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Shock-induced flow through particle clouds

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Preface

This thesis is submitted in partial fulfillment of the degree of *philosophiae doctor* (Ph.D.) at the University of Oslo. The work has been partially funded and carried out at the Norwegian Defence Research Establishment (FFI).

The thesis consists of an introduction and the following four papers:

Paper I: Osnes, A. N., Vartdal, M., Pettersson Reif, B. A.: Numerical simulation of particle jet formation induced by shock wave acceleration in a Hele-Shaw cell. *Shock Waves* 28(3) (2018)

Paper II: Vartdal, M., Osnes, A. N.: Using particle-resolved LES to improve Eulerian-Lagrangian modeling of shock-wave/particle-cloud interactions. *Proceedings of the summer program 2018*. Centre for Turbulence Research, Stanford University

Paper III: Osnes, A. N., Vartdal, M., Omang, M. G., Pettersson Reif, B. A.: Computational analysis of shock-induced flow through stationary particle clouds. *International Journal of Multiphase Flow* 114 (2019)

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Vartdal, M., Osnes, A. N.: Linear motion of multiple superposed fluids. *Physical Review E*, 99(4) (2019)

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Contents

Preface	i
Acknowledgements	iii
1 Background and motivation	1
1.1 Multiscale interactions in particle-laden flow	3
1.2 Thesis objectives	4
1.3 Thesis outline	5
2 High-speed particle-laden flow	7
2.1 Dimensionless numbers	7
2.2 Flow around a sphere	8
2.3 Shock-wave interaction with particle clouds	12
2.4 Particle jet formation in shock-induced flow	22
3 Governing equations	25
3.1 Single phase compressible flow	25
3.2 Particle motion	25
3.3 Volume-averaged continuous phase equations	26
3.4 Momentum transfer	30
4 Computational methods and grids	33
4.1 Computational methods	33
4.2 Particle-resolved computational grids	34
5 Summary of papers	37
5.1 Numerical simulation of particle jet formation induced by shock wave acceleration in a Hele-Shaw cell – (Osnes et al., 2018)	37
5.2 Using particle-resolved LES to improve Eulerian-Lagrangian modeling of shock-wave/particle-cloud interactions – Vartdal and Osnes (2018)	38
5.3 Computational analysis of shock-induced flow through stationary particle arrays – (Osnes et al., 2019a)	39
5.4 Particle-resolved simulations of shock-induced flow through particle clouds at different Reynolds numbers – (Osnes et al., 2019c)	39
6 Concluding remarks and future perspectives	41

Bibliography	43
7 Paper I	55
8 Paper II	67
9 Paper III	79
10 Paper IV	99

Chapter 1

Background and motivation

Understanding flow dispersion of gases, liquids, and particles is important for modern societies. Toxic chemicals and harmful biological substances are widely used in industry and agriculture, and accidents can therefore expose people to these substances. Especially in urban areas, this can have drastic consequences, such as in the Bhopal disaster. In that accident, half a million people were exposed to methyl isocyanate gas, which caused more than 3800 direct deaths, and many times more premature deaths and injuries (Broughton, 2005). It is therefore of key importance to be able to predict substance concentrations, transport velocities, and how to respond to such an event. Increased knowledge and preparedness for dispersal events can improve the safety of people living in relatively high-risk areas. Understanding contaminant dispersal is also important for handling predictable releases, such as air pollution due to road traffic.

An unforeseen dispersal event typically consists of a few different flow regimes. First, there is a release of a substance from some source, for example a broken pipe, a pressurized container, or due to an explosion in close proximity to a container of a harmful substance. The initial flow dispersal is strongly affected by source characteristics, and the environment in immediate proximity of the source (Wingstedt et al., 2017). This flow regime typically determines the flow dispersal up to a spatial scale of a few meters. Next, geometries at a larger scale become important for the flow. Buildings, roads, and small hills are common examples of such geometries. If the substance is a gas, or consisting of sufficiently small particles, it might also be dispersed at atmospheric scale. This thesis is part of a broad research effort to fill knowledge gaps in this multi-scale, multi-physics problem. The focus of this work is to understand the flows and dispersal characteristics when particles are dispersed as a result of an explosion.

Explosions release a very high amount of energy concentrated in a short time window, and within a small volume. This results in the formation of shock waves that propagate outwards from the explosion through the air (Needham, 2010). Shock waves are supersonic waves with nearly instantaneous jumps in density, velocity, temperature, and pressure. They impose very large forces and high temperatures when they impinge on an object, and for this reason, they are a major safety concern. Due to the large forces, shock waves are able to accelerate objects to very large velocities. In some cases, large objects thrown by shock waves might be the most dangerous aspect of an explosion. Explosives can disperse particles over large distances in a short amount of time. The extreme accelerations and temperatures that the particles will be exposed to can, however, be high enough to neutralize harmful substances (Gottiparthi et al., 2014). Characterization of the loads that particles are exposed to during

explosive dispersal is therefore also important. Combined with high-quality dispersal modeling, this can provide accurate predictions of the risks related to explosive dispersal.

The ability to accurately model the interaction between high-speed flows and dense particle suspensions has numerous other applications. Such interactions are widely used in engineering systems. For instance, in liquid fuel combustion engines for aerospace applications, fuel is injected as a liquid jet into a high-speed crossflow (Li and Soteriou, 2014; Bravo et al., 2015). Research is being conducted to enable combustion of easily available fuels, such as liquid ethanol or liquid kerosene, as options for scramjet propulsion (Nakaya et al., 2015; Tian et al., 2015). The injection of a liquid jet into a supersonic flow generates shock waves around the jet. The dynamics and shapes of these shocks are related to the interaction between the incident flow and the liquid jet. When exposed to the crossflow, the jet will break down through various flow instability mechanisms. During the breakup and the mixing of fuel and air, the fuel volume fraction diminishes, and passes through the dense dispersed flow regime (Liu et al., 2016). Subsequent dispersal, evaporation, and mixing of fuel and air therefore depend on the physics of high-speed flow through dense droplet suspensions. Models that accurately capture this process enable design of improved high-speed propulsion systems.

Other technological applications include thrust-vectoring of high-speed vehicles (Perurena et al., 2009), solid-fuel rocket motors (Cai et al., 2003; Shimada et al., 2006), noise reduction in jet engines and rocket launch pads (Krothapalli et al., 2003; Ignatius et al., 2008; Nagata et al., 2016), operation of turbomachinery in particle-laden flows (Hamed et al., 2006), spray deposition (Dolatabadi et al., 2004; Samareh and Dolatabadi, 2008), mining safety (Ugarte et al., 2017), heterogeneous explosives (Zhang et al., 2001), and drug-delivery systems using micro shock-tubes (Truong et al., 2006).

Dense high-speed particle-laden flows also occur in nature. For example in volcanic eruptions, shock particle interaction occur during decompression of magma chambers, and the subsequent flow of ash and steam (Wohletz et al., 1984; Valentine and Wohletz, 1989). Sustained explosive eruptions can lead to fountaining multiphase mixtures, that transition from dilute to dense mixtures as they impact on the ground (Valentine and Sweeney, 2018). Similarly, snow avalanches feature dense suspensions of rapidly moving snow particles (Hopfinger, 1983). Another occurrence is found in atmospheric entry of near-earth objects. Meteoroids on the scale of tens of meters, such as the one in the Chelyabinsk event, break up in the atmosphere and cause blast waves. Early detection of such meteoroids is very difficult, and air-blasts caused by meteoroids can pose a threat to human lives. The threat is both direct, through damage from the blast wave and heat pulse, and indirect, by causing accidents such as dam breaks, damage to nuclear reactors, etc. (Artemieva and Shuvalov, 2016). Accurate modeling of the dense, particle-laden flow during meteoroid breakup is central to understanding the risks associated with such events (McMullan and Collins, 2019).

This thesis increases the knowledge about high-speed flow through dense

particle clouds, and how to properly model such flows. This is achieved by the use of numerical simulations of shock-induced flow through particle layers. Both simplified models and highly resolved simulations are used to investigate these flows. By using the present state-of-the-art simplified dispersed flow models, model shortcomings are identified. The highly resolved simulations are then used to obtain accurate data, and model improvements are suggested based on these. Additionally, these simulations provide a novel dataset describing high-speed flow through dense particle clouds. Analysis of this data reveals important details concerning the dynamics at particle scale in these flows.

1.1 Multiscale interactions in particle-laden flow

Particle laden flows often feature particles of much smaller sizes than the systems of interest. Typical particle sizes can range from micrometers to millimeters, while system scales can be up to kilometers in certain natural phenomena. Accurate predictions of the behavior of a particle requires simulations that resolve the flow around it. Particles are accelerated by the pressure forces and viscous friction acting on their surfaces, and these are directly dependent on flow conditions in immediate proximity of the particle. The local flow is related to the bulk flow, and this relationship is captured by simulations that resolve the flow at particle scale. This methodology demands too much computational resources to be applicable to full-scale problems.

Statistical descriptions and simplified dispersed flow models are therefore necessary in studies of dispersed flows. Simplified dispersed flow models consist of equations that describe the flow at large scale, with terms that represent the effect of the unresolved, small-scale, physics. In some problems, such as the ones considered in this work, these terms are important for bulk flow dynamics and must therefore be properly modeled. Changes in bulk flow can also feed back to the small-scale processes. This scale interaction is a major challenge in dispersed flow studies. A model that can be applied to the problem at full scale is incapable of resolving the microscale features. On the other hand, a model that resolves microscale features cannot be applied to the full-scale problems, due to excessive computational costs. An accurate model must properly represent the flow at all scales, and to do this, models must be tailored specifically for the flow conditions relevant to each problem. For this purpose, it is necessary to consider the flow conditions at particle scale for each problem.

In this thesis, two different aspects of shock-wave particle cloud interaction are considered. The first paper investigates the development of particle jets in a quasi two-dimensional setting. The other papers focus on the flow within stationary random particle arrays. A common denominator for these studies is that physical processes occurring at spatial scales much smaller than the bulk length scales of the problem, lead to large-scale flow features. Properties of these large-scale flow features are dependent on the bulk parameters of the problem, such as the length of the particle layer.

Specifically, the large particle-jets observed during explosive dispersal of par-

ticles are the result of processes beginning at particle scale. The process is currently not well understood, and multiple hypotheses for particle jet formation have been proposed. Accurate modeling of particle jet formation requires models that are able to capture the statistical results of particle collision, forces on the particles, and the flow fluctuations at particle scale.

Papers II-IV are concerned with the shock-induced flow within planar particle layers. The study by Theofanous and Chang (2017) demonstrated that most dispersed flow models predict accumulation of particles near the downstream edge of the particle cloud in these problems. In contrast, experimental works show that particles near the downstream edge are subjected to stronger forces than those further in. The particle layer is therefore diluted at the downstream edge, which is the opposite of the effect predicted by the dispersed flow models. In this case, particle-scale flow phenomena inhibit the particle accumulation, and accounting for these effects is necessary in dispersed flow models, in order to obtain accurate predictions of the particle dispersion.

This thesis investigates the importance of particle scale effects in shock-wave particle cloud interaction. In paper I, we explore different models for particle scale effects and examine how these influence particle jetting. This approach yields an understanding of the large-scale features that are possible outcomes when different particle-scale models are employed. In papers II-IV, we perform simulations that resolve the particle scale physics, and analyze the importance and statistics of the terms in the governing equations. The simulation data, which are highly resolved both in space and in time, enable investigation of the unclosed terms in the simplified dispersed flow models. Derivations of simplified models are usually based on averaging of flow equations, for example through volume averaging or ensemble averaging. Any of these approaches are possible to apply to data from particle-resolved simulations, which gives access to the exact closures. The remaining challenge is to develop models that accurately represent these data, either through algebraic expressions (Mehrabadi et al., 2015), additional equations, tabulated data (Akiki et al., 2017a), or machine learning-based approaches (Sen et al., 2015, 2018). Thorough understanding of the important physical processes is essential for assessing the physicality and quality of any proposed model. Data from particle-resolved simulations are therefore especially important when investigating shock-wave particle cloud interactions.

1.2 Thesis objectives

The main objectives of this thesis are:

- I:** Improve the understanding of how particles are dispersed by shock waves.
- II:** Use particle-resolved simulations of shock waves passing through particle clouds to characterize the three-dimensional, time-dependent, flow field within the particle cloud.

III: Propose improvements to simplified dispersed flow models based on the findings from the particle-resolved simulations.

1.3 Thesis outline

This thesis is organized as follows. Chapter 2 introduces particle laden flows and discusses the physical processes that are relevant for shock-wave particle cloud interaction. Chapter 3 contains the governing equations for compressible flow, as well as the volume-averaged equations used to describe the bulk behavior of high-speed dense dispersed flows. Chapter 4 specifies the computational approach used for the simulations in this thesis. Summaries of the four papers in this thesis are found in chapter 5. Finally, chapter 6 contains general conclusions based on the findings of this thesis, and suggestions for future studies.

Chapter 2

High-speed particle-laden flow

Flows where particles are suspended or transported in a fluid are called particle-laden flows. Particle-laden flows cover a huge range of different physical problems, and are important in a number of natural and industrial processes. Particles can interchange mass, momentum, and energy with the flow, and in some cases react chemically or undergo phase transitions. Particle-laden flows are often inherently multi-scale, due to small particles in combination with relatively large systems. Shimada et al. (2006), in the context of flow within solid fuel rocket motors, stated that "It is a general feature of multiphase flow that micro-scale phenomena at phase interfaces affect fluid-dynamic phenomena of macro scale." The multi-scale coupling makes particle-laden flows challenging to study and model. Particles are transported by the fluid, and interact with it in a complicated fashion, which necessitates a careful analysis of which processes are relevant for a given problem. High-speed particle laden flows often feature particles that respond slowly to changes in the flow. Therefore, the relative phase velocities can be high, which leads to strong interfacial forces and rapid energy transfer. In some cases, the relative phase velocity can exceed the speed of sound in the fluid, and in such flows, the dispersed phase generates shock waves in the fluid. This is the case for shock-induced flows through particle clouds, which is the focus of this thesis

This chapter discusses the physics governing the interaction of shock waves and particle clouds, and introduces relevant literature. First, the dimensionless numbers that characterize such flows are introduced. The following section is concerned with the flow around an isolated sphere. Next, shock-wave interaction with particle clouds is discussed, along with flow fluctuations. The final section of this chapter introduces the phenomenon of particle jet formation.

2.1 Dimensionless numbers

An important parameter for description of the response of a particle to changes in the flow around it is the Stokes number, St . The Stokes number is the ratio of the particle relaxation time to the characteristic flow time scale. It is commonly approximated as

$$St = \frac{\rho_p |\mathbf{u} - \mathbf{v}| D_p}{18\mu}, \quad (2.1)$$

where ρ_p is the particle mass density, $\mathbf{u}$ is the fluid velocity, $\mathbf{v}$ is the particle velocity, D_p is the particle diameter, and μ is the dynamic viscosity of the fluid. High Stokes numbers imply that the particle will respond slowly to changes in the flow around it. For low Stokes numbers, the particle responds quickly and follows the flow. In this and the following expressions, the appropriate fluid

phase variables are those that would be found at the particle location in the absence of the particle, i.e. "undisturbed" fluid variables.

Another important dimensionless number is the particle Reynolds number, Re_p , which is used to characterize the flow state around a particle. The particle Reynolds number is

$$\text{Re}_p = \frac{\rho |\mathbf{u} - \mathbf{v}| D_p}{\mu}, \quad (2.2)$$

where ρ is the fluid mass density. It is an approximation of the ratio of inertial forces to the viscous forces of the flow in immediate proximity of the particle.

For the flows studied in this thesis, the relative velocities between the particles and the fluid are very large, and this results in important compressibility effects. The dimensionless number used to characterize this is the particle Mach number, Ma , which is the ratio of the relative velocity to the speed of sound in the fluid. This is given by

$$\text{Ma} = \frac{|\mathbf{u} - \mathbf{v}|}{c}, \quad (2.3)$$

where c is the speed of sound in the fluid. For isolated particles at high Reynolds numbers, sonic flow occurs on the sphere at $\text{Ma} \approx 0.58$ (Kaplan, 1940). Past this value, shocks form in the vicinity of the particle and significantly affect the forces acting on it. The Mach number is also used to describe local flow states, and the strength of shock waves. In those cases, the relative velocity in eq. (2.3) should be replaced by the fluid velocity or the shock wave velocity, respectively.

In rarefied flows, or for very small particles, the ratio of the mean free path length of fluid molecules to particle diameter can become small. This is characterized by the Knudsen number, which in general can be written

$$\text{Kn} = \frac{L_{\text{mfp}}}{L}, \quad (2.4)$$

where L_{mfp} is the mean free path length of fluid molecules, and L is a representative length scale of the problem under investigation, for example the particle diameter. If $\text{Kn} \ll 1$, then the continuum approximation is appropriate. In the opposite case, non-continuum effects might be important, especially at the phase boundary.

Finally, for dense particle suspensions, the ratio of the volume of particles to the volume of the fluid is important. It is referred to as the particle volume fraction, and will be denoted by α_p in this thesis. When formulating equations describing particle-laden flows, it is more convenient to use the volume fraction of the fluid phase. Here, it will be denoted by α . The two volume fractions sum to unity.

2.2 Flow around a sphere

Flow around a sphere is a canonical flow configuration that has received much attention in the past. Incompressible isolated particle flows are characterized by the particle Reynolds number. Compressible flows also need to be considered

in terms of the Mach number, as well as the Knudsen number if the particle is very small. The following discussion briefly describes the qualitative changes in the flow as a function of Reynolds and Mach numbers.

At very low flow speeds, $Re_p \ll 1$, the flow is called Stokes flow. In this regime, inertial forces are negligible compared to the viscous forces in the flow, and the equations of motion can be simplified accordingly. In Stokes flow around a sphere, the flow is steady and symmetric around an axis aligned with the flow direction through the center of the sphere. As the Reynolds number increases, the flow loses its front-back symmetry (Le Clair et al., 1970), but is still steady, and does not separate from the sphere. The fraction of the drag force due to pressure increases as the Reynolds number increases. At $Re_p \approx 20$, the flow separates from the sphere, and a recirculation region appears behind it (Magnaudet et al., 1995). The length of the circulation region increases when the Reynolds number increases (Taneda, 1956). Between $Re_p \approx 130 - 280$, the axisymmetric flow state becomes unstable. As a result, the flow becomes unsteady, first by circulation-length oscillation and later by vortex shedding (Taneda, 1956; Magnaudet et al., 1995; Sansica et al., 2018).

While vortex shedding can occur in laminar flows, the vortices break down in the particle wake and the flow becomes turbulent. The breakdown happens closer to the sphere with increasing Reynolds number (Tiwari et al., 2019). When the Reynolds number is increased from $Re_p \approx 280$ to 6000, there are several qualitative changes in the vortex shedding pattern and the breakdown to turbulence. A detailed discussion of these changes can be found in Sakamoto and Haniu (1990). Up to $Re_p \approx 2 \times 10^5$, the flow is in a state where the boundary layer is laminar until it separates from the sphere (Rodriguez et al., 2011). The separation point is about 80 – 90 degrees measured from the front of the sphere (Constantinescu and Squires, 1999). Above $Re_p \approx 1000$, the separated shear layer breaks down into turbulence within a few diameters downstream of the sphere. The flow has large-scale, slow and periodic vortex shedding, and the wake exhibits a helical pattern (Rodriguez et al., 2011).

At even higher Reynolds number, $Re_p \approx 2 \times 10^5$, the boundary layer at the sphere becomes turbulent before it separates. As a result of the turbulent boundary layer, the flow sticks to the sphere surface much longer, and does not separate until about 120 degrees (Constantinescu and Squires, 2004). This results in a significantly reduced drag coefficient, and the phenomenon is called the drag crisis. The pressure has a local maximum within the separation region (Geier et al., 2017), which results in a sharp drop in drag to about 20% of its value before the drag crisis.

The above results are for incompressible flows. If the flow Mach number is non-negligible, it affects flow stability, turbulent transition, and can introduce additional flow phenomena such as shocks. Supersonic flow around an isolated particle results in a bow shock in front of the particle. Due to flow acceleration around the sphere, shocks also occur at subsonic mean flow speeds. At a critical incident flow Mach number, the flow becomes supersonic around the sphere. At very high Re_p , this occurs at $Ma \approx 0.58$ (Kaplan, 1940), while at lower Reynolds numbers, the shock formation happens at slightly higher Mach numbers. The

Figure 2.1: Compressible flow around an isolated particle, illustrated by density gradient contours, at three different Mach numbers. The particle Reynolds number is 5000.

supersonic region is terminated by a shock at about 90 degrees (Jaikrishnan et al., 1977), and this is also where the boundary layer separates from the sphere. Consequently, the separation point is no longer delayed by the development of a turbulent boundary layer (Jaikrishnan et al., 1977), and thus there is no drag crisis in this regime. An illustration of the flow field around a single sphere in the low Mach, transonic, and supersonic regimes is shown in fig. 2.1. This figure is for $Re_p = 5000$. At this Reynolds number and $Ma = 0.9$, the flow has an extended supersonic region that terminates around the location where the wake breaks down. At $Ma = 2.6$, the bow shock is clearly visible in front of the particle. It can also be observed that the particle wake changes with Mach number.

Compressibility effects have a strong effect on particle drag. Bailey and Hiatt (1971) characterized the average drag forces on an isolated sphere over $Re_p = 2 \times 10^2 - 10^5$ and $Ma = 0.1 - 6$. In general, increasing Mach numbers up to $Ma \approx 1.5 - 2$ tend to increase drag coefficients, while further increases tend to decrease the drag coefficients. Just below $Ma = 1$, in the transonic regime, the drag coefficient increases rapidly with Mach number. Above $Ma = 1$, the bow shock forms in front of the sphere, and further increases in Mach number have a much weaker effect on the drag coefficient.

Flow stability, wake structure, and vortex shedding are also affected by Mach number. Compressibility effects increase the stability of the flow, and as a result, the onset of vortex shedding occurs at higher Reynolds numbers with higher Mach numbers. Nagata et al. (2016, 2018) performed direct numerical simulations of flow around isolated spheres between $Re_p = 50 - 1000$ and $Ma = 0.3 - 2$, and characterized the transition between different flow regimes within this range. An extended, and significantly more detailed, review of the different flow regimes for single particles can be found in Tiwari et al. (2019). Further complicating factors, such as wall proximity, flow stratification, free flow

Figure 2.2: Illustration of a $Ma = 2.6$ shock wave passing over a single particle, visualized by the density gradient. The particle Reynolds number based on post-shock flow properties is 5000.

turbulence, and more are discussed in that review.

In the context of shock-induced flow, the transient following the interaction of a shock wave and a sphere is also of importance, due to the rapid exchange of momentum and kinetic energy during this process. An illustration of the transient following shock wave impact on a sphere at $Re_p = 5000$ is shown in the image series in fig. 2.2. When the shock wave first impacts on the sphere, a regular shock reflection is formed. As the shock wave propagates further, a Mach reflection is formed (Sun et al., 2005), which can be observed in the third image in fig. 2.2. On the downstream side, the shock wave converges, creating a high-pressure region immediately behind the sphere. Further on, the flow field becomes increasingly complicated to characterize, due to the shock-wave particle-wake interaction, as can be observed in the figure. Experimental works have characterized shock-wave particle interaction, see e.g. Britan et al. (1995); Zhang et al. (2017), and it has also been studied using numerical simulations (Sun et al., 2005; Sridharan et al., 2015). Sun et al. (2005) demonstrated that the ratio of viscous and pressure forces acting on the particle increases with decreasing Reynolds number, and that viscous forces can be important, for example by counteracting the temporary negative pressure drag coefficient that results when the shock wave converges behind the sphere. Models of the forces acting on the sphere during this interaction can be found in Parmar et al. (2009).

Flow around isolated particles is, despite the simple geometry, incredibly complicated. Exact relations or very good approximations for particle drag, and the flow around a particle, can be obtained in low Reynolds number regimes. Such results become increasingly hard to obtain as the particle Reynolds number increases. The Mach number further complicates the flow, and becomes very important for particle drag when it approaches or exceeds unity. If there are other particles or obstacles nearby, the results for isolated particles no longer apply. Configurations with dense suspensions of particles within a high-speed flow is the topic of this thesis. These problems feature all the difficulties mentioned,

and therefore require detailed investigations of the flow at particle scale.

2.3 Shock-wave interaction with particle clouds

Interactions between shock waves and particle clouds are of interest for numerous safety applications as well as industrial processes. Shock-wave mitigation systems in storage facilities for explosives, or other locations where explosions may occur, can utilize dust suspensions or geometrical configurations of obstacles to reduce safety distances (Igra et al., 1987; Suzuki et al., 2000; Chaudhuri et al., 2013). Metallic particles can be utilized in heterogeneous explosives to enhance blast properties (Balakrishnan and Menon, 2011), and such methods have been suggested for neutralization of bacterial spores (Henderson et al., 2015). Additionally, the bacterial spores themselves interact non-trivially with the shock wave (Gottiparthi et al., 2014). High velocity oxy-fuel thermal spray and cold gas-dynamic spray processes feature a particle jet in an overexpanded nozzle. Detailed modeling of the interaction of the particle jet and the shock diamonds in these configurations can be used to optimize deposition efficiency (Dolatabadi et al., 2004; Samareh and Dolatabadi, 2008).

When a shock wave impinges on a cloud of particles, there is rapid transfer of momentum and kinetic energy between the phases. If the particle suspension is dense, the forces imposed on the gas-phase will be very large during the initial phase of the interaction. The upper volume fraction limit where the statistical behavior of particles are the same as for isolated particles, was estimated in Crowe et al. (2011) as 0.1%, while Zhang et al. (2001) considered volume fractions below 1% as dilute. Experimental studies have shown that suspensions with volume fractions as low as 1% can generate reflected shocks as a result of bow-shock coalescence (Boiko et al., 1997; Nourgaliev et al., 2004; Theofanous et al., 2018). Even thinner suspensions can form a reflected shock wave through a series of compression waves, that over time form a shock wave (Blagosklonov et al., 1979), as cited in Boiko et al. (1997). Non-dilute particle flows also feature particle collision. While particle collision is important in shock-wave particle cloud interaction, investigation of this effect is considered outside the scope of this thesis.

As the shock wave travels through the particle cloud, it impacts successively on new particles. This results in a weakening of the shock wave during its passage through the particle cloud. If the particle layer is sufficiently long, the shock wave can decay into a compression wave (see also the discussion in Mehta et al. (2018)). The cases that are studied within this thesis do not feature long enough particle clouds for this phenomenon to occur. Therefore, a transmitted shock wave emerges from the downstream edge of the particle cloud (Boiko et al., 1997; Wagner et al., 2012; DeMauro et al., 2017; Theofanous et al., 2016). The transmitted shock wave is always weaker than the incident shock wave, due to the interphase momentum and energy transfer, as well as the kinetic energy dissipation within the particle cloud.

The creation and propagation of the various waves in shock-wave particle

Figure 2.3: $x - t$ diagram for $\text{Ma} = 2.6$, $\alpha_p = 0.1$, $\text{Re}_p = 5000$, showing the location of the incident, reflected and transmitted shock waves, upstream and downstream contact discontinuities, and upstream propagating acoustic waves. The gray region indicates the extent of the particle layer. Here, t_0 denotes the time when the shock wave impacts on the particle cloud, and τ_L is the time it takes for the incident shock wave to travel a distance equal to the particle cloud length.

cloud interaction can be conveniently summarized using $x - t$ diagrams, as in e.g. Regele et al. (2014); Mehta et al. (2019b). An $x - t$ diagram based on a numerical simulation of a $\text{Ma} = 2.6$ incident shock wave and an $\alpha_p = 0.1$ particle layer at $\text{Re}_p = 5000$, based on post-shock flow variables, is shown in fig. 2.3. In addition to the shock waves, there are contact discontinuities originating from the upstream and downstream particle layer edges. These waves feature density and temperature jumps, but there is no change in either streamwise velocity or pressure. Upstream-directed acoustic waves originating around the downstream layer edge are also shown in fig. 2.3. The leftmost acoustic signals are first stationary, then propagate leftwards. This indicates that the flow is roughly sonic at these locations immediately after the shock wave passes, and then becomes subsonic. The three next acoustic waves propagate to the right, and thus the flow at the location of these waves is supersonic. Necessarily, there exists a transonic region between these sets of waves. The drag coefficients on the particles in the transonic regime are drastically higher than in subsonic or supersonic flows (Bailey and Hiatt, 1971; Nagata et al., 2016). Therefore, the particles in the transonic region will experience higher acceleration than those further upstream, and the particle concentration will diminish at the downstream edge (Theofanous et al., 2018). Similarly, particle cloud elongation has also been observed in shotgun ammunition, where the shot

cloud travels at transonic speeds (Compton et al., 1998).

Additionally, the three right-most acoustic waves can be seen to converge, coinciding with the appearance of an upstream directed, but rightward propagating, shock wave immediately downstream of the particle layer. Thus, there is a build-up of pressure and a corresponding pressure gradient over time. The pressure gradient eventually sharpens into a shock wave. As the contact waves, featuring density jumps, propagate through the pressure gradient region, they are subject to gas-dynamic instabilities. The downstream contact is subject to Rayleigh-Taylor instabilities, where the initially dominant perturbation wavelength is set by the particle diameter and inter-particle distance. The upstream contact contains similar initial perturbations, but is subject to Richtmyer-Meshkov instabilities, since it encounters the upstream-directed shock wave downstream of the particle cloud. As the particle layer begins to move, its edges are also potentially subject to multiphase instabilities, which are analogous to Richtmyer-Meshkov and Rayleigh-Taylor instabilities (Black et al., 2018). These are caused by misalignments in average particle concentration gradients and the gradients of the forces acting on the particles.

Experimental investigations of shock-wave particle cloud interaction have provided reference data that can be used to assess the accuracy of dispersed flow models. Important flow properties that have been measured are the strengths of the reflected and transmitted shocks, pressure histories upstream and downstream of the particle cloud, particle cloud acceleration and expansion, and flow fluctuations away from the particle cloud (Boiko et al., 1997; Rogue et al., 1998; Wagner et al., 2012, 2015; Theofanous et al., 2016; DeMauro et al., 2017). These works have also examined trends when particle sizes, particle volume fractions, and shock-wave Mach numbers are varied. The particle cloud has been observed to expand as the particles move downstream. Theofanous et al. (2016) found that the cloud expansion behavior with time can be decomposed into a constant acceleration regime, where the rate of expansion increases with time, and a constant velocity regime, in which the expansion rate is constant. They also provided an estimate of a characteristic time scale for these two regimes. It remains a challenge for experimental works to obtain data within the particle cloud. Such data are crucial in order to understand the physical processes driving the particle acceleration, and for development of simplified dispersed flow models.

Dispersed flow models have also been employed to study shock-wave particle cloud interaction (Boiko et al., 1997; Ling et al., 2012; Regele et al., 2014; Houim and Oran, 2016; McGrath et al., 2016; Saurel et al., 2017; Theofanous and Chang, 2017; Utkin, 2017; Shallcross and Capecelatro, 2018). These studies have shown that shock-wave particle cloud interaction includes phenomena that are not captured with models based on single-particle studies. The particle concentration is not robustly predicted in dispersed flow models (Theofanous and Chang, 2017; Theofanous et al., 2018). Theofanous and Chang (2017) argue that the problem is partly due to ill-posed models, as also discussed in Lhuillier et al. (2013), and partly due to missing important physical processes at the particle scale. There is, at the present time, no general agreement on what

the correct continuous-phase equations are, nor on how to properly model the interphase exchange terms. Additionally, there are few available models for continuous phase subgrid-scale fluctuations that have been developed specifically for shock-induced flow through dense particle suspensions. The latter problem is devoted much attention in this thesis.

Access to spatially and temporally resolved data within particle clouds can be obtained with particle-resolved simulations. Such simulations accurately capture the flow around each particle and the interface coupling. Such approaches have recently become popular, due to the ability to include a large enough number of particles in a simulation for flow statistics to be representative of the problem at large scale. Studies that have used particle-resolved simulations for investigation of shock-wave particle cloud interaction are, e.g., Regele et al. (2014); Sridharan et al. (2015); Mehta et al. (2016a,b, 2018, 2019a,b); Das et al. (2017); Sen et al. (2017, 2018); Theofanous and Chang (2017); Theofanous et al. (2018); Hosseinzadeh-Nik et al. (2018). This is also the simulation approach that is used in papers II-IV in this thesis. The relevant parameter space to map out with such simulations is large, consisting of Reynolds number, incident shock wave Mach number, particle volume fraction, particle cloud length, and more. An outcome of the simulations in papers II-IV in this thesis is a database containing highly resolved data in time and space for a range of Mach numbers, particle Reynolds numbers, and volume fractions. This database provides a basis for development of improved dispersed flow models for shock-wave particle cloud interaction.

2.3.1 Fluctuations in shock-wave particle cloud interaction

The unsteady or turbulent nature of most flows makes it necessary to use statistical descriptions to obtain useful information. When describing a complete multiscale system, it is generally impossible to resolve all spatial and temporal scales relevant to the problem. Therefore, it is necessary to account for the average effect of unresolved scales. This is the basis of both Reynolds-averaged Navier-Stokes (RANS) and large-eddy simulations (LES). In the RANS method, ensemble averaging is used to formulate equations that describe expected flow dynamics, reflecting the fact that it is impossible to avoid uncertainties in initial and boundary conditions. RANS therefore models a part of the flow dynamics at all scales. LES is based on spatial filtering of flow fields. As a result, length scales smaller than the filter width must be modeled. Any form of averaging implies the existence of fluctuations, and the fluctuations represent different concepts for different averaging methods.

In this thesis, volume averaging is used for both model development and analysis of simulation results. In paper IV, ensemble averaging is used in combination with volume averaging to obtain a larger dataset within each averaging volume. When the flow equations are averaged over a volume containing both gas and particles, multiple fluctuation correlation terms appear in the resulting equations. In the LES framework, such terms are referred to as subgrid terms. The most important subgrid terms in the momentum conservation equations,

Figure 2.4: Contours of various flow fluctuation products for flow around a single particle, where fluctuations are defined as deviations from volume-averaged flow quantities. Here, the averaging volume has a streamwise length of $D_p/2$, and spans the domain in the spanwise directions. The averaging volume edges can be discerned as discontinuous jumps in the fluctuations at certain streamwise positions. The dashed line in each colorbar indicates the color corresponding to a value of zero.

apart from the interphase momentum transfer terms, are the velocity fluctuation correlations, which will be referred to as Reynolds stresses. Note that the velocity fluctuation correlations are not Reynolds stresses in the same sense as the velocity correlations in the RANS equations, but rather terms that arise from an analogous sequence of algebraic manipulations. There are also subgrid terms resulting from correlations between viscosity and velocity gradient fluctuations, but these are not important in the problems considered in this thesis. The energy conservation equation contains subgrid terms representing fluctuating advection of internal and kinetic energy, mean advection of velocity fluctuation correlations, fluctuating pressure work, fluctuating heat convection and more. Their relative importance in shock-wave particle cloud interaction is not well known.

2.3.1.1 Continuous phase fluctuations

For shock-wave particle cloud configurations that have been the focus of recent studies, e.g. Wagner et al. (2012); DeMauro et al. (2017); Theofanous et al. (2016), the particle Reynolds number is typically in the range $10^3 - 10^5$. Based on isolated particle studies, this range is within the subcritical regime. Each particle induces a separated flow behind it, and the flow has relatively large-scale unsteadiness, as well as turbulent motion, in the particle wake.

When the flow is averaged over volumes that are larger than a particle, each particle induces subgrid flow-phenomena in the region close to itself. This is illustrated for a single particle in fig. 2.4, where the fluctuating streamwise momentum advection ($\rho u_1'' u_1''$), fluctuating spanwise momentum advection ($\rho u_3'' u_3''$), fluctuating pressure work ($p' u'$), and fluctuating internal energy advection ($\rho e'' u_1''$) are shown. The mathematical notation and derivation of these terms are discussed in chapter 3. Clearly, the particle induces fluctuations, which are mostly confined within a limited region in its proximity. The different terms are distributed differently around the particle. The fluctuating streamwise momentum advection is primarily located within the particle wake, while the fluctuating spanwise momentum advection is primarily located around the upstream face of the particle and in the vortex-shedding region further downstream. The fluctuating pressure work and the fluctuating internal energy advection are found both directly in front of the particle and in its wake.

Similar flow fluctuations to those shown in fig. 2.4, exist around each particle within the particle cloud during, and after, the passage of the shock wave. However, there might be significant distortion caused by nearby particles, and the fluctuations in dense particle suspensions might therefore be very different from fluctuations around isolated particles. Local area contraction and expansion can cause flow acceleration or deceleration, particle wakes can impinge on other particles, particle wakes can interact, particles can collide, etc. These phenomena generate a seemingly chaotic flow, whose statistical properties are the focus of much of the work in this thesis.

There are a few published works that have investigated flow fluctuations in shock-wave particle cloud interaction. Regele et al. (2014), based on two-dimensional inviscid simulations, found that root-mean-square (RMS) velocity fluctuations were comparable to the mean flow speed within the particle cloud. In a follow-up study, Hosseinzadeh-Nik et al. (2018) performed viscous simulations of a similar setup, and found that viscosity dampens the RMS velocity fluctuations slightly. The RMS velocity fluctuations were still more than 50% of the mean velocity. Additionally, the fluctuating kinetic energy was comparable to the mean kinetic energy. Similarly, using two-dimensional inviscid simulations, Sen et al. (2018) found that for a strong shock ($Ma = 3.5$), the fluctuating kinetic energy was the same order as the mean kinetic energy, within a square array of cylinders at a volume fraction of 0.1. Lower volume fractions reduced the ratio of fluctuating to mean kinetic energy. They also found that at 10% volume fraction, the fluctuating to mean kinetic energy ratio is quite similar for $Ma = 1.1$, 2.3 and $Ma = 3.5$. For the $Ma = 1.1$ shock wave, however, the

fluctuating kinetic to mean kinetic energy ratio is initially higher and decays faster over time than for $Ma = 2.3$ and 3.5 .

Two-dimensional flow around cylinders is in many ways similar to three-dimensional flow around spheres, but there are important differences in boundary layer separation point, vortex shedding behavior, transition numbers, etc. (Regele et al., 2014). Two-dimensionality limits the flow dynamics, which results in significantly stronger vorticity generation (Mehta et al., 2019a). Using inviscid three-dimensional simulations, Mehta et al. (2019a) found RMS velocity fluctuations that were between 10-50% of the mean flow velocity, which is lower than the two-dimensional fluctuations at corresponding flow conditions. Mehta et al. (2019a) also investigated the fluctuating internal energy advection, as well as the fluctuating pressure work. They found that the magnitudes of these terms were small compared to the corresponding mean flow fields. As mentioned in their study, it is the gradients of these terms that are present in the conservation equations, and therefore an assessment of the magnitudes of the fluctuation correlations is insufficient for determining their importance. Viscous and inviscid simulations are also fundamentally different due to flow dynamics that depend on viscosity, such as flow separation and turbulence. Therefore, the findings in inviscid flows need to be tested in viscous flows.

While it is the variation of velocity fluctuations that imposes effective forces on the flow, the magnitudes of the fluctuations are also important. Fundamentally, any flow process must conserve mass, momentum and energy. Therefore, it is necessary to know how fluctuating motions are generated, and how much energy that is deposited in the velocity fluctuations. In computational approaches, it is common to solve the total energy equation as part of compressible flow simulations. Pressure fields are subsequently obtained from the equation of state. To obtain the internal energy, which is part of the equation of state, both the mean and fluctuating kinetic energies must be subtracted from the total energy. This was clearly demonstrated by Regele et al. (2014), who performed both one-dimensional and two-dimensional simulations of a shock wave passing through an array of cylinders. In their one-dimensional simulations, the pressure was overestimated compared to the two-dimensional simulations. When the fluctuating kinetic energy from the two-dimensional simulations was added to the pressure, the simulations agreed very well.

The equations governing the interactions between the internal energy, mean kinetic energy, and fluctuating kinetic energy, in the volume-averaging framework, are presented in section 3.3. Figure 2.5 shows schematically the various energy exchange mechanisms that exist for dispersed flows with inert particles in statistically one-dimensional problems. The different energy transfer terms are not independent. For example, if there are relative phase velocities, there also exist stagnation points on the particles. Therefore, there are regions of fluctuating compression work. The work due to relative phase velocities is the only interaction type in fig. 2.5 that is exclusive to dispersed flows. In shock-wave particle cloud interaction, this term is especially important due to the extreme relative phase velocity, and is responsible for rapid generation of fluctuating kinetic energy.

Figure 2.5: Energy transfer paths for the flow problems considered in papers II-IV. Note that the viscous dissipation paths are one-way processes. Terms that require spanwise flow gradients are not present because the problems are statistically one-dimensional.

2.3.1.2 Dispersed phase fluctuations

In dense, high-speed flows, different particles can be exposed to very different forces and temperatures. As a result, they attain a range of velocities and temperatures. Due to the enormous number of particles or droplets in typical applications, their behavior must be described statistically. Variations in particle forces are especially important, since they lead to particle distribution inhomogeneities. Such fluctuations also imply a variation of the production and dissipation of fluctuating kinetic energy, through the relative phase velocity work term, c.f. fig. 2.5. Particles can be exposed to different forces as a result of large-scale carrier phase variations, carrier phase turbulence, particle-induced carrier phase fluctuations, or particle collisions.

In shock-wave particle cloud interaction, dispersed phase fluctuations are primarily the result of variations induced by the dispersed phase itself. The forces acting on a particle are strongly dependent on the relative position of other particles in the particle's proximity (Boiko et al., 2002; Theofanous et al., 2004; Zarei et al., 2011; Mehta et al., 2018). When the shock wave passes through the particle cloud, each particle interacts with the shock wave in approximately the same way as illustrated in fig. 2.2. However, the shock wave might be distorted by other particles located further upstream and reflected waves from nearby particles can lead to important differences over time. A particle located in the shock-wave focusing region behind an upstream particle will be exposed to much higher pressures due to the presence of the upstream particle. Other configu-

Figure 2.6: Dimensionless forces on particles within a particle cloud (F_p^*) as a function of non-dimensional time (t^*), where unit t^* is the time it takes for the shock wave to propagate one particle diameter, when exposed to a $\text{Ma} = 2.6$ shock wave. Black lines show the forces on a sample of particles. The white line represents the mean value for all particles, while the dark grey and light grey regions indicate one and two standard deviations, respectively.

rations might lead to weakening of the forces on the particles, and in random configurations, there will be a large variation in forces due to these effects. In inviscid simulations of a one-dimensional streamwise array of particles, Sridharan et al. (2015) found that a particle separation of slightly less than one particle diameter was optimal for amplification of maximal particle force, in agreement with the experimental study by Boiko et al. (2002). Zarei et al. (2011) found that steady-state forces on a pair of cylinders in supersonic flow can be increased or decreased depending on their relative configuration, and certain configurations could lead to attraction or repulsion of the cylinders. Entrainment of a cylinder in another cylinder's wake was observed to be more likely to occur at higher Mach numbers. Mehta et al. (2016a) found that particles in a transverse array experienced the same forces as isolated particles when the particle spacing was above three particle diameters. Three-dimensional arrays have been shown to display both amplification and reduction of maximal particle forces, as well as temporarily negative drag coefficients (Mehta et al., 2016b, 2018).

The temporal variation of particle forces is also large, as a result of nearby particles. An example of the variation of the particle forces during the interaction of a $\text{Ma} = 2.6$ shock wave and a 10% volume fraction cloud is shown in fig. 2.6. Here, the forces are normalized by the flow properties behind the incident shock, and the projected area of the particles. Time is normalized based on the particle diameter and the shock wave speed. The variation of the particle

forces over time is large, and at late time, the standard deviation is as large as the mean value.

In dense suspensions of particles, the relative arrangement of particles has more degrees of freedom than can reasonably be analyzed. It is therefore necessary to use a statistical description of the variation of particle forces. Probability distributions of particle forces are appropriate for this purpose, and their dependence on bulk-flow properties is possible to characterize. Akiki et al. (2016) provided scattered data of particle forces in incompressible flows for different particle Reynolds numbers and volume fractions. Mehrabadi et al. (2018) provided particle acceleration probability density functions in decaying isotropic turbulence at low volume fraction. Mehta et al. (2018, 2019b) provided peak particle force distributions during shock wave interaction with particle clouds at different Mach numbers and volume fractions.

Models for the effect of subgrid effects on particle forces often take the form of a modified drag law, see for example Gidaspow (1994); Tenneti et al. (2011); Tang et al. (2015). Such approaches account for the increased drag due to the density of particles, but do not usually account for the attraction or repulsion of particles in close proximity. There are some notable exceptions, such as the pairwise interaction extended point-particle (PIEP) model of Akiki et al. (2017a,b), which is based on a mapping of the perturbation flow of isolated particles as a function of bulk-flow parameters. It is also possible to use stochastic models to account for the force variations (Compton et al., 1997; Tenneti et al., 2016), and in this context, probability distribution functions of particle forces are essential. These extensions ensure that the particle velocity variance can remain non-zero, as is required in many flows. A more recent alternative is to use models that rely on statistical learning (Lu et al., 2012; Sen et al., 2017).

In the context of a two-fluid description of the dispersed flow, as in e.g. Theofanous and Chang (2017); Saurel et al. (2017), the particles are assumed to move with a single velocity at each point. At volume fractions where particles are not in constant contact, this can be a poor assumption. If that is the case, particle-velocity fluctuation correlations need to be modeled, which has not been common in the context of shock-wave particle cloud interaction. Similar fluctuations exist if particle parcels are used in Lagrangian descriptions. This is not addressed in this thesis.

It is clear from the above discussion that dense high-speed dispersed flows contain various flow phenomena that occur at a scale comparable to the size of the particles. In an averaged description, these phenomena manifest as fluctuations. A flow model applicable to full-scale simulations of dense particle-laden flows must accurately account for particle-scale fluctuations, since they are dynamically important. Nourgaliev et al. (2004) remark that "In a truly multi-physics multi-scale problem where scale-to-scale interactions do matter, sub-grid scale phenomena may greatly affect and even alter global behaviour". Altered global behavior can in turn affect the subgrid scale processes. These multi-scale interactions are very challenging to model, due to the necessity of proper models for unresolved physics, which can only depend on resolved flow quantities. The dispersive behavior of shock-wave particle cloud interaction in

Figure 2.7: Particle jet formation during explosive dispersal of silicon carbide powder. Reprinted by permission from Springer Nature: Shock Waves, Terminal velocity of liquids and granular materials dispersed by a high explosive, Loiseau, J., Pontalier, Q., Milne, A. M., Goroshin, S., and Frost, D. L. (Loiseau et al., 2018), Copyright 2018.

planar geometries (Theofanous and Chang, 2017) is one example of a large-scale flow phenomenon that depends on particle-scale physics. Another example is particle jetting during explosive dispersal. The latter is discussed in the following section.

2.4 Particle jet formation in shock-induced flow

Impulsively accelerated layers of liquids and/or particles in diverging geometries develop strong inhomogeneities in the form of radially aligned jets. The jets appear as spines on the surface of the expanding particle shell. Particle jet formation can be seen in fig. 2.7, which shows an image series of an explosive dispersal experiment by Loiseau et al. (2018). These macroscale features develop from particle-scale inhomogeneities. Since particle jetting is a robust phenomenon when shock waves interact with sufficiently thick particle layers, it is important to understand the origin of particle jetting (Ritzel et al., 2009), and modeling of explosive dispersal must account for jets. Increased understanding of particle jets can potentially be used to improve shock mitigation systems (Pontalier et al., 2018) or jets can be utilized in engineering applications to either disseminate substances homogeneously, or heterogeneously, depending on the needs of the application. Particle jetting has a role in naturally occurring phenomena, such as meteorite breakup in the atmosphere (Svetsov et al., 1995; Artemieva and Shuvalov, 2001) and volcanic eruptions (Valentine and Wohletz, 1989). Since this thesis is focused on flows with solid particles, the discussion in this section will be focused on particle jetting. However, many points are equally valid for formation of jets of liquid droplets.

Particle jetting can be described as a preferential alignment of particles in

the radial direction. Such clustering of particles can reduce the deceleration of particles within the cluster relative to that which would occur in the absence of clustering (Zarei et al., 2011). As a result, particles can be dispersed over a larger volume due to particle jetting. Particle jets can even attain high enough speeds to overtake the shock wave (Ritzel et al., 2009). Because particle jetting implies that there are particles distributed over large radial distances, the particles are exposed to very different accelerations and temperatures, depending on whether they are in the front, middle, or rear of a jet. Subsequent dispersal by for example thermal lift might primarily affect particles furthest in. It is therefore important to be able to accurately predict particle jetting when considering the risk related to explosive dispersal of harmful substances. This is not achieved by most full-scale computational models today.

Explosive particle jet formation is challenging to investigate because of the short time and small spatial scales governing the process, combined with the relatively long times and large spatial scales that describe the bulk flow. Another challenge is that well-resolved temporal and spatial measurements of the internal structure of the particle layer are unattainable with present experimental techniques. It has, however, been observed that the development of jets begins during or shortly after the shock wave passes through the particle layer (Milne et al., 2014; Xue et al., 2019; Fernández-Godino et al., 2019). To circumvent the difficulty of obtaining measurements within an explosively dispersed particle layer, a simpler model for explosive dispersal has been investigated in recent studies. In this model, a cylindrical shell of particles inside a Hele-Shaw cell was accelerated with the use of a shock tube (Rodriguez et al., 2013, 2014, 2016; Xue et al., 2018). The Hele-Shaw cell allows high-speed imaging of the internal structure of the particle layer. In this configuration, the sequence of events leading to particle jet formation could be divided into three parts. First, radially aligned structures appear around the inner particle layer edge. Next, small outer jets appear on the outer layer edge. Due to geometric expansion, the pressure drops in the central region and eventually the particle layer is decelerated. Later on, large outer jets appear, and Rodriguez et al. (2016) proposed that this was due to lower drag experienced within the previously formed, radially aligned, particle clusters.

The formation of particle jetting in explosive dispersal is not necessarily governed by the same processes as observed in the Hele-Shaw model. Importantly, the Hele-Shaw model features significantly milder shock pressures and temperatures than the explosive case. Therefore, there are additional physical processes that can occur in explosive dispersal that will not be captured in the Hele-Shaw model, in particular processes relating to particle deformation. Various candidate processes have been proposed for the origin of explosive particle jetting, such as sintering of particles and subsequent fragmentation (Loiseau et al., 2018), microscale gas jets (Xu et al., 2013), and particle force-chain dynamics (Xue et al., 2019). Inelastic collisions reduce lateral particle spreading (Nourgaliev et al., 2004), and can therefore create or reinforce particle jets. Wake dynamics, such as entrainment of particles and particle-induced shock-wave interactions, are further possibilities (Ritzel et al., 2009; Carmouze et al.,

2018).

In our study, we focus on the Hele-Shaw model, and investigate how model choices affect the development of particle jets in this configuration. The formation of particle jets in our study, as well as in Balakrishnan (2014); Fernández-Godino et al. (2019), is due to flow instability originating from misalignment of average particle forces and effective density gradients. Fernández-Godino et al. (2019) observed a related effect using two-dimensional simulations of an explosively dispersed particle layer. Particles in locally low particle density regions attain higher velocities than those in high volume fraction regions. As these particles propagate radially outwards, they migrate into regions of higher volume fractions. They labeled this as a channeling instability. In general, such instabilities are referred to as multiphase gas-dynamic instabilities (McFarland et al., 2016). Multiphase flow instabilities share many properties with classical interface instabilities, such as Rayleigh-Taylor and Richtmyer-Meshkov instabilities. In multiphase instabilities, however, there are a number of additional complicating factors, such as relative phase velocities, particle inertia, particle shapes, and particle collision. Furthermore, development of multiphase flow instabilities in numerical simulations depends on details of the coupling between the gas phase and the dispersed phase (Black et al., 2018). The study of multiphase flow instability is a less developed field than classical interface instability, and is likely to see significant developments in coming years.

Multiphase flow instabilities have previously been rejected as the mechanism for particle jet formation in explosive dispersal. The basis of this rejection was that classical gas-dynamic instability growth rates were not comparable to the experimentally observed jet growth rate (Milne et al., 2010), and this was backed up by a two-dimensional simulation. However, to the author’s knowledge, no theory exists for multiphase flow instability in diverging geometries with two interfaces. It is known that multiple interfaces affect the growth rates of classical instabilities (Mikaelian, 1982, 1990), and one can expect this to be the case also for multiphase instabilities. The rejection of this mechanism, while it might be correct, is therefore lacking sound theoretical basis.

Despite the considerable number of studies that have investigated particle jetting, the understanding of and ability to model the phenomenon remain limited. The multiple ways which particle jetting can emerge, and their ability to co-exist, indicate that jetting results as a combination of many different physical processes. The importance of particle jetting for safety and industrial processes, natural phenomena, as well as simply being a very interesting phenomenon, continues to drive research into particle jetting and dense high-speed dispersed flows in general.

Chapter 3

Governing equations

3.1 Single phase compressible flow

Single-phase high-speed flow is governed by the compressible Navier-Stokes equations, which express the conservation of mass, momentum, and energy. In the following, ∂_t denotes temporal partial differentiation, ∂_i denotes partial differentiation with respect to the i 'th spatial coordinate, and Einstein's summation convention is used. The Navier-Stokes equations can be written

$$\partial_t \rho + \partial_j (\rho u_j) = 0, \quad (3.1)$$

$$\partial_t (\rho u_i) + \partial_j (\rho u_i u_j) = -\partial_i p + \partial_j \sigma_{ij}, \quad (3.2)$$

$$\partial_t (\rho E) + \partial_j (\rho E u_j) = -\partial_j (u_j p) + \partial_j (u_j \sigma_{ij}) - \partial_j (\lambda \partial_j T), \quad (3.3)$$

where $p(\mathbf{x}, t)$ is the pressure, $\sigma_{ij}(\mathbf{x}, t) = \mu (\partial_j u_i + \partial_i u_j - 2\partial_k u_k \delta_{ij}/3)$ is the viscous stress tensor, $E(\mathbf{x}, t) = \rho(e + u_i u_i/2)$ is the total energy per unit volume, $e(\mathbf{x}, t)$ is the internal energy per unit mass, $\lambda(\mathbf{x}, t)$ is the thermal conductivity and $T(\mathbf{x}, t)$ is the temperature. In this thesis, the temperature dependence of the viscosity is modeled as a power law, where $\mu(\mathbf{x}, t) = \mu_0 (T/T_0)^{0.76}$. Thermal conductivity and dynamic viscosity are related by a constant Prandtl number of 0.7. For all simulations, we assume that the continuous phase is described by the ideal gas equation of state, i.e.,

$$p = (\gamma - 1) \rho e, \quad (3.4)$$

where γ is the heat capacity ratio.

3.2 Particle motion

In this thesis, the problems considered feature rigid particles that do not interchange mass or thermal energy with the fluid phase. The equations governing the motion of a particle are then

$$d_t x_{p,i} = v_i, \quad (3.5)$$

$$m_p d_t v_i = F_{p,i} + F_{pp,i} + F_{body,i}, \quad (3.6)$$

where d_t denotes the rate of change following the particle, x_p is the particle position, m_p is the particle mass, F_p is the total force exerted by the fluid on the particle, F_{pp} is the sum of forces due to particle collision, and F_{body} is the sum of body forces, such as gravity, acting on the particle. The forces on the particles will be further discussed in section 3.4. In papers II-IV, the particles are locked in place.

3.3 Volume-averaged continuous phase equations

In both analysis and modeling of particle-laden flows, it is useful to consider the conservation equations applied to a control volume of finite size. The resulting equation set can be considered a version of large eddy simulation. The differences from standard LES equation sets are the presence of the volume fraction and the interphase coupling terms, as will be discussed below.

The validity of the volume-averaged equations as a point-wise description depends on the spatial scale of the variations in particle concentration, and of the continuous phase variables. As discussed in Crowe et al. (2011), a particle volume fraction is well defined only for a volume with $\mathcal{O}(10^5)$ particles. This requirement defines a minimum size of the control volumes that can be used in a simulation. Simultaneously, the control volume must be smaller than the scale over which bulk-flow parameters vary. These two requirements are not simultaneously realizable for many problems, and then the volume-averaged equations, as a point-wise description, are not valid for those problems.

It is possible to relax the scale requirements if one considers the integral form of the conservation equations. Volume fractions and volume-averaged flow properties are always well defined as integral measures. It is then important to keep in mind that all variables are averages over a volume, and that fluctuations within the volume can be dynamically important. Flux computations, fluctuation models, and particle force models must be formulated in a manner that reflects that all available flow variables are volume averages. Similarly, when volume averaging is used as a framework for data analysis, the scale requirements are not necessary.

Let $\bar{\cdot}$ denote a volume averaged quantity. If the particles do not exchange mass or thermal energy with the continuous phase, the volume averages of temporal and spatial gradients are (Crowe et al., 2011; Schwarzkopf and Horwitz, 2015)

$$\overline{\partial_t A} = \partial_t \bar{A} + \frac{1}{V} \int_{S_d} A v_i n_i dS, \quad (3.7)$$

$$\overline{\partial_i A} = \partial_i \bar{A} - \frac{1}{V} \int_{S_d} A n_i dS, \quad (3.8)$$

where A denotes any continuous phase variable, V denotes the averaging volume, and S_d is the dispersed phase boundary with normal vector n , pointing into the continuous phase. In addition, the volume average and the phase average of a quantity are related by

$$\bar{A} = \alpha \langle A \rangle, \quad (3.9)$$

where $\langle A \rangle$ denotes the phase average of A , and α is the volume fraction of the continuous phase. Let also $\tilde{A} = \langle \rho A \rangle / \langle \rho \rangle$ denote a Favre-averaged variable. The deviations from the phase-average and Favre-average will be denoted by A' and A'' , respectively. The volume averaged conservation equations are

$$\partial_t (\alpha \langle \rho \rangle) + \partial_i (\alpha \langle \rho \rangle \tilde{u}_i) = 0, \quad (3.10)$$

$$\begin{aligned} \partial_t (\alpha \langle \rho \rangle \tilde{u}_i) + \partial_j (\alpha \langle \rho \rangle \tilde{u}_j \tilde{u}_i + \alpha \langle p \rangle \delta_{ij}) &= \partial_j (\alpha \langle \sigma \rangle_{ij}) - \partial_j (\alpha \langle \rho \rangle \tilde{R}_{ij}) \\ &+ \frac{1}{V} \int_{S_d} p n_i dS - \frac{1}{V} \int_{S_d} \sigma_{ij} n_j dS, \end{aligned} \quad (3.11)$$

$$\begin{aligned} \partial_t (\alpha \langle \rho \rangle \tilde{E}) + \partial_j (\alpha \langle \rho \rangle \tilde{E} \tilde{u}_j + \alpha \langle p \rangle \tilde{u}_j) &= \partial_j (\alpha \langle \sigma_{ij} \rangle \tilde{u}_i) - \partial_j (\alpha \langle \lambda \partial_j T \rangle) \\ &- \partial_j (\alpha \langle \rho e'' u_j'' \rangle) - \partial_j (\alpha \langle \rho \rangle \tilde{R}_{ij} \tilde{u}_i) + D^u + D^p + D^\mu + D^{ap} + D^{a\mu} \\ &+ \frac{1}{V} \int_{S_d} p u_j n_j dS - \frac{1}{V} \int_{S_d} \sigma_{ij} u_j n_i dS + \frac{1}{V} \int_{S_d} (\lambda \partial_j T) n_j dS. \end{aligned} \quad (3.12)$$

Here, $\tilde{R}_{ij} = \widetilde{u_i'' u_j''}$ is the velocity fluctuation correlation tensor, which for single-phase flows is the Reynolds stress tensor. The integrals represent the forces acting on the dispersed phase. $D^u = -0.5 \partial_j (\alpha \langle \rho u_i'' u_i'' u_j'' \rangle)$ is the turbulent diffusion, $D^p = -\partial_j (\alpha \langle p' u_j' \rangle)$ is the pressure diffusion, $D^\mu = \partial_x (\alpha \langle u_j' \sigma_{ij}' \rangle)$ is the turbulent viscous diffusion, $D^{ap} = \partial_j (\alpha a_j \langle p \rangle)$ is the pressure-diffusion effect due to the density-velocity correlation, where $a_j = -\langle \rho' u_j' \rangle / \langle \rho \rangle$, and $D^{a\mu} = -\partial_j (\alpha a_i \langle \sigma \rangle_{ij})$ is the analogous viscous diffusion effect. We use the label "turbulent" for these terms only to signify that they result from the same algebraic manipulations that are used to derive classical LES and RANS equation sets. They do not necessarily represent the effect of turbulence in particle-laden flows, because the fluctuations can be laminar flow phenomena induced by the particles. Equations (3.10) to (3.12) are the point-wise descriptions of the volume-averaged conservation equations. In this thesis, they should only be interpreted as a convenient notation for their corresponding integral formulations.

The equations governing the mean kinetic energy, the fluctuating kinetic energy and mean internal energy can be derived from eqs. (3.10) to (3.12). The mean kinetic energy and the fluctuation kinetic energy equations are, respectively, half the traces of

$$\begin{aligned} \partial_t (\alpha \langle \rho \rangle \tilde{u}_i \tilde{u}_j) + \partial_k (\alpha \langle \rho \rangle \tilde{u}_i \tilde{u}_j \tilde{u}_k) &= -\alpha \tilde{u}_j \partial_i \langle p \rangle - \alpha \tilde{u}_i \partial_j \langle p \rangle + \alpha \tilde{u}_j \partial_k \langle \sigma_{ik} \rangle \\ &+ \alpha \tilde{u}_i \partial_k \langle \sigma_{jk} \rangle - \partial_k (\alpha \langle \rho \rangle \tilde{u}_j \tilde{R}_{ik}) - \partial_k (\alpha \langle \rho \rangle \tilde{u}_i \tilde{R}_{jk}) \\ &+ \alpha \langle \rho \rangle \tilde{R}_{ik} \partial_k \tilde{u}_j + \alpha \langle \rho \rangle \tilde{R}_{jk} \partial_k \tilde{u}_i + \frac{\tilde{u}_j}{V} \int_{S_d} p' n_i dS \\ &+ \frac{\tilde{u}_i}{V} \int_{S_d} p' n_j dS - \frac{\tilde{u}_j}{V} \int_{S_d} \sigma'_{ik} n_k dS - \frac{\tilde{u}_i}{V} \int_{S_d} \sigma'_{jk} n_k dS, \end{aligned} \quad (3.13)$$

and

$$\begin{aligned} \partial_t (\alpha \langle \rho \rangle \tilde{R}_{ij}) + \partial_k (\alpha \langle \rho \rangle \tilde{R}_{ij} \tilde{u}_k) &= -\alpha \langle \rho \rangle \tilde{R}_{ik} \partial_k \tilde{u}_j - \alpha \langle \rho \rangle \tilde{R}_{jk} \partial_k \tilde{u}_i \\ &+ \alpha (a_j \partial_i \langle p \rangle + a_i \partial_j \langle p \rangle) + \alpha \langle p' \partial_i u_j' + p' \partial_j u_i' \rangle \\ &- \alpha (a_j \partial_k \langle \sigma_{ik} \rangle + a_i \partial_k \langle \sigma_{jk} \rangle) - \alpha \langle \sigma'_{ik} \partial_k u_j' + \sigma'_{jk} \partial_k u_i' \rangle \\ &- \partial_i (\alpha \langle p' u_j' \rangle) - \partial_j (\alpha \langle p' u_i' \rangle) + \partial_k (\alpha \langle \sigma'_{ik} u_j' \rangle) + \partial_k (\alpha \langle \sigma'_{jk} u_i' \rangle) \\ &+ \frac{1}{V} \int_{S_d} (p' u_j'' n_i + p' u_i'' n_j - \sigma'_{ik} u_j'' n_k - \sigma'_{jk} u_i'' n_k) dS. \end{aligned} \quad (3.14)$$

3. Governing equations

Equation (3.14) does not agree completely with the fluctuating kinetic energy equation in paper II. Equation (3.14) implies a production of fluctuating kinetic energy by the terms $\alpha a_i \partial_i \langle p \rangle$ and $\alpha a_i \partial_j \langle \sigma_{ij} \rangle$, whereas in paper II, the corresponding terms are claimed to be $a_i \partial_i (\alpha \langle p \rangle)$ and $a_i \partial_j (\alpha \langle \sigma_{ij} \rangle)$. The differences are the terms $a_i \langle p \rangle \partial_i \alpha$ and $a_i \langle \sigma \rangle_{ik} \partial_k \alpha$. For the results presented in paper II, the difference in the fluctuating kinetic energy production due to these errors is negligible, and does not affect the conclusions in the paper. In addition, in paper II it is claimed that there is a production of fluctuating kinetic energy by the terms

$$-\frac{\tilde{u}_k}{V} \int_{S_d} p n_k dS, \quad -\frac{\tilde{u}_k}{V} \int_{S_d} \sigma_{ik} n_k dS, \quad (3.15)$$

where the integrands should not have the full pressure or the full viscous stress tensor, but only their fluctuating components. In the results of paper II, the forces on the particles are used, and the results presented for the production terms are therefore correct, but inconsistent with their definitions in the paper.

The volume-averaged internal energy equation is

$$\begin{aligned} \partial_t \alpha \langle \rho \rangle \tilde{e} + \partial_k (\alpha \langle \rho \rangle \tilde{e}) &= \partial_k \left(\alpha \langle \rho \rangle \widetilde{e'' u_k''} \right) - \alpha \langle p \rangle \partial_k \tilde{u}_k + \partial_k (\alpha a_k \langle p \rangle) \\ &\quad - \alpha a_k \partial_k \langle p \rangle - \alpha \langle p' \partial_k u_k' \rangle + \alpha \langle \sigma_{ik} \rangle \partial_k \tilde{u}_i - \partial_k (\alpha a_i \langle \sigma_{ik} \rangle) \\ &\quad + \alpha a_i \partial_k \langle \sigma \rangle_{ik} + \alpha \langle \sigma'_{ik} \partial_k u_i' \rangle - \partial_k (\alpha \langle \lambda \partial_k T \rangle) \\ &\quad + \frac{\langle p \rangle}{V} \int_{S_d} u_k'' n_k - \frac{\langle \sigma_{ik} \rangle}{V} \int_{S_d} u_i'' n_k + \frac{1}{V} \int_{S_d} (\lambda \partial_k T) n_k dS. \end{aligned} \quad (3.16)$$

Pairwise comparison of eqs. (3.13), (3.14) and (3.16) reveals the energy exchange mechanisms that are shown in fig. 2.5. The expressions for the energy exchange mechanisms are

$$\begin{aligned} \text{Mean flow compression} &= -\alpha \langle p \rangle \partial_k \tilde{u}_k + \frac{\langle p \rangle}{V} \int_{S_d} u_k'' n_k dS, \\ \text{or expansion work} & \end{aligned} \quad (3.17)$$

$$\begin{aligned} \text{Dissipation of mean} &= \alpha \langle \sigma \rangle_{ik} \partial_k \tilde{u}_i - \frac{\langle \sigma_{ik} \rangle}{V} \int_{S_d} u_i'' n_k dS, \\ \text{kinetic energy} & \end{aligned} \quad (3.18)$$

$$\begin{aligned} \text{Reynolds stress} &= -\alpha \langle \rho \rangle \tilde{R}_{ik} \partial_k \tilde{u}_i, \\ \text{production} & \end{aligned} \quad (3.19)$$

$$\begin{aligned} \text{Work due to} &= -\frac{\tilde{u}_i}{V} \int_{S_d} (p' n_i - \sigma'_{ik} n_k) dS, \\ \text{relative phase velocity} & \end{aligned} \quad (3.20)$$

$$\begin{aligned} \text{Dissipation of fluctuating} &= -\alpha (a_i \partial_k \langle \sigma_{ik} \rangle + \langle \sigma'_{ik} \partial_k u_i' \rangle), \\ \text{kinetic energy} & \end{aligned} \quad (3.21)$$

$$\begin{aligned} \text{Fluctuating compression} &= -\alpha (a_k \partial_k \langle p \rangle + \langle p' \partial_k u_k' \rangle). \\ \text{or expansion work} & \end{aligned} \quad (3.22)$$

In eq. (3.17), the integral can be expressed as

$$\frac{\langle p \rangle}{V} \int_{S_d} u_k'' n_k dS = -\langle p \rangle \tilde{u}_k \partial_k \alpha + \frac{\langle p \rangle}{V} \int_{S_d} u_k n_k dS, \quad (3.23)$$

Figure 3.1: Particle at a control volume boundary, and the definition of the surface sections.

and thus eq. (3.17) can be combined with the term $\alpha \tilde{u}_k \partial_k \langle p \rangle$ in the mean kinetic energy equation to form a conservative flow work term. The remaining integral represents the work done by change in particle volume fraction, which can be seen by rewriting the individual parts of the integral as integrals over separate particle surfaces and replacing u_k with each particle's velocity. Similar considerations hold for eq. (3.18). In addition, there is a transfer of kinetic energy to the dispersed phase through the integral terms in eq. (3.13) and eq. (3.14). For the pressure, these terms sum to

$$\frac{1}{V} \int_{S_d} (p' \tilde{u}_k + p' u_k'') n_k dS = \frac{1}{V} \int_{S_d} p' u_k n_k dS, \quad (3.24)$$

which is the work done by the dispersed phase on the continuous phase through pressure forces, since $u_i = v_i$ on each particle surface. Again, similar relations hold for the viscous forces.

3.3.1 The pressure integral

The interphase coupling terms, i.e., the integral terms in eq. (3.11), deserve special attention. For a given control volume, they consist of the sum of individual integrals over particle surfaces within that volume. For particles entirely contained within the control volume, the pressure integral represents the momentum transfer due to pressure forces, and is appropriately closed by a drag law. For particles located at the boundary, the drag law is insufficient as a model closure. For those particles, the pressure distribution at the particle surface must be considered, since only a part of the particle surface is contained within the control volume. This is illustrated in fig. 3.1. In general, if the particle is not in equilibrium with the surrounding flow, the average pressure at the particle surface is not equal to the average pressure of the surrounding gas (Seidl et al., 1997; Rodriguez et al., 2011). Therefore, the gas phase is subject to a pressure that is not equal to the volume-averaged pressure, at a part of the control volume surface.

For each particle at the boundary, the pressure at the part of the control volume boundary covered by the particle can be defined in terms of the pressure

at the part of the particle surface inside the control volume (Crowe et al., 2011). Let $S_{b,i}$ denote the part of the particle surface inside the control volume, and $S_{b,b}$ the part of the control volume surface covered by the particle, as indicated in fig. 3.1. Then the following relation holds for the pressure at $S_{b,b}$,

$$\int_{S_{b,i}} p n_i dS = \langle p \rangle_{b,i} \int_{S_{b,i}} n_i dS = -\langle p \rangle_{b,i} \int_{S_{b,b}} n_i dS, \quad (3.25)$$

where $\langle p \rangle_{b,i}$ is the average pressure at $S_{b,i}$, and the last identity follows because the integral of the normal vector over a closed surface is zero (note the difference between i and i in this expression). In the case of multiple particles at the control volume boundary, each particle has its own distinct value of $\langle p \rangle_{b,i}$. The pressure integral on a control volume surface is therefore, without approximation,

$$\int_{S_{CV}} p n_i = \int_{S_g} p n_i + \sum_{j=0}^{N_{p,b}} \langle p \rangle_{b,i}^j \int_{S_{b,b}^j} n_i dS, \quad (3.26)$$

where S_{CV} denotes the control volume surface, S_g denotes the part of the control volume surface that is not covered by any particle, $N_{p,b}$ denotes the number of particles that overlap the surface and superscripts are used to denote properties belonging to particle j . The sum of S_g and all $S_{b,b}^j$ is the total control volume surface, S_{CV} .

If the pressures $\langle p \rangle_{b,i}^j$ are assumed to be equal to the average pressure at S_g , then the total pressure force on the control volume is the same as if there were no particles. This is the approximation we have used in paper I. This is generally incorrect, and is therefore a limitation of that work. The approximation is poor when there is a large velocity difference between the particles and the gas. In addition, the approximation is likely to get worse with increasing particle volume fraction, and is also problematic under strong volume fraction gradients, where the number of particles at each side of the control volume can vary significantly. These issues are interesting topics for future studies.

Similar relations hold for the integral of the viscous stress tensor. The properties of this integral will not be elaborated here.

3.4 Momentum transfer

When particles move relative to the surrounding fluid, momentum is transferred between the phases by forces acting on the particle surfaces. Fundamentally, these forces are due to pressure and viscous friction acting on the surface. The total force exerted on a particle by the fluid is

$$F_{p,i} = - \int_{S_p} (p n_i - \sigma_{ij} n_j) dS, \quad (3.27)$$

where S_p denotes the particle surface.

The force on a single particle can be decomposed into separate contributions due to different physical effects. Parmar et al. (2012) decomposed the forces as

$$F_p = F_{qs} + F_{iu} + F_{vu} + F_{bg}, \quad (3.28)$$

where the right-hand side terms represent the quasi-steady force (F_{qs}), the inviscid unsteady force (F_{iu}), the viscous unsteady force (F_{vu}), and the buoyancy/gravity force (F_{bg}). Such decompositions are useful for modeling because the relative importance of the terms can be assessed. Terms with insignificant contributions can then be ignored in specific problems. It also aids understanding of the flow.

The quasi-steady drag is often the dominant term, as exemplified for shock-wave particle cloud interaction in Ling et al. (2012). It is usually written in terms of the drag-coefficient C_D as

$$F_{qs,i} = \frac{1}{2} \rho C_D \frac{\pi D_p^2}{4} |u_i - v_i| (u_i - v_i). \quad (3.29)$$

There exist plenty of models for C_D that are valid for different flow configurations and ranges of particle Reynolds numbers. In this thesis, two different correlations are used; the correlation developed by Clift (1970) (as cited in Crowe et al. (2011)), and a correlation with a correction due to particle volume fraction (Gidaspow, 1994). The expressions for these correlations are given in paper I. It has also been found that the quasi-steady drag depends on other flow parameters, such as Mach number (Nagata et al., 2016, 2018), and flow blockage (Achenbach, 1974; Akutsu, 1977).

The buoyancy/gravity force represents the force due to pressure variations in an undisturbed flow as well as the force of gravity, and is sometimes also referred to as the pressure gradient force (Ling et al., 2012). In absence of gravity, it can be expressed as

$$F_{bg,i} = \frac{\pi}{6} D_p^3 \partial_i p, \quad (3.30)$$

where the divergence theorem has been used to convert the surface integral of the pressure into a volume integral, and the pressure gradient has been assumed constant over the particle. The inviscid unsteady and viscous unsteady forces in eq. (3.28) have not been addressed or used for drag modeling in this thesis, and will therefore not be discussed here.

Chapter 4

Computational methods and grids

4.1 Computational methods

The simulations in this thesis are computed using finite volume methods. Such methods are discretizations of the conservation equations, c.f. sections 3.1 and 3.3, in integral form. Finite volume methods are appropriate for studies of shock waves, since the integral relations hold even for a volume containing a shock wave.

All simulations in this thesis have been conducted using the "CharLES" code developed by Cascade Technologies (Brès et al., 2011, 2017, 2018). CharLES is a control-volume based finite-volume method for large eddy simulations on unstructured grids. The solution is advanced in time by a third order Runge-Kutta scheme.

In paper I, we use a modified version of CharLES to solve the volume-averaged conservation equations. The extension of the solver from a standard LES code to a solver for the volume-averaged equations has been conducted as part of this thesis. Papers II-IV use the unmodified CharLES version 5.0.0.

In the simulations of paper I, the particles are not locked in place as for the simulations in papers II-IV. Here, the particle positions are advanced in time by a Crank-Nicholson scheme. Second order interpolation is used to obtain gas variables at each particle position. The interphase coupling is only applied to the control volume containing each particle. It has been shown that it is necessary to apply the interphase coupling terms with specified filter widths, in order to obtain simulation results that converge with grid size. Unbounded volume fractions can also occur with the omission of such filters (Shallcross and Capecehatro, 2018). Since the model used in the simulations in paper I does not apply such a filter, this is a limitation of that study.

4.1.1 Fluxes

A crucial part of finite volume methods is the computation of fluxes between control-volumes. In this thesis, two different methods are used. The first is the Harten-Lax-van Leer-Contact (HLLC) Riemann solver developed by Toro et al. (1994). The second is an entropy-stable Lax-Friedrich flux scheme. The HLLC method is based on the analytical solution of a Riemann problem, which is approximated by a set of three waves. Specifically, the HLLC solver utilizes the Rankine-Hugoniot relations for the fastest leftward and rightward propagating signals, combined with relations that hold for the contact discontinuity between them. Determination of the direction of these three waves is used to define the state at each control volume face, and the flux is subsequently computed based on that state. The HLLC solver was originally developed for the Euler

equations, but is here applied to the volume-averaged conservation equations, which include the gas-phase volume fraction as a variable. The problem is split so that the HLLC solver is used for the conservative part of the gas-fluxes, and the non-conservative part is handled implicitly in the particle advancement. With this approach, the extension of the original HLLC solver to the equation set containing the gas volume fraction is straightforward. The details are discussed in paper I.

4.1.2 Entropy stable schemes

Most computational methods for compressible flows are formulated in a manner that conserves mass, momentum, and energy. In addition to these conservation principles, any flow phenomenon also obeys the second law of thermodynamics; flow processes must conserve or increase entropy, but this is not necessarily obeyed by numerical formulations of mass-, momentum-, and energy-conserving fluxes (Chandrashekar, 2013).

Failure to obey the second law of thermodynamics can lead to numerical instabilities and admit non-physical solutions. Quirk (1997) discusses problems occurring with many common schemes. Some approaches have introduced artificial viscosity in order to dampen numerical instabilities. However, by doing so, the numerical methods can become too dissipative to accurately represent flow phenomena of interest, such as turbulence.

Papers II-IV in this thesis use an entropy stable flux scheme. The flux is computed with a modified Lax-Friedrich scheme (Masquelet et al., 2017), with minimal dissipation of kinetic energy.

4.2 Particle-resolved computational grids

Paper II-IV utilize particle-resolved simulations to study the flow through random arrays of particles. Two different approaches are taken for generating the computational mesh. In papers II and III, the mesh consists of structured regions around each particle, and an unstructured mesh in the rest of the domain. This is illustrated in fig. 4.1, where the left image shows the mesh around a single particle. In paper IV, the structured region around each particle was omitted. The reason for this difference is due to practical problems. We could not successfully combine periodic boundary conditions and the structured meshes with the specific version of the meshing tool. In paper IV, we prioritize periodic boundary conditions.

Grid sensitivity studies are performed in paper III, using the single particle force history as a measure. We also consider the grid resolution in terms of viscous shear length scales, and find that the grid size is appropriate for an LES simulation. For the grids in paper IV, the grid sizes are determined based on the results of paper III, and on a previous grid sensitivity study for a related problem (Osnes et al., 2019b).

The difference between the structured and unstructured grids is not addressed in the papers, but is shown in fig. 4.2. The figure shows a comparison of

Figure 4.1: Illustration of the computational grids around the particles in papers II and III (left), and paper IV (right). The grid shown on the left contains a structured region around the sphere, where the control volume size increases with distance from the particle surface.

the forces on a single particle subjected to a $Ma = 2.6$ shock wave at $Re_p = 5000$ in a square channel with slip walls. The figure also shows the velocity fluctuations around it. The results are compared against high-resolution simulations with both grid types. The grid-size used in the simulations in papers II-IV has roughly 28 control volumes per particle diameter, while the highly resolved simulation shown in fig. 4.2 has 84. The highly resolved simulations agree very well, and it can be seen that the low-resolution structured grid matches the high-resolution results better than the low-resolution unstructured grid. The unstructured low-resolution grid underpredicts both the viscous force on the particle, and the velocity fluctuations around it. If the trends with grid size and type are the same for particle clouds as for the single particle, this indicates that forces on the particles might be overpredicted by a few percent in papers II-IV, and that the fluctuations in the simulations of paper IV might be slightly underpredicted.

Figure 4.2: Comparison of drag coefficients (left) on a single particle in a rectangular channel, where $C_{D,p}$ is the pressure drag coefficient and $C_{D,\mu}$ is the viscous drag coefficient, and streamwise velocity fluctuations (right) around it, with different grids. Here, the structured and unstructured grids with resolutions corresponding to those used in the papers are respectively denoted SLR and ULR, while high-resolution structured and unstructured grids are denoted SHR and UHR. u_{IS} is the post-shock velocity.

Chapter 5

Summary of papers

5.1 Numerical simulation of particle jet formation induced by shock wave acceleration in a Hele-Shaw cell – (Osnes et al., 2018)

Particle jet formation under rapid acceleration of particle layers is a phenomenon that is not well understood. Recent experiments of shocked cylindrical shells of particles in a Hele-Shaw cell have allowed observation of particle distributions during jet formation. However, exploring the mechanisms leading to jet formation is difficult in an experimental setting. The goal of this study is to explore the capability of present numerical methods to simulate particle jet formation, and to examine the flow fields within the particle layer during the particle jet formation. To this end, we simulate the flow in a problem similar the one studied in the recent experimental works of Rodriguez et al. (2013, 2014, 2016).

In this study, we use an Eulerian-Lagrangian method for solving the volume-averaged, three-dimensional time-dependent Navier-Stokes equations. We derive the characteristic wave speeds of the equations, and show that the wave-speeds are real if the particle volume fraction is lower than the close-packing limit used in the particle collision model.

We find that particle jets are obtained using an Eulerian-Lagrangian method. The jet formation is robust to choice of drag law, whether or not particle volume fraction is accounted for, and to including particle collision. The only approaches that do not result in particle jet formation are when one-way coupling between the phases is used, or the naïve approach where the particle layer is modeled as a dense gas. For the models that predict particle jetting, we find that the particle jets differ in number and heterogeneity for the different modeling choices and shock-wave Mach number. For weak shock waves, we find that the late-time particle jets appear after the passage of a second shock wave through the particle layer, while the cases with stronger incident shock waves develop jets prior to the secondary shock interaction.

We explore the possibility that multiphase instabilities can be a contributing factor to the formation of particle jets. The results show that flow configurations during particle jet formation are consistent with both classical flow instabilities and multiphase instabilities. We identify the angular location of late-time particle jets and the dilute regions between them. Differences in flow velocity between these regions can be discerned much earlier than differences in particle distributions.

This study demonstrates that Eulerian-Lagrangian simulations can predict at least one form of particle jet formation, although there are considerable uncertainties about how model details affect the number, heterogeneity, and devel-

opment over time of the jets. It also improves the understanding of multiphase flow instabilities, and their relevance to high-speed particle dispersal.

5.2 Using particle-resolved LES to improve Eulerian-Lagrangian modeling of shock-wave/particle-cloud interactions – Vartdal and Osnes (2018)

This study simulates the shock-induced flow through stationary arrays of particles, in order to obtain knowledge about the flow inside such configurations. Usage of Eulerian-Lagrangian (or Eulerian-Eulerian) models to simulate interaction between shock-waves and particle suspensions has been shown to produce incorrect particle distributions (Theofanous and Chang, 2017). It has been proposed that this is either a result of the use of models with complex wave speeds, or that the models are incapable of representing important physical processes in these flows. In particular, particle-scale velocity fluctuations are commonly ignored in simulations of shock-wave particle cloud interactions, and one of the goals of this study is to investigate whether this can be justified.

This study utilizes particle-resolved simulations, which give access to detailed space- and time-resolved data. We perform simulations of different particle volume fractions, particle sizes, and shock-wave Mach numbers. Bulk-flow properties, such as the transmitted and reflected shock-wave strengths, are examined, as well as the level of fluctuating kinetic energy within the particle cloud. We find that the fluctuating kinetic energy contains between 20-40% of the local total kinetic energy, and it is therefore unreasonable to neglect its influence on the flow.

The production and dissipation of fluctuating kinetic energy are examined. The production is dominated by a term related to the pressure forces on the particles. The dissipation is comprised mainly of the pressure-dilatation correlation and viscous dissipation. At the downstream particle cloud edge, coupling of mean and fluctuating kinetic energy through mean flow velocity gradients is also important, and transfers energy from fluctuating kinetic energy to mean flow kinetic energy.

We use the data from the resolved simulations to develop an extension of standard Eulerian-Lagrangian models. The extension is comprised by an equation for the fluctuating kinetic energy. Using this model in combination with a curve-fitted, time-dependent, drag law from the resolved simulations, yields results in much better agreement with the resolved simulations, than a reference simulation that is representative of common models used in other studies.

The results imply that particle-scale velocity fluctuations are an important component of the flow dynamics in shock-wave particle cloud interaction. Including their effect accounts for some of the missing physical processes that might be the source of the erroneous particle distributions observed by Theofanous and Chang (2017).

5.3 Computational analysis of shock-induced flow through stationary particle arrays – (Osnes et al., 2019a)

This study expands the analysis of the data from the particle-resolved simulations that are the basis of the study described in section 5.2.

We report the mean flow fields over time as the shock wave passes through the particle layer. These fields are of interest for understanding which forces and temperatures the particles are exposed to, and how that depends on the particle location within the cloud.

We observe that some combinations of particle sizes and volume fractions give very similar results for the shock-wave attenuation. The mean flow fields within the particle cloud are also similar for these combinations. We therefore hypothesize that this is related to how much the flow is being deflected per distance, and as a proxy for that value, we use a parameter we label as a sight-length (its definition is given in the paper). This parameter turns out to be described to within an error of 1.5% by a simple algebraic expression. This expression can be used to estimate combinations of particle volume fractions and particle diameters that can be expected to give similar flow fields during, and for some time after, the shock wave passage through the particle layer.

We find that the gradient of streamwise Reynolds stress is important for the momentum balance at the particle cloud edges. Crucially, this means that the Reynolds stress affects the strength of the reflected shock wave. The Reynolds stress is comprised primarily of the separated flow in the wake of each particle. We propose an algebraic Reynolds stress model which, when applied to the data from the resolved simulations, predicts the fluctuation magnitude very well. This model requires specification of a single parameter (or function), which determines the average volume of the separated flow regions. We find that this parameter varies most strongly with particle volume fraction within the parameter ranges we consider.

This study improves the understanding of high-speed flow through particle clouds. The results reported in the paper are important for development of simplified models, e.g. as we do in paper II, that can be applied to full-scale problems. The Reynolds stress model, in particular, is an important development, and it is simple enough to implement in the most common models in use today.

5.4 Particle-resolved simulations of shock-induced flow through particle clouds at different Reynolds numbers – (Osnes et al., 2019c)

Particles of different sizes interact differently with high-speed flows. This is because the relative importance of viscous and inertial forces on the particle changes as the particles become smaller or larger. This study addresses the effect of different particle sizes, by varying the particle Reynolds number.

In this study, we perform particle-resolved large eddy simulations of the shock-induced flow through particle clouds. We simulate $\text{Re}_p = 500, 2000, 5000$, and 10000 , and for each Reynolds number, we perform an ensemble of simulations, in order to reduce the dependency of flow statistics on the particle configurations.

When the particles become smaller, the attenuation of the primary shock wave increases, and the strength of the reflected shock wave increases. As a result, the flow behind the reflected shock wave attains higher pressures, higher densities, and lower velocities, for lower particle Reynolds numbers. We find that velocity fluctuations, defined as deviations from the volume-averaged, density-weighted velocity, have a non-monotone dependency on particle Reynolds number. This is in contrast to the monotone trends found for the mean flow fields. Both the streamwise and spanwise velocity fluctuations vary almost proportionally to the square of the volume-averaged velocity. Surprisingly, this proportionality is insensitive to flow field gradients and magnitudes over this Reynolds number range.

We also investigate how the forces on the particles depend on the particle Reynolds number. We find that maximal forces have only a moderate Reynolds number dependency, and that their variation is almost independent of Reynolds number. This indicates that maximal particle forces are controlled by processes that are not highly affected by viscosity, such as shock-wave reflection, focusing and diffraction. Both the variation of time-averaged particle drag and the temporal variation are strongly dependent on Reynolds number, after the initial shock-related transient.

The results in this study contribute to the understanding of the fundamental processes occurring during shock-wave particle cloud interaction. How these change as a function of particle size is important for the design of systems involving interactions between shock waves and particle suspensions. This is especially important when the particle size varies with time, for instance in liquid- and solid-fuel combustion engines.

Chapter 6

Concluding remarks and future perspectives

Shock-wave particle cloud interaction occurs in a range of industrial and natural processes, and has implications for societal safety and security. This thesis contributes to the understanding and ability to model this complex, multi-scale problem. Multiphase flows, in general, are inherently multi-scale and challenging to model. Physics at particle scale lead to complex bulk-flow behavior, which can in turn affect particle-scale processes. Detailed investigations of particle-scale physics are necessary for development of models that represent the statistical effect of small-scale physics, at large scale.

This thesis has investigated shock-wave particle cloud interaction using numerical simulations. In papers II-IV, we have used simulations that resolve the physics at particle scale. Particle-resolved numerical simulations give access to highly resolved data in space and time. These simulations complement experimental investigations by providing data in regions where measurements are difficult. The first-of-a-kind viscous three-dimensional simulations of shock-wave particle cloud interaction in papers II-IV in this thesis have provided a database which can be used to improve state-of-the-art dispersed flow models.

This thesis has advanced the research in high-speed particle laden flows, in particular by demonstrating the usefulness of performing particle-resolved simulations. There is a large potential for this approach to further improve the understanding of dense particle-laden flows. Future studies can for example investigate the dynamical effects caused by volume fraction gradients and multimodal particle distributions, or investigate statistically steady-state flows in order to further characterize the effect of particle volume fraction on particle wakes, particle forces and particle force variations.

The effect of different approximations of the pressure at the particle surfaces, for the particles located at control volume boundaries, should be examined. This is particularly interesting for flows with volume fraction gradients, because the importance of the pressure approximation will vary in space.

Extended simulations, which account for particle movement, can be used to investigate entrainment of particles within particle clouds. In combination with accurate representation of particle collision, this can help illuminate the generation of particle jets, as well as their development over time.

The database generated with particle-resolved simulations can be used for development of dispersed flow models. This is a natural extension of the research in this thesis. The velocity fluctuation model proposed in paper III reproduced the simulation results well *a priori*, but should be evaluated as part of an Eulerian-Eulerian or Eulerian-Lagrangian simulation. This model represents

the effect of particle wakes, and is therefore not exclusive to shock-wave particle cloud interaction. Its applicability to other flows featuring dense particle suspensions should be investigated.

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Chapter 7

Paper I

I

Numerical simulation of particle jet formation induced by shock wave acceleration in a Hele-Shaw cell

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Abstract The formation of jets from a shock-accelerated cylindrical shell of particles, confined in a Hele-Shaw cell, is studied by means of numerical simulation. A number of simulations have been performed, systematically varying the coupling between the gas and solid phases in an effort to identify the primary mechanism(s) responsible for jet formation. We find that coupling through drag is sufficient for the formation of jets. Including the effect of particle volume fraction and particle collisions did not alter the general behaviour, but had some influence on the length, spacing and number of jets. Furthermore, we find that the jet selection process starts early in the dispersal process, during the initial expansion of the particle layer.

Keywords Impulsive dispersion · Granular media · Numerical simulation · Particle jetting · Dispersed flow

1 Introduction

The use of explosives to disperse granular media typically results in the formation of coherent structures in the form

of jets or fingers. The physical mechanism responsible for the formation of such jets is not well understood and has been the subject of several investigations, e.g., [11, 13, 25, 31]. Through these studies some trends have been discovered. Firstly, the number of jets generated depends on the mass ratio between the explosive and the dispersed material [12]. Secondly, there appears to be a minimal layer velocity below which jetting does not occur [24]. Another interesting experimental observation is that most, but not all, configurations result in jet formation, as demonstrated in the work by Loiseau et al. [17]. Their experimental study of the dispersal of a thin layer of hardened steel particles did not display the jetting behaviour, while similar masses of weaker materials like iron and brass did form jets. Xu et al. [30] suggested that the dominant mechanisms for jet formation are formation of particle clusters due to microscopic gas jets between particles at the inner layer of the particle bed and inelastic collisions between the particles. However, in Milne et al. [20] it is stated that the fragment size appears to be linked to the macroscopic flow and bulk material properties. They also claim that the number of fragments has only a weak dependence on original grain size.

According to [21], the growth rate of the jets formed during explosive dispersal of liquids is significantly larger than those of the classical gas-dynamic Rayleigh–Taylor (RT)/Richtmyer–Meshkov (RM) instabilities which one initially might suspect as a generating mechanism. Dispersed flows with varying particle concentrations display instabilities with much of the same behaviour as RT and RM instabilities [23], but there are also important differences between these instabilities due to particle inertia, such as faster breakdown of RT bubbles [7] and less deposition of circulation on the interface [18]. Particle-induced RT and RM instabilities may not be the sole sources of the particle jetting during explosive particle dispersal, but they are present in the problem under

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Fig. 1 Sketch of the problem set-up. A Hele-Shaw cell, consisting of two horizontal and parallel plates separated by a 4-mm gap, is located above a shock tube. The shock tube is entering the Hele-Shaw cell from below. Around the shock tube exit there is a cylinder shell of solid particles, as indicated by the grey ring. The proportions in the figure are altered for illustration purposes

investigation, which involves the much lower pressures in a gas shock tube, and likely play some role in the development of particle jets.

Recently, experiments on a geometrically quasi-two-dimensional model problem were considered by Rodriguez et al. [26–28]. The experiments consisted of the radial dispersion of a cylindrical shell of particles in a Hele-Shaw cell, using a shock tube, fitted in the centre of the particle shell, as a source for the impulse (see Fig. 1). Although not in the same gas- and thermodynamic regime as explosive dispersal in terms of Mach number, etc., this configuration also results in the formation of jets, making it a viable experimental candidate as a simplified analogue to explosive dispersal.

Additionally, the geometrically quasi-two-dimensional set-up makes it possible to observe the formation of the jets in greater detail than its explosive counterparts, making it easier to analyse.

In the present study, we investigate the formation of particle jets in a Hele-Shaw cell, similar to that of Rodriguez et al., by means of numerical simulation. It is an extension of the work presented in [22]. We have undertaken a number of simulations where the coupling between the gas and solid phases has been systematically varied in an effort to identify the primary mechanism(s) responsible for jet formation. Most of the simulations employ an Euler–Lagrange-type formulation where the gas phase is represented as a continuum, while the particles are modelled as Lagrangian parcels. The results from these computations are also compared to those obtained using an Euler–Euler-type simulation where the solid particles are modelled as a continuum.

We emphasize here that even though the motivation for this work comes from explosive dispersal, the results obtained here are in a situation where the overpressure is orders of magnitude smaller than in the explosive case. Care must therefore be taken before extrapolating these results to the explosive regime as there are likely effects in the explosive regime that are not captured here.

The remainder of this article is structured as follows: in Sect. 2, the governing equations are presented. In Sect. 3 the numerical method is described, and Sect. 4 contains a description of the problem set-up. Section 5 contains the base flow results, while a description of the circumferential variations can be found in Sect. 6. Finally, the results are summarized along with concluding remarks in Sect. 7.

2 Governing equations

2.1 Gas phase

The equations governing the motion of the gas phase are the volume-averaged compressible Navier–Stokes equations, which are derived in [9]. These are

$$\partial_t \alpha \langle \rho \rangle + \nabla \cdot (\alpha \langle \rho \rangle \tilde{\mathbf{u}}) = 0, \quad (1)$$

$$\begin{aligned} \partial_t \alpha \langle \rho \rangle \tilde{\mathbf{u}} + \nabla \cdot (\alpha \langle \rho \rangle \tilde{\mathbf{u}} \tilde{\mathbf{u}} + \langle p \rangle \mathbf{I}) &= \nabla \cdot \left[\mu (\nabla \tilde{\mathbf{u}} + \nabla \tilde{\mathbf{u}}^T) \right] \\ &- \nabla \cdot \boldsymbol{\tau} - \frac{1}{V} \sum_i \frac{1}{8} \rho C_d \pi D_p^2 |\tilde{\mathbf{u}} - \mathbf{v}_i| (\tilde{\mathbf{u}} - \mathbf{v}_i), \end{aligned} \quad (2)$$

$$\begin{aligned} \partial_t \alpha \tilde{E} + \nabla \cdot (\alpha \tilde{\mathbf{u}} \tilde{E} + \alpha \tilde{\mathbf{u}} \langle p \rangle) &= \nabla \cdot ((1 - \alpha) \langle \mathbf{v} \rangle \langle p \rangle) \\ &+ \nabla \cdot \left[\alpha \mu (\nabla \tilde{\mathbf{u}} + \nabla \tilde{\mathbf{u}}^T) \cdot \tilde{\mathbf{u}} \right] - \nabla \cdot (k \nabla T) - \xi \\ &- \frac{1}{V} \sum_i \frac{1}{8} \rho C_d \pi D_p^2 |\tilde{\mathbf{u}} - \mathbf{v}_i| (\tilde{\mathbf{u}} - \mathbf{v}_i) \cdot \mathbf{v}_i, \end{aligned} \quad (3)$$

where $\langle \cdot \rangle$ denotes a phase-averaged variable, $\tilde{\cdot} = \langle \rho \cdot \rangle / \langle \rho \rangle$ denotes a Favre-averaged quantity, α is the gas-phase volume fraction, ρ is the mass density of the gas, $\mathbf{u}$ is the gas velocity vector, p is the pressure, μ is the dynamic viscosity, $\boldsymbol{\tau}$ is the sub-grid stress tensor, $E = \rho e + 0.5 \rho \tilde{\mathbf{u}} \cdot \tilde{\mathbf{u}}$ is the total energy, where e is the internal energy, $\mathbf{v}_i$ is the velocity of particle i , V is the averaging volume, k is the heat conductance of the gas, T is the gas temperature, and ξ contains any sub-grid terms in (3). Quantities related to the viscous drag law are defined in Sect. 2.2. The particle volume fraction is capped at 0.7, and thus, the gas-phase volume fraction has a lower bound of 0.3. Thermal coupling between the gas and particles and buoyant forces on the particles have been omitted. The phase average of a variable is defined as the average of that variable over the volume of that phase and is related to the volume average by $\langle \cdot \rangle = \tilde{\cdot} / V$, where $\tilde{\cdot}$ denotes a volume-averaged variable. The $\tilde{\cdot}$ and $\langle \cdot \rangle$ notations are omitted later for notational convenience.

We assume that the gas phase can be described by the ideal gas equation of state, which is

$$\rho e = p / (\gamma - 1), \quad (4)$$

where γ is the adiabatic index. Furthermore, the temperature dependence of the gas viscosity is neglected. In this work,

we also examine one simulation with two different gases, and for this purpose we employ the five-equation model of [2].

The growth of jets is initiated by growth of perturbations around radial base profiles. The growth of the perturbations is accompanied by increase in vorticity, which is governed by

$$\begin{aligned} \partial_t \boldsymbol{\omega} = & -\mathbf{u} \cdot \nabla \boldsymbol{\omega} - \boldsymbol{\omega} \nabla \cdot \mathbf{u} + \boldsymbol{\omega} \cdot \nabla \mathbf{u} \\ & - \frac{1}{(\alpha\rho)^2} \nabla p \times \nabla (\alpha\rho) - \frac{1}{(\alpha\rho)^2} \mathbf{F} \times \nabla (\alpha\rho) \\ & - \frac{1}{\alpha\rho} \nabla \times \mathbf{F} + \nu \nabla^2 \boldsymbol{\omega} + \boldsymbol{\psi}, \end{aligned} \quad (5)$$

where $\boldsymbol{\omega}$ is the vorticity, ν is the kinematic viscosity, $\mathbf{F}$ is the sum in (2), and $\boldsymbol{\psi}$ contains all sub-grid terms. Note that the volume fraction appears in the baroclinic torque term. Compared to the standard vorticity equation, there are additional sources of vorticity due to misalignment of the drag force and the gradient of the volume-averaged gas density, i.e., term five on the right-hand side, as well as the possibility of drag-induced torque, term six.

2.2 Particles

The equations governing the motion of the particles are

$$d_t \mathbf{X} = \mathbf{v}, \quad (6)$$

$$\begin{aligned} m_p d_t \mathbf{v} = & \frac{1}{8} \rho C_d \pi D_p^2 |\mathbf{u} - \mathbf{v}| (\mathbf{u} - \mathbf{v}) \\ & - (\nabla \tau_p) m_p / (\alpha_p \rho_p), \end{aligned} \quad (7)$$

where $\mathbf{X}$ is the particle position, m_p is the particle mass, $\mathbf{v}$ is the particle velocity vector, C_d is the drag coefficient, D_p is the particle diameter, τ_p is the inter-particle stress, and $\alpha_p = 1 - \alpha$ is the particle volume fraction.

We use two different particle drag laws in this work. The first drag law is that of [8] (as cited in [9]), where the drag coefficient is

$$C_d = 24f/\text{Re}_p, \quad (8)$$

where

$$f = 1 + 0.15\text{Re}_p^{0.687} + 0.0175 \left(1 + 4.25 \times 10^4 \text{Re}_p^{-1.16} \right)^{-1} \quad (9)$$

is the drag factor, and $\text{Re}_p = \rho_g D_p |\mathbf{u} - \mathbf{v}| / \mu$ is the particle Reynolds number. The second drag law [14] includes a correction for densely packed particles. Here, the drag factor is given by

$$\begin{aligned} f = & \left(1 + 0.15\text{Re}_p^{0.687} \alpha^{-1.8} \right), \quad \text{Re}_p < 1000, \\ f = & 0.44\alpha^{-1.8}, \quad \text{Re}_p \geq 1000. \end{aligned} \quad (10)$$

The particle Reynolds numbers encountered in this problem are typically in the range $\text{Re}_p \in [0, 100]$ which is within the range where these drag laws are calibrated. More sophisticated drag laws are available in the literature, see e.g., [16], but these are not considered here. The particle collision model used in this work was proposed by [15], where the inter-particle stress is modelled as

$$\tau_p = P_s \alpha_p^\beta / (\alpha_c - \alpha_p), \quad (11)$$

where P_s is a constant defining the scale of the particle stress, β is a constant, and α_c is the particle close-packing limit. For the constants, we use the values $P_s = 10 \text{ Pa}$, $\beta = 3.0$, and $\alpha_c = 0.73$.

We list here the equations governing the motion of the effective fields α_p and $\langle \mathbf{v} \rangle$, where $\langle \mathbf{v} \rangle$ is the mass-averaged particle velocity within the control volume, which are needed in the characteristic analysis in the next section. The particle volume fraction is governed by

$$\partial_t (\alpha_p) + \nabla \cdot (\alpha_p \langle \mathbf{v} \rangle) = 0. \quad (12)$$

The mass-averaged particle velocity is governed by

$$\partial_t (\alpha_p \langle \mathbf{v} \rangle) + \nabla \cdot (\alpha_p \langle \mathbf{v} \rangle \langle \mathbf{v} \rangle) = \frac{F}{\rho_p} - \frac{\nabla \cdot \tau_p}{\rho_p} - \nabla \cdot \boldsymbol{\theta}, \quad (13)$$

where ρ_p is the particle mass density and $\boldsymbol{\theta} = \alpha_p \langle \mathbf{v} \rangle \langle \mathbf{w} \rangle - \alpha_p \langle \mathbf{v} \rangle \langle \mathbf{v} \rangle$ is a “particle Reynolds stress”, and $\langle \mathbf{w} \rangle$ is the momentum-averaged particle velocity. Note that the Lagrangian formulation of the particle equations provides exact closure of the particle Reynolds stress in the limit where each parcel represents one particle.

2.3 Characteristic analysis

The characteristics of the system of (1)–(3) and (12)–(13) can be found by examining the Jacobian of the equations in primitive form. The following analysis is written in one-dimension for compactness. Using the primitive variables $(\rho, u, p, \alpha, \langle v \rangle)$ we find the Jacobian

$$\mathbf{J} = \begin{bmatrix} u & \rho & 0 & \frac{\rho}{\alpha} (u - \langle v \rangle) & \frac{\rho}{\alpha} (1 - \alpha) \\ 0 & u & (\alpha\rho)^{-1} & 0 & 0 \\ 0 & \rho c^2 & u - A & \rho c^2 \frac{(u - \langle v \rangle)}{\alpha} & \rho c^2 \frac{(1 - \alpha)}{\alpha} \\ 0 & 0 & 0 & \langle v \rangle & -(1 - \alpha) \\ 0 & 0 & 0 & -B & \langle v \rangle \end{bmatrix}, \quad (14)$$

where c is the sound speed in the gas,

$$A = \left(\frac{\partial p}{\partial e} \right)_\rho \frac{(u - \langle v \rangle)(1 - \alpha)}{\alpha \rho}, \quad (15)$$

and

$$B = \frac{P_s \alpha_p^\beta}{\rho_p (\alpha_c - \alpha_p)^2} \left[\beta \left(\frac{\alpha_c}{\alpha_p} - 1 \right) + 1 \right]. \quad (16)$$

Here, we have assumed that the buoyant force on the particles is negligible relative to the viscous forces acting on the particles. This was already assumed in (7) and is reasonable for small particles. The eigenvalues of $\mathbf{J}$ are

$$\begin{aligned} \lambda_1 &= u, \\ \lambda_{2,3} &= u - \frac{A \pm \sqrt{A^2 + 4c^2/\alpha}}{2}, \\ \lambda_{4,5} &= \langle v \rangle \pm \sqrt{\alpha_p B}. \end{aligned} \quad (17)$$

The eigenvalues are real since B is positive for $\alpha_p < \alpha_c$ and the system is hyperbolic. However, the eigenvalues deviate from the pure gas eigenvalues when the particle volume fraction and relative phase velocities become significant. The deviation has two parts, one which is proportional to the relative phase velocities and one which is proportional to the particle volume fraction. The term A does not contribute much to the wave speed for the problem considered here, since the relative phase velocities are small. The second correction, due to volume fraction, can contribute up to a factor $1/\sqrt{0.3}$ to the effective sound speed. We note here that the inclusion of buoyant forces on the particles eliminates the term A from the Jacobian, but makes its eigenvalues imaginary.

3 Numerical method

The numerical method used for the gas phase is a control volume-based, low dissipation and dispersion, finite volume method developed for large eddy simulations on unstructured grids [6]. The Harten–Lax–van Leer–Contact (HLLC) Riemann solver [29] is used to compute fluxes between neighbouring cells, and the solution is advanced in time by a third-order explicit Runge–Kutta scheme. The HLLC Riemann solver, with gas volume fraction included, gives the convective flux as

$$\mathcal{F} = \begin{cases} \mathbf{F}_L, & \text{if } 0 \leq S_L \\ \mathbf{F}_L + S_L(\mathbf{U}_{*L} - \mathbf{U}_L), & \text{if } S_L \leq 0 \leq S_* \\ \mathbf{F}_R + S_R(\mathbf{U}_{*R} - \mathbf{U}_R), & \text{if } S_* \leq 0 \leq S_R \\ \mathbf{F}_R, & \text{if } S_R \leq 0 \end{cases}, \quad (18)$$

where subscripts denote the state from which a quantity is computed (either left or right state), $\mathbf{F}$ is the convective flux, S is the largest wave speed, S_* is the middle wave speed, $\mathbf{U} = (\alpha \rho, \alpha \rho u_1, \alpha \rho u_2, \alpha \rho u_3, \alpha E)^T$ is the vector of state variables, and $\mathbf{U}_*$ is the vector of intermediate states in the HLLC solver. To obtain a similar treatment of the pressure in both the momentum and energy equations we rewrite the pressure term in the momentum equation as $\nabla p = \nabla(\alpha p) + \nabla([1 - \alpha]p)$, in which the latter is treated as a source term. Rewriting the momentum equation this way separates the fluxes due to gas–gas interaction and gas–particle interaction. This splitting is similar to the approach used in [1,4], but we do not explicitly consider the gas–solid Riemann problem. The equation set can now be written as $\partial_t \mathbf{U} + \nabla \cdot \mathbf{F} = \mathbf{D}$, where

$$\mathbf{F} = \begin{pmatrix} \alpha \rho \mathbf{u} \\ \alpha \rho \mathbf{u} \mathbf{u} + \alpha p \\ \alpha \rho E \mathbf{u} + \alpha p \mathbf{u} \end{pmatrix}, \quad (19)$$

and $\mathbf{D}$ contains the right-hand side of (1)–(3) and the term $-\nabla([1 - \alpha]p)$ in the momentum equation. We apply the HLLC solver to solve the equation $\partial_t \mathbf{U} + \nabla \cdot \mathbf{F} = 0$, which has characteristic wave speeds $\lambda_1 = u$, $\lambda_{2,3} = u \pm c$. The term $\mathbf{D}$ is then computed in a way consistent with the HLLC solver by evaluating it with the same pressure and velocity as used in the HLLC flux. The intermediate state used in the HLLC solver is

$$\mathbf{U}_{*K} = \alpha_K \frac{S_K - q_K}{S_K - S_*} \begin{pmatrix} \rho_K \\ \rho_K \mathbf{u}_K + \left(\frac{p_* - p_K}{S_K - q_K} \right) \mathbf{n} \\ E_K + \frac{p_* S_* - p_K q_K}{\alpha_K (S_K - q_K)} \end{pmatrix}, \quad (20)$$

where $K = L, R$ and $\mathbf{n}$ is the face-normal unit vector, whereas $q = \mathbf{u} \cdot \mathbf{n}$ is the face-normal velocity and p_* is the same intermediate state pressure as in the original HLLC solver. We use the wave-speed estimates recommended by Batten et al. [5]:

$$\begin{aligned} S_L &= \min[q_L - c_L, \tilde{q} - \tilde{c}], \\ S_R &= \max[q_R + c_R, \tilde{q} + \tilde{c}], \end{aligned} \quad (21)$$

where $\tilde{\cdot}$ denotes Roe-averaged variables.

The source term $\nabla \cdot ((1 - \alpha) \langle \mathbf{v} \rangle \langle p \rangle)$ is computed as a surface integral, and the quantity $\langle \mathbf{v} \rangle$ is computed from the particles crossing each face. On each face this term is computed as

$$\begin{aligned} (1 - \alpha_L) \langle \mathbf{v} \rangle \cdot \mathbf{n} p_*, & \text{if } \langle \mathbf{v} \rangle \cdot \mathbf{n} > 0, \\ 0, & \text{if } \langle \mathbf{v} \rangle = 0, \\ (1 - \alpha_R) \langle \mathbf{v} \rangle \cdot \mathbf{n} p_*, & \text{if } \langle \mathbf{v} \rangle \cdot \mathbf{n} < 0. \end{aligned} \quad (22)$$

Table 1 Description of the cases examined in this study

Case	Type	Coupling
I	Standard	One-way through drag
II	Standard	Two-way through drag
IIIa	Standard	Two-way drag and volume
IIIb	Standard	Two-way drag and volume
IIIc	Standard	Two-way drag and volume
IIId	Standard	Two-way drag and volume
IV	Standard	Two-way drag and volume
V	Standard	Two-way drag and volume
VI	Continuum	Tracer particles

The momentum and energy coupling between the particles and the gas is computed by a zeroth-order particle-in-cell method. See [10] for an evaluation of methods for computing particle-based quantities.

4 Problem set-up

We consider the radial dispersion of a cylinder shell of particles by a shock wave in a pseudo-two-dimensional geometry. The particle cylinder shell is located in the centre of a Hele-Shaw cell. A shock tube is fitted in the centre of the cell through one of the walls, and its diameter corresponds to the inner diameter of the cylinder shell. Figure 1 shows a sketch of the geometry. The solid particles have an average particle diameter of $10 \pm 1 \mu\text{m}$ and a mass density of 1530 kg/m^3 , corresponding to the values for the flour that was used in the experiments. We further assume that the particles are spherical.

The cases considered in this study are summarized in Table 1. Each case has a different coupling between the gas and particles, with the exception of cases IIIa to IIId, which vary only in initial conditions. There are two different types of set-ups, which we label as the standard type and the continuum type. The standard type refers to the cases where the particles are modelled using a Lagrangian approach, and the continuum type refers to the case where the particle cloud is modelled as a continuum. The difference between cases IIIa and IV is the drag law used, which in case IV is given by (10) and this case is the only one that uses this drag law. Case V includes the particle-collision model. In order to obtain a one-to-one comparison with the other cases, we add tracer particles to the continuum case.

4.1 Computational set-up

We use a computational domain that represents one quadrant of the cylindrically symmetric geometry. The full

length of the shock tube is included in the simulation. The geometry can be split into two parts, the Hele-Shaw cell and the shock tube. The dimensions of the Hele-Shaw cell are $(L_r, \Delta\theta, L_z) = (0.65 \text{ m}, \pi/2, 0.004 \text{ m})$, and the dimensions of the shock tube are $(L_r, \Delta\theta, L_z) = (0.016 \text{ m}, \pi/2, 1.155 \text{ m})$. The computational domain is discretized into a total of 2.9×10^6 control volumes. Within the Hele-Shaw cell the mesh is approximately aligned with the radial and circumferential directions. The number of control volumes is $(N_r, N_\theta, N_z) = (400, 90, 20)$ in the radial, circumferential and vertical directions, respectively, in the Hele-Shaw cell, and in the shock tube we use $(N_r, N_\theta, N_z) = (69, 90, 350)$. The particles are represented by computational particle packets where each packet represents 3864 real particles. In case IIId we use twice as many computational particles; thus, each computational particle represents 1932 real particles. The total number of particles corresponds to 3.9×10^9 real particles. The boundary conditions used are slip conditions on all boundaries, except on the outer boundary of the Hele-Shaw cell, where a zero-gradient boundary condition is used. We use no sub-grid scale model in this work.

4.2 Initial conditions

The initial conditions of cases I–IIIa, IIId and IV–VI consist of a $M = 1.26$ shock wave travelling through the shock tube. In cases IIIb and IIIc, the shock wave has a Mach number of 1.32 and 1.39, respectively. The state of the ambient gas in front of the shock corresponds to air at atmospheric pressure and room temperature. At $t = 0$, the shock wave is located at $z = -0.03 \text{ m}$. To approximate the experimental conditions we have first computed the state in the shock tube by a 1D simulation where the initial conditions are a high-pressure region (driver section) and a low-pressure region (driven section), similar to the experiments. That being said, this study is not an attempt to replicate the experimental results (since sufficient details for a complete replication are not available), but rather an attempt to identify the physical mechanisms involved in the formation of particle jets.

The particles are initialized by drawing random positions within the designated volume of the cylinder shell, until the total volume of the particles is equal to the volume of the cylinder shell. Because of the large number of particles used, the volume fraction variation within the shell is less than 2%, and even smaller in case IIId. The particles are initially at rest. For the simulation with the continuum approximation, we assume that the entire cylinder shell is filled with the “particle–gas” and that this gas is at atmospheric pressure, room temperature and has a density of 1530 kg/m^3 . We superimpose density perturbations of 2% with a white-noise spectrum to mimic the perturbations obtained with the particles.

5 Base flow

The primary gas-dynamic features are the shocks originating from the shock tube. At $t = 0$, the primary shock is located at $z = -0.03$ m and travelling upwards. As the shock exits the tube, the gas and particles in the Hele-Shaw cell are accelerated outwards. The shock reflects from the upper horizontal wall and starts propagating back down into the shock tube. It is again reflected from the bottom and starts moving upwards. This process repeats once more in the time interval considered here. As the first shock travels through the particle cloud, the particles accelerate outwards. The particle cloud is first compacted radially, followed by an expansion before the second shock impacts on the cloud, as shown in Fig. 2. Similarly to the case of explosive dispersal, there are multiple shock waves passing through the layer of particles. However, the principal mechanism for generating these shock waves is different, and they are significantly weaker. Whereas in the explosive case, the subsequent shock wave(s) is due to over-expansion of the detonation products, here it is due to reflection of the primary shock wave.

The radial position of the centre of mass of the particle clouds for the different cases is shown in Fig. 3. Initially, the particles are accelerated outwards and the acceleration is similar for all cases with the same shock wave Mach number, except case I. The acceleration phase lasts up to about $t = 2.5$ ms. Thereafter the particle cloud expands. On average the particles move faster than the gas and are therefore decelerated. The second shock passes through the particles at about 6 ms, initiating a new acceleration phase that lasts up to approximately 7.5 ms. After 9 ms the particle cloud mass centre of case II falls behind the mass centres of the other cases. This is likely due to the increased permeability of the particle cloud, compared to the other cases, which reduces

Fig. 2 Locations of shocks (dashed lines) and cloud boundaries (solid lines) over time for case IIIa. The cloud boundaries are defined as enclosing 90% of the particles

Fig. 3 Radial position of the centre of mass of the particle cloud over time for the different cases

the period of positive radial impulse. In addition, we observe that cases IIIa and IIId differ quite a bit during the later stages of the dispersal process. This indicates that the processes are sensitive to initial conditions, which suggests the use of an ensemble average when analysing this problem. However, this is outside the scope of the current study.

While the test case was designed to be geometrically two-dimensional in terms of particle dispersion, the sharp corner at the inlet generates significant three-dimensional variations in the gas. To assess this effect we consider the circumferentially averaged radial gas velocity and particle positions. The resulting fields at $t = 1.25, 5$ and 15 ms, are found in Fig. 4. Clearly, significant variations are present in both fields. This is particularly clear at late times where the particles have separated into layers near the bottom and top of the cell, with the majority of the particles located near the bottom. This observation is important for interpreting the results in the next section, which discusses the circumferential variations, as particle jets may lie in different layers. Note that the accumulation of particles near the bottom is not due to gravity as the gravitational force is not included in this study. Interestingly, we can observe from Fig. 4c that the radial gas velocity exhibits a peak that coincides with the maximum particle concentration near the lower horizontal wall of the cell. At this position, the particle momentum exceeds that of the gas and drives it outwards, switching roles compared to the initial acceleration phase.

6 Development of circumferential inhomogeneities

The average behaviour of the particle cloud was described in the previous section. However, the simulations also display significant circumferential variations appearing at different stages of the dispersal process. Figure 5 shows scatter plots of

Fig. 4 Particle positions and radial gas velocity contours at three points in time for case IIIa. Dashed lines indicate negative contours

the six cases with initial shock wave Mach number 1.26 at a late stage in the dispersal process. Significant circumferential inhomogeneities are clearly visible in all cases. Case I is, as expected, very different from the other cases, but even in this case we observe circumferential variations. This shows that the flow configuration is susceptible to instabilities even without particles and demonstrates that the timescale required for the gas-dynamic instabilities to develop is comparable to the timescales associated with the dispersion. In Case I, these instabilities are artificial, i.e., results of numerical errors and grid imperfections, since this configuration is axisymmetric. At $t = 1.25$ ms, it can be observed that the dominant circumferential wavelength of these instabilities is comparable to the sizes of the jets observed in the other cases. While we do expect some grid dependence in the results of cases II–VI, mostly due to the way α_p and the particle–gas interaction terms in the gas equations are computed, the variation within cases II–VI cannot be explained by grid effects.

Cases II–V all show large outer jets, with some variation in the number, spacing and length of jets. The difference between cases I and II is that the gas loses momentum and

Fig. 5 Scatter plots of the different cases at $t = 1.25$ ms for case I and at $t = 15$ ms cases II–VI

energy by accelerating the particles, and this appears to be sufficient for late-time jets to develop. Interestingly, the continuum model (case VI) does not display a similar jetting behaviour at this late stage even though the movement of the “particle” mass centre was similar to cases IIIa, IV and V. This indicates that the presently chosen continuum model is insufficient for predicting particle jetting, but the average “particle” movement is captured by the model. This does not mean that continuum models per se cannot predict particle jetting. The present continuum model treats the particles as a dense gas where no relative phase velocity is possible and thus circumferential variations will only appear through classical gas-dynamic instabilities. Relative phase velocity may be a necessary component in the particle jet formation, and therefore, it is not surprising that the radial and circumferential particle distributions are not well reproduced. Examples of continuum models more suitable for the present problem that include relative phase velocities are models based

on the Baer–Nunziato equations [3] and variations thereof, e.g., [19]. Investigations on the use of these models are postponed to future studies.

The process leading up to the generation of the late-time outer jets is further discussed below. The discussion has been divided into distinct flow phases, where different processes take place, as will be shown. We observe a similar sequence of events as Rodriguez et al. reported in their experimental work, that is the formation of inner jets, short-wavelength outer jets and late-time large outer jets.

6.1 Early time, $t \lesssim 2.5$ ms

Inner circumferential inhomogeneities appear during the initial acceleration of the particle cloud. They occur in all the cases with two-way coupling, but not in case VI. Figure 6 shows scatter plots of cases IIIa and VI at $t = 1.0$ ms where inner structures have developed in case IIIa. These structures quickly attain a length comparable to the thickness of the particle layer, and their circumferential extent is very limited. As is evident from the figure, case IIIa also has much larger inhomogeneities throughout the particle cloud than case VI. The circumferential fluctuations of particle distribution are negatively correlated with fluctuations in the radial gas velocity, signifying that vorticity in the gas is present around these structures. Because the inner structures appear in case II, which does not include α in the gas-phase equations, the simplified term five, $(\mathbf{F} \times \nabla \rho) / \rho$, and term six, $(\nabla \times \mathbf{F}) / \rho$, of (5), are likely important for the initial generation of the inner structures. However, once the perturbations have formed, the dominant term in (5) is the standard baroclinic torque term.

6.2 Intermediate time, $2.5 \lesssim t \lesssim 6.0$ ms

After the initial acceleration of the particle cloud and the generation of inner structures, the particles enter a phase where

Fig. 6 Scatter plots of cases III and VI at $t = 1.0$ ms. Case IIIa shows significant circumferential variations in the inner part of the particle cloud, while case VI only has very small-amplitude perturbations on the inner interface

Fig. 7 Scatter plots of cases II–V at $t = 5.0$ ms, where short-wavelength outer jets have appeared

they move as fast, or faster, than the gas. As noted earlier, the particles start decelerating at about 2.5 ms. At this point, outer short-wavelength jets appear, which is consistent with a Rayleigh–Taylor-like instability originating from term five in (5). Slightly later, the pressure gradient also changes sign, making the outer edge of the particle cloud susceptible to classical Rayleigh–Taylor instabilities. The structures generated in this way continue to develop until the time of the secondary shock. Although structurally similar, some variation exists between cases II–V, as displayed in Fig. 7. Case II has a more diffuse outer interface, while IIIa and IV are qualitatively similar. Case V appears to have generated slightly longer outer structures with shorter wavelengths. In addition, radially aligned structures appear within the central area of the particle cloud. These are most visible in Fig. 7b, c.

6.3 Late time, $t \gtrsim 6.0$ ms

In the cases with initial shock wave Mach number 1.26 the late-time jets appear after the passage of the secondary shock. Again the whole particle cloud is accelerated, but some particles attain significantly higher velocities than the average and move out in front of the particle cloud to form the outer late-time jets. These jets are not simply the radially aligned structures formed during the intermediate time, but structures generated by the interaction of the secondary shock with the particle cloud and the gas within it. This behaviour is consistent throughout all simulations with initial shock wave Mach number 1.26 and two-way coupling between the

Fig. 8 Contours of particle volume fraction at $t = 11.25$ ms in case IIIa with contour levels adjusted to emphasize the particle jets. The dashed lines indicate the jets (black) and voids (white) used to compute the profiles shown in Figs. 9 and 10. Dark blue and white contours are areas of low and high particle volume fraction, respectively

phases. However, the length, spacing and particle concentration of the jets vary slightly. In the cases with higher shock wave Mach numbers, the outer particle jets form prior to the secondary shock passage. In these cases, the effect of geometric expansion is stronger since the initial acceleration of the particles is higher, which appears to lead to a quicker formation of large outer jets. Additionally, the effect of the secondary shock on the particle jets is less significant and decreasing with stronger initial shock wave Mach number.

To investigate the development of the late-time jets, we have identified the circumferential position of the jets by visual inspection and computed the averaged radial profiles of pressure, density, radial gas velocity, particle volume fraction and average particle velocity along bands from the origin through the jets. Figure 8 shows the estimated positions of the jets and voids for case IIIa. These have subsequently been compared with the average profiles and the profiles through the voids between the jets. The quantities that show the largest difference between the three profiles are particle volume fraction and radial gas velocity, which are shown for case IIIa in Figs. 9 and 10, respectively. The volume fraction profiles are initially very similar, but differences are visible at $t = 3$ ms, which is during the expansion of the particle layer after the initial compaction.

Figure 10 shows the radial gas velocity profiles at the same times as the particle volume fraction profiles in Fig. 9. Even the earliest profile displayed in Fig. 10 shows qualitative differences between the jet and void profiles. This bears resemblance to observations made by Milne et al. [21] in the explosive regime that the jet generation process starts very early in the dispersal process. The jet profiles are in a state of expansion relative to the mean profiles, where gas closer to the origin is moving slower than gas further out. The void

Fig. 9 Normalized particle volume fraction averaged over jets (solid lines), voids (dashed lines) and full circumferential average (dotted lines) in case IIIa, for times (from left to right): $t = 1.5$ ms, $t = 3$ ms, $t = 5$ ms, $t = 8$ ms, and $t = 11$ ms

Fig. 10 Difference between the circumferentially averaged radial gas velocity and jet averaged (solid lines) and void averaged (dashed lines) in case IIIa for times (from top to bottom): $t = 1.5$ ms, $t = 3$ ms, $t = 5$ ms, $t = 8$ ms, and $t = 11$ ms

profiles show the opposite behaviour. This is the case for all the simulations that show jetting behaviour. We observe that the radial gas velocity profiles start to deviate before any differences can be discerned in the volume fraction profiles.

After the outer jets have formed, the outer parts of the velocity profiles show a clear peak for the jets and a trough for the voids. This shape persists for a long time due to energy and momentum transfer through drag on the particles in the jets, which at these times move faster than the gas. The gas velocity in the void profiles in fact becomes negative during the later stages of the dispersal process due to overexpansion of the gas. In the jets, the momentum of the particles continues to drive both the particles and the surrounding gas forward. Since any particle in the void areas is driven inward during this stage, while the particles in the jets continue outwards, the jets stretch and become more and more pronounced.

Fig. 11 Scatter plots of cases IIIa (left), IIIb (middle) and IIIc (right) at the points in time when the particle mass centre is at 23.3 cm, which corresponds to $t = 20$ ms in case IIIa

Cases IIIa, b, c differ in the strength of the initial shock wave, and this significantly affects the number of jets in the simulations. Figure 11 shows scatter plots of these three cases at times when their particle mass centre is at $r = 23.3$ cm, which in case IIIa corresponds to $t = 20$ ms. As mentioned above, in the cases with stronger initial shock waves, the large outer jets form prior to the secondary shock passage, and due to this there appears to be fewer outer jets in cases IIIb, c than in IIIa, although counting the jets is a very approximative procedure. Case IIIc has more outer jets than case IIIb, which is consistent with the trend observed by Rodriguez et al., that stronger initial shock waves lead to a higher number of outer jets. The cases with initial $M = 1.26$ shock waves undergo a different jet generation process, which is likely why they do not fit this trend.

7 Summary and concluding remarks

The formation of jets from a cylindrical shell of particles resulting from shock acceleration has been studied by means of numerical simulation. We have performed a number of simulations where the coupling between the gas and solid phases has been systematically varied in an effort to identify the primary mechanism(s) responsible for jet formation. The majority of the simulations employed an Euler–Lagrange-type formulation where the gas phase is represented as a continuum, while the particles are modelled as Lagrangian point parcels. The results from these computations were also compared to those obtained using an Euler–Euler-type simulation where the solid particles were modelled as a continuum.

We observed that particle jets formed, even in the simulation where the coupling between the phases was limited to the effect of drag alone. Including the effect of particle volume fraction and particle collisions did not alter the general behaviour, but had some influence on the length, spacing and number of jets. The simulation with the particles represented as a continuum did not show jet formation, and we hypothesize that this is due to the omission of relative phase velocities in the model employed here. It should be noted that, even in

the case where the gas phase was unaffected by the particles, circumferential variations appeared on a timescale comparable to those of the jet formation in the other cases. However, these variations were not of the same nature as those observed in the cases with two-way coupling.

The process leading up to the generation of the late-time outer jets was found to consist of three distinct temporal phases. The first phase consists of an acceleration and compaction of the particle shell. During this phase, we observed generation of structures on the inner interface, which had the same appearance for all the cases with two-way coupling. The second phase starts after the initial acceleration is complete. The particle layer travels outwards, expands and short-wavelength outer jets appear. These jets continue to develop as long as the particles decelerate. We also observed the formation of radially aligned structures extending through the central area of the particle layer during this phase. The final phase consists of the secondary shock and the appearance of large outer jets. In the cases with initial shock wave Mach number 1.26 the large outer jets did not appear until after the secondary shock wave had passed through the particle cloud. In the cases with a stronger initial shock wave the large outer jets appeared prior to the secondary shock acceleration, and this shock had little effect on the particle distribution. The signature of the outer jets was found to be observable in the radial gas velocity profiles prior to any discernible differences in the volume fraction profiles.

In summary, the flow phases observed here correspond well to the sequence of events observed in the experimental work of Rodriguez et al. [26–28]. We found that the formation of the outer jets starts during the initial expansion of the particle layer. However, for the limited range of Mach numbers tested here, we do not see the same trend in number of jets with increasing acceleration. A wider range of Mach numbers should be examined before conclusions are drawn regarding this trend.

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Chapter 8

Paper II

II

Using particle-resolved LES to improve Eulerian-Lagrangian modeling of shock-wave/particle-cloud interactions

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We perform particle resolved large-eddy simulations of a shock wave passing through a random array of stationary particles, varying incident shock Mach number, particle number density and volume fraction. The variation of the mean flow is quantified by fitting the reflected and transmitted shock wave Mach numbers as power laws of these parameters. We analyze the fluctuations from locally volume averaged quantities, and find that the fluctuating kinetic energy is generated primarily by the forces on the particles, and reaches values as high as two thirds of the mean kinetic energy. We use the data from the particle-resolved simulations to close the volume averaged equations, in which the present problem can be formulated in one dimension, and demonstrate that correct drag laws and sub-grid closures are necessary for reliable predictions.

1. Introduction

The interaction of a shock wave with a cloud of particles is a canonical high speed multiphase flow problem that has recently received some attention in both numerical (Houim & Oran 2016) and experimental studies (Ling *et al.* 2012; Theofanous *et al.* 2016). Interactions of this type play an important role in several applications of practical interest, such as explosive blast mitigation, design of combustion systems and atmospheric dissemination of powders and liquids. Resolved simulations of such systems are typically not possible due to the extremely large scale separations. This means that appropriate model equations are needed in order to provide useful predictions.

A particularly challenging case is high-speed particle laden flows with moderate particle volume fractions, i.e. ranging from 1% to 10-15%, as the models employed for either low or high volume fractions are inapplicable, and a model for the intermediate regime has not yet been established. A number of studies have considered either Eulerian-Eulerian models or Eulerian-Lagrangian models for the intermediate regime, but in the past these have had a number of issues. Careful derivation of the model equations are needed to ensure that the equations are well posed (Lhuillier *et al.* 2013; McGrath *et al.* 2016), and additionally the models might be missing important physical processes which are crucial in order to obtain correct particle distributions (Theofanous & Chang 2017).

Recently, a few studies have considered resolved simulations of shock-wave particle-cloud interactions to investigate the particle scale physics in order to improve the simplified models. The Euler equations were employed in resolved simulations with both structured arrays (Mehta *et al.* 2016) and random arrays (Mehta *et al.* 2018). Regele *et al.* (2014) and Hosseinzadeh-Nik *et al.* (2018) considered viscous two-dimensional simulations of shock waves passing through arrays of cylinders and examined the genera-

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tion of vorticity by baroclinic torque and vorticity-dilatation. Theofanous *et al.* (2018) considered an effective boundary method for the Euler equations and obtained particle distribution results in good agreement with experiments. The current work extends the previous studies by performing particle-resolved LES simulations of a shock-wave passing through a particle-cloud and quantifying the particle scale fluctuations. Specifically, we generate datasets containing all the terms in the volume averaged equations of motion, including the equation for the fluctuating kinetic energy. We vary the incident shock wave Mach number, particle number density and volume fraction. The resulting dataset spans a parameter space that has not been explored in any other study. Furthermore, we develop a closure of the volume averaged equations in an attempt to improve the predictive capability of the Eulerian-Lagrangian models for the statistically 1D configuration. The proposed closure consists of an additional equation for the unresolved kinetic energy and a turbulence length scale.

2. Governing equations and computational method

In the following, $\bar{\cdot}$ denotes a volume averaged quantity, $\langle \cdot \rangle$ denotes a phase averaged quantity and $\tilde{\cdot} = \langle \rho \cdot \rangle / \langle \rho \rangle$ denotes a Favre-averaged quantity. The volume and phase average of continuous phase quantities are related by $\alpha \langle \cdot \rangle = \bar{\cdot}$, where α is the continuous phase volume fraction. We utilise both Reynolds and Favre decomposition, where we use the notation $u_i = \langle u \rangle_i + u'_i$ for the former and $u_i = \tilde{u}_i + u''$ for the latter. The Favre- and Reynolds averaged velocities are related by $\tilde{u}_i - \langle u \rangle_i = a_i$, where $a_i = -\langle u'' \rangle_i = \langle \rho' u'_i \rangle / \langle \rho \rangle$ is commonly referred to as the turbulent mass flux. For a description of the volume averaging procedure, including the effects of density fluctuations, consult Schwarzkopf & Horwitz (2015). We use subscripts IS, RS and TS to refer to quantities related to the incident shock, reflected shock and transmitted shock, respectively.

2.1. Governing equations

The resolved simulations in this work are described by the conservation equations for mass, momentum and energy. These are expressed in differential form as

$$\partial_t \rho + \partial_k (\rho u_k) = 0, \quad (2.1)$$

$$\partial_t (\rho u_i) + \partial_k (\rho u_i u_k) = -\partial_i p + \partial_j \sigma_{ij}, \quad (2.2)$$

$$\partial_t (\rho E) + \partial_k (\rho E u_k + p u_k) = \partial_j (\sigma_{ij} u_i) - \partial_k (\lambda \partial_k T), \quad (2.3)$$

where ρ is the mass density, u is the velocity, p is the pressure, $\sigma_{ij} = \partial_j [\mu(\partial_j u_i + \partial_i u_j - 2\partial_k u_k \delta_{ij}/3)]$ is the viscous stress tensor, μ is the dynamic viscosity, $E = \rho e + 0.5 \rho u_k u_k$ is the total energy per unit mass, e is the internal energy per unit mass, λ is the thermal conductivity, and T is the temperature. The system of equations is closed by an ideal gas equation of state, a constant specific heat capacity, a power law dependence of viscosity on temperature with an exponent of 0.76, and a Prandtl number of 0.7. The pre-shock state is air at standard conditions.

In the statistically one-dimensional cases considered here, the application of volume averaging to the governing equations, assuming stationary inert particles, yields

$$\partial_t (\alpha \langle \rho \rangle) + \partial_x (\alpha \langle \rho \rangle \tilde{u}_0) = 0, \quad (2.4)$$

$$\begin{aligned} \partial_t (\alpha \langle \rho \rangle \tilde{u}_0) + \partial_x (\alpha \langle \rho \rangle \tilde{u}_0 \tilde{u}_0 + \alpha \langle p \rangle) &= \partial_x (\alpha \langle \sigma \rangle_{00}) - \partial_x (\alpha \langle \rho \rangle \tilde{R}_{00}) \\ &+ \frac{1}{V} \int_S p n_0 dS - \frac{1}{V} \int_S \sigma_{0k} n_k dS, \end{aligned} \quad (2.5)$$

$$\begin{aligned} \partial_t (\alpha \langle \rho \rangle \tilde{E}) + \partial_x (\alpha \langle \rho \rangle \tilde{E} \tilde{u}_0 + \alpha \langle p \rangle \tilde{u}_0) &= \partial_x (\alpha \langle \sigma_{00} \rangle \tilde{u}_0) - \partial_x (\alpha \langle \lambda \partial_x T \rangle) \\ &- \partial_x (\alpha \langle \rho e'' u''_0 \rangle) - \partial_x (\alpha \langle \rho \rangle \tilde{R}_{00} \tilde{u}_0) + D^u + D^p + D^\mu + D^{ap} + D^{a\mu}. \end{aligned} \quad (2.6)$$

Here, $\tilde{R}_{00} = \widetilde{u''_0 u''_0}$ is a turbulent stress analogous to the classical Reynolds stresses, V denotes the averaging volume, $D^u = -1/2 \partial_x (\alpha \langle \rho u''_i u''_i u''_0 \rangle)$ is the turbulent diffusion, $D^p = -\partial_x (\alpha \langle p' u'_0 \rangle)$ is the pressure diffusion, $D^\mu = \partial_x (\alpha \langle u'_j \sigma'_{j0} \rangle)$ is the viscous diffusion, $D^{ap} = \partial_x (\alpha a_0 \langle p \rangle)$ is the pressure-diffusion effect due to the density-velocity correlation, $D^{a\mu} = -\partial_x (\alpha a_0 \langle \sigma \rangle_{00})$ is the analogous viscous diffusion effect and S denotes the continuous phase boundary. For discussion purposes we also define the mean kinetic energy per unit mass $\tilde{K} = 0.5 \tilde{u}_k \tilde{u}_k$.

The 1D volume averaged model includes a transport equation for the fluctuating kinetic energy, $k = 0.5 \widetilde{u''_k u''_k}$, which is of the form

$$\begin{aligned} \partial_t (\alpha \langle \rho \rangle k) + \partial_x (\alpha \langle \rho \rangle \tilde{u}_0 k) &= D^u + D^p + D^\mu + D^{ap} + D^{a\mu} \\ &+ P + M^p + M^\mu + \Pi - \varepsilon + A + B, \end{aligned} \quad (2.7)$$

where $P = -\alpha \langle \rho \rangle \tilde{R}_{00} \partial_x \tilde{u}_0$ is a production term due to velocity gradients, $\varepsilon = \alpha \langle \sigma'_{jk} \partial_k u'_j \rangle$ is the viscous dissipation, $M^p = -\alpha \langle p \rangle \partial_x a_0$ is a pressure driven production term due to divergence of the density-velocity correlation, $M^\mu = \alpha \langle \sigma \rangle_{00} \partial_x a_0$ is the analogous viscous production term, and $\Pi = \alpha \langle p' \partial_k u'_k \rangle$ is the pressure-dilatation correlation. This leaves

$$A = -\frac{\tilde{u}_0}{V} \int_S p n_k dS, \quad B = \frac{\tilde{u}_0}{V} \int_S \sigma_{jk} n_k dS, \quad (2.8)$$

which are the production due to the pressure and viscous forces on the particles, respectively.

2.2. Computational method

The resolved simulations are performed using the CharLES solver from Cascade Technologies (Bres *et al.* 2018). It is an entropy-stable Voronoi-mesh based solver with third order Runge-Kutta based time-stepping. For the one-dimensional simulations, we use an in-house code that solves Eqs. (2.4)-(2.7). It uses first order reconstruction of primitive variables at the control-volume faces and the fluxes are computed using a Lax-Friedrich type method. Time-stepping is computed by a third order Runge-Kutta scheme. The closure models used for the numerous unclosed terms in Eqs. (2.4)-(2.7) will be discussed below.

3. Resolved simulations

We have simulated the passage of a shock wave through particle clouds of volume fractions in the range $\alpha \in [0.05, 0.1]$. Figure 1 shows a sketch of the problem setup. The particle cloud is located between $x/L = 0$ and $x/L = 1$, where $L = 1.94088 \times 10^{-3}$ m, and the span-wise extent is $L_y = L_z = 2L/3$ for the cases with the largest particle

Case	Ma	r	α_p	$Re_{p,IS}$	n [mm ⁻³]	D_p [μm]	$\Delta p_{RS}/p_{IS}$	$\Delta p_{TS}/p_{atm}$	Ma_{RS}	Ma_{TS}
I	2.2	1.235	0.1	6160	191.0	100	0.9103	2.948	1.334	1.878
II	2.4	1.235	0.1	7091	191.0	100	1.127	3.593	1.402	2.020
III	2.6	1.235	0.1	7927	191.0	100	1.334	4.279	1.464	2.160
IV	2.8	1.235	0.1	8666	191.0	100	1.527	5.053	1.519	2.309
V	3.0	1.235	0.1	9309	191.0	100	1.700	5.900	1.567	2.461
VI	2.6	1.445	0.1	6292	382.0	79.4	1.365	3.881	1.473	2.080
VII	2.6	1.726	0.1	4994	763.9	63.0	1.396	3.582	1.482	2.018
VIII	2.6	1.903	0.075	4537	763.9	57.2	1.313	3.957	1.458	2.096
IX	2.6	2.180	0.05	3964	763.9	50	1.160	4.486	1.412	2.201
X	2.2	2.097	0.1	3080	1528	50	0.9908	2.261	1.360	1.714
XI	2.6	2.097	0.1	3964	1528	50	1.429	3.313	1.492	1.960
XII	3.0	2.097	0.1	4654	1528	50	1.803	4.669	1.596	2.236

TABLE 1. The different simulations considered in this study and key parameters. $Re_{p,IS}$ is the particle Reynolds number based on post incident shock values, and n is the number density.

diameters. We keep the ratio of span-wise extent to particle diameter constant for all the simulations. The position of the spheres are drawn randomly, with a minimum distance between the sphere centers of $1.5 D_p$ and a minimum distance between the spheres and the boundaries of $D_p/20$. We use body fitted structured meshes around each sphere extending $D_p/5$ out from the particle surface. These body fitted meshes have 10 points in the sphere normal direction with a growth ratio of approximately 1.1. The rest of the computational mesh is a Voronoi mesh with approximately uniform density matching the outer cell dimensions of the body fitted meshes. The overall mesh consists of 50-70 million cells depending on the number of particles involved. No-slip boundary conditions are applied on the particles and slip elsewhere. A grid-sensitivity test was conducted with twice and half the number of points for $Ma = 3$, $\alpha_p = 0.1$ and $D_p = 100 \mu m$, and the results were not found to be grid-sensitive within this range.

The statistics of the flow are quantified by computing a moving volume average. The averaging volume extends $\sqrt[3]{4}D_{p,max}$ in the streamwise direction and span both lateral directions, where $D_{p,max}$ is the largest particle diameter considered in this study. This gives a minimum of 50 particles per averaging volume.

The general flow structure is the same for all cases considered. Figure 2 shows the position of the incident, transmitted and reflected shock waves, upstream and downstream contact lines and acoustic waves emanating from $x/L = 0.25$, $x/L = 0.5$, $x/L = 0.75$, $x/L = 0.98$ and $x/L = 1$ for case VII. Time is non-dimensionalised by $\tau_L = L/u_{IS}$, which is the time it takes for the shock to travel a distance equal to the particle cloud length. The transmitted shock is attenuated as it passes through the particle cloud, while the reflected shock is strengthened continuously over the time-frame considered here. The acoustic wave emanating from $x/L = 0.98$ can be seen to have an infinite slope, which indicates that the flow chokes at this point and becomes supersonic further downstream, as can be seen by the acoustic wave emanating at $x/L = 1$. There is also a quasi-stationary shock downstream of the particle cloud, but this shock is very irregular and takes some time to develop, thus it is not shown in the figure.

The different simulations and key parameters describing the bulk behavior are shown in Table 1. Ma_{RS} and Ma_{TS} are the average shock wave Mach numbers of the reflected shock between $x/L = -0.2$ and $x/L = -0.01$, and the transmitted shock between $x/L = 1$

FIGURE 1. Sketch of the 3D simulation problem setup. A shock wave, shown in the left part of the figure passes through the cloud of particles located between $x/L = 0$ and $x/L = 1$.

FIGURE 2. Wave diagram showing the positions of the incident, transmitted and reflected shock waves (solid lines), upstream and downstream contacts (dashed lines) and acoustic waves (dotted lines) in case VII. The particle cloud is indicated by the grey region.

and $x/L = 1.3$, respectively. With increasing incident shock wave Mach number we see a strengthening of both the reflected and transmitted shocks. Increasing the theoretical mean minimal particle separation,

$$r = \frac{1}{N_p D_p} \sum_p \min_{i \neq p} \|x_i - x_p\|, \quad (3.1)$$

which is a non-dimensional measure of number density, increases the reflected shock strength and decreases the transmitted shock strength. Decreasing particle volume fraction increases Ma_{TS} and decreases Ma_{RS} . We fit the reflected and transmitted shock Mach numbers as power laws of incident shock Mach number, r and volume fraction. The resulting functions are

$$Ma_{RS} = 1.035 \alpha_p^{0.0768} r^{0.03865} Ma^{0.5395}, \quad (3.2)$$

and

$$Ma_{TS} = 0.6566 \alpha_p^{-0.1726} r^{-0.1813} Ma^{0.8716}. \quad (3.3)$$

In addition to the dependencies described above, the strength of the transmitted and reflected shocks depend in a non-trivial manner on the regularity of the particle distribution (Mehta *et al.* 2016, 2018).

To estimate the importance of the velocity fluctuations, we consider the ratio of fluctuating kinetic energy to mean kinetic energy. Figure 3 shows the ratio of fluctuating kinetic energy to total kinetic energy for $(t - t_0)/\tau_L = 0.5, 1$ and 2 , where t_0 is the time when the incident shock impacts the particle cloud. Clearly, k contains a significant amount of

FIGURE 3. Ratio of fluctuating kinetic energy to total kinetic energy at $(t-t_0)/\tau_L = 0.5$ (black), 1, (grey) and 2 (light grey). Solid lines: case III, dashed lines: case VII, solid line and disks: case XI.

FIGURE 4. Mean fluctuating kinetic energy over $x/L = 0.1$ to $x/L = 0.9$. Solid black line: case I, black dashed line: case II, black dotted line: case III, black dash-dotted line: case IV, black dashed and double-dotted line: case V, black line and circles: case VI, black squares: case VII, dark grey squares: case VIII, light grey squares: case IX, grey solid line: case X, grey dashed line: case XI, grey dotted line: case XII.

the kinetic energy, peaking at about $2/3$ of $\tilde{K}$. We observe that k peaks a few particle diameters behind the primary shock wave, and subsequently decays to a value that stays roughly constant throughout the particle cloud. Figure 4(a) shows the mean fluctuating kinetic energy over $x/L = 0.1$ to $x/L = 0.9$ normalised by the kinetic energy behind the incident shock for the cases with $n = 191 \text{ mm}^{-3}$ and those with $n = 1528 \text{ mm}^{-3}$. The average value peaks after the shock has passed through the particle cloud, and for the largest particle size the timing of the peak value collapses when scaled by τ_L . For the smallest particles, we observe that the timing of the peak does not collapse with the shock-associated time scale, and that the peak is earlier for the higher Mach numbers. The normalised fluctuating kinetic energy magnitude can be seen to decrease with Mach number, but this should not be confused with a decrease in absolute values of the fluctuation intensity. A similar plot for the cases with $Ma = 2.6$ is shown in Figure 4(b). We note that the timing of the peak does not collapse when scaled by τ_L here either, but the deviation is small. Higher number densities (or r) result in a delayed and smaller peak value. As a higher number density corresponds to a larger particle surface area within the particle cloud, we could expect more intense fluctuations, since (as will be shown below)

FIGURE 5. Source terms in Eq. (2.7) for case VII at (a) $(t - t_0)/\tau_L = 1$ and (b) $(t - t_0)/\tau_L = 2$, non-dimensionalised by $\mathcal{P}$. Black solid line: A , black dashed line: B , grey solid line and triangles: ε , black solid line and squares: Π , black dotted line: M^{ap} , grey line and disks: M^{am} , light grey solid line: P .

the dominant fluctuation production is due to forces on the particle surfaces. What we find instead is a lower fluctuation intensity, and this is likely due to the smaller scales introduced into the flow by the smaller particles. This leads to increased dissipation, and this increase is stronger than the increase of production.

The generation and dissipation of fluctuating kinetic energy is governed by seven terms in Eq. (2.7). Understanding the relative importance of these terms is essential if we want to model the evolution of k . To this end, we examine the production and dissipation terms in one of our simulations. Figure 5 shows the source terms of k for case VI at $(t - t_0)/\tau_L = 1$ and 2, non-dimensionalised by $\mathcal{P} = \rho_{IS} \bar{K}_{IS} u_{IS} / D_p$. Clearly, A , the production due to the pressure on the particles is the dominant term, while B , Π and ε are also important. Figure 5(b) shows the source terms at $(t - t_0)/\tau_L = 2$, at which point the flow has established a quasi-steady regime, where the streamwise distribution of the source terms do not vary much in time. Terms A , B and Π are roughly constant over $0.1 < x/L < 0.80$, and ε is slightly increasing in magnitude over this region. In the region close to the downstream edge of the particle cloud, the relative importance of the source terms change quite significantly. The production term due to Reynolds stresses attains a higher magnitude than all the other source terms except A , primarily due to the transition to supersonic flow which significantly increases the streamwise velocity. We observe that A and Π are negatively correlated, and we find that the Pearson correlation coefficient for A and Π averages above 0.8 for all the simulations, and is strongest for the highest values of r .

4. 1D simulations

In this section, we consider 1D simulations of a Mach 2.6 shock wave impacting on a particle cloud with volume fraction $\alpha_p = 0.1$ and particle number density of 763.9 mm^{-3} , i.e. case VII. As a baseline, we consider the most basic version of Eqs. (2.4)-(2.6) where all unclosed terms are set to zero. The computational domain is discretized into 1920 control volumes and extends from $x/L = -5/3$ to $x/L = 10/3$. The volume fraction field is generated by seeding 16000 particles uniformly over $0 \leq x/L \leq 1$, and the control volume height and width are chosen to match the desired volume fraction. Since the control volume length does not match exactly an integer number of particle separations there

FIGURE 6. Pressure at $(t - t_0)/\tau_L = 1.5$ for case VII (solid line) and corresponding 1D simulations. No sub-grid closures and Clift & Gauvin's drag law: dashed line, no sub-grid closures and exact drag law: dotted line, sub-grid closures and exact drag law: solid grey line.

are small variations in the local volume fraction through the particle cloud. Although the particles are locked in space, the choice of drag law affects the flow through the appearance of the particle forces in the momentum equation. The force due to drag on each particle is applied only to the control volume containing the particle. We include the quasi-steady drag force and the Archimedes force on each particle. The quasi-steady drag is computed from the drag law of Clift and Gauvin, as cited in Schwarzkopf *et al.* (2011), where the drag coefficient is

$$C_d = \frac{24}{Re_p} [1.0 + 0.15 Re_p^{0.687} + 0.0175 Re_p (1 + 4.25 \times 10^4 Re_p^{-1.16})^{-1}]. \quad (4.1)$$

Figure 6 shows the pressure from the 3D- and 1D-simulation at $(t - t_0)/\tau_L = 1.5$. We note that the basic wave-structure is the same in both cases, c.f. Figure 2. However, there are a number of differences between the 3D and 1D results. The reflected shock wave can be seen to be much stronger in the 3D case, and as a result its location is much further upstream than the reflected shock in the 1D case. We see that at $x/L = 0$ the pressure begins to decrease with x , sharply at first and then more slowly, with a constant negative gradient, over most of the cloud length. The 1D simulation shows a too steep and narrow initial pressure gradient, followed by a too weak constant pressure gradient region. At the downstream end of the particle cloud the 1D simulation does show an expansion region, but it is less pronounced than its 3D counterpart. Since the reflected shock is too weak, the transmitted shock is too strong, and we find elevated pressure levels downstream of the particle cloud.

We now demonstrate the effect of a few improvements to the simple 1D model. As a first iteration, we replace the drag law by a curve fit of the forces exerted on the particles in the 3D simulation. We refer to this approach as using an exact drag law. As can be seen in Figure 6, the resulting pressure distribution is much closer to the 3D simulation data than the results with Clift & Gauvin's drag law. We note that the pressure within the particle layer is quite a bit higher than it should be, but the gradient matches the 3D data well. The difference originates at the upstream edge of the particle cloud, where the 3D data has a rapid drop in pressure. Downstream we see the same problem as with the previous drag law. The pressure drop in the expansion region is not strong enough, but we see that the pressure even further downstream is now closer to the 3D data.

Finally, we include the sub-grid scale fluctuating kinetic energy and propose closures for R_{00} , P , A , B , Π and ε . We emphasise that these closures are specific to this case and are not recommended for general uses. Terms M^p and M^μ are neglected, as are all

the transport terms labeled $D^{(\cdot)}$. R_{00} is closed by specifying the turbulence anisotropy, which we observe from the data to give roughly $R_{00} = 6k/5$. A and B are closed by the drag law. Π was found to be significantly correlated with the forces on the particles, and we set it simply to $\Pi = -0.3(A + B)$. For ε , we use a simple length scale model so that

$$\varepsilon = \frac{\rho k^{3/2}}{l}, \quad (4.2)$$

where l is the dissipation length scale. We use the 3D data to estimate the dissipation length scale, and as a first approach use a constant value of 10^{-4} m, i.e. slightly larger than the particle diameter. The resulting pressure distribution is shown in Figure 6. Clearly, the additional terms bring the simulation closer to the 3D data. The reflected shock is now well represented, and the distribution throughout the particle cloud is very good. There are still deviations close to the upstream and downstream edges of the particle cloud, but these are smaller than for the other two models.

Based on experimentation with different closures for the various unclosed terms in Eqs. (2.4)-(2.6) and the drag-law, we make the following observations;

(I) The drag law is important for the strength of the reflected shock. A stronger drag imposes a stronger force on the gas phase, in addition to increasing the production of fluctuating kinetic energy. We believe that capturing the initial spike in the drag coefficient is important for obtaining a correct reflected shock strength. Commonly applied drag-laws, including the one used here, does not capture this spike. Other studies that have investigated particle drag in the shock-particle cloud setting, e.g. Mehta *et al.* (2016, 2018), are therefore very important for simulation of these problems.

(II) The level of the fluctuating kinetic energy has an appreciable impact on the pressure field when it is computed from the total energy and kinetic energy fields, which is the most common solution method for both the Euler and Navier-Stokes equations. Neglecting the fluctuating kinetic energy leads to erroneous pressure gradients, and thus wrong mean flow.

(III) The Reynolds stress contribution in the momentum equation is significant. It affects the strength of the reflected shock wave, and in turn all the fields downstream. By tuning the anisotropy of the Reynolds stress tensor, we can to some extent adjust the reflected shock strength and the mean field profiles throughout the particle layer. A proper model for the Reynolds stress is thus necessary.

5. Conclusions

We have conducted three-dimensional resolved simulations of shock waves passing through particle clouds for varying Mach numbers, particle number densities and volume fractions. We investigated the bulk effect of the particle cloud and fitted power laws for the transmitted shock and reflected shock wave Mach numbers. We have also investigated the development of fluctuating kinetic energy, and found that it reaches values as high as two thirds of the local mean kinetic energy. The primary source of fluctuating kinetic energy is the forces on the particles, and both viscous dissipation and pressure-dilatation are significant sinks. We performed 1D simulations, corresponding to one of the 3D simulations, and demonstrated that a naive approach which ignores the unresolved fluctuations has several problems. Adding the exact drag law, taken from the 3D data, significantly improved the 1D simulations, but this approach still does not reproduce the 3D data very well. We included the fluctuating kinetic energy equation, provided closures for its sources and sinks, and the results from this extended equation

set were significantly improved compared to the previous 1D simulations. The remaining deviations from the 3D data were located close to the upstream and downstream edge of the particle cloud.

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Chapter 9

Paper III

III

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Computational analysis of shock-induced flow through stationary particle clouds

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ABSTRACT

We investigate the shock-induced flow through random particle arrays using particle-resolved Large Eddy Simulations for different incident shock wave Mach numbers, particle volume fractions and particle sizes. We analyze trends in mean flow quantities and the unresolved terms in the volume averaged momentum equation, as we vary the three parameters. We find that the shock wave attenuation and certain mean flow trends can be predicted by the opacity of the particle cloud, which is a function of particle size and particle volume fraction. We show that the Reynolds stress field plays an important role in the momentum balance at the particle cloud edges, and therefore strongly affects the reflected shock wave strength. The Reynolds stress was found to be insensitive to particle size, but strongly dependent on particle volume fraction. It is in better agreement with results from simulations of flow through particle clouds at fixed mean slip Reynolds numbers in the incompressible regime, than with results from other shock wave particle cloud studies, which have utilized either inviscid or two-dimensional approaches. We propose an algebraic model for the streamwise Reynolds stress based on the observation that the separated flow regions are the primary contributions to the Reynolds stress.

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1. Introduction

Interaction between shock waves and particle clouds are of interest in a number of different natural phenomena, as well as industrial applications and safety measures such as shock wave mitigation using porous barriers (Suzuki et al., 2000; Chaudhuri et al., 2013). It also finds applications in heterogeneous explosives (Zhang et al., 2006) and explosive dissemination of powders and liquids (Zhang et al., 2001; Milne et al., 2010; Rodriguez et al., 2017). In coal mines, enhanced or secondary explosions due to coal dust is a major safety concern (Ugarte et al., 2017; Shimura and Matsuo, 2018). Shock wave particle interaction also occurs in a number of natural phenomena, with volcanic eruptions (Bower and Woods, 1996) as the prime example. There are also astrophysical examples such as ejection of stellar dust from supernovae (Silvia et al., 2012). More generally, high-speed multiphase flow has important industrial applications, such as liquid and solid fuel engines and

fluidized beds. Gas-turbines operating in regions with suspensions of sand particles in the air are subject to substantial degradation due to particle deposition on turbine blades (Hamed et al., 2006). Water injection systems have been used to reduce sound intensity at rocket launch pads (Ignatius et al., 2008), and it might be possible to utilize similar systems to reduce jet noise (Krothapalli et al., 2003), which is especially important around air-crafts during take-off.

Shock wave interaction with particle clouds has been extensively studied over the last fifty years. The dilute particle cloud and the granular flow regimes are quite well understood, but the intermediate regime has proven challenging to model (Theofanous and Chang, 2017). The intermediate volume fraction regime is where particles neither display the same statistical properties as isolated particles, nor as particles in the granular regime. In Crowe et al. (2011), flows with particle volume fractions above 0.1% were considered to belong to this regime, while Zhang et al. (2001) used a lower limit of 1%. The difficulty in modeling these flows stems from the complex interaction between the flow field and the particle distribution. The particles occupy a volume that is large enough that their collective nozzle effect is one of the dominating

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dynamical effects in the flow (Mehta et al., 2018b), but they are not close enough that particle collision exclusively determines the movement of the particles. Each particle deflects the flow around it, causing local flow acceleration and deceleration that depends on the local particle configuration. Additionally, boundary layers develop over the particle surface, and the flow separates behind the particle. When the shock wave passes over a particle there is a reflection from the front of the particle, and a focusing of the shock wave behind it (Tanno et al., 2003). The reflected shock interacts with the upstream particles and their wakes, and also with reflected shocks from other nearby particles. These complex flow dynamics lead to a large variation in drag forces that depends on the local particle configuration.

The intermediate particle volume fraction regime has recently become feasible to study in much greater detail than was previously possible. In experiments, the short time-scales and the limited possibility of recording data in the regions of interest have presented significant difficulties. Recent improvements to experimental techniques have enabled experimentalists to accurately characterize the wave system and particle distribution when a shock wave passes through a curtain of particles (Wagner et al., 2012; Ling et al., 2012). Even more recently, DeMauro et al. (2017) used high speed, time-resolved, particle image velocimetry to measure velocity fields in front of and behind the particle curtain. The new sets of experimental data have resulted in a renewed effort to study these problems using numerical simulations, in particular using the Eulerian–Lagrangian framework (Houim and Oran, 2016; Shallcross and Capecelatro, 2018; Theofanous and Chang, 2017), but also Eulerian–Eulerian models (McGrath et al., 2016; Saurel et al., 2017; Utkin, 2017).

Some quantities are very difficult to measure experimentally, such as flow field distributions inside the particle cloud and fluctuations at the particle scale. Instead, these can be obtained using particle-resolved numerical simulations. Such simulations are computationally expensive, since a large number of particles must be used to obtain meaningful statistics. A limiting factor is the very large scale separation between the dynamically important particle scale physics and the global length scale of the problems. However, a number of studies have recently been able to investigate shock-wave particle cloud interaction using two-dimensional (Regele et al., 2014; Hosseinzadeh-Nik et al., 2018; Sen et al., 2018) and three-dimensional (Sridharan et al., 2015; Mehta et al., 2016; 2018a; 2018b; Theofanous et al., 2018) numerical simulations. In particular, particle resolved simulations can be used to investigate closures for unresolved terms that appear in Eulerian–Lagrangian or Eulerian–Eulerian models due to averaging of products of fluctuations. Volume averaging is one form of filter used in Large Eddy Simulations, and is also used in the formulation of most Eulerian–Lagrangian methods. Volume averaging does not commute with spatial or temporal derivatives. Therefore, the averaging operation introduces new terms in the volume averaged equations, as discussed in e.g. Schwarzkopf and Horwitz (2015). Volume averaging can be applied to data from particle-resolved simulations to investigate the unclosed terms, both the terms that appear in single-phase models and those that are specific to dispersed flow models.

In the intermediate particle volume fraction regime, the inter-particle distance and the particle size are of the same order. The spatial extent of the flow field fluctuations is comparable to the inter-particle distance, and we will refer to these as particle scale fluctuations. It is common to divide the flow fluctuations into pseudo-turbulent and turbulent structures, and refer to the kinetic energy in these as pseudo-turbulent kinetic energy (PTKE) and turbulent kinetic energy (TKE), respectively. The flow perturbations induced by the particles are considered to be pseudo-turbulent effects. Pseudo-turbulent flow structures might have very different time and spatial scales than turbulent structures. For this reason it

is a useful technique for analyses and modeling purposes to distinguish between the two (Mehrabadi et al., 2015). In the setting of shock waves passing through particle clouds, PTKE is caused primarily by three effects. Firstly, shock wave reflection from individual particles causes very large differences between the region affected by the reflected shock and the surrounding regions, with correspondingly high PTKE values. Secondly, flow deflection around particles causes local flow accelerations and decelerations, resulting in both streamwise and spanwise fluctuations. In addition, flow separation behind particles also causes a significant deviation from the mean flow speed. This last effect in particular will be discussed in this paper. As evident from these examples, pseudo-turbulent flow fluctuations are quite different from classical turbulence. However, pseudo-turbulent fluctuations might themselves generate classical turbulent fluctuations. This is expected to occur as a result of the strong velocity shear in the particle wakes. The processes generating TKE and PTKE are very different phenomena, and should therefore be modeled differently. Both TKE and PTKE enter the volume averaged momentum equations through a term that is analogous to the classical Reynolds stress, and for convenience we will use the term Reynolds stress for this term throughout this paper.

The velocity fluctuations in shock-particle interaction have previously been examined in two-dimensional flows using both inviscid (Regele et al., 2014) and viscous simulations (Hosseinzadeh-Nik et al., 2018). In those flows, the PTKE was found to be slightly higher in the inviscid simulations, but of the same order as the mean flow kinetic energy in both cases. Regele et al. (2014) additionally demonstrated the importance of capturing the PTKE in volume-averaged simulations in order to obtain correct pressure fields. In contrast, Mehta et al. (2018a) found very low values of PTKE, demonstrating a significant difference between the two-dimensional and inviscid three-dimensional simulations. The Reynolds stress plays an important role in the dynamics around the particle cloud edges, and in particular it influences the (time-dependent) strength of the reflected shock wave. Since the incoming flow field is altered by the reflected shock wave, phenomena such as particle drag, pressure drop through the particle cloud and even the transmitted shock strength depend directly on the strength of the reflected shock, and therefore also on the Reynolds stress.

Recent studies have recognized that an issue for Eulerian–Lagrangian methods is that the forces imposed on the continuous phase by a particle disturbs the flow around the particle. Calculation of drag by standard drag laws is incorrect if continuous phase variables within the disturbed flow region is used, because most drag-laws are calibrated against undisturbed flow quantities. Methods for handling this problem exactly in the zero Reynolds number limit have been proposed and even shown to yield good results in finite Reynolds number flows (Horwitz and Mani, 2016; 2018; Balachandar et al., 2019). Accounting for how the particle influences the local flow field was also done in Moore and Balachandar (2018), who used a linear superposable wake to approximate continuous phase fluctuations within a particle cloud for incompressible flow. So far, no such model has been proposed for the compressible flow inside a particle cloud. However, using knowledge about how the particles disturb the flow in their vicinity to improve drag computation can be done even in this complex setting, as will be shown.

In this work we perform three-dimensional, time dependent, viscous simulations of a shock wave passing through a random particle array. The particles are assumed to be inert and stationary. We vary the incident shock wave Mach number between 2.2 and 3, the particle volume fraction between 0.05 and 0.1, and the particle diameter between 50 μm and 100 μm . Preliminary results from these simulations were reported in Vartdal and Osnes (2018).

We utilize volume averaging to define the mean flow and the fluctuations from that mean. Key flow properties such as mean velocity, pressure and density, as well as the Reynolds stress and its anisotropy, are examined.

The purpose of this work is twofold. Firstly, we analyze trends in mean flow properties over different combinations of volume fractions and Mach numbers than those that have been reported previously. In addition, we vary the particle diameter, which has not been done before. This analysis improves the understanding of the bulk effect of particle cloud properties on shock wave particle cloud interaction. The second purpose is to analyze statistics of the Reynolds stresses and their anisotropy, as well as their importance in the flow dynamics. To the authors' knowledge, this has not yet been investigated for viscous simulations of three-dimensional random particle arrays. Such data are crucial to the development of Reynolds stress closure models for shock wave particle cloud interaction.

This paper is organized as follows. In Section 2 we briefly introduce the basic flow patterns occurring when the shock wave passes over a group of particles. The governing equations and the volume averaged equations used for analysis are described in Section 3. Section 4 describes the computational method and the set-up of the problems under consideration. Section 5 presents the simulation results. First the grid-quality is checked by examination of particle drag and resolution of viscous shear layers. Next, we discuss the shock wave attenuation as it passes through the particle layer. We then examine the mean fields, i.e. density, velocity, pressure and Mach number distributions throughout the particle layer, and discuss trends as we change particle volume fractions, particle diameters and incident shock wave Mach numbers. Next we discuss the velocity fluctuations and their anisotropy. We discuss the momentum balance around the upstream edge of the particle cloud, to highlight the dynamic importance of the velocity fluctuations. The discussion of the simulation results is finalized by an examination of the particle drag coefficients and the average particle forces obtained in the different simulations. In Section 6 we utilize the data from the resolved simulations to propose models that capture some of the observed properties of the flow. We provide an algebraic expression for combinations of particle diameter and particle volume fractions that result in the same shock wave attenuation. We also propose an algebraic Reynolds stress model based on the effect of separated flow behind particles on volume averaged equations, and compare this model to the streamwise velocity fluctuation intensity obtained in the simulations. Finally, concluding remarks are given in Section 7.

2. Shock-induced flow around particles

In this section, we present a brief overview of the flow during and after the shock wave passes over a group of particles. In Fig. 1, numerical schlieren images (Quirk, 1997) and instantaneous streamwise velocities are shown for a time-series in one of the simulations (case VII) that will be described in Section 4. The time sequence covers the shock wave pattern and the subsequent development of particle wakes. Initially, a planar shock impacts on the first particle, and a regular shock reflection is formed at the front of the particle (first frame). As the shock propagates, a Mach reflection is obtained, which can be discerned in the second frame. During this time, the pressure difference between the front and the back of the particle is very large. Due to the presence of multiple particles, the individual reflected shocks coalesce and form a reflected shock (Boiko et al., 1997; Wagner et al., 2012), which over time becomes nearly planar and propagates upstream. The particles also cause shock wave diffraction, as clearly seen by the curved front in the third frame. Behind each particle, the shock is focused and a high-pressure region is created (fourth frame).

Viscous forces become more important for the flow around particles when the particle Reynolds number is reduced. This is relevant also for shock particle interaction, since smaller particles correspond to lower particle Reynolds numbers. Henceforth, “particle Reynolds number” and “Reynolds number” will be used interchangeably. Sun et al. (2005) showed that depending on the Reynolds number, the high-pressure region created by shock focusing can create temporary negative drag-coefficients. This phenomena was only observed for particle Reynolds numbers of the order 10^3 . For lower Reynolds numbers, viscous forces counteracted this effect, and the total drag-coefficient remained positive. As they varied the particle Reynolds number from 4900 to 49, the importance of viscous forces increased drastically, and for the lower Reynolds number, the late-time viscous forces was almost twice the magnitude of the pressure forces.

The particle Reynolds number is often used to characterize the flow, and it is typically based on undisturbed flow, or incident flow, quantities. It is likely that characterization based on incident flow properties are less reliable in the shock wave particle cloud setting, due to the generation of a collective reflected shock wave. The strength of this shock wave determines the properties of the gas that enters the particle cloud, and is highly dependent on properties of the cloud. In addition, particles within the cloud are exposed to the pseudo-turbulent flow induced by upstream particles, which is very likely to affect statistical properties of the wake.

The development of flow separation and particle wakes can be seen in the middle frames in Fig. 1. Boundary layers develop over the particle surfaces, and the flow separates. The particle wakes are highly distorted due to the presence of other particles, even for the first particles in the cloud. For isolated particles with Reynolds numbers in the range 50 – 300, Nagata et al. (2016) found that for increasing Reynolds numbers, the separation line moves forward along the particle surface. They also found that higher Reynolds numbers resulted in longer separated flow regions. Within a particle cloud, the length of the separated flow region is significantly affected by the presence of other particles, as is the case for the wake behind the leftmost particle in Fig. 1. This phenomena cannot be described solely based on Reynolds number and Mach numbers.

The bottom frame of Fig. 1 shows a snapshot of the flow over the whole particle cloud. The different effects discussed above are visible in this frame, occurring at different spatial locations throughout the particle cloud.

3. Governing equations

The gas-dynamic processes considered in this work are governed by the conservation equations of mass, momentum and energy. In differential form these are

$$\partial_t \rho + \partial_k (\rho u_k) = 0, \quad (1)$$

$$\partial_t (\rho u_i) + \partial_k (\rho u_i u_k) = -\partial_i p + \partial_j \sigma_{ij}, \quad (2)$$

$$\partial_t (\rho E) + \partial_k (\rho E u_k + p u_k) = \partial_j (\sigma_{ij} u_i) - \partial_k (\lambda \partial_k T), \quad (3)$$

where ρ is the mass density, u is the velocity, p is the pressure, $\sigma_{ij} = \mu(\partial_j u_i + \partial_i u_j - 2\partial_k u_k \delta_{ij}/3)$ is the viscous stress tensor, μ is the dynamic viscosity, $E = \rho e + 0.5 \rho u_k u_k$ is the total energy per unit volume, e is the internal energy per unit mass, λ is the thermal conductivity, and T is the temperature. We utilize the ideal gas equation of state, with $\gamma = 1.4$, and relate internal energy and temperature by a constant specific heat capacity. We assume a power law dependence of viscosity on temperature, with an exponent of 0.76, and we relate the thermal diffusivity to the viscosity by assuming a constant Prandtl number of 0.7.

Fig. 1. Numerical schlieren images (top and bottom row) and streamwise velocities (middle row) in a cut plane, when a shock wave impacts on and passes through a cloud of particles. Flow direction is from left to right. Frames are taken at times $(t - t_0)/\tau_p = 0.13, 0.69, 1.25, 1.79, 2.86, 4.81, 6.77, 8.73, 10.63, 12.47, 26.82$. t_0 denotes the time when the shock wave is at $x = 0$ (upstream particle cloud edge) and τ_p is defined in Eq. (7). In the middle frames, the colormap is linear between -900 m/s (black) and 900 m/s (white). The red dashed square shows the location of the zoomed view in the upper rows. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

In the analysis of the results, we consider the volume averaged equations of motion. These are obtained by applying the volume averaging operator to Eqs. 1, 2, 3. We use the notation $\bar{\cdot}$ for volume averaging, $\langle \cdot \rangle$ for phase-averaging, and $\tilde{\cdot}$ for Favre-averaging. The deviations from the phase-averaged and Favre-averaged values are denoted by $\cdot'$ and $\cdot''$, respectively. Phase averaging and volume averaging are related by $\alpha \langle \cdot \rangle = \bar{\cdot}$, where α denotes the gas phase volume fraction. We use the symbol α_p for the particle volume fraction. The problem under consideration is statistically homogeneous in the y and z directions and therefore the volume averaged equations can be expressed in one dimension. The volume averaged equations are then

$$\partial_t(\alpha \langle \rho \rangle) + \partial_x(\alpha \langle \rho \rangle \tilde{u}_1) = 0, \quad (4)$$

$$\begin{aligned} \partial_t(\alpha \langle \rho \rangle \tilde{u}_1) + \partial_x(\alpha \langle \rho \rangle \tilde{u}_1 \tilde{u}_1 + \alpha \langle p \rangle) \\ = \partial_x(\alpha \langle \sigma \rangle_{11}) - \partial_x(\alpha \langle \rho \rangle \tilde{R}_{11}) \\ + \frac{1}{V} \int_S p n_1 dS - \frac{1}{V} \int_S \sigma_{1k} n_k dS, \end{aligned} \quad (5)$$

$$\begin{aligned} \partial_t(\alpha \langle \rho \rangle \tilde{E}) + \partial_x(\alpha \langle \rho \rangle \tilde{E} \tilde{u}_1 + \alpha \langle p \rangle \tilde{u}_1) \\ = \partial_x(\alpha \langle \sigma_{11} \rangle \tilde{u}_1) - \partial_x(\alpha \langle \lambda \partial_x T \rangle) \\ - \partial_x(\alpha \langle \rho e'' u_1'' \rangle) - \partial_x(\alpha \langle \rho \rangle \tilde{R}_{11} \tilde{u}_1) \\ + D^u + D^p + D^\mu + D^{ap} + D^{a\mu}. \end{aligned} \quad (6)$$

In the equations above, $\tilde{R}_{11} = \overline{u_1' u_1'}$ is a stress due to velocity fluctuations, analogous to the classical Reynolds stress and we refer to this term as Reynolds stress throughout this paper. The continuous phase boundary is denoted by S , V is the averaging volume, and the integrals represent the forces acting on the particle surfaces. $D^u = -1/2 \partial_x(\alpha \langle \rho u_1' u_1' u_1' \rangle)$ is the turbulent diffusion, $D^p = -\partial_x(\alpha \langle p' u_1' \rangle)$ is the pressure diffusion, $D^\mu = \partial_x(\alpha \langle u_1' \sigma_{j1}' \rangle)$ is the turbulent viscous diffusion, $D^{ap} = \partial_x(\alpha \langle a_1 \langle p \rangle \rangle)$ is the pressure-diffusion effect due to the turbulent mass flux $a = \langle \rho' u' \rangle / \langle \rho \rangle$, and $D^{a\mu} = -\partial_x(\alpha \langle a_1 \langle \sigma \rangle_{11} \rangle)$ is the analogous viscous diffusion effect. An investigation of the energy

balance during shock wave particle cloud interaction is outside the scope of this work, but we include the equation for completeness. The Reynolds stress appears in both Eqs. (5) and (6), and the terms containing it represent the forces due to velocity fluctuations and the work done by those forces, respectively. Those fluctuations can be both shear turbulence and pseudo-turbulent fluctuations. The physical processes represented by the Reynolds stress will be discussed in this paper in order to guide closure modeling.

4. Computational method and set-up

4.1. Computational method

The simulations in this work are performed using the compressible flow solver “CharLES”, developed by Cascade Technologies. The governing equations are solved with an entropy-stable scheme on a Voronoi-mesh (Bres et al., 2018), and a third order Runge-Kutta method for time stepping. A discussion of entropy stable schemes can be found in e.g. Tadmor (2003); Chandrashekar (2013).

4.2. Problem set-up

We perform numerical simulations of shock waves passing through a fixed cloud of particles, with varying shock wave Mach number, particle size and particle volume fraction. Fig. 2 shows a sketch of the computational domain and the particle distribution. The particle cloud has length L , and spans the domain in the y and z directions. We denote the particle diameter by D_p . The particle configuration in the figure is the configuration used for the simulations with the largest particle diameter. The computational grid consists of structured grids around each particle, which extend $0.2D_p$ out from the particle surface, and an approximately uniform Voronoi-grid in the rest of the domain. Within this structured region, the control volume size increases geometrically with distance to the particle surface. Fig. 3 provides an impression of

Fig. 2. Sketch of the computational domain and the particle configuration used for the simulations with the largest particles. The particles are located at $0 \leq x \leq L$, where $L = 1.2\sqrt[3]{4}$ mm, and the computational domain extends $2L/3$ upstream and $L/3$ downstream of the particle cloud. The axis directions are indicated at the origin. The span-wise extent is set to a constant multiple of the particle diameter, so that $\Delta y = \Delta z = 8\sqrt[3]{4}D_p$, and therefore varies depending on the particle size.

Fig. 3. Illustration of the mesh around particle, where the faces of each control-volume in this cut-plane are shaded according to the direction of their normals. There is a structured mesh around each particle extending $0.2D_p$ out from the particle surface, and a Voronoi-grid in the rest of the domain. Note that the control volume sizes in this figure are adjusted for illustration purposes.

the mesh around each particle. The particle positions are drawn from a uniform random distribution, so that any position within $0 \leq x/L \leq 1$ has equal probability of containing a particle. We accept a particle position if it is not closer than $1.5D_p$ to any other particle center. This ensures that the structured grids do not overlap, and that there is a small distance between the structured grids where the Voronoi-grid can create a smooth transition between the two structured regions. In addition, we require that structured grids do not intersect the spanwise domain boundaries. Particles are drawn in this way until the particle volume fraction reaches the desired value. For the simulations considered in this study, the minimal number of particles in any simulation is 586 and the maximal number is 1173. The size of the control volumes in the Voronoi part of the mesh matches approximately the outer layer of the structured grid around each particle, and it is slightly coarsened in the regions away from the particle cloud. The total number of control volumes is roughly 6×10^7 for all the simulations here. On 300 cores, each simulation took roughly 24 hours to complete. The initial condition consists of two homogeneous regions separated by a shock wave, where the pre-shock conditions are set to $\rho^0 = 1.2048 \text{ kg/m}^3$, $u^0 = 0 \text{ m/s}$ and $p^0 = 1.01325 \times 10^5 \text{ Pa}$.

Table 1

The different simulations considered in this study and key parameters. Ma is the incident shock wave Mach number, $Re_{p,IS}$ is the particle Reynolds number based on post incident shock values, and n is the number density. L_s is the sight-length, as defined in Section 5.2.

Case	Ma	L_s/L	α_p	$Re_{p,IS}$	$n \text{ [mm}^{-3}\text{]}$	$D_p \text{ [}\mu\text{m]}$
I	2.2	0.196	0.1	6160	191.0	100
II	2.4	0.196	0.1	7091	191.0	100
III	2.6	0.196	0.1	7927	191.0	100
IV	2.8	0.196	0.1	8666	191.0	100
V	3.0	0.196	0.1	9309	191.0	100
VI	2.6	0.157	0.1	6292	382.0	79.4
VII	2.6	0.125	0.1	4994	763.9	63.0
VIII	2.6	0.163	0.075	4537	763.9	57.2
IX	2.6	0.226	0.05	3964	763.9	50
X	2.2	0.099	0.1	3080	1528	50
XI	2.6	0.099	0.1	3964	1528	50
XII	3.0	0.099	0.1	4654	1528	50

The post-shock conditions are determined from the shock wave strength. Post-shock quantities are used for normalization, and will be denoted with a subscript IS. For the post-shock gas velocity we omit the numeric component subscript for notational convenience. The shock wave propagates in the x-direction. The upstream boundary is set to the post-shock condition and the downstream boundary is set to a zero-gradient outlet. We apply symmetry conditions at the y and z boundaries.

Table 1 provides an overview of the parameter combinations we simulate. The simulations will be referred to as Case I, II, ..., XII. We vary the incident shock wave Mach number between 2.2 and 3, particle size between 50 μm and 100 μm and particle volume fraction between 0.05 and 0.1.

The analysis is conducted using the volume averaging framework. We define averaging volumes spanning the domain in the y and z directions, with a streamwise extent of $L/60$. These bins contain both the gas phase and the particles, and thus the particle volume fraction within a bin might deviate from the bulk particle volume fraction. The flow quantities are averaged over these bins, and we subsequently compute a moving average with a window of five bins to reduce the sensitivity of the results to the local particle configuration.

We utilize two time-scales to compare the simulation results. These are

$$\tau_L = L \left(Ma \sqrt{\gamma \frac{p^0}{\rho^0}} \right)^{-1}, \quad \tau_p = D_p \left(Ma \sqrt{\gamma \frac{p^0}{\rho^0}} \right)^{-1}, \quad (7)$$

where τ_L is the time it takes for the incident shock wave to travel a distance equal to the particle cloud length, τ_p is the time it takes for the incident shock wave to pass over a particle and Ma is the Mach number. Unless otherwise specified, the time-scale is computed using the incident shock wave Mach number in each simulation, so that the time-scales are different for the different simulations. We let t_0 denote the time when the shock wave is at $x = 0$.

5. Results

All simulations considered here feature the same basic flow pattern, which has been reported in a number of previous experimental and numerical studies. The most important features are the generation of the reflected shock, the generation of particle wakes, and the continuous weakening of the primary shock as it impacts on particles throughout the layer. It should be noted that the particle layer considered here is not long enough to completely dissipate the shock wave, and therefore a transmitted shock emerges from the downstream edge of the particle cloud. After the trans-

Fig. 4. Drag coefficient for an isolated particle subjected to a $Ma = 2.6$ shock wave with different grid resolutions. Here, N denotes the number of points at the particle surface.

mitted shock has moved away from the particle cloud, a flow expansion region occurs around the downstream edge of the particle cloud, where the flow transitions from subsonic ($Ma \approx 0.5 - 0.8$) to supersonic ($Ma \approx 1.2 - 1.6$). The expansion region is terminated by a shock wave a short distance downstream of the particle cloud.

5.1. Grid resolution

Previous studies of shock interaction with particle arrays have estimated grid qualities by examining the drag-coefficient on a single particle (Mehta et al., 2016; 2018b; Hosseinzadeh-Nik et al., 2018). It is important that the particle forces are well reproduced in the simulation, since they are central to the problem under investigation. Following the same approach, we conduct simulations of a single particle with diameter $63 \mu\text{m}$, subjected to a $Ma = 2.6$ shock wave with various number of faces at the particle surface. This parameter combination is chosen because it is in the middle of the range of Mach numbers and particle sizes we have simulated. Fig. 4 shows the drag coefficient, as defined in Eq. (15), as a function of time for five different grid resolutions. The drag-coefficient with $N = 2252$ deviates roughly 2% from the highest resolution, and is a feasible resolution in terms of computational cost for the particle cloud simulations. Therefore, we apply this resolution to the simulations considered in this paper.

In addition to the drag-coefficient, we also examine the grid-resolution in terms of the parameter

$$l^+ = \sqrt[3]{V_{CV}}/l_{\text{viscous}}, \quad (8)$$

which is the non-dimensional grid-length scale relative to the local viscous length scale of the flow. Here $\sqrt[3]{V_{CV}}$ is the length scale of the control volume,

$$l_{\text{viscous}} = \sqrt{\frac{\mu}{\rho(2S_{ij}S_{ij})^{1/2}}}, \quad (9)$$

is the viscous length scale (Wingstedt et al., 2017) and $S_{ij} = 0.5(\partial_j u_i + \partial_i u_j)$ is the strain rate tensor. The viscous length scale can be interpreted as the smallest length scale of the local shear flow. Thus, if the grid size is comparable to or smaller than this length scale, it is reasonable to assume that the flow is well resolved locally. The viscous length scale can be utilized independent of the state of the flow (turbulent or laminar). It should be noted that the values obtained for l_{viscous} depends on the grid-size,

Fig. 5. Histogram of l^+ for case VII, with $(Ma, \alpha_p, D_p) = (2.6, 0.1, 63 \mu\text{m})$, at $(t - t_0)/\tau_L = 1.36$.

and l^+ therefore only serves as a post-simulation measure of grid-quality, as opposed to a value that can be used quantitatively to refine a mesh. Fig. 5 shows a histogram of the l^+ values for case VII, with $(Ma, \alpha_p, D_p) = (2.6, 0.1, 63 \mu\text{m})$, at $(t - t_0)/\tau_L = 1.36$. The middle 98% of the distribution is located between $l^+ = 30$ and $l^+ = 114$. The highest values are located in the shear layer around each particle and their wakes. For problems where it is critical to resolve the turbulent energy cascade, the grid size should be comparable to l_{viscous} , or if larger grid sizes are used, the smaller scales should be appropriately modeled. In this problem, it is unlikely that details of the energy cascade are very important. Therefore the requirement on l^+ can probably be slightly relaxed here without affecting the results considerably. Some phenomena, such as wake-wake interaction, and shock-wake interaction, might require finer resolutions than we use. However, it is not the purpose of this work to explore these phenomena in detail, and it is likely that they only have a minor effect on the results presented here.

The viscous length scales in this case are distributed between 20 nm and 200 nm. This means that the smallest viscous length scales are only about an order larger than typical mean free paths of air molecules. The Knudsen number based on the viscous length scale is given by

$$Kn = \frac{l_{\text{free}}}{l_{\text{viscous}}} = \left(\frac{k_B T}{\sqrt{2}\pi p D_{p,\text{air}}} \right) \frac{1}{l_{\text{viscous}}}, \quad (10)$$

where l_{free} is the mean free path of the molecules, k_B is the Boltzmann constant and $D_{p,\text{air}} = 3.84 \times 10^{-10} \text{ m}$ is the effective diameter of an air molecule. Throughout most of the particle layer, the Knudsen number takes values around 0.1. In the expansion region at the downstream end of the particle cloud, the Knudsen number increases, and around the very last particles we find values up to two. This indicates that the wakes and shear layers around particles at the downstream end of the particle cloud might be influenced by non-continuum effects, but we do not expect those effects to be very large.

We conclude that the grid-resolution used in this study is sufficient to obtain reliable particle forces, and that it represents the local flow gradients in a satisfactory manner.

5.2. Shock wave attenuation

As the shock wave passes through the particle cloud, it is attenuated by shock reflection from the particles. The amount of

Fig. 6. Difference between undisturbed shock arrival time, x/u_s , where u_s denotes the incident shock wave speed, and the obtained shock arrival time, t_s , as a function of position within the particle cloud for an incident $Ma = 2.6$ shock wave. The shock arrival time is defined as the time when the average pressure within the bin first exceeds 3 bar.

attenuation depends on particle size and particle volume fraction, as well as the regularity of the particle distribution. As will be shown, the shock wave attenuation and certain mean flow trends are well characterized by a single parameter depending only on geometric properties of the particle cloud.

Fig. 6 shows the shock arrival time as a function of distance within the particle cloud for the cases with $Ma = 2.6$. Cases VI and VIII, with $(\alpha_p, D_p) = (0.1, 79.4 \mu\text{m})$ and $(0.075, 57.2 \mu\text{m})$ respectively, have very similar shock speeds during the passage of the shocks through the particle clouds. Cases III and IX, with $(\alpha_p, D_p) = (0.1, 100 \mu\text{m})$ and $(0.05, 50 \mu\text{m})$ respectively, appear quite similar in this plot, but it can be seen that the difference between them increases with distance. The shock wave reflection imposes a strong transient force on the particles, and therefore shock wave attenuation serves as a measure of the average initial particle drag, and vice versa. The simulations do indeed show that summing up the forces on the particles during the first τ_p after the shock hits each particle, yields approximately the same result for cases VI and VIII.

The regularity of the particle distribution can affect the shock attenuation through statistical differences in shock focusing and particle forces. For this reason, it is necessary to estimate the effect of our non-random particle distribution. We generate the particle distributions by drawing random positions satisfying two criteria that makes the particle distribution slightly more regular than a completely random distribution, as discussed in Section 4. To quantify this effect, we examine the area in the y - z plane that is occluded by the particles as a function of distance. The occluded area at a streamwise coordinate x is the projection of all particles with streamwise coordinates less than x , onto a plane, accounting for overlap between the projections. We refer to the ratio of the non-occluded area to the total area as opacity, and compute it for the different geometries that we have used in the numerical simulations. Fig. 7 shows the opacity as a function of position inside the particle cloud, where each line is the mean of 8192 realizations. The dashed lines are the corresponding opacities by only requiring that the particles are completely inside the assigned domain. The opacity for the less restrictive distribution is always slightly higher than the opacity for our particle distribution. Our particle distributions are possible realizations of the less restrictive distribution, but as there is not too much overlap between the stan-

Fig. 7. Opacity for the different geometry parameters used in the simulations, as a function of distance into the particle cloud. The solid lines are the results for the particle drawing method used in this study and the dashed lines are the results for distributions without the inter-particle distance restriction. The shaded areas indicate the standard deviations for each line. The dotted lines indicate L_s for the different parameter combinations.

dard deviation regions, it is clear that they are very unlikely. Since our distribution occludes more of the area over a given distance, we expect slightly stronger shock reflection and a slightly weaker transmitted shock. The effect of the restriction that the particles should not overlap the spanwise domain boundaries is examined in Section 6.1. The result is that it increases the opacity, and is more important than the inter-particle distance. The results within this work should be interpreted with these effects in mind. Additionally, it must be emphasized that only a single realization of the particle distribution is used for the flow simulation for each parameter combination. We also note that the curves have slight bumps near $x = 0$ and $x/L = 1$, due to the constraints imposed on the particle distribution. We expect a similar effect for the distribution close to the spanwise domain boundaries.

The opacities for $\alpha_p = 0.01$, $D_p = 79.4 \mu\text{m}$ and $\alpha_p = 0.075$, $D_p = 57.2 \mu\text{m}$ are very similar. These parameter combinations also resulted in a very similar shock wave attenuation, which indicates that the opacity might be used to predict some properties of shock-wave particle cloud interaction. Since the opacity curves do not seem to intersect, we use the length at which the opacity equals 0.5 as a unique number that represents the opacity. We refer to it as the sight-length, and use the symbol L_s . The sight-length for each configuration is given in Table 1, and marked in Fig. 7 for the cases with $Ma = 2.6$. We see that this classification indicates that the parameter combinations $(\alpha_p, D_p) = (0.1, 79.4 \mu\text{m})$ and $(\alpha_p, D_p) = (0.075, 57.2 \mu\text{m})$ should be very similar, as we do observe. However, the results would indicate a larger difference between $(\alpha_p, D_p) = (0.1, 100 \mu\text{m})$ and $(\alpha_p, D_p) = (0.05, 50 \mu\text{m})$ than we observe. It should be noted that there is considerable standard deviation in the sight length because of the number of particles we use, so the apparent similarity between the latter two parameter combinations could be exaggerated by the specific particle distributions. A larger number of particles or an ensemble of simulations could be used to examine this in greater detail, but that is outside the scope of the current work.

The results indicate that it is possible to characterize some properties of shock wave particle cloud interaction using the sight-length. For this reason, we provide an algebraic expression that approximates this quantity in Section 6.1.

Fig. 8. Mean flow velocity with $Ma = 2.6$ and different particle sizes and volume fractions at $(t - t_0)/\tau_L = 0.5, 1.0, 1.5$ and 2.0 from left to right. The particle cloud is located between $0 \leq x/L \leq 1$.

Fig. 9. Mean flow velocity with $D_p = 100 \mu\text{m}$, $\alpha_p = 0.1$ and different incident shock wave Mach numbers at $(t - t_0)/\tau_L = 2$.

5.3. Mean flow

In this section we examine the flow field during and after the shock has passed through the particle cloud. The flow quantities are phase-averaged, or Favre-averaged where appropriate, over volumes spanning the domain in the y and z directions.

Fig. 8 shows the normalized velocity at $(t - t_0)/\tau_L = 0.5, 1.0, 1.5$ and 2.0 for the cases with $Ma = 2.6$. In the first two frames the shock wave is located inside the particle cloud. The reflected shock is visible as a sharp drop in velocity slightly before $x = 0$, and the recovery shock is present around $x/L = 1.1$ in the last two frames. For a given particle volume fraction, the reflected shock wave is stronger for smaller particles. This is expected based on the behavior of the primary shock discussed above, since there is a higher attenuation of the shock wave in these cases. At the upstream particle cloud edge, the mean flow speed increases rapidly over a distance equal to a few particle diameters and then has a gentler slope throughout the central region of the particle cloud. At the downstream particle cloud edge there is a strong flow expansion, and the flow speed roughly doubles over $0.9 \leq x/L \leq 1.05$ at late times. As seen in the two rightmost frames, the strength of the expansion increases with time after the shock has exited the particle layer. As noted in the discussion of grid-size above, the expansion region might be subject to non-continuum effects due to the increasing mean free path of the air molecules over the expansion

region. We obtain stronger expansions for higher volume fractions and smaller particles. Thus it might be necessary to account for non-continuum effects if the volume fraction is increased or the particle diameter is decreased. The flow speed varies with volume fraction and particle sizes in the same manner as the shock speed discussed above. Again we find that the parameter combinations $(\alpha_p, D_p) = (0.1, 79.4 \mu\text{m})$ and $(\alpha_p, D_p) = (0.075, 57.2 \mu\text{m})$ are approximately equal, but there are slight differences between these cases in the region upstream of the particle cloud and within the expansion region.

The variation of the mean velocity with incident shock wave Mach number is shown in Fig. 9. The normalized flow velocity within the particle layer decreases with increasing Mach number. However, the normalized velocity within a few particle diameters of the shock wave has a very weak dependence on the incident shock Mach number. The expansion region accelerates the flow to about $1.2u_{IS}$ in all cases, and therefore the relative strength of the acceleration is larger for stronger incident shock waves. The reflected shock has a larger jump in normalized velocity with increasing Mach number. We note that the strength of the reflected shock wave increases with time over the time-frame considered here (Vartdal and Osnes, 2018).

It is of interest to compare the results here to those obtained in the inviscid simulation in Mehta et al. (2018b). Fig. 10 shows the results from case V, with $(Ma, \alpha_p, D_p) = (3.0, 0.1, 100 \mu\text{m})$, at

Fig. 10. Comparison of normalized velocity for case V, with $(Ma, \alpha_p, D_p) = (3.0, 0.1, 100 \mu\text{m})$, and the inviscid simulations of Mehta et al. (2018b) at three times. Black lines are the results from the simulations in this work, and orange lines are the inviscid simulation results. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

three times and the corresponding results from the inviscid simulations of Mehta et al. (2018b) with the same incident shock wave Mach number and particle volume fraction. On a qualitative level, the two simulations agree quite well. However, there appears to be a non-negligible difference in the reflected shock strength between the inviscid and viscous simulations, where the viscous simulations feature a stronger reflected shock wave. We emphasize again that our particle configuration is slightly more regular than that in Mehta et al. (2018b), which we expect to affect the reflected shock strength. This was also observed when comparing the simulations of the inviscid face-centered cubic array in Mehta et al. (2016) to the random array. We also expect that the viscous effects increase the reflected shock strength, since there will be both stronger particle drag and also a much stronger effect of Reynolds stresses. The effect of the Reynolds stress will be discussed below.

The mean pressure and density profiles are shown for the different geometries in Fig. 11. Both quantities display much the same behavior as the velocity field. There is a rapid change around the upstream particle cloud edge, followed by an approximately monotonic decrease throughout most of the particle cloud until quite close to the shock wave position. For the cases shown here, the pressure tends to the same level around the downstream particle cloud edge, but the pressure drop over the expansion region is significantly smaller for the lowest volume fraction case. The density profiles intersect inside the particle layer, and the configurations with higher L_s have lower densities at low x and higher densities at higher x . It can be seen that the velocity, pressure and density profiles vary predictably with the sight-length. For lower L_s there is a higher mean velocity inside the particle layer, lower pressure and flatter density profiles. We find that case IX, with $(Ma, \alpha_p, D_p) = (2.6, 0.05, 50 \mu\text{m})$, deviates slightly from the trend observed for the other cases. This might indicate that some of the trends we observe may be slightly different at low volume fractions, or it may be an effect of the specific particle distribution.

Fig. 12 shows the local flow Mach number for the cases with incident shock wave Mach number 2.6. As we vary the particle volume fraction and particle diameters, we find, as expected, that the Mach number is lower for the cases where we observed a lower shock wave speed inside the particle layer. The Mach number stabilizes about $0.2L$ behind the shock wave, and has a slight positive gradient over the interior region of the particle cloud. The local Mach number drops to values around 0.5–0.6 for late times in these cases. However, it increases drastically over the expansion region, attaining values up to 1.4 in the latest frame shown here. The transition to supersonic flow happens about one or two particle diameters upstream of the downstream cloud edge.

Fig. 13 shows the local flow Mach number for the cases with $\alpha_p = 0.1$, $D_p = 100 \mu\text{m}$. When compared using the time-scale based on incident shock wave speed, we find that higher incident shock wave Mach numbers result in higher local Mach numbers within the particle cloud and downstream. The expansion region is stronger for higher Mach numbers, but it appears to converge for the highest values. However, when we compare the local Mach number at the same physical time, as shown in the lower panels,

Fig. 11. Mean flow pressure (top) and density (bottom) with $Ma = 2.6$ and different particle sizes and volume fractions at $(t - t_0)/\tau_l = 0.5, 1.0, 1.5$ and 2.0 from left to right. Line colors are as in Fig. 8.

Fig. 12. Local Mach number for different geometries with incident shock wave Mach number 2.6 at $(t - t_0)/\tau_L = 0.5, 1.0, 1.5$ and 2.0 from left to right. Line colors are as in Fig. 8.

Fig. 13. Local Mach number with varying incident shock wave Mach numbers with $\alpha_p = 0.1$ and $D_p = 100 \mu\text{m}$ at $(t - t_0)/\tau_L = 0.5, 1.0, 1.5$ and 2.0 from left to right (top). The bottom panels show the results at the same physical time, corresponding to using the τ_L scaling with $Ma = 2.6$, i.e. the same times as shown in Fig. 12. Line colors are as in Fig. 9.

we find that after the strong transient following the shock wave passage at each location, all the simulations attain the same local Mach number. We also see that the reflected shock wave has the same jump in Mach number for these simulations. In the expansion region, the results differ, and the increase in Mach number is much stronger for higher incident shock wave Mach numbers.

Regele et al. (2014) reported an average local Mach number about 0.4 for their inviscid two-dimensional simulations with a $Ma = 1.67$ shock wave and a particle volume fraction of 0.15. Our results indicate that the local Mach number does not depend much on the incident shock wave Mach number, but has a strong dependence on particle size. The lowest average Mach number within the cloud in our cases with $Ma = 2.6$ happens for $\alpha = 0.1$ and $D_p = 50 \mu\text{m}$, where the average value at late time is 0.55. We expect that, in addition to differences caused by the two-dimensionality, the regularity of the particle configuration in

Regele et al. (2014) strengthens the reflected shock wave and results in a lower local Mach number than for a random configuration.

In summary, we find that within the central part of the particle cloud, variation of mean flow properties with particle volume fraction and particle diameter is well represented by the sight-length, which characterizes the area blockage per distance. At the downstream edge, we observe a strong flow expansion, and we find that there is a region around the upstream cloud edge that behaves differently than the central region. In these regions, which have a streamwise extent of a few particle diameters, the behavior is not predicted by the sight-length. This is because the flow field fluctuations are dynamically important in these regions, and they depend differently on volume fraction and particle diameters than the mean flow fields. This will be further discussed in the next section.

Fig. 14. Normalized streamwise Reynolds stress for different particle sizes and volume fractions at $(t - t_0)/\tau_L = 0.5, 1.0, 1.5$ and 2.0 from left to right. Line colors are as in Fig. 8.

5.4. Velocity fluctuations

Fig. 14 shows the Reynolds stresses, $\tilde{R}_{ij}$, which are the single-point, density weighted (Favre averaged), velocity fluctuation correlations, i.e.

$$\tilde{R}_{ij} = \frac{\langle \rho u_i'' u_j'' \rangle}{\langle \rho \rangle}. \quad (11)$$

Only the streamwise component of the Reynolds stress enters the volume averaged momentum balance in this problem, but we plot the spanwise components as well since these contribute to the fluctuation kinetic energy. It can be seen that the Reynolds stress is higher at the upstream edge than in the interior of the particle cloud. It is also stronger close to the shock wave than further behind it. Upstream of the particle cloud it is zero as expected, except around the location of the reflected shock wave where the apparent Reynolds stress is an artifact of the volume averaging. The Reynolds stress is significantly higher at early times than late, and the relative magnitude does not follow the same trend as the mean fields. It has a strong dependence on the particle size, but also on the volume fraction, and it increases with both parameters. Notably, it does not vary with L_s in the same manner as the mean flow fields. This suggests that the characterization of the flow in terms of L_s only holds for a limited time, because the fluctuations should eventually affect the flow throughout the domain. In the two right-most frames, it can be seen that the Reynolds stress drops sharply over the downstream particle cloud edge. This is related to the fact that there are no longer any wakes further downstream, which are the primary contributions to the streamwise Reynolds stress in this flow. This will be discussed in more detail in Section 5.5 and Section 6.2. Similarly, the spanwise components drop because there are no particles to deflect the flow. While the Reynolds stress drops sharply, it does not vanish completely. This means that there are flow fluctuations that are advected downstream from the particle cloud.

It is worth noting the considerable magnitude of $\tilde{R}_{11}$. When scaled by twice the kinetic energy behind the incident shock wave, it reaches about 0.15 for a particle volume fraction of 0.1 for the early times, and decays to between 0.05 and 0.1 at the latest times shown here. The role of the Reynolds stress in the momentum balance is through streamwise gradients of $\tilde{R}_{11}$, and as can be seen in Fig. 14, the gradients are very sharp around the particle cloud

edges. We thus expect the Reynolds stress to play an important part of the mean flow dynamics in the regions around the upstream and downstream particle cloud edges.

The magnitudes of the spanwise components are less than half of that of the streamwise component. We note that the off-diagonal components of the Reynolds stress in this problem are zero since the problem is constructed to have no difference between the y and z directions, and no dependence on the y and z coordinates. The velocity fluctuations are therefore statistically axisymmetric, and the coordinate axes coincide with the principal axes of the fluctuations. Fig. 15 shows the Reynolds stress anisotropy,

$$b_{ij} = \tilde{R}_{ij}/\tilde{R}_{kk} - \delta_{ij}/3. \quad (12)$$

Since $\tilde{R}_{22} = \tilde{R}_{33}$, the anisotropy tensor satisfies $b_{ij} = 0$ if $i \neq j$ and $b_{22} = b_{33} = -b_{11}/2$. There is a strong anisotropy throughout the particle cloud, and it increases significantly with time. Where for the early time we observe that the maximal value of b_{11} is about 0.3, we find values as high as 0.4 around the upstream particle cloud edge at late times, and roughly 0.225 through most of the particle cloud. The streamwise fluctuation component increases faster with distance from the upstream edge than the other components, which ramp up over a distance of $0.2L$. We notice that the anisotropy increases towards the downstream particle cloud edge at late times, which is likely due to the strengthening of the flow expansion. This causes the difference between the velocity in the separated flow regions behind the particles in this region and the mean flow to increase, and since the spanwise fluctuations are not increased similarly, the anisotropy increases.

The importance of particle scale fluctuations in shock-wave particle-cloud interaction was previously examined in two-dimensional configurations using inviscid simulations by Regele et al. (2014), and viscous simulations by Hosseinzadeh-Nik et al. (2018), where the particle volume fraction was 0.15. Both studies featured a $Ma = 1.67$ shock wave, which is significantly weaker than the shock waves studied here. In the two-dimensional simulations, the intensity of the velocity fluctuations were comparable to the mean flow. In the inviscid simulations, the pseudo-turbulent fluctuations were approximately isotropic. Viscous effects preferentially reduced the fluctuation magnitude, with a larger reduction for the spanwise fluctuation component. An anisotropic behavior is therefore observed in both two-dimensional and three-dimensional

Fig. 15. Reynolds stress anisotropy for different particle sizes and volume fractions at $(t - t_0)/\tau_L = 0.5, 1.0, 1.5$ and 2.0 from left to right. Line colors are as in Fig. 8.

Fig. 16. Root-mean square of velocity fluctuations normalized by the mean flow density and velocity for the geometry variation at $(t - t_0)/\tau_L = 0.5, 1.0, 1.5$ and 2.0 from left to right. Line colors are as in Fig. 8, and the dashed lines are the spanwise velocity fluctuations.

viscous simulations, but the anisotropy is substantially stronger in the three-dimensional case.

The square root of the Reynolds stress, normalized by the mean flow velocity, is shown in Fig. 16 for both the Mach number variation and the geometry variation with $Ma = 2.6$. We note that we use bins that are longer in the streamwise direction than those used in the two-dimensional studies, which should result in larger velocity fluctuations. The normalized velocity fluctuations are insensitive to Mach number within the range we have investigated (results not shown). The streamwise fluctuation component is in addition insensitive to particle size, but the particle volume fraction has a considerable effect on the magnitude of the normalized fluctuations. By extrapolation of the trend observed with volume fraction increase, we would obtain normalized streamwise components between 0.5 and 0.6 for $\alpha_p = 0.15$ at late times, which is significantly lower than that reported in Hosseinzadeh-Nik et al. (2018). The results here differ from the previous studies which have examined fluctuations in the shock wave-particle cloud setting; we find lower fluctuation intensities than the two-dimensional studies, but significantly higher than reported for three-dimensional inviscid simulations (Mehta et al., 2018a). However, our results are quite close to that of Mehrabadi et al. (2015), who performed incompressible simulations of flow through particle suspensions up to Reynolds number 300. They reported a ratio of fluctuating to mean kinetic energy just above 0.2

for a particle volume fraction of 0.1 and a Reynolds number of 300. This ratio is slightly above 0.3 for our simulations at $\alpha_p = 0.1$, and we also know that it decays in time. In fact, since the local Mach numbers are not very high after about $1.5\tau_L$, it is not unreasonable to assume that the flow within the particle layer is dominated by incompressible flow phenomena after the shock-induced transients have passed.

5.5. Upstream edge momentum balance

The reflected shock is generated by the coalescence of the bow shocks from each particle, but it is sustained and strengthened by the forces acting on the flow by the particles over time. Capturing the reflected shock strength is essential for modeling shock wave particle cloud interaction since it determines the incoming flow field. If the reflected shock wave is not appropriately captured in a simulation, the mean flow fields downstream of it become incorrect, and properties such as particle drag will be computed from erroneous mean flow fields. Then only additional errors that can yield results that approximate experimental results, by introducing effects that act opposite the effect of the erroneous reflected shock wave. This situation is clearly not ideal, and we therefore stress the importance of the reflected shock wave. As will be shown, the Reynolds stress has an appreciable impact on the momentum balance around the upstream and downstream particle cloud edges.

Fig. 17. Momentum balance over time at $x/D_p \approx 2$. For $(t - t_0)/\tau_p < 3.5$ the data consist mostly of artifacts from volume averaging when the shock is within the averaging volume.

The Reynolds stress has traditionally been neglected in simulations of particle dispersion by shock waves. The results here indicate that assuming that the Reynolds stresses are negligible cannot be justified.

We investigate the process behind the generation of the reflected shock in detail by examining the volume averaged momentum balance around the front edge of the particle cloud. Fig. 17 shows the terms in Eq. (5) in a bin centered at $x/D_p \approx 2$ as a function of time for $(Ma, \alpha_p, D_p) = (2.6, 0.1, 63 \mu\text{m})$. The bin size is $L/60$, but the values are averaged over five bins so the values presented here are influenced by a volume spanning about $2.5D_p$ in the streamwise direction. The terms are normalized by

$$F_0 = (\rho u)_{IS}/\tau_p. \quad (13)$$

We choose to show the results for this particular parameter combination because it is in the middle of the range of incident shock wave Mach numbers and particle sizes we have simulated, and the observations made for this case are representative of the other cases. Until $(t - t_0)/\tau_p \approx 3.5$, the shock is within the region influencing this bin, and during this time, the results are dominated by artifacts from the averaging method. The most important processes occurring during this time are the shock wave reflections

by the particles within the bin. Since the reflected shock waves do not have time to interact with each other, except where the particles are very close to each other, the resulting flow field is essentially just a superposition of individual shock wave-sphere interactions. After the shock has passed out of the bin, we find that the momentum-balance can be split into two different time-intervals. In the first interval there is a transient in the strength and relative importance of the different terms in the volume averaged momentum equation. The second has a slow decay of the strength of all the terms over time. It can be seen that the largest terms are the pressure gradient and the drag on the particles. The Reynolds stress contribution is initially quite a bit lower than the particle drag and pressure gradient, but it decays less over time than the other terms. After the strong initial transient it becomes comparable to the particle drag.

An impression of the processes occurring during the first transient can be obtained using numerical schlieren images, as shown in Fig. 18. These images are of an xy-plane through the middle of the domain at $(t - t_0)/\tau_p = 2, 4, 8$ and 16. In the fourth image, the size and location of the averaging region used in Fig. 17 are indicated by the red dashed lines. The first time-interval, in which the strength of the momentum balance terms change quickly, is similar to the time-period spanned by these plots. During this time, there are numerous reflected shocks within the averaging volume, but they are almost completely gone at $(t - t_0)/\tau_p = 16$. As the reflected shocks from the particles propagate upstream, the pressure rapidly builds up upstream of the bin. Subsequently, the pressure within the bin builds up due to the bow-shocks from particles further downstream. This process causes the rapid change in pressure gradient around the minimum at $(t - t_0)/\tau_p \approx 8$. Over the same time, the mean flow velocity decreases, and therefore the magnitudes of the particle forces are reduced.

The build-up of particle wakes also occurs during this time period, as can be seen in Fig. 18. The particle wakes and the shock reflections are the main contributions to the velocity fluctuations within each bin, and thus make up the Reynolds stress in the volume averaged equations. Insight into which processes that contribute to the Reynolds stress can be obtained by consideration of the function $f(u_1'')$, defined as

$$\langle\rho\rangle\tilde{R}_{11} = \frac{1}{V_{\text{gas}}} \sum_{i=1}^{N_{\text{CV}}} (\rho u_1'' u_1'')^i V_{\text{CV}}^i \approx \int_{-\infty}^{\infty} f(u_1'') du_1''. \quad (14)$$

Here V_{gas} is the volume of the gas within the bin, N_{CV} is the number of control volumes in each bin, and the superscript i denotes

Fig. 18. Numerical schlieren-images on a slice through the middle of the domain for the case with $(Ma, \alpha_p, D_p) = (2.6, 0.1, 63 \mu\text{m})$ at times $(t - t_0)/\tau_p = 2, 4, 8$, and 16, from left to right. In the fourth image, the red dashed lines show the size and location of one of the averaging volumes used in the analysis of the flow field. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Fig. 19. Contour plot of the function f , as defined in Eq. (14), as a function of velocity fluctuation and time. The lower panel shows the total contribution to $\tilde{R}_{11}$ by positive and negative velocity fluctuations.

control volume number i . This function is the contribution to the streamwise Reynolds stress by streamwise fluctuations of a certain magnitude. Contours of f as a function of u_1' and time are shown in Fig. 19. The figure also shows the total contribution to the integral by positive and negative fluctuations. Until $(t - t_0)/\tau_p \approx 8$ there is a comparable contribution to $\tilde{R}_{11}$ by negative fluctuations with magnitudes from 100 m/s to 1000 m/s, due to shock wave reflection from the particles. There is also a narrow band of positive fluctuations making up about 30% of $\tilde{R}_{11}$. Later, the contribution by negative fluctuations are primarily by fluctuations between -200 m/s and -600 m/s. The very high fluctuation magnitudes can only be caused by the particle wakes, since at late times there are no longer any shocks within the particle layer. The lower panel shows that more than 70% of $\tilde{R}_{11}$ can be attributed to the negative fluctuations, and the percentage increases slowly with time. The contribution to $\tilde{R}_{11}$ from positive fluctuations are predominantly due to two effects. The first of these effects is the local flow acceleration around particles in regions where the local particle distribution is denser than average. The second effect is caused by the separation regions behind each particle, which when added together amount to quite large regions with very low flow speeds. These regions shift the average velocity away from the “free” flow velocity. As a consequence, there are very few regions in the flow which have velocities equal to the mean velocity, and this results in contributions to $\tilde{R}_{11}$ from regions of smooth “free” flow. This has consequences for modeling since the mean slip velocity, if assumed to be equal to the volume-averaged velocity, is lower than it should be. There is a similarity between this problem and the self-induced flow disturbance problems examined in (Horwitz and Mani, 2016; Balachandar et al., 2019), in the sense that flow disturbance induced by the particle, i.e. the separated flow, affects how particle drag should be calculated. In Section 6.2, we propose a simple model for the Reynolds stress that also provides a ratio of the average flow speed to the free flow speed. The free flow speed is higher than the average flow speed, and it may be more suitable for calculating particle drag.

It is clear that the momentum balance around the upstream particle cloud edge has strong contributions from both particle drag and Reynolds stress. Together these balance about two-thirds of the pressure gradient. The (time-dependent) strength of the reflected shock wave thus depends strongly on the particle forces and the velocity fluctuations caused by shock wave reflection and flow separation. In Eulerian–Lagrangian or Eulerian–Eulerian meth-

ods, these quantities require careful modeling so that the reflected shock wave, and therefore the incoming flow, is correct. The viscous simulations show fluctuations with much higher magnitudes than inviscid simulations because of flow separation. Therefore viscosity has an appreciable effect on the reflected shock strength.

5.6. Particle drag

The forces acting on the particles are one of the most important aspects in modeling of dispersed flows when the particle relaxation time is large compared to the mean flow time scale. The initial force history, and the distribution of peak drag coefficients, in shock wave particle cloud interaction has been characterized in Mehta et al. (2018b). Theofanous et al. (2018) performed particle-resolved inviscid simulations with an immersed boundary method, and found a dispersive behavior at the downstream end of the particle cloud, in agreement with experimental results. They also pointed out that the opposite behavior is typically seen in Eulerian–Lagrangian or Eulerian–Eulerian simulations of shock-wave particle interaction, i.e. a particle accumulation at the downstream edge. Those previous studies both utilized inviscid simulations. It is clear from the discussion above that viscous effects affect the flow field. The particle wakes in particular differ in viscous and inviscid simulations, and therefore the particle forces differ after the particle wake has developed. For this reason, we examine the particle drag during the time where the particle wakes have developed.

The particle drag coefficient is defined as

$$C_d = \frac{\int_{S_i} (p + \sigma_{1k}) n_k dS_i}{0.5 \langle \rho \rangle \tilde{u}_i^2 A_p}, \quad (15)$$

where A_p is the projected area of the particle in the direction of the flow, and S_i denotes the surface of the particle. The time-averaged drag-coefficient, averaged in time starting at $0.5\tau_L$ after the shock wave has passed, is shown in Fig. 20 for $(Ma, \alpha_p, D_p) = (2.6, 0.1, 63 \mu\text{m})$ as a function of position. The drag coefficient increases slowly with distance throughout the particle cloud, until about $x/L = 0.9$, where the drag coefficient abruptly increases and reaches a maximum of 2.25. While the average drag coefficient increases with distance, the averaged particle forces decrease with distance, because the kinetic energy of the flow decreases with

Fig. 20. Black disks: time-averaged drag-coefficients over the time interval after $0.5\tau_L$ after the shock wave has passed each particle in the case with $(Ma, \alpha_p, D_p) = (2.6, 0.1, 63 \mu\text{m})$ as a function of position. Solid red line: mean flow Mach number at $(t - t_0)/\tau_L = 2$. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Fig. 21. Total force exerted on the particles per unit volume at $(t - t_0)/\tau_L = 0.5, 1.0, 1.5$ and 2.0 , for $Ma = 2.6$ and the different geometries (top), and different Mach numbers for $\alpha_p = 0.1$, $D_p = 100 \mu\text{m}$ (bottom). Line colors are as in Figs. 8 and 9.

distance. Similarly, Mehta et al. (2018b) found that the peak particle forces decrease with distance within the particle cloud. So for most of the particle layer, the peak acceleration and the averaged forces decrease with distance. There is a slight difference between the very first particles and those a bit further in, because the first particles are exposed to the smooth incident flow rather than the chaotic flow further inside the particle cloud. The abrupt increase in drag-coefficient around the downstream edge can be explained by looking at the mean flow Mach number, which is shown as a red line in Fig. 20. The increase in drag-coefficient coincides with an increase in local Mach number as the flow expands and becomes supersonic. The abrupt increase in drag in the transonic region is consistent with previous findings that have examined single-particle drag as a function of Mach number (Bailey and Hiatt, 1971; Nagata et al., 2016). We obtain significantly higher drag coefficients than reported in those single-particle studies. The wide distribution of drag coefficients is caused by the random particle distribution, which creates local flow acceleration and deceleration. However, only the minimal drag coefficients we obtain are close to those reported in the mentioned studies, so there is a clear difference between isolated particle drag and the drag within a particle cloud. However, in Section 6.2 we propose a correction to the particle drag. Using this correction, the particle drag coefficients are reduced, which brings them closer to the single particle drag-coefficients.

The total streamwise forces exerted on the particles per unit volume, normalized by post-shock momentum per τ_L , i.e.

$$F_p = \frac{\tau_L}{V(\rho u)_{IS}} \int_S p n_1 + \sigma_{1k} n_k dS, \quad (16)$$

as a function of distance at $(t - t_0)/\tau_L = 0.5, 1.0, 1.5$ and 2.0 , is shown in Fig. 21. The particle force per unit volume increases with increasing particle volume fraction and with decreasing particle diameter. The variation with particle volume fraction is stronger than with particle size within the range we have simulated. The particle force is significantly higher at early times than late. Furthermore, it increases drastically at the downstream cloud edge at late times. The exception to this trend is the case with $(Ma, \alpha_p, D_p) = (2.6, 0.05, 50 \mu\text{m})$. In that case, which has the lowest particle volume fraction, and the smallest particles, the increase at the

downstream edge is quite moderate. The variation with incident shock wave Mach number is shown in the lower panels of Fig. 21. As the Mach number is increased, the particle forces increase, and when normalized by post-shock momentum and a time-scale based on the shock speed, the forces are very similar, especially at the later times.

6. Modeling

In this section, we propose two algebraic models based on the observations made in the preceding sections. The first model is for the sight-length, and can be used to estimate combinations of α_p and D_p that behave similarly. We also use this model to quantify the effect of the regularity of the particle distribution used in the flow simulations. The second model is an algebraic, single-parameter expression for the streamwise Reynolds stress. It reliably predicts the streamwise Reynolds stress intensity over time for all the simulations in this work. Accurate Reynolds stress models are important in Eulerian–Lagrangian and Eulerian–Eulerian models for dispersed flow, due to the importance of the fluctuations in the flow dynamics.

6.1. Sight-length

Based on the results presented in Section 5.2, we found that the shock wave attenuation throughout the particle cloud could be well characterized by the sight-length. Simulations with similar sight-lengths had similar shock wave attenuation over a given distance. Many of the mean flow quantities were also found to be predictable based on the sight-length. We thus seek an expression for the sight length in terms of the particle volume fraction and the particle diameter. To this end, we compute the sight-length for a range of particle volume fractions between 0.05 and 0.1 and particle sizes between $50 \mu\text{m}$ and $100 \mu\text{m}$, by sampling the particle distribution 10,240 times for each parameter combination. We fit a model on the form

$$L_s = (A + B/\alpha_p) D_p, \quad (17)$$

where A and B are the model constants to be fitted to the data. We do this using a non-linear least squares method. This model

Table 2

Best fit for the constants A and B in Eq. (17) with and without restrictions on inter-particle distance and spanwise domain boundaries.

Restrictions	A	B
Inter-particle distance and spanwise boundaries	−1.012	0.4775
Inter-particle distance	−0.5191	0.4098
Spanwise boundaries	−0.5313	0.4703
None	−0.3317	0.3957

Fig. 22. Sight-length into the particle cloud for various particle sizes and particle volume fractions. The black lines are data contour lines, while the white dashed lines are the corresponding contours of Eq. (17).

form goes to infinity as the particle volume fraction goes to zero, and to 0 for a particle volume fraction of $\alpha_p = |B/A|$. The model is however not intended for volume fractions outside the range studied in this work, and so the latter limit is of little consequence. To quantify the effect of the additional constraints we have put on the particle distribution, we also sample the particle distributions in a much larger spanwise domain and compute the sight-length in a subset of this larger domain. We refer to this setting as having no spanwise domain boundaries. The width and height of the subset are $8\sqrt{4}D_p$, as in the flow simulations. We also remove the restriction on the inter-particle distance with and without spanwise domain boundaries. The best fit for the different combinations of restrictions are given in Table 2. Fig. 22 shows a contour plot of the resulting sight-lengths for the range of particle volume fractions and particle diameters we use in the flow simulations. The figure also shows the contour lines of Eq. (17) with the model constants when all particle distribution restrictions are applied. The model fits the data with a maximal relative error of 1.5%, and the maximal errors occur for low particle volume fraction and low particle diameter. Within the range of volume fractions we have simulated, the longest sight length is obtained with spanwise boundaries and no restriction on inter-particle distance. Compared to the case without restrictions, the case with spanwise boundaries has 17% longer sight-length at $\alpha_p = 0.05$ and 15% longer at $\alpha_p = 0.1$. The inter-particle distance changes the sight-length with just 1% at both ends of the volume fraction range. When both restrictions are combined, the sight-length is increased by 13% at $\alpha_p = 0.05$ and by less than 1% at $\alpha_p = 0.1$. Overall, the effect of the slightly increased regularity of the particle distribution is to increase the sight-length, but the effect is not very strong. When the particle volume fraction is doubled, the sight-length is almost halved. Therefore, variation of the sight length with changes in particle volume fraction is much more important than the variation with particle distribution restrictions used here.

6.2. Modeling the streamwise Reynolds stress

In this section we propose a model for the streamwise Reynolds stress based on the observations made in Section 5.5. Most importantly, we found that the Reynolds stress is caused mainly by separated flow behind the particles.

The gas within a separation region behind a particle has a velocity about the same as the particle, which in our case is zero. This is a few hundred m/s lower than the mean flow speed, and therefore the contribution to $\bar{R}_{11}$ by separated flow regions will quickly become very large with increasing volume of the separation region. A simple model for this effect is the following: We assume that the separation region can be approximated as a region with velocity equal to the particle velocity. The rest of the volume then contains gas with an average velocity that is higher than $\tilde{u}$, and related to $\tilde{u}$ by a function of the volume of the separated flow. The sum of the volume of separated flow regions within a bin occupies a fraction of the volume which we denote by α_{sep} . If the mean velocity in the bin is known, in absence of any other sources of Reynolds stress, the streamwise velocity correlation is given as

$$\langle u''_1 u''_1 \rangle = \tilde{u}_1^2 \frac{\alpha_{sep}}{\alpha - \alpha_{sep}}. \quad (18)$$

Here, α_{sep} is the volume fraction of the separation regions, which is a function that must be determined. These assumptions also imply that the mean velocity in the rest of the gas volume is

$$u_{free} = \tilde{u}_1 \frac{\alpha}{\alpha - \alpha_{sep}}. \quad (19)$$

We further assume that the triple-correlation part of

$$\bar{R}_{11} = \langle u''_1 u''_1 \rangle + \langle \rho' u''_1 u''_1 \rangle / \langle \rho \rangle, \quad (20)$$

is negligible, in line with the principle of receding influence, so that $\bar{R}_{11}$ is directly given by Eq. (18). We evaluate α_{sep} for the various simulations at every location between $0.2 \leq x/L \leq 0.8$, for the time interval between $15\tau_p$ after the shock has passed that location until the end of the simulation. This time-delay is introduced so that the shock-induced transient does not affect the results. The average separation volume fraction for each simulation is given in Table 3. It was found to be insensitive to the location within $0.2 \leq x/L \leq 0.8$, and insensitive to the incident shock wave Mach number. It varies slightly with particle diameter and drastically with volume fraction, which is to be expected. The ratio α_{sep}/α_p increases significantly as α_p is reduced. This is likely caused by the increasing inter-particle distance, which allows the separation regions to develop with less disturbances than for higher particle volume fractions. Fig. 23 shows the normalized Reynolds stress obtained in the simulations, averaged over $0.2 \leq x/L \leq 0.8$ as a function of time, and the Reynolds stress computed from Eq. (18). The model captures the magnitude and general trend of the Reynolds stress well. In each case, there is a transient during and slightly after the shock wave passes through the particle cloud that the model does not represent. During this time, the shock reflection from individual particles comprise a significant portion of the observed Reynolds stress. Since the Reynolds stress model represents the effect of particle wakes only, we expect a deficiency when shock-reflection is still occurring. Fig. 23 does indeed show that between $0.5 \leq (t - t_0)/\tau_L \leq 1.5$ the observed Reynolds stresses are higher than the model predicts. However a large portion of the Reynolds stress is also captured during this phase, because particle wakes develop for a large number of the particles before the shock exits the particle cloud. The model also increases too rapidly early on, since it is directly proportional to the mean velocity, while the separation regions take some time to develop. This model

Table 3
Volume fraction of separated flow, α_{sep} , for the various simulations in this study.

Case	(Ma, α_p, D_p)	α_{sep}	Case	(Ma, α_p, D_p)	α_{sep}
I	(2.2, 0.1, 100 μm)	0.152	VII	(2.6, 0.1, 63.0 μm)	0.142
II	(2.4, 0.1, 100 μm)	0.152	VIII	(2.6, 0.075, 57.2 μm)	0.131
III	(2.6, 0.1, 100 μm)	0.153	IX	(2.6, 0.05, 50 μm)	0.115
IV	(2.8, 0.1, 100 μm)	0.153	X	(2.2, 0.1, 50 μm)	0.148
V	(3.0, 0.1, 100 μm)	0.152	XI	(2.6, 0.1, 50 μm)	0.148
VI	(2.6, 0.1, 79.4 μm)	0.152	XI	(3.0, 0.1, 50 μm)	0.148

Fig. 23. Normalized streamwise Reynolds stress averaged over $0 \leq x/L \leq 0.8$, as a function of time for the simulations with $\alpha_p = 0.1$, $D_p = 100 \mu\text{m}$ (left) and $Ma = 2.6$ and various geometries (right). Line colors are as in Figs. 8 and 9. Dashed lines are the corresponding fluctuations computed from Eq. (18).

apparently captures the majority of the Reynolds stress, but it does not represent flow structures that are not associated with the particles, such as vortices being advected by the flow. We thus expect that the volume fractions reported in Table 3 are slightly too high. Additional models should be used to capture the other phenomena causing velocity fluctuations. The model represents the velocity fluctuations caused by the separated flow regions behind each particle, and the additional velocity “fluctuations” that appear since the averaged flow velocity is shifted away from the free flow speed.

As a Reynolds stress model to be used in Eulerian–Lagrangian simulations of shock particle interaction, the form of Eq. (18) is attractive, since it can be associated with the Lagrangian particles. It does not involve any gradient operations or additional interpolations than what must be used to compute particle drag. However, in Eulerian–Lagrangian simulations, the model is limited to situations where the control volumes are considerably larger than a single particle.

The assumptions made about the flow in the immediate proximity of the particles in the derivation of Eq. (18) has implications for the calculation of particle drag. The model for $\tilde{R}_{11}$ suggested above showed that between 10% and 15% of the volume could be considered to belong to separation regions. We assumed that the average velocity of a separation region was zero. The large volume in these separated flow regions means that the average velocity is not the appropriate velocity to use for computing the drag. If u_{free} is used instead of $\tilde{u}_1$ to compute the drag coefficient, it will be lower than if it is computed directly from $\tilde{u}_1$. The velocity correction factor is $\alpha/(\alpha - \alpha_{\text{sep}})$, and since the denominator in Eq. (15) contains $\tilde{u}_1^2$, the drag coefficient becomes about 30% lower when we include this correction. The model also implies a correction to the free flow Mach number, since the Mach number is proportional to $\tilde{u}_1$. Standard drag laws correlate the particle forces to the undisturbed flow quantities, but since the notion of an

undisturbed flow is meaningless inside a particle cloud, it is still an open question how to calculate drag in Eulerian–Lagrangian models. However, this model does partly explain why the average drag coefficients appear to be very high in this flow.

The Reynolds stress model, based on an assumed separated flow in the particle wake with a given volume and an average velocity of zero, approximates the bulk streamwise Reynolds stress well. It is easily applicable in both Eulerian–Lagrangian and Eulerian–Eulerian models of dispersed flow, and only needs an estimate of α_{sep} , since the other model inputs are already known. The model implies corrections to mean flow properties, due to the non-negligible volume fraction of the separated flow. It is clear that improvements to this model can be obtained by detailed examination of the statistical properties of particle wakes in the shock particle setting, and this is a possible direction for future work.

7. Concluding remarks

In this work, we have investigated the flow fields during the passage of a shock wave through a random array of particles, using viscous three-dimensional numerical simulations. The flow field variation with different incident shock wave Mach numbers, particle volume fractions and particle diameters was investigated using the volume averaging framework. It was found that many mean flow features could be predicted based on the sight-length, which relates particle volume fractions and particle diameters. Flows at a given particle volume fraction were found to have many similarities to higher or lower particle volume fractions if the particle diameter was increased or decreased so that the sight-length remained the same. This characterization was found to work best within the interior of the particle layer. At the upstream and downstream particle cloud edges, we found that flow field fluctuations play an important role in the mean flow dynamics. The variation of

the fluctuations was not found to be predicted by the sight-length parameter. In agreement with this, we observed that the quantities that varied predictably with sight-length in the interior of the particle cloud did not follow the same variation at the edges.

The regularity of the particle distribution has a non-negligible effect on the flow. This work utilized structured meshes around each particle, in order to best facilitate the prediction of the viscous shear layers. For this reason, a slightly increased regularity of the particle distribution was necessary. In the cases considered in this work, the regularity increased the sight-length. However, the change in sight-length due to regularity was found to be small compared to the change when the particle volume fraction was varied. In general, the specific realization of any particle distribution plays a role in the flow statistics, unless the number of particles in the spanwise directions is very large. Ensemble averaging can serve as a substitute for large computational domains, and is therefore recommended for future works.

We observed that the flow expansion at the downstream edge of the particle cloud featured an increase in the mean free path of the air molecules. For the case with a $Ma = 2.6$ incident shock wave, $\alpha_p = 0.1$ and $D_p = 63 \mu\text{m}$, we found that the Knudsen number of the local shear flow attained values above one around the particles furthest downstream. Different combinations of volume fractions and particle sizes might result in situations where non-continuum effects become significant, and should be treated carefully.

The Reynolds stress was found to be dynamically important at the particle cloud edges. The magnitudes of the Reynolds stresses were significantly higher than those found in the inviscid simulations of Mehta et al. (2018a). Since the flow dynamics around the upstream particle cloud edge affect the reflected shock, this implies that the reflected shock is strengthened due to viscous effects. Around the particle cloud edges, the Reynolds stress gradients were of the same order as the particle forces. The Reynolds stress is caused primarily by shock wave reflection and separated flow behind the particles. It contains a significant part of the kinetic energy of the flow, and it is strongly anisotropic. Based on which physical phenomena that are the causes of the Reynolds stress, we proposed an algebraic Reynolds stress model. It uses the mean flow speed and the particle volume fraction, in addition to an estimate of the volume fraction of separated flow. The model could predict the magnitude of the Reynolds stress and its evolution in the interior of the particle cloud fairly well. By comparison to previous particle-resolved studies, the pseudo-turbulent kinetic energy magnitude was found to be more similar to results from incompressible simulations than to the results from previous shock wave particle cloud simulations. The previous shock wave particle cloud simulations were either inviscid or two-dimensional, and this has strong implications for the fluctuations within the particle cloud. We also found that the local Mach number was not very high within the particle layer after the shock-induced transient had ended. These observations suggest that the dynamics governing the flow fluctuations in the interior of the particle cloud are primarily incompressible flow phenomena.

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Chapter 10

Paper IV

IV

Particle-resolved simulations of shock-induced flow through particle clouds at different Reynolds numbers

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This study investigates the Reynolds-number dependence of shock-induced flow through particle layers at 10% volume fraction, using ensemble-averaged results from particle-resolved large eddy simulations. The advantage of using large eddy simulations to study this problem is that they capture the strong velocity shears and flow separation caused by the no-slip condition at the particle surfaces. The shock particle cloud interaction produces a reflected shock wave, whose strength increases with decreasing particle Reynolds number. This results in important changes to the flow field that enters the particle cloud. The results show an approximate proportionality between the mean flow velocity and the flow fluctuation magnitudes. Maximum particle drag forces are in excellent agreement with previous inviscid studies, and we complement these results with statistics of time-averaged particle forces as well as the variation of temporal oscillations. The results of this work provides a basis for development of improved simplified dispersed flow models.

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I. INTRODUCTION

Interactions between shock waves and dense suspensions of particles occur in many engineering applications and industrial processes. Some examples are liquid and solid fuel engines^{7,12,32}, heterogeneous explosives⁴⁸, blast mitigation^{8,25} and dust-explosion safety measures³⁸. Natural occurrences of shock-wave particle cloud interactions include volcanic eruptions⁹ and supernovae^{17,39}.

The process of shock wave particle cloud interaction has recently received attention in both experimental^{13,42,46} and numerical studies^{16,20,37,40,41}. Numerical studies have primarily utilized two different approaches. The first type employs Eulerian-Eulerian or Eulerian-Lagrangian methods to simulate flows with a large number of particles. The model equations are formulated to account for the volume and density of the dispersed phase. There are numerous issues with such simplified dispersed flow models, such as non-hyperbolic equation sets, as discussed in Lhuillier et al.¹⁹, Theofanous and Chang⁴¹. The second approach circumvents these problems by utilizing particle-resolved simulations. This is the method utilized in this study. Particle-resolved simulations are valuable because they provide highly resolved data, in both space and time, which enables a comprehensive analysis. The primary limitation of such simulations is that only small-scale problems are computationally feasible.

There is a considerable body of work investigating shock wave particle cloud interaction using particle-resolved inviscid simulations^{22–24,31,36,43}. The number of studies that have included viscous effects in such simulations is, however, limited. Particle-resolved studies that have included viscous effects are, e.g., the two-dimensional simulations of Hosseinzadeh-Nik et al.¹⁵, Naiman and Knight²⁸ and the three-dimensional simulations of Osnes et al.²⁹, Vartdal and Osnes⁴⁵. Viscous effects have not been analyzed directly in experimental studies either. There is, however, a moderate range of particle Reynolds numbers Re_p where experimental results exist. Based on the shock wave strength, the particle Reynolds numbers in Wagner et al.⁴⁶ are approximately 2650 – 4200. The study of DeMauro et al.¹³ spans $Re_p \approx 900 - 5700$, whereas Theofanous et al.⁴² investigated configurations in the range $Re_p \approx 7000 - 70000$. Since these studies vary Reynolds number simultaneously with Mach number and ratio of layer thickness to particle diameter, isolating the Reynolds-number effects is difficult.

The Reynolds number is a measure of the relative importance of inertial to viscous forces

within the flow. Viscosity has an effect on the flow field even at very high particle Reynolds numbers, as long as the flow remains in the continuum regime. In particular, viscous effects are responsible for flow separation behind particles. This is in fact an important phenomenon in shock wave particle cloud interaction, as will be shown in this study.

This study considers particle Reynolds numbers in the range $500 - 10000$. In incompressible, single-particle flows, this particle Reynolds number range spans three different flow regimes, by their definitions in Tiwari et al.⁴⁴. These flow regimes are commonly labeled the vortex shedding regime ($270 \leq Re_p \leq 800$), the separating vortex regime ($800 < Re_p \leq 3000$), and the sub-critical regime ($3000 < Re_p < 3.4 \times 10^5$). Sakamoto and Haniu³⁴ discusses the flow properties over this range and draws the following conclusions. In the vortex shedding regime, laminar vortices are shed periodically. Above $Re_p = 800$, vortex tubes and vortex loops are formed in the vortex sheet, and can interact with the large scale laminar vortices, introducing irregularity in the vortex shedding. Above $Re_p = 3000$, the vortex sheet becomes turbulent, and the turbulence intensity increases with Re_p . As a result of this, the Strouhal number, i.e., the non-dimensional vortex shedding frequency, decreases with Reynolds number. At $Re_p = 6000$ and above, the vortex sheet is fully turbulent and the Strouhal number is approximately constant.

Compressible flows over isolated particles in this Reynolds number range have not received nearly as much attention. Nagata et al.^{26,27} investigated $50 \leq Re_p \leq 1000$. Notably, the drag coefficient increases by more than a factor of two when the flow goes from subsonic to supersonic in this Re_p range. The Mach number, Ma , also has a stabilizing effect on the flow, and Nagata et al.²⁷ found that at $Ma = 2$ the flow is stable to at least $Re_p = 1000$.

It is not straightforward to apply these findings to shock-wave particle cloud interaction. Importantly, the incident flow becomes subsonic due to the generation of a planar, upstream propagating, reflected shock^{4,13,46}. The strength of this shock determines which flow conditions the particles are exposed to, and these flow conditions define a particle Reynolds number and a local Mach number that is not known *a priori*. These parameters are likely more appropriate for classification of the flow through the particle cloud after the initial shock-induced transient than the ones based on flow properties behind the incident shock. Additionally, the flow Mach number increases with downstream distance within the particle cloud^{29,31,43} in a manner similar to that observed in Fanno flows¹⁴. The presence of nearby particles also affects the flow around each particle by changing the direction of the incoming

flow, exposing it to particle wakes, etc.

As will be shown in this study, the particle Reynolds number affects the level of particle-scale fluctuations within the particle cloud. These fluctuations are defined here as the deviations from the volume averaged velocity, and need not be turbulent fluctuations; a laminar particle wake generates significant fluctuations. When the particle concentration increases, the impact of the wake-induced fluctuations also increases. In particular, particle wakes start to comprise a significant part of the volume within the cloud. This causes a problem for models based on volume averaging. The volume averaged velocity is shifted towards the average particle velocity, and as a result, it represents neither the flow in immediate proximity of each particle, nor the freer flow between them. In the current work, we explore what this means for the fluctuation levels and particle drag coefficients.

The current study is concerned with how the particle Reynolds number affects shock-wave particle cloud interaction. To this end, we perform particle resolved, three-dimensional, viscous simulations of the passage of a shock wave through a particle layer with volume fraction 0.1. The particle positions are assumed to be fixed over the time frame considered. We examine shock wave attenuation and reflection, mean flow fields and fluctuation statistics. We also explore the Reynolds number dependence of forces acting on the fixed particles, including both maximal values, time-averages and distributions of the drag coefficients. The results from the current study are important as a baseline for development of closures for simplified dispersed flow models, as well as the formulation of particle force models for shock-wave particle cloud interaction.

This paper is structured as follows. In section II we describe the equations governing the flow through the particle cloud, the mathematical framework used in the flow analysis and the computational method. Section III specifies the problem under investigation. The simulation results are presented and discussed in section IV, and section V contains concluding remarks.

II. GOVERNING EQUATIONS AND COMPUTATIONAL APPROACH

The motion of the fluid is governed by the compressible Navier-Stokes equations, which can be written

$$\partial_t \rho + \partial_k (\rho u_k) = 0, \tag{1}$$

$$\partial_t (\rho u_i) + \partial_k (\rho u_i u_k) = -\partial_i p + \partial_j \sigma_{ij}, \quad (2)$$

$$\partial_t (\rho E) + \partial_k (\rho E u_k + p u_k) = \partial_j (\sigma_{ij} u_i) - \partial_k (\lambda \partial_k T), \quad (3)$$

where $\rho(\mathbf{x}, t)$ is the mass density, in which $\mathbf{x}$ is the spatial coordinate vector and t denotes time, $u(\mathbf{x}, t)$ is the velocity, $p(\mathbf{x}, t)$ is the pressure, $\sigma_{ij}(\mathbf{x}, t) = \mu(\partial_j u_i + \partial_i u_j - 2\partial_k u_k \delta_{ij}/3)$ is the viscous stress tensor, $\mu(\mathbf{x}, t)$ is the dynamic viscosity, $E(\mathbf{x}, t) = \rho e + 0.5\rho u_k u_k$ is the total energy per unit volume, $e(\mathbf{x}, t)$ is the internal energy per unit mass, $\lambda(\mathbf{x}, t)$ is the thermal conductivity, and $T(\mathbf{x}, t)$ is the temperature. Here, ∂_t denotes partial differentiation with respect to time and $\partial_{i,j,k}$ denotes partial differentiation with respect to space. The subscripts denote tensor components, and repeated indices imply summation from 1-3. Internal energy, pressure and density are related by the ideal gas equation of state, with $\gamma = 1.4$. Temperature and internal energy are related by a constant specific heat capacity. We assume that the viscosity varies with temperature as $\mu(\mathbf{x}, t) = \mu^0 (T/T^0)^{0.76}$, where μ^0 is the viscosity at $T = T^0$. We further relate the thermal diffusivity to the viscosity through a constant Prandtl number of 0.7.

The analysis in this work is based on the volume averaged momentum conservation equations. A discussion of volume averaging for flows containing particles can be found in, e.g., Crowe et al.¹¹, Schwarzkopf and Horwitz³⁵. Since the configuration is statistically one-dimensional in space, only the streamwise momentum equation is relevant. It can be expressed

$$\begin{aligned} \partial_t (\alpha \langle \rho \rangle \tilde{u}_1) + \partial_x (\alpha \langle \rho \rangle \tilde{u}_1 \tilde{u}_1 + \alpha \langle p \rangle) &= \partial_x (\alpha \langle \sigma \rangle_{11}) \\ -\partial_x (\alpha \langle \rho \rangle \tilde{R}_{11}) + \frac{1}{V} \int_S p n_1 dS - \frac{1}{V} \int_S \sigma_{1k} n_k dS, \end{aligned} \quad (4)$$

where α is the gas volume fraction, $\tilde{R}_{ij}(\mathbf{x}, t) = \widetilde{u_i'' u_j''}$ is the velocity fluctuation correlation tensor, V denotes the averaging volume, n is the normal vector pointing into the continuous phase, and S denotes the continuous phase boundary. Here, $\langle \cdot \rangle$ denotes a phase average, $\tilde{\cdot}$ denotes a Favre average, and fluctuations from the Favre average are denoted $''$. Furthermore, we denote the fluctuating kinetic energy per unit volume, $\langle \rho \rangle \tilde{R}_{ii}/2$, by k , and mean kinetic energy per unit volume by K . The particle volume fraction is denoted by α_p .

In the analysis of the computational results, the temporal evolution is discussed in terms of a time-scale related to the passage of the shock through the particle layer. This time-scale is

$$\tau_L = L/u_s, \quad (5)$$

where u_s is the speed of the incident shock wave and L is the length of the particle cloud. Furthermore, we use t_0 to denote the time point when the shock wave is at $x = 0$.

The particle drag coefficient will be used in the discussion of particle forces. It is

$$C_D = \frac{\int_{S_p} (pn_1 - \sigma_{1k}n_k) dS}{0.5\langle\rho\rangle\tilde{u}_1^2 A_p}, \quad (6)$$

where S_p is the particle surface and A_p is the projected area of the particle in the flow direction.

A. Computational method

The present simulations are conducted using the compressible flow solver "CharLES"⁶, developed by Cascade Technologies. The compressible, filtered, Navier-Stokes equations are solved on an unstructured Voronoi-based grid⁵. CharLES is a finite volume large-eddy simulation code. It computes fluxes between control volumes based on an entropy-stable modified Lax-Friedrich flux. A more detailed discussion of the entropy stable scheme can be found in Masquelet et al.²¹. A third order explicit Runge-Kutta scheme is applied to advance the solution in time.

III. SET-UP AND COMPUTATIONAL GRID

We consider the interaction between a planar shock wave and a cloud of particles at different Re_p . Figure 1 shows a sketch of the computational set-up. The computational domain is $-0.9L \leq x \leq 2L$, $0 \leq y \leq 8\sqrt[3]{4}D_p$ and $0 \leq z \leq 8\sqrt[3]{4}D_p$, where D_p is the particle diameter. The particles are located within $0 \leq x \leq L$, and the particle volume fraction is 0.1. In all configurations, the length of the particle layer and the particle diameter are related by $L = 12\sqrt[3]{16}D_p$. The particles are drawn randomly within this range, and we require that no particle boundary extends outside $0 \leq x \leq L$. The minimum distance between each particle is set to roughly $0.05D_p$. The shock wave position is initially $-0.1L$, and is indicated by the thick line in the figure. Its direction of propagation is from left to right.

The computational grid is an unstructured Voronoi-based grid, which is body-fitted to the particles. We use three different refinement levels, as indicated by the roman numerals in fig. 1. Refinement level I has control volumes eight times larger (by volume), than level II,

FIG. 1. Sketch of the computational set-up and domain. The particle layer is located between $0 \leq x \leq L$, where the particle volume fraction is $\alpha_p = 0.1$. The thick solid line indicates the initial position of the shock wave, and the arrow shows its propagation direction. The roman numerals indicate the level of grid refinement, where the control volumes in region I are eight times larger than those in region II, and those in region II are again eight times larger than those in region III (by volume). The dashed lines indicate the boundaries between the refinement levels. Note that the vertical axis has been stretched for illustration purposes.

and similarly for levels II and III. The length scale of the smallest control volumes (level III) is roughly $0.036D_p$. Due to the density of the particles, most of the region $0 \leq x \leq L$ contains level III control volumes. The total number of control volumes is roughly 10^8 . The control volume sizes are similar to those used in Osnes et al.^{29,30}. Those studies investigated grid sensitivity based on the grid-convergence of the particle forces, resolution of viscous shear length scales, and convergence of spanwise velocity fluctuation correlations.

This study investigates the effect of particle Reynolds number over the range $500 - 10000$ on the shock-induced flow through particle clouds. The particle Reynolds number is defined as

$$\text{Re}_p = \frac{\rho u D_p}{\mu}. \quad (7)$$

Throughout this paper, the Reynolds number is based on flow properties behind the incident shock wave, unless otherwise specified. Subscript IS will be used to denote post-shock values for the other flow variables. The Reynolds number is systematically varied by altering the viscosity, rather than varying the particle diameter or the shock wave strength. This enables the use of the same computational grid for different Reynolds numbers.

The initial conditions consist of two homogeneous spatial regions, which are separated by the shock wave at $x = -0.1L$. The pre-shock conditions are chosen to correspond to air at atmospheric conditions, i.e., $\rho^0 = 1.2048 \text{ kg/m}^3$, $u^0 = 0 \text{ m/s}$, $p^0 = 1.01325 \times 10^5 \text{ Pa}$. The viscosity μ^0 , is varied to obtain the desired particle Reynolds number. At $\text{Re}_p = 5000$, this corresponds approximately to the viscosity of air at standard atmospheric conditions ($\mu^0 \approx 1.8 \times 10^{-5} \text{ kg/ms}$). The Mach number of the incident shock wave is 2.6, and behind it is a homogeneous flow with the post-shock state, which is $\rho_{\text{IS}} = 4.16 \text{ kg/m}^3$, $u_{\text{IS}} = 633 \text{ m/s}$, and $p_{\text{IS}} = 782 \text{ kPa}$. At the $x = -0.9L$ boundary, we apply constant inflow conditions, corresponding to the post-shock state. At $x = 2L$, we use a zero-gradient outlet. The spanwise boundaries are periodic. The spanwise domain lengths are both roughly 13 particle diameters, and this should be sufficient to hinder any periodic artifacts. The simulations are run for a total time of $3.75\tau_L$.

Flow field statistics are obtained by averaging flow variables over predetermined volumes. In the current work, we utilize volumes spanning the computational domain in the y and z directions, with a streamwise length of $L/60 \approx 0.5D_p$.

A large number of particles is required in the spanwise directions to achieve well resolved statistics of the time-dependent flow field. Since only a limited number of particles is feasible to include in a single simulation, we perform an ensemble of simulations at each Re_p . The gas-phase variables are presented in terms of volume averaged quantities. The volume averages from the simulations are averaged over the ensemble of simulations, so that for example

$$\langle \rho \rangle(\mathbf{x}, t) = \frac{1}{N_{\text{sim}}} \sum_{i=0}^{N_{\text{sim}}} \frac{1}{V^i(x)} \sum_{j=0}^{N_{\text{CV}}^i(x)} \rho^j(t) V_{\text{CV}}^j, \quad (8)$$

where N_{sim} is the number of simulations (ten in this study), N_{CV} is the number of control volumes within the averaging volume $V(x)$ and superscripts denote quantities belonging to simulation i or control volume j . Fluctuation correlations are computed implicitly as the difference between the products of the averages and the averages of the products. Thus, the velocity correlations are

$$\widetilde{u_i'' u_j''} = \widetilde{u_i u_j} - \tilde{u}_i \tilde{u}_j. \quad (9)$$

We consider only statistics up to second order moments, and we therefore use the convergence of the fluctuating kinetic energy, k , to estimate the required ensemble size. We find that the tenth simulation changes the statistics of k by about 0.5% on average. We therefore

consider an ensemble of ten simulations at each Re_p sufficient for the current analysis.

IV. RESULTS

This section presents the simulation results. Section IV A examines the attenuation of the main shock wave and the strength of the reflected shock wave. Section IV B discusses mean fields and fluctuations in the gas phase. Finally, Section IV C presents particle drag coefficient trends and distributions.

A. Shock-wave attenuation and reflection

Figure 2 shows the main shock position as a function of time. The results are plotted as the deviation from the hypothetical trajectory of a shock wave with constant Mach number 2.6. This deviation is due to shock wave attenuation caused by the presence of the particle cloud. Both shock wave reflection and particle drag contributes to the attenuation. The arrival time at a given location is delayed for lower Reynolds numbers.

If there is to be a considerable effect of Re_p on the shock wave attenuation, the impulse from viscous forces must be non-negligible on a time-scale comparable to the passage of the shock wave over a particle. Viscous forces are caused by the no-slip condition at the particle surface, which sets up a strong velocity gradient around the particle. An estimation of the importance of viscous forces on the shock wave attenuation can be obtained by comparing viscous and pressure forces acting on the particles during the time when the shock interacts with them. The average ratio of the viscous to pressure forces on the particles during the shock-particle interaction is given in table I. It can be seen that for the lower Reynolds numbers, the viscous forces are appreciable even during the initial phase.

The Mach number of the transmitted shock wave, based on the average transmitted shock wave speed over $L \leq x \leq 2L$, is also given in table I. The Mach number is reduced by 5.3% as Re_p decreases from 10000 to 500. For the particle layer lengths examined here, the additional shock wave attenuation by viscous effects is only moderate, but it might become significant if longer layers are considered.

The position of the reflected shock wave as a function of time is also shown in fig. 2. Since the incident flow is supersonic, the reflected shock wave moves slowly in this reference

FIG. 2. (a) Main shock and (b) reflected shock position as a function of time for different Re_p . As opposed to the reflected shock, the variation in main shock position with Re_p is small and is therefore plotted as the deviation from the trajectory of a hypothetical $Ma = 2.6$ shock wave with no attenuation.

TABLE I. Average ratio of viscous to pressure forces acting on the particles (force ratio) over the time frame where the shock wave interacts with each particle, the Mach numbers of the transmitted (Ma_{TS}) and the reflected (Ma_{RS}) shock waves, the particle Reynolds number based on the flow state behind the reflected shock wave ($Re_{p,RS}$), and the local Mach number of the flow behind the reflected shock wave (Ma^*).

Re_p	Force ratio	Ma_{TS}	Ma_{RS}	$Re_{p,RS}$	Ma^*
500	0.142	2.076	1.580	360	0.379
2000	0.059	2.139	1.558	1495	0.404
5000	0.028	2.174	1.530	3904	0.435
10000	0.015	2.192	1.516	7967	0.451

frame. Its strength increases with decreasing Reynolds number. This is expected, since the magnitude of the particle drag increases with reduced Reynolds number. There is a larger resistance for the flow to pass through the particle layer due to the viscous forces, which builds up pressure in the flow. Therefore the reflected shock strength must increase. Note that the strength of the reflected shock increases with time.

The average Mach number of the reflected shock is given in table I. It is based on the

average speed of the reflected shock wave over the time-frame where it is located upstream of $x = -0.1L$. The lower Reynolds numbers have higher reflected shock Mach numbers, and the difference between $\text{Re}_p = 10000$ and $\text{Re}_p = 500$ is 4%.

Table I also shows the particle Reynolds number and the local Mach number of the flow based on the properties behind the reflected shock, assuming a constant reflected shock Mach number. For classification of the late-time flow field in the particle cloud, these two parameters are more appropriate than the Mach number behind the incident shock wave and Re_p based on ρ_{IS} , u_{IS} and μ_{IS} . The change in Reynolds number is moderate, and does not imply any qualitative changes in the flow, based on the characterization in single-particle studies. The change in local Mach number is more important because the flow behind the incident shock is supersonic while the flow behind the reflected shock is subsonic with a relatively low Mach number.

B. Flow fields and fluctuations

Figure 3 shows the normalized streamwise velocity, pressure and fluctuating kinetic energy at three different time points. The fluctuating kinetic energy is normalized by the inflow kinetic energy. Similarly, fig. 4 shows the Mach number, particle Reynolds number and normalized average streamwise particle forces, i.e.,

$$F_p = \frac{1}{0.5N_p(x)(\rho u^2)_{\text{IS}}A_p} \sum_{j=0}^{N_p(x)} \int_{S_j} (pn_1 - \sigma_{1k}n_k) dS, \quad (10)$$

where $N_p(x)$ is the number of particles within the control volume centered at x , and S_j is the surface of particle j .

The fluctuating kinetic energy is the only flow quantity in figs. 3 and 4 that has a non-monotone dependence on Re_p . The highest level of fluctuating kinetic energy is found for $\text{Re}_p = 2000$. The three highest Reynolds numbers are very similar at early time points, but the difference increases with time.

The Mach number plots reveal that the flow becomes sonic just upstream of the downstream particle cloud edge. Similar observations have been made in other studies^{29,41,43}, and this behaviour is very similar to that found in Fanno flows. As discussed in Emanuel and Jones¹⁴, the Mach number increases with downstream distance in Fanno flows due to the

FIG. 3. Streamwise velocity, pressure and fluctuating kinetic energy at three times for different Re_p . The first column shows a time where the shock wave is still inside the particle layer, the second where it has recently exited the layer, and the final column is close to the end of the simulation.

decreasing pressure. If the duct is sufficiently long, the flow chokes at the downstream exit, just like we observe here.

In fig. 4 it can be seen that the particle forces increase drastically at the downstream layer edge for the two latest time points shown. The Reynolds number increases slightly as well, but is insufficient for explaining the increase in particle forces. Instead, the higher particle forces are due to the increased Mach number.

An important part of the high speed flow through particle clouds is the particle-scale fluctuations. These are commonly neglected in Eulerian-Lagrangian and Eulerian-Eulerian simulations of shock-wave particle cloud interactions, see , e.g., Houim and Oran¹⁶, Ling et al.²⁰, Sugiyama et al.⁴⁰, Theofanous and Chang⁴¹. The gradient of the streamwise velocity

FIG. 4. Mach number, local particle Reynolds number, and average normalized particle forces at three time points for different Re_p . The first column shows a time point where the shock wave is still inside the particle layer, the second where it has recently exited the layer, and the final column is close to the end of the simulation.

fluctuations is an integral part of the momentum balance around the particle cloud edges. Osnes et al.²⁹ showed that at the upstream particle cloud edge, the streamwise Reynolds stress gradient is of equal importance as the particle forces after the initial shock-related transient. As can be seen in fig. 3, the fluctuating kinetic energy has a very sharp gradient, and its magnitude is considerable, especially at early times. Figure 5 shows the ratio of fluctuating kinetic energy to total kinetic energy, integrated over the interior of the particle cloud, as a function of time. It can be seen that the ratio exceeds 0.25 for all Reynolds numbers around $(t - t_0)/\tau_L = 0.5$, i.e., when the shock wave is slightly less than halfway through the particle cloud. When the shock wave exits the cloud, the ratio decays slowly

over time. The trend with Re_p is not monotone, which is also the case for the fluctuating kinetic energy, c.f. fig. 3. Regele et al.³¹ showed that the pressure field computed in a one-dimensional Eulerian-Lagrangian simulation of shock-wave particle cloud interaction corresponded to the sum of the volume averaged pressure and the Reynolds stress in their two-dimensional simulations. The overestimation of the pressure in their one-dimensional simulations is therefore the result of neglecting the energy deposited in velocity fluctuations. For the current simulations, the ratio k/p takes values up to 0.25 when the shock wave is inside the particle cloud. It remains non-negligible even at late times, where the value is between 0.02 and 0.14 within the particle cloud. The ratio is lower for $\text{Re}_p = 500$ than the other Reynolds numbers, which are quite similar.

FIG. 5. Ratio of fluctuating to total kinetic energy integrated over the particle layer, as a function of time, for different Reynolds numbers.

Currently, there are very few models for flow field fluctuations that have been developed specifically for shock-wave particle cloud interaction. It is therefore useful to accurately identify flow phenomena that contribute to the fluctuation correlations, so that model development can be based on a fundamental understanding of the flow. In the current work, we consider only the velocity fluctuations. Figure 6 shows the contribution to the Reynolds stress by velocity fluctuations of different magnitudes at $t = 3.75\tau_L$. The figure shows the function f , which is defined by

$$\langle \rho \rangle \tilde{R}_{11} = \int_{-\infty}^{\infty} f(u'') du''. \quad (11)$$

FIG. 6. Contribution to (a) the streamwise Reynolds stress and (b) the spanwise Reynolds stresses by different velocity fluctuations for different Reynolds numbers. Data for $0.25 \leq x/L \leq 0.75$ at $t = 3.75\tau_L$.

FIG. 7. Contours of f at $t = 3.75\tau_L$ for one realization at each Re_p . The color indicates the velocity fluctuation and f is used to set the color saturation, as indicated by the curve in each colorbar located below the plot. Thus areas with high color saturation have the highest contribution to the Reynolds stress.

f is a measure of the importance of velocity fluctuations of a given amplitude with regards to the velocity fluctuation correlations. For $Re_p = 500$, the peak in f is very sharp, and the contribution from negative fluctuations below the peak is negligible. As the Reynolds number increases, the peak decreases. It moves towards more negative fluctuations because

the mean flow velocity increases. The peak also broadens, and the contribution from strong negative fluctuations increases. The total contribution by negative fluctuations increases with Reynolds number, comprising 62.9%, 67.1%, 69.0% and 69.2% for Reynolds numbers 500, 2000, 5000 and 10000, respectively. The contribution from positive fluctuations can be seen to have a non-monotone dependence on Reynolds number over the range studied here. The peak value is very similar for the two lowest Reynolds numbers. When the Reynolds number is increased further, the peak value decreases to about 80% and 65% of the $Re_p = 2000$ peak. Similar to the negative fluctuations, the curve broadens, but the effect is small.

A similar plot of f was used in Osnes et al.²⁹ to argue that the bulk contribution to the Reynolds stress was due to the circulation region behind each particle. Those results were for a flow configuration very similar to the $Re_p = 5000$ case considered here. Figure 7 shows contours of f in space and confirms that the circulation regions are those with the highest contributions to the streamwise Reynolds stress. The flow in the circulation region has an average velocity of zero and therefore differs drastically from the mean flow speed. This implies that the volume of the circulation region is an important parameter for determining the streamwise Reynolds stress magnitude. It is also evident that most of the flow volume contains velocities that are higher than the volume averaged velocity. This effect arises because the separation regions shift the average velocity away from the velocity of the flow between the particles. At $Re_p \geq 2000$ there are very few areas within the particle cloud that have a velocity equal to the volume-averaged velocity.

Figure 6 also shows the contribution to the spanwise Reynolds stresses by spanwise velocity fluctuations of different magnitudes. The function $g(|w''|)$ is the analogue to $f(u'')$ for spanwise fluctuations, and is averaged over the two spanwise velocity components. Additionally, since $g(|w''|)$ should be symmetric around $w'' = 0$, we plot the contribution as a function of the fluctuation magnitude. The shapes of the curves are quite similar for all Reynolds numbers, but the magnitude is significantly lower for $Re_p = 500$. The location of the peak value is at 0.08 for $Re_p = 500$ and around 0.135 for the other Reynolds numbers. The trend with Re_p is non-monotone, and the highest magnitude is obtained at $Re_p = 2000$. This is similar to the trend for positive streamwise fluctuations, but the reduction at higher Re_p is less significant for the spanwise fluctuations.

The areas that contribute most to the spanwise Reynolds stress components are shown in

FIG. 8. Contours of g at $t = 3.75\tau_L$ for one realization at each Re_p . The color indicates the velocity fluctuation and g is used to set the color saturation, as indicated by the curve in each colorbar located below the plot. Thus areas with high color saturation have the highest contribution to the Reynolds stress.

fig. 8. It can be seen that at $Re_p = 500$, the fluctuations are located in large coherent regions. These are significantly larger than a single particle, which indicates that it is the inter-particle spacing rather than the particle size that is important for the spanwise Reynolds stress components. The same phenomenon is seen for the higher Reynolds numbers, but to a lesser degree. At $Re_p = 10000$, the scale of the coherent regions only appears slightly larger than a single particle. The regions contributing to the spanwise fluctuations are not the same as those that are important for the streamwise fluctuations. The streamwise fluctuations are primarily particle wakes, whereas the spanwise fluctuations are mostly due to flow deflection around particles and streaming through channels between them. The spanwise fluctuations are therefore located slightly in front and to the side of each particle, as well as in the open spaces within the cloud.

In Figure 9 and Figure 10, the streamwise and spanwise Reynolds stress contributions are plotted at different streamwise locations within the particle layer. $Re_p = 2000$ and 10000 have very similar trends as $Re_p = 5000$ and are therefore not shown. It can be seen that negative streamwise fluctuations at $Re_p = 500$ have very little variation with streamwise position. On the other hand, positive fluctuations shift towards higher magnitudes as distance increases, and the curve broadens. This is also the case for $Re_p = 5000$, although the shifts

FIG. 9. Contribution to the streamwise Reynolds stress by different velocity fluctuations at $t = 3.75\tau_L$ for different streamwise positions. (a) $Re_p = 500$. (b) $Re_p = 5000$.

FIG. 10. Contribution to the spanwise Reynolds stress by different velocity fluctuations at $t = 3.75\tau_L$ for different streamwise positions. (a) $Re_p = 500$. (b) $Re_p = 5000$.

are slightly lower. The shift in positive direction is related to the flow acceleration, which is stronger for $Re_p = 500$ than for $Re_p = 5000$. For $Re_p = 5000$, the shape of the curve for negative fluctuations changes with downstream distance. Smaller magnitudes become more important, presumably due to increasingly turbulent flow.

For spanwise fluctuations, we find that at $Re_p = 500$, the magnitude increases with downstream distance throughout the particle cloud. Additionally, the peak location shifts towards higher fluctuation magnitudes. At $Re_p = 5000$, the trend is similar up to $x/L = 0.5$,

FIG. 11. (a) α_{sep} and (b) the analogous function for spanwise fluctuations for different Re_p , at $t = 3.75\tau_L$.

but further downstream distance has little effect on the fluctuations.

Osnes et al.²⁹ found that the streamwise fluctuations in the interior of the particle cloud could be represented by

$$\langle u_1'' u_1'' \rangle = \tilde{u}_1^2 \frac{\alpha_{\text{sep}}}{\alpha - \alpha_{\text{sep}}}, \quad (12)$$

where α_{sep} is an estimate of the average volume of the circulation region behind each particle. This model approximates the flow as two constant states. One is the flow between the particles and the other is the separated flow behind a particle, where the velocity is assumed to be zero. We note that this model does not predict zero velocity fluctuations when α goes to one, nor is it Galilean invariant, and therefore needs a modification if it is to be used in simplified dispersed flow models. A way to correct this is to replace $\tilde{u}_1$ by the relative velocity between the particles and the gas, and replace α_{sep} by $\alpha_p C$ in eq. (12), where C is a constant or a function of dimensionless flow variables. Figure 11 shows α_{sep} at the end of each simulation, estimated from the simulation results using eq. (12). α_{sep} changes rapidly close to the cloud edges, but over the interior of the cloud it has an approximately constant value. $\text{Re}_p = 500$ deviates slightly more from a constant value than the higher Reynolds numbers. The trend with Re_p is monotone over this range, and lower Reynolds numbers have larger separation volumes. The trends found here agree qualitatively with observations from single sphere studies in the incompressible regime, where the separation length, i.e., the average distance from the particle to the end of the separated flow region, was found

to be roughly 30% shorter at $\text{Re}_p = 10000$ than at $\text{Re}_p = 3700$ ³³. Indications of a similar trend were also found for compressible flows, where $\text{Re}_p = 1000$ at $\text{Ma} = 0.8$ and 1.2 had a shorter separation length than $\text{Re}_p = 750$ ²⁷.

Figure 11 also shows the analogous function to α_{sep} for the spanwise fluctuations. It can be seen that this function has little variation over $0.2 \leq x/l \leq 0.95$. It does not follow from the derivation of eq. (12) that the spanwise fluctuations should vary this way. The results should be interpreted as confirming that the velocity fluctuations vary proportionally to the mean streamwise flow velocity throughout most of the particle layer. We note that for the spanwise fluctuations, there is a longer distance at the start of the layer where the function increases with distance. We suspect that this is because spanwise fluctuations are more related to inter-particle distance than particle diameter. If this is the case, it is not surprising that the build-up distance is longer, since the inter-particle distance is larger than the particle diameter on average. In contrast to the monotonous behavior of α_{sep} with Re_p , there is a non-monotone trend for the spanwise fluctuations. We also find that for $\text{Re}_p = 10000$, the function begins to increase towards the end of the layer. We suspect that this is the result of increasingly turbulent flow.

The simple relationship between the mean flow velocity and the velocity fluctuations is surprisingly robust across different flow conditions. The flow field within the particle cloud features rapidly varying velocity-, pressure- and density-magnitudes as well as varying gradients. Additionally, the Mach numbers vary from 0.3 to 1. The insensitivity to these variations is encouraging for development of velocity fluctuation correlation models that can be used as closures for simplified dispersed flow models.

C. Particle drag

Accurate description of particle forces is of key importance in dispersed flow simulations. In dense particle suspensions, the local particle configuration can lead to large variations in the directions and magnitudes of the particle forces. The maximal drag for each particle occurs during its interaction with the shock wave. The behaviour of maximal drag forces has been examined in inviscid simulations by Mehta et al.^{23,24}. We compare the peak streamwise drag forces in the current simulations to their inviscid simulations in fig. 12. The figure shows the trend in average peak streamwise drag forces with downstream distance and

FIG. 12. (a) Least squares first order polynomial fit of peak streamwise drag-coefficients, denoted $P_x^1 [\max(C_{D,x})]$, as a function of x for different Reynolds numbers. (b) Best normal distribution fit to the deviation of the peak drag coefficients from $P_x^1 [\max(C_{D,x})]$. The plots also show the results obtained in inviscid $Ma = 3$ simulations by Mehta et al.²⁴. In order to compare against those results, only particles between $0 \leq x/D_p \leq 12.5$ have been included for the simulations in this work. Note that for the results shown in this figure, drag coefficients are based on ρ_{IS} and u_{IS}

the distribution of peak streamwise drag forces. Note that for the results shown in fig. 12, the drag forces are presented as a drag coefficient using ρ_{IS} and u_{IS} . In figs. 12 to 15, subscripts x and y are used to indicate streamwise or spanwise drag coefficients, respectively. The shock wave Mach number is 2.6 in the current simulations and 3 in the inviscid simulations. We thus expect slightly higher drag coefficients in our simulations. The lower Reynolds number simulations show higher peak drag forces, and this is to be expected because the contribution from viscous forces increases. It can also be seen that the slope is steeper for the lower Reynolds numbers. This is due to the stronger shock wave attenuation occurring for lower Reynolds numbers. The distribution of the deviation of peak drag forces from the linear trend with x is also shown in fig. 12. The results are in excellent agreement with the inviscid simulations. It can also be seen that the distribution only has an inconsequential dependence on Reynolds number. This means that the peak drag variation is controlled by processes that are almost unaffected by viscosity, such as shock wave focusing and diffraction.

After the initial shock-induced transient, the importance of viscosity increases. It is therefore of interest to investigate how the distributions of instantaneous and time-averaged

FIG. 13. Distribution of the time-averaged drag coefficients for $t > 1.875\tau_L$. (a) Streamwise drag coefficient. (b) Spanwise drag coefficient. The linear trend with x has been subtracted. Note the different scale in the plots.

drag coefficients depend on Reynolds number. Figure 13 shows the distribution of the drag coefficients averaged over $1.875 \leq t/\tau_L \leq 3.75$. Starting at $t = 1.875\tau_L$ ensures that any shock-related transients have decayed. The linear trend with x has been subtracted from the drag coefficients and they are also normalized with that function. For the spanwise distributions, we have normalized the drag coefficients based on the linear trend of the streamwise drag coefficients. The highest Reynolds number has a wider distribution of streamwise drag coefficients than the lower Reynolds numbers. The other three are very similar, but it seems that the distribution for $Re_p = 2000$ is slightly higher and narrower than those for $Re_p = 500$ and 5000 . The distributions are slightly skewed. This is most pronounced for $Re_p = 10000$. The spanwise distributions are more similar for all Re_p . The highest Reynolds number has the widest distribution, and the distributions for the two middle Re_p are almost equal.

Figure 14 shows the distribution of the deviation of the instantaneous drag coefficients from a linear trend in time. For each particle, the linear trend in time is also used for normalization. Since the trend in time has been subtracted, these distributions reflect the magnitude and frequency of temporal oscillations. The trend with Re_p is similar for both the streamwise and spanwise drag-coefficients, where higher Re_p result in wider distributions. Note that the spanwise drag coefficient distribution is about twice as wide as that

FIG. 14. Distribution of instantaneous drag coefficients for $t > 1.875\tau_L$. (a) Streamwise drag coefficient. (b) Spanwise drag coefficient. The linear trend with t for each particle, denoted $P_t^1(C_D)$ has been subtracted.

of the streamwise drag coefficient. The trends are more pronounced for the distribution of instantaneous than mean drag coefficients.

Both mean flow and instantaneous drag coefficient distributions have a dependency on particle Reynolds number. There are separate implications for drag modeling from each of these distributions. The distributions of time-averaged drag coefficients imply that drag models should incorporate terms that depend on the local particle configuration. These models can be based on the relative position of nearby particles or on the particle density. The PIEP model developed in Akiki et al.² is an example of the former model type. In the latter model type, the distributions shown in fig. 13 can be used directly by imposing random fluctuations drawn from these distributions. The results here also imply that the importance of including such distributions increases with Reynolds number since the distribution is widest at $Re_p = 10000$.

The distribution of instantaneous drag coefficients is a result of temporal flow fluctuations, and these have strong Reynolds number dependencies. It is likely that a part of these distributions is related to the shedding of vortices from both the particle itself and the nearby particles. The variation imposed by vortex shedding from nearby particles could be modeled based on the local particle configuration, although this is likely quite challenging. In addition to the trends with Reynolds number observed here, the distributions are likely

FIG. 15. Average drag coefficient at $t = 3.75\tau_L$ for various Re_p , based on local (volume averaged) flow properties. The standard deviation in Re_p and $C_{D,x}$ are indicated by the horizontal and vertical error bars, respectively. The results of Nagata et al.^{26,27} as well as the drag correlation of Clift and Gauvin¹⁰ are also shown.

dependent on the particle volume fraction. Investigating this effect is a topic for future studies.

Figure 15 shows the streamwise drag coefficient at $t = 3.75\tau_L$. The figure also shows the drag coefficients where a modified flow velocity, defined as

$$u_{\text{free}} = \tilde{u} \frac{\alpha}{\alpha - \alpha_{\text{sep}}}, \quad (13)$$

is used to calculate the drag coefficient. The modified velocity was suggested in Osnes et al.²⁹ and attempts to correct for the contributions of the circulation regions behind the particles, which shift the average velocity away from the "free" velocity within the particle layer. Also shown in the figure are the single-particle drag coefficients obtained by Nagata et al.^{26,27} and the drag correlation by Clift and Gauvin¹⁰. For reference, the average Mach numbers within the particle cloud are in the range 0.3–0.7, c.f. fig. 4. Here, the lower Mach number is for $Re_p = 500$ and the highest Mach number is for $Re_p = 10000$, where the velocity correction has also been used for the Mach number. Even with the correction, which reduces the drag coefficients, the current simulations result in significantly higher drag coefficients than predicted by models based on single-particle results. The single-particle simulation

results of Nagata et al.^{26,27} only cover the lower two Reynolds numbers considered here. However, if the trend from these single particle simulation results can be extrapolated, it seems that the deviation is larger for low particle Reynolds numbers than high.

Other studies have found that confinement has a strong effect on the drag on single particles^{1,3,18,47}. For Re_p up to about 300, Akutsu³ found that a 30% area blockage increased the drag coefficient by more than a factor of two. At Re_p above 3×10^4 , Achenbach¹ found a 10% increase for 50% blockage. We expect that a similar effect occurs due to the presence of nearby particles. If a correction for this is combined with the corrections due to Mach number and separation volume, it is likely that the average drag coefficients will approach the values seen in isolated particle studies.

V. CONCLUDING REMARKS

This study has investigated the propagation of a Mach 2.6 shock wave through particle clouds with particle volume fraction 0.1. Particle resolved large-eddy simulations were utilized, and the particle Reynolds number, based on the incident shock state, was varied between 500 and 10000.

The results show that the shock wave attenuation increases with decreasing particle Reynolds number, but the effect is small over this Reynolds number range. The strength of the reflected shock wave increases with decreasing Reynolds number. This results in considerable changes in the flow quantities upstream of and inside the particle layer, i.e., higher pressures, lower velocities and lower Mach numbers with reduced particle Reynolds numbers.

We examined the development of fluctuations from the volume averaged flow quantities within the particle layer. The velocity fluctuation intensity has a non-monotone dependency on particle Reynolds number. The most intense velocity fluctuations were found at $Re_p = 2000$. Streamwise velocity fluctuations are located in the particle wakes, and most importantly in the circulation region behind each particle. Spanwise fluctuations are located in the inter-particle regions, and consist of coherent regions that extend further than the size of single particles. As the Reynolds number increases, the sizes of these regions decrease. We find an approximate proportionality between the mean flow velocity and the flow fluctuations at late times. This relationship holds for both the streamwise and the spanwise

fluctuations. Interestingly, the proportionality factor varies monotonously with Re_p for the streamwise fluctuations, but not for the spanwise fluctuations.

The distributions of particle forces were examined. Maximal drag forces and their spatial variation agree well with the inviscid simulations of Mehta et al.²³. In the late-time flow field, we find that both the variation of time-averaged particle forces and the temporal variation increases with particle Reynolds number. The trend with particle Reynolds number is more pronounced for the temporal variation than the time-averaged distribution. These distributions provide a basis for development of particle force variation models, that can be used in simplified dispersed flow models.

The particle drag coefficients within the particle cloud were found to be higher than isolated particle drag coefficients on average, and the largest deviation occurred for the lowest Reynolds number. We demonstrated that utilizing a correction to the mean flow velocity yields drag coefficients closer to the single-particle results. A combination of this correction with drag correlations that incorporate Mach number and flow blockage effects, can possibly reproduce the observed average drag coefficients in shock-wave particle cloud interactions.

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