot-wire anemometry. *Philosophical Transactions of the Royal Society of London. Series A, Containing Papers of a Mathematical or Physical Character*, pages 373–432.


List of publications

Publications


8. Z. Li, T.C.E. Janssen, Kay A. Buist, N.G. Deen, M. van Sint Annaland, J.A.M. Kuipers., Experimental and simulation study on heat transfer in fluidized beds with heat production, in preparation


Presentations, Conference Proceedings and Posters


Curriculum Vitae


Kay startte in 2005 met de bachelor Chemische Technologie aan de Universiteit Twente. Waarna hij zijn opleiding voorzette aan dezelfde universiteit met een master Chemical Engineering. In het kader van deze master heeft hij een stage afgerond bij HoSt BV.

In 2012 is hij afgestudeerd voor de master Chemical Engineering bij de Universiteit Twente met een onderzoek naar ontwikkeling van een meetmethode voor segregatie van deeltjes in gefluidizeerde bedden bij de vakgroep Multiphase Reactors bij de Technische Universiteit Eindhoven.


Per augustus 2016 is Kay werkzaam als assistant proffesor bij de leerstoel Multi-Scale Modelling of Multiphase Flows, met als hoofdthema non-invasive monitoring of multiphase chemical reactors.
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