Analysis of Stochastic Methods for Predicting Particle Dispersion in Turbulent Flows

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ANALYSIS OF STOCHASTIC METHODS FOR PREDICTING PARTICLE DISPERSION IN TURBULENT FLOWS

A Thesis Presented

by

Kyle Paul Sala

to

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of

The University of Vermont

In Partial Fulfillment of the Requirements
for the Degree of Master of Science
Specializing in Mechanical Engineering

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November 5, 2012
Abstract

The current research seeks to develop a computational model that accurately describes particle dispersion in turbulent flow. Current particle dispersion models do not accurately predict the small-scale clumping of particles in turbulent flow that occurs due to interaction with turbulent eddies. A new stochastic vortex structure (SVS) model was developed and compared with current stochastic Lagrangian models (SLM) for turbulent flows. To examine what characteristics of the fluid flow field that lead to dispersion of particles, a number of non-trivial measures were used. A discrete-element model is used to transport particle locations for cases with and without adhesive forces. Direct numerical simulations (DNS) are used as a baseline for comparison between the two models. Initial results show that the SVS model matches the spatial structure of the flow field of DNS reasonably well, while the SLMs do not. Investigation of particle collision rate suggest that while SVS matches the large length scales of flow, it omits the smaller scales of the flow.
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I am also thankful for the existence of LATEX which made writing this thesis much more enjoyable than the alternative.

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Chapter 1

Introduction

Turbulent fluid motion is a ubiquitous phenomenon that has been studied extensively over the past century. On the surface, turbulence appears to be chaotic but scientists have found ways of describing the motion. Turbulence can be thought of as an energy dissipation process over a wide range of length scales. The large scale structures look like large vorticies, or eddies, that swirl chaotically. As the scale gets smaller, so do the eddies. Kolmogorov (1941) defined the smallest scale of these turbulent eddies, which is now known as the Kolmogorov length scale. Theoretically no eddies beyond this scale exist in the flow as the viscous forces completely dissipate the remaining energy. Scientists are now able to fully simulate simple turbulent flows at low Reynolds numbers down to the Kolmorogov length scale with very high resolution (Hackl et al., 2011).

Of particular interest in the current study, is the dynamics of particles in turbulent flows. Particles with mass are known to disperse in turbulent flows, meaning they don’t follow the path of the fluid (Yudine, 1959). Particle dispersion in turbulent flow is a widely studied field that has many applications, such as blood and
digestive flows, suspended microalgae and associated biofuel processes, shale oil separation, sediment transport, meteorology, nanoparticle and microparticle dispersion in manufacturing processes, dust fouling of electronic equipment, ash collection from combustion processes, and smoke particle respiration and associated lung problems.

Depending on the application, different descriptions of the fluid turbulence, and subsequently particle dispersion, are used. For highly simplified flows with modest Reynolds number, it is possible to solve for all scales of the turbulent motion using a so-called direct numerical simulation (DNS) approach. As the Reynolds number increases or the flow becomes more complex, however, the variation of length and time scales in the problem quickly makes such a direct solution infeasible. Large eddy simulation (LES) methods have been developed in which the largest scales of turbulent motion are directly computed and the smaller scales are modeled. LES can be used for a broader range of problems than DNS, but LES is still extremely demanding in terms of computational resources. Consequently, most practical engineering problems are solved with some type of Reynolds Averaged Navier-Stokes (RANS) model, of which there are a large number. Among the simplest RANS models is the popular $k - \epsilon$ model, which solves the Navier-Stokes equations with the effect of the sub-grid scale turbulence modeled as an eddy viscosity, together with additional equations for turbulence kinetic energy $k$ and dissipation rate $\epsilon$, from which one can deduce the dominate time and length scales of the turbulent motion.

It is not necessary to introduce a particle dispersion model for DNS computations, since effect of the large turbulent eddies on the particle motion can be directly computed. However, when using a RANS or LES model for the turbulence it is necessary to introduce an additional model to account for the dispersion of the particles by the unresolved turbulent motion. Common approaches for particle dispersion simply
add a Gaussian-distributed random perturbation onto the particle velocity to mimic the effects subgrid turbulence (Gosman & Ioannides, 1983). The time interval for changing this random particle velocity is often correlated with the turbulent eddy time scales. An improvement on this model is the use of velocity-based stochastic Lagrangian models of the Langevin type to approximate the subgrid-scale turbulent fluid motion, such that the particle motion is solved by direct solution of the particle momentum equation (Cai et al., 2006). Both of these approaches tend to produce a scattered cloud of particles in turbulent flows, due to the fact that there is no correlation between the random “turbulent” motion of neighboring particles. Thus, such approaches can adequately capture the “bulk” dispersion of the particle field, in which the averaged concentration is treated as a smoothly-varying function of position and time, but they cannot capture the fine-scale heterogeneity of the concentration field.

An example of such heterogeneity is shown in Figure 1.1 for the problem of inertial particles dispersed from the core of a turbulent vortex (Marshall, 2005). This heterogeneity arises due to the effects of centrifugal forces which act to throw particles out of the turbulent eddies, causing the particles to collect in high concentration sheets lying between the energy-containing eddies. Modeling of this small-scale heterogeneity is important for accurate prediction of particle collision rate and adhesion. This is vital for description of problems such as growth of agglomerates of adhesive particles (Marshall, 2007, 2009) and temperature intermittency in particulate combustion processes.

Recent advancements have been made by using acceleration-based stochastic Lagrangian methods (Sawford, 1991b; Reynolds, 2003). These methods have been constructed to model the statistics of the acceleration field, which is known to be responsible for particle clustering (Csanady, 1963). The Sawford model has been shown to
Figure 1.1: Series of contour plots at time a) $t = 0$, b) 20, c) 40, and d) 60, of the concentration of particles from a slice of a turbulent vortex core. At $t = 0$ all the particles are within the vortex core, and $t = 60$ we can see the high concentration particle sheets. From Marshall (2005).

produce a Gaussian distribution of acceleration, when it has been shown experimentally that the acceleration field is non-Gaussian (LaPorta et al., 2001; Mordant et al., 2004). The Reynolds model accurately captures the non-Gaussian statistics of the acceleration field. However, a statistical equivalency in the acceleration field doesn’t imply that the correct turbulent structures will form (Lee, 2005). Further modeling efforts are required for applications involving small scale structures.

Current research in this field has focused primarily on fluid elements, rather than inertial particles. Cases that do consider particles with inertia often treat the particles as point-particles and neglect effects of particle collision and adhesion as well as other fluid forces that act on particles with finite volume. When particle aggregates form,
they essentially form a larger particle which reacts differently in the flow than the smaller particles.

1.1 Objective and Scope

The objectives of this research are to examine the effectiveness of current stochastic Lagrangian methods and the new stochastic vortex structures method for simulating particles dispersion and determine the characteristics of a fluid field that lead to dispersion. In order to evaluate the current methods it was necessary to develop non-trivial metrics of the flow field. Direct numerical simulations are used as a baseline for comparison between the models.
2.1 Particle dispersion

It is well-known that particle dispersion in turbulent flows is highly heterogeneous when viewed on a sufficiently small scale (Squires & Eaton, 1991; Falkovich & Pumir, 2004; Grits et al., 2006; Bec et al., 2007). This heterogeneity arises in part due to the effects of particle inertia. If a particle is more dense than the carrier fluid, then the particle will drift relative to the Lagrangian trajectory of fluid elements (Yudine, 1959). This phenomenon is referred to as the inertia effect. The fluid exerts a drag force on the particle due to the relative velocity, and this imposes an acceleration on the particle (Csanady, 1963). An important parameter that is characteristic of particle drift is the Stokes number. The Stokes number is defined as the ratio of the characteristic particle response time, $\tau_P$, over the characteristic time scale of the fluid, $\tau_F$. Expressed mathematically (Tang et al., 1992),

$$St = \frac{\tau_P}{\tau_F} = \frac{\rho_p d_p^2 U}{18 \mu L}$$  \hspace{1cm} (2.1)
where $\rho_p$ is the particle density, $d_p$ is the particle diameter, $\mu$ is the dynamic fluid viscosity, $U$ is the characteristic fluid velocity, and $L$ is the characteristic length scale. For small Stokes numbers ($St \ll 1$) the particle follows the carrier fluid, and the particle drift is negligible. Conversely, at large Stokes numbers ($St \gg 1$), the particles are barely affected by the carrier fluid. At intermediate Stokes numbers ($St \approx 1$) particles are observed to drift relative to the fluid. Figure 2.1 shows the particle drift dependence on Stokes number. For the case of turbulent flow at small Stokes number, the particles will follow the turbulent fluctuations.

![Image](image_url)

Figure 2.1: Particle dispersion patterns for flow past a bluff body at different Stokes numbers. (From Tang et al., 1992).

The drift force is caused by the fluid acceleration which implies the acceleration field of the fluid is related to particle clustering (Bec et al., 2007). The trajectories
of inertial particles that drift ($St \leq 1$) have been shown to over-sample areas of low vorticity and high strain rate (Maxey, 1987; Squires & Eaton, 1991; Ayyalasomayajula et al., 2008). Physically, this clustering is due to the centrifugal force which acts to throw inertial particles out of the turbulent eddies, causing the particles to collect in high concentration sheets lying between the energy-containing eddies (Druzhinin, 1994; Marshall, 2005). This phenomenon is known as preferential concentration or preferential clustering and will be referred to as such. Preferential clustering of particles is displayed in Figure 2.2, where particle positions are plotted against the vorticity field.

Figure 2.2: Particle positions plotted with contours of vorticity at $St = 1$. (From García, 2009).

Experiments have been conducted to examine the statistical nature of acceleration within a turbulent flow. Mordant et al. (2004) performed a comprehensive experimental and numerical study of Lagrangian statistics of high Reynolds number turbulence. They found that the probability density function (PDF) of the velocity field is Gaussian (Figure 2.3a) whereas the PDF of the acceleration field is highly non-Gaussian (Figure 2.3b). From Figure 2.3b we can see that some fluid elements
experience very large accelerations, up to 30 times that of the root mean square value of acceleration. This has been confirmed by multiple investigators (LaPorta et al., 2001; Mordant et al., 2004; Lee, 2005). These large accelerations occur over very brief periods of time, on the order of microseconds, and over distances of micrometers as seen in Figure 2.4. Given these results, it becomes obvious why it is so difficult to fully resolve turbulent motion. These effects, although small when looking at the gross flow, and negligible for some applications, create intermittency in the flow field variables.

Figure 2.3: (a) PDF of one component of velocity (solid line) at $Re_\lambda = 810$ compared to a Gaussian distribution with the same variance (dashed). (From Mordant et al., 2004). (b) Probability density functions of normalized acceleration at different Reynolds numbers. The solid line is a parameterization of $Re_\lambda = 970$ data. The dashed line is a Gaussian distribution with the same variance. (From LaPorta et al., 2001).

Mordant et al. (2004) also observed that vorticity has a strong influence on acceleration. Inertial particles experience the largest rates of change when in regions of high vorticity. This was confirmed by computing the components of acceleration that are parallel and perpendicular to the local vorticity field along the particle trajectory and the acceleration induced by vorticity. When these values were compared, it was
shown that the acceleration perpendicular to the local vorticity vector is almost equal to the full acceleration. This is shown in Figure 2.5. The accelerations induced by the regions of high vorticity were among the highest.

Figure 2.5: (a) Total acceleration, (b) acceleration due to vorticity, (c) perpendicular acceleration and (d) parallel acceleration (From Mordant et al., 2004).

Given that vorticity has a strong correlation with local acceleration, researchers have become interested in the connection between coherent turbulent structures and the acceleration. This relationship becomes particularly important when constructing models to reproduce particle dispersion. Lee (2005) investigated the relationship
between vorticity, entrosphy, dissipation, and acceleration. It was found that large accelerations always point towards the rotational axis of a vortex filament, which aligns with the findings of Mordant et al. (2004). The pressure gradient also points into the center of vortical structures, as shown in Figure 2.6. The centripetal force produced by these vortices has values up to 20 times its root-mean square value. Thus, it can be suggested that the coherent structures are the main sources of acceleration intermittency. However a statistical equivalence of the acceleration field does not imply that you will have the correct vortex structures, or the correct particle dispersion.

![Figure 2.6: Isosurface of entrophy at $Re_\lambda = 44$ with its corresponding cross section, in which the pressure gradient is shown in arrows. (From Lee, 2005).](image)

### 2.2 Particle collisions

Particle collisions have been the subject of research for many applications. Of interest here is the effect of fluid structures on particle collisions. Over the years collision
rate models of varying complexity have been developed, from pure fluid elements to spherical particles with finite inertia in a highly turbulent flow field. Overall, the multiple effects of turbulence on the collision of particles has been shown to enhance the collision rate (de Jong et al., 2010).

The development of particle collision rate models often deals with specific mechanisms of particle dynamics pre-collision, during-collision, and post-collision. The isolation of these mechanisms, such as drift and Stokes number effects, is helpful in determining which fluid characteristics play an important role in dispersion. It also illustrates the need for an accurate solution of particle motion.

### 2.2.1 Collision rate modeling

The collision rate of particles in a suspension has a large effect on the properties of that suspension (Abrahamson, 1975). Particles may aggregate, collisions could break up aggregates and they can transfer energy, such as electrical charge or thermal energy. Another phenomenon that has a profound effect on suspension dynamics is agglomeration of particles. Ayyalasomayajula et al. (2008) described the effect of filtering, which is associated with effects that scale with the Stokes number. If an agglomerate of particles forms it effectively has a larger Stokes number than a single particle (Mei & Hu, 1999).

Smoluchowski (1917) considered the case in which particles followed the fluid streamlines in a laminar flow. The assumptions in his analysis were that the particles are the same size, that all collisions leads to agglomerates, that all collisions are between only two particles, and that collisions occur according to an assumed analytic expression. A visual example of the result of these assumptions is shown in Figure 2.7a. Saffman & Turner (1956) extended this model for the case of isotropic turbu-
lence. This expression is accurate when the sum of the radii of colliding particles is small when compared to the smallest eddies in the flow so that particles close to each other experience correlated velocities. This analysis is in the limit of zero Stokes number.

![Diagram](image)

Figure 2.7: Particle motion and mechanism of collision at two different times for the case of (a) no particle drift and (b) particles with different inertias that are allowed to drift. (From Kruis & Kusters, 1997).

For particles with intermediate Stokes number and/or a highly turbulent fluid, particles drift relative to the fluid velocity. Abrahamson (1975) noted the limitations of the assumptions of the previous researchers, and formulated an expression for the collision rate in a vigorous and highly dissipative turbulent flow with the assumptions that (i) at any given time each particle has a velocity independent of other particles, see Figure 2.8, and (ii) that the velocity fluctuations are isotropic. While this model accounts for particles that drift, due to the assumption of uncorrelated velocities it cannot account for particles with small Stokes numbers.

Williams & Crane (1983) developed a theory that tried to bridge the two extremes of small non-inertial particles, $St \to 0$, (Saffman & Turner, 1956) and large inertial particles in a vigorously dissipative flow, $St \to \infty$, (Abrahamson, 1975) by accounting
Figure 2.8: Inertial particles colliding that experience uncorrelated velocities. (From Kruis & Kusters, 1997).

for particles with intermediate Stokes numbers. More specifically, they took into account the relative difference in velocity between the fluid and the inertial particles. While this model did present some advantages over previous models, it was not able to accommodate particles with somewhat-correlated velocities (inertial subrange of turbulence). Furthermore, the added mass effects of particles moving through the fluid were ignored.

Independently of Williams & Crane (1983), Yuu (1984) formed a model that takes into consideration the added mass effects. However, both of these models were shown by Kruis & Kusters (1997) to not be applicable for particles within the inertial subrange and they fail to approach the limit calculated by Saffman & Turner (1956).

Kruis & Kusters (1997) sought to provide a general expression for particle collision rates. The analysis took into account the effects of inertia of particles over the full range of Stokes numbers, the difference in density between the fluid and particles, and the relative velocity between two particles due to turbulent acceleration in liquid or gaseous system. Most of the previous derivations were for gaseous systems, and thus were not universally applicable. The particle-velocity correlation is applicable for particles with highly correlated velocities completely entrained by the smallest eddies, all the way to particles with completely independent velocities, including the
cases of somewhat correlated velocities. The theory of Kruis & Kusters (1997) reduces to that of Saffman & Turner (1956) in the limit of non-inertial particles, and to that of Abrahamson (1975) for particles with very large Stokes numbers. In between these two extremes, an interpolating formula was used that included both the effects of fluid shear, and the acceleration of the particles due to inertia.

Up to this point, none of the collision rate models took into account the effects of preferential particle concentration due to particle dispersion. Sundaram & Collins (1997) performed DNS calculations that showed preferential concentration enhanced the particle collision rate, shown as a function of Stokes number in Figure 2.9. They noted that at the two extremes of Stokes numbers (zero and infinity), their results matched with the theory of Saffman & Turner (1956) and Abrahamson (1975). They related the behavior of the intermediate Stokes numbers to two effects: (i) preferential concentration and (ii) particle inertia effects on the correlation of two nearby particles, thus altering their relative velocities. Both of these effects increase the collision rate. Subsequently, Reade & Collins (2000) showed that the amount of preferential clustering increases as Reynolds number increases.

Mei & Hu (1999) looked at a rapidly sheared homogeneous turbulent flow and examined the collision rate dependence on the spatial structure of the turbulence. At time $t = 0$ the turbulence is isotropic; however, the rapid shearing quickly deforms the flow resulting in highly anisotropic turbulence. Figure 2.10 shows the relationship between collision rate and the mean shear rate of the turbulence. It was concluded that the collision rate is dependent on the structure of the turbulence.

Wang et al. (2000) generalized the conclusions of Reade & Collins (2000) regarding the two main effects which largely govern particle collisions: the large scales of the turbulence induce relative velocities on colliding particles, called the turbulent
transport phenomenon, and the small scales of the turbulence which lead to preferential concentration. They performed detailed DNS to examine these two effects independently. The maximum effect of the turbulent transport phenomenon scales with the square of $Re\lambda$. The effect of preferential concentration was found to be a maximum at a Stokes number equal to one, later confirmed again by Bec et al. (2005). Both effects scale with Reynolds number, and a model accounting for both effects was constructed.

Figure 2.11 shows a comparison between the model predictions and DNS for low $Re\lambda$. Note that for these $Re\lambda$ there is an overlap of both effects, and thus one peak is present. However, at higher $Re\lambda$ there is a larger gap between the flow timescales, and two peaks are present. This is shown in Figure 2.12a and illustrates the independent effects of the large and small scales of turbulence. At high $Re\lambda$ the preferential concentration effects are dominant, which reinforces the notion that the physical structures of turbulence play a key role in particle dynamics. This model was subsequently
Figure 2.10: Normalized collision rate as a function of the ratio of the mean shear rate to the turbulence characteristic shear rate, $\Gamma/(\epsilon/\nu)^{1/2}$ for four shear rates. $\Gamma$ is made dimensionless by the initial isotropic state turbulence characteristic shear rate $(\epsilon_0/\nu)^{1/2}$. $\Gamma$ increases with time and total shear, thus illustrating that the collision rate is dependent of the structure of the turbulence. (From Mei & Hu, 1999).

extended by Zhou et al. (2001) to incorporate particles of different inertias.

Shown in Figure 2.12b is the difference in collision rate between the model of Wang et al. (2000) and models that don’t account for preferential concentration effects. The disparity between the models grows as the $Re_\lambda$ increases.

Zhou et al. (2001) continued the work of Wang et al. (2000) using DNS. One of the important conclusions of this work was the confirmation that particles with different Stokes number sample the flow field differently. Furthermore, particles of the same inertia are more likely to collide with particles of different inertias. This was also confirmed by Fayed & Ragab (2012).
2.3 Stochastic Lagrangian methods

Stochastic Lagrangian methods (SLM) have long been used to track the dispersion of Lagrangian particles in high Reynolds number turbulence (Pope, 1994, 2000). The Markov property is assumed in these methods, namely, the next state of the system only depends on the present state. All SLM use a statistical random variable with zero mean and a variance on the order of the time step. In the simplest sense, they account for the mean fluid motion via the following equation for velocity,

\[ du = -\frac{u}{T} dt, \]

\[ (2.2) \]
Figure 2.12: (a) The dimensionless collision kernel plotted against the Stokes number. The first peak corresponds to the maximum effect of preferential concentration. The arrows correspond to where the turbulent transport phenomenon is at a maximum. In (b) the difference in model predictions for collision frequency as a function of Reynolds number is plotted for the model of Wang et al. (2000) and models that do not account for preferential concentration. (From Wang et al., 2000).

where $T$ is the Lagrangian time scale. To account for the random fluctuations in a turbulent flow, a stochastic part is added to the equation,

$$du = -\frac{u}{T}dt + d\mathcal{R},$$

(2.3)

where $d\mathcal{R}$ is a random variable.

Pope (1985) made the argument that any turbulent fluid property can be treated as a random variable, such as velocity. Even in two experiments with the ‘exact same’ initial and boundary conditions, the results will be different. The smallest differences in any condition of the system will be amplified by the turbulence, thus leading to a different solution.

Here we examine three stochastic Lagrangian methods, starting with the simplest.
2.3.1 The Thomson model

Thomson (1987) proposed criteria for the selection of stochastic models of Lagrangian particle dispersion in turbulent flow. Including the assumption of the Markov property, Thomson also noted that if the Reynolds number is sufficiently large, then the effects of molecular diffusion on the ensemble mean concentration field is very small. This approximation allows us to satisfactorily treat the Lagrangian particles as if they were fluid elements. This is the first criteria proposed by Thomson and is the so-called well-mixed condition. This criteria states that the density functions of the distribution of Lagrangian particles and fluid elements should be equal.

The class of SLMs considered by Thomson are concerned with the evolution of velocity, \( \mathbf{u} \), and subsequently position, \( \mathbf{x} \). Mathematically, they are represented by

\[
du_i = c_i(\mathbf{x}, \mathbf{u}, t)dt + b_{ij}(\mathbf{x}, \mathbf{u}, t)d\xi_j
\]

\[
d\mathbf{x} = \mathbf{u}dt
\]

where \( c_i \) and \( b_{ij} \) are functions of \( \mathbf{x}, \mathbf{u}, \) and \( t \) and the subscript \( i \) denotes different dimensions. \( d\xi_i \) is an independent random variable with zero mean and variance \( dt \).

This equation is the basis for all velocity-based stochastic Lagrangian methods. A simple model for Gaussian turbulence has the form of a Langevin equation,

\[
du_i = -\frac{u_i}{\tau}dt + \left(\frac{2\sigma_u^2}{\tau}\right)^{\frac{1}{2}}d\xi_i
\]

where \( \sigma_u^2 \) is the velocity variance. This model is valid for homogeneous, statistically stationary turbulence in one dimension with no mean flow. Others have extended this model to account for some inhomogeneity and non-stationarity (Wilson et al.,
1983; Thomson, 1984). A simple way to extend to three dimensions is to assume that equation (2.6) is independent in each dimension.

Figure 2.13 shows a sample application of equation (2.6). Fluid element paths are plotted for the case of stationary homogeneous turbulence. Due to the independent random forcing term, fluid elements with the same initial conditions will have different paths.

A favorable consequence of the Markov assumption is that after sufficient time the initial conditions are “forgotten.” As long as the time scales are prescribed correctly, any discontinuities with the initial conditions will vanish. However, this assumption is such that the model cannot accurately resolve particle trajectories over the order of the Kolmorgorov timescale, $\tau_\eta$.

Equation (2.6) has been extended to describe more complicated situations such as nonhomogeneous turbulence (Thomson, 1987; Mito & Hanratty, 2002). Mito & Hanratty (2002) performed a numerical study of turbulent dispersion in a channel flow using a modified form of (2.6). Figure 2.14 shows the dispersion of fluid elements.
released from different distances from the wall, $x_2^+$. These results match well with DNS results, and show the usefulness and power of this model.

![Dispersion of fluid elements in a channel flow](image)

Figure 2.14: Dispersion of fluid elements in a channel flow originating at a distance, $x_2^+ = 300$ in the wall-normal direction. (From Mito & Hanratty, 2002).

### 2.3.2 The Sawford model

Sawford (1991b) proposed an acceleration-based stochastic Lagrangian model. The motivation for developing an acceleration-based method is so that the acceleration field is not a random variable. With the velocity-based methods the acceleration field is perturbed by a random variable, and is dependent on the time step. Sawford gives a physical interpretation of the different model orders which is shown in table 2.1. In

<table>
<thead>
<tr>
<th>Markov Variables</th>
<th>White-noise variable</th>
<th>Order of $U$ equation</th>
<th>Time scale</th>
</tr>
</thead>
<tbody>
<tr>
<td>Diffusion equation</td>
<td>$x$</td>
<td>$u = \frac{dx}{dt}$</td>
<td>0</td>
</tr>
<tr>
<td>Langevin equation</td>
<td>$x, u$</td>
<td>$a = \frac{du}{dt}$</td>
<td>1</td>
</tr>
<tr>
<td>Sawford’s model</td>
<td>$x, u, a$</td>
<td>$\frac{da}{dt}$</td>
<td>2</td>
</tr>
</tbody>
</table>

Table 2.1: Table showing model hierarchy of stochastic Lagrangian models. (Adapted from Sawford, 1991b).
this table $T$ is the Lagrangian time scale, and $\tau_\eta$ is the Kolmogorov time scale. The diffusion equation contains no time scale whereas the Langevin equation contains $T$, which represents the energy-containing scales of motion. The addition of $\tau_\eta$ in the second order model, which is representative of the dissipative scales, helps alleviate a flaw with the Markovian assumption of the Thomson model.

The Sawford model is given by

$$
d a + \alpha_1 a dt + \alpha_2 \int_0^t a(t') dt' dt = \sqrt{2\alpha_1 \alpha_2 \sigma_u^2} d\xi
$$

(2.7)

where $\sigma_u^2$ is the velocity variance, $\alpha_i$ are coefficients chosen to ensure that $u$ and $a$ are asymptotically stationary, and $d\xi$ is a random variable with zero mean and variance $dt$. Equations for velocity and position are obtained by successively integrating equation (3.2) in time.

Pope (2011) presented the Sawford model with coefficients for homogeneous turbulence, given by

$$
da = - \left( 1 + \frac{\eta_c}{\tau_c} \right) \frac{a}{\eta_c} dt - \frac{u}{\tau_c \eta_c} dt + \left[ 2a'^2 \left( \frac{1}{\eta_c} + \frac{1}{\tau_c} \right) \right]^\frac{1}{2} d\xi
$$

(2.8)

where $a'^2$ is the root mean squared acceleration, $\tau_c$ and $\eta_c$ are related to the integral time scale and Kolmogorov time scale, respectively. $a_0$ and $C_0$ are constants that can be fit from DNS data.

By design, Sawford’s model produces Gaussian velocity and acceleration statistics. However, acceleration statistics of turbulent flow are shown to have highly non-Gaussian statistics (Mordant et al., 2004; Lee, 2005; Ayyalasomayajula et al., 2008). Despite this shortcoming, Figure 2.15 shows that Sawford’s model does reasonably...
well at reproducing the velocity structure function when compared to DNS.

Figure 2.15: Comparision of velocity structure function for equation (2.7) and DNS from Yeung & Pope (1989). (From Sawford, 1991a).

2.3.3 The Reynolds model

Reynolds (2003) assembled an acceleration-based SLM to produce the non-Gaussian statistics observed in DNS and experiments. The model incorporates an instantaneous dissipation rate, which means that each particle has a unique dissipation rate modeled by an independent stochastic equation (Pope & Chen, 1990).

Pope and Chen assumed that the evolution of the logarithm of the normalized dissipation rate, \( \chi = \ln(\epsilon/\langle \epsilon \rangle) \), is a stationary Markovian process and can be modeled by a Uhlenbeck-Ornstein process

\[
d\chi = -\left(\chi - \langle \chi \rangle\right) \frac{dt}{T_\chi} + \left(\frac{2\sigma^2_\chi}{T_\chi}\right)^{1/2} dW \tag{2.9}
\]

where \( \chi = \chi(t) \), \( dW \) is a Gaussian random variable with zero mean and variance
\[ dt, \epsilon = \epsilon(t) \text{ is the local dissipation rate, and } \langle \epsilon \rangle \text{ is the mean dissipation rate. The Reynolds model for acceleration is} \]

\[
da = - \left( \frac{1}{\tau_c} + \frac{1}{\eta_c} - \frac{1}{\sigma_a} \frac{d\sigma_a}{dt} \right) a dt - \frac{u}{\tau_c \eta_c} dt + \sqrt{2\sigma_u^2 \left( \frac{1}{\tau_c} + \frac{1}{\eta_c} \right) \frac{1}{\tau_c \eta_c}} d\xi \]

(2.10)

where \( \tau_c, \eta_c \) are related to the Lagrangian time scale and Kolmogorov time scale, respectively; and \( \sigma_u^2 \) and \( \sigma_a^2 \), are the variance of velocity and acceleration, respectively. Again, the constants \( a_0^* \) and \( C_0 \) are fit from DNS data.

In this model, the time scale parameters, \( \tau_c \) and \( \eta_c \), change at each time step due to the evolution of the local dissipation rate \( \epsilon \). Also, the acceleration variance \( \sigma_a^2 \) is conditional on the local dissipation rate, and can be expressed as \( \sigma_a^2 = \sigma_a^2 | \epsilon \). This says that for a given dissipation rate there exists a distribution of accelerations.

The advantage of this model over the Sawford model, is that it produces non-Gaussian statistics of acceleration. Figure 2.16 shows the probability density function for normalized acceleration for the Sawford model, Reynolds model, and experimental data. Reynolds model produces the characteristic fat tails of the acceleration PDF.

### 2.4 The vortex model

Ayyalasomayajula et al. (2008) introduced a model to simulate 2D flow that uses an array of potential vortices of time-varying strength. The model was constructed in an effort to produce a flow field in which preferential concentration of inertial particles occurred.

The parameters of the model are based on the physical scales of the flow. The spacing between the vortices is fixed and is equal to the integral length scale. The
vortices have a viscous core with a radius of the Kolmogorov length scale. Outside of the core 2D inviscid potential flow theory is invoked to compute the velocity. The circulation of a single vortex is given by a random Gaussian function with zero mean and standard deviation equal to integral length scale squared over the integral time scale, $\sigma_\Gamma = L^2/T_L$ where $L$ is the integral length scale and $T_L$ is the integral time scale. Figure 2.17 shows how inertial particles selectively sample the flow field by clustering in regions away from the vortex centers.

Figure 2.16: Probability density functions for Lagrangian accelerations produced by equation (2.10) (solid line), and equation (2.7) (dotted line). Experimental data (LaPorta et al., 2001) for the tail of the distribution for $Re_\lambda = 200$ (circles) and $Re_\lambda = 970$ (squares). (Adapted from Reynolds, 2003).
Figure 2.17: PDF of particles distances from vortex centers for fluid elements (line) and inertial particles with various Stokes numbers produced by the vortex model of Ayyalasomayajula et al. (2008). Fluid particles are seen to be nearly uniformly distributed whereas inertial particles have a tendency to cluster in regions away from the vortex centers. (From Ayyalasomayajula et al., 2008).
Chapter 3

Computational methods

3.1 Stochastic Lagrangian models

Presented in this section are the details of the three stochastic Lagrangian models; one velocity-based and two acceleration-based. The numerical solution is presented for the Sawford model, and the others can be found in Appendix B.

3.1.1 The Thompson model

Thomson (1987) proposed a fairly simple model for homogeneous turbulence, which is based on the generalized Langevin equation. In this model the \( i^{th} \) component of the velocity is approximated by solution of the stochastic differential equation

\[
du_i = -\frac{u_i}{T} dt + \left( \frac{4q_i}{T} \right)^{1/2} d\xi
\]

where \( q_i = \overline{u_iu_i}/2 \) is the turbulence kinetic energy associated with the \( i^{th} \) component of the fluctuating velocity field (no sum on the repeated index) and \( T \) is the integral
time scale, which is related to the turbulence dissipation rate $\epsilon$ and the total turbulent kinetic energy $q = q_1 + q_2 + q_3$ by $T = q/3\langle \epsilon \rangle$. The differential $d\xi$ is a Gaussian distributed random variable with zero mean and variance equal to the time step $dt$. The tensor index convention does not apply for 3.1. It is assumed that both $\epsilon$ and $q_i$ are known as functions of position from a RANS solution for the turbulent flow field. The initial conditions are $u_i(x, 0) = \sigma_u d\xi$ where $\sigma_u = \sqrt{2q/3}$ is the velocity variance.

### 3.1.2 The Sawford model

Sawford (1991b) modeled the fluid acceleration of stationary homogeneous isotropic turbulence using a second-order autoregressive equation. A version of the equation for homogeneous turbulence was proposed by Pope (2011) as

$$da_i = -\left(1 + \frac{\eta_c}{\tau_c}\right) \frac{a_i}{\eta_c} dt - \frac{u_i}{\tau_c \eta_c} dt + \left[2a_i^2 \left(\frac{1}{\eta_c} + \frac{1}{\tau_c}\right)\right]^{\frac{1}{2}} d\xi \tag{3.2}$$

where $a = a(t)$ is the Lagrangian acceleration, $a_i^2 = u_i^2/(\tau_c \eta_c)$ is the root-mean-squared acceleration, the time scales $\tau_c = 4T/C_0$ and $\eta_c = C_0 \eta/2a_0$ are related to the integral time scale $T$ and Kolmogorov time scale $\eta$, respectively. The coefficient $a_0$ is fit using DNS and is represented by the power law, $a_0 = 0.13 \cdot Re_\lambda^{0.64}$, where $Re_\lambda = \sigma_u^2 (15/\nu \epsilon)^{1/2}$ is the Taylor microscale Reynolds number. The coefficient $C_0$ is the Kolmogorov constant, which is also obtained by a fit from direct numerical simulation data as $C_0 = 7$ (Sawford, 1991b). The initial conditions are $u_i(x, 0) = \sigma_u d\xi$, and $a_i(x, 0) = u_i/(\tau_c \eta_c)$. 

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3.1.3 The Reynolds model

Pope & Chen (1990) assumed that the evolution of the logarithm of the normalized dissipation rate, \( \chi = \ln(\epsilon / \langle \epsilon \rangle) \), is a stationary Markovian process and can be modeled by a Uhlenbeck-Ornstein process, such that

\[
d\chi = - (\chi - \langle \chi \rangle) \frac{dt}{T_\chi} + \left( \frac{2\sigma^2 \chi}{T_\chi} \right)^{\frac{1}{2}} dW
\]

(3.3)

where \( \chi = \chi(t) \), \( dW \) is a Gaussian random variable with zero mean and variance \( dt \), \( \epsilon = \epsilon(t) \) is the local dissipation rate, and \( \langle \epsilon \rangle \) is the mean dissipation rate. Since \( \chi \) is Gaussian and normalized so that \( \langle \exp(\chi) \rangle \) is unity, its mean is given by \( \langle \chi \rangle = -\sigma^2 / 2 \).

The time scale is given by \( T_\chi = 2\sigma^2 / C_0 \langle \epsilon \rangle \) and the variance is fit from DNS data, yielding \( \sigma^2 = -0.354 + 0.289 \ln(Re_\lambda) \), where \( Re_\lambda = \sigma_u \lambda / \nu \) is the Reynolds number based on the Taylor microscale \( \lambda = \sqrt{15\nu \sigma^2_u / \langle \epsilon \rangle} \). The Reynolds model for acceleration is,

\[
da_i = - \left( \frac{1}{\tau_c} + \frac{1}{\eta_c} - \frac{1}{\sigma_{a|\epsilon}} \frac{d\sigma_{a|\epsilon}}{dt} \right) a_i dt - \frac{u}{\tau_c \eta_c} dt + \sqrt{2\sigma^2_u \left( \frac{1}{\tau_c} + \frac{1}{\eta_c} \right) \frac{1}{\tau_c \eta_c}} d\xi
\]

(3.4)

where \( \tau_c = 4T / C_0 \) is representative of the energy-containing scales and \( \eta_c = C_0 \tau_c / 2a_0 \) is representative of the dissipative scales of motion. The variance of velocity and acceleration are \( \sigma^2_u = 2q / 3 \) and \( \sigma^2 = a_0^* \epsilon / \eta_c \), respectively. The constants \( a_0^* = 3.3 \) and \( C_0 = 7 \) are fit from DNS data (Yeung & Pope, 1989), and \( a_0^* \) is a universal constant related to \( a_0 \) by the relationship \( a_0 = a_0^* \exp(\frac{2}{9} \sigma^2) \) (Reynolds, 2003). The differential \( d\xi \) is also a Gaussian random variable with zero mean and variance \( dt \), but it is independent of the variable \( dW \). The conditional acceleration variance \( \sigma_{a|\epsilon} \) depends on \( \chi(t) \). For each set of fluid particles with a given \( \epsilon \), there are many different
accelerations, which is why the acceleration variance is conditional on $\epsilon$. The variance is defined by
\[
\sigma_{a|\epsilon} = a_0^2 (\epsilon/\langle \epsilon \rangle)^3/2 a_\eta^2
\] (3.5)
where $a_\eta = (\langle \epsilon \rangle^3/\nu)^{1/4}$ is the Kolmogorov acceleration scale. The values of $\sigma_{a|\epsilon}^2$, $\tau_c$, and $\eta_c$ depend on the local dissipation rate $\epsilon$ and change in time for the Reynolds model. The initial conditions for these equation are $\chi(x, 0) = \sigma \chi dW$, $\epsilon(x, 0) = \langle \epsilon \rangle \exp[\chi(x, 0)]$, $u_i(x, 0) = \sigma_u d\xi$, and $a_i(x, 0) = \sigma_{ai} d\xi$.

### 3.1.4 Numerical solution

In this section the numerical formulation for the Sawford model is presented. The numerical method used for the other stochastic Lagrangian methods are similar, and are presented in Appendix B.

Beginning with equation (3.2) we seek to solve for acceleration and subsequently velocity via integration of $du/dt = a$. To aid in the clarity of the analysis the following constants are defined, $c_1 \equiv -1/(\eta_c + 1/\tau_c)$, $c_2 \equiv -1/(\tau_c \eta_c)$, and $c_3 \equiv [2a_\eta^2(1/\eta_c + 1/\tau_c)]^{1/2}$. Replacing the parameters in equation (3.2) with these constants and multiplying by an integration factor of $\exp(-c_1 t)$ we have,
\[
\frac{d}{dt}[\exp(-c_1 t) a] = \exp(-c_1 t) \left( c_2 u + c_3 \frac{dW}{dt} \right).
\] (3.6)
A predictor-corrector algorithm is used to advance the solution. The predictor steps, denoted by $^*$, are,
\[
a_{n+1}^* = \Delta t \left( (c_2 u_n + c_3) \frac{dW}{dt} \right) \exp(c_1 \Delta t) + \exp(c_1 \Delta t) a_n
\] (3.7)
\[ u_{n+1}^* = \Delta t a_n + u_n \]  

(3.8)

and the corrector steps are,

\[ a_{n+1} = \Delta t \left[ \frac{c_2}{2} (u_n + u_{n+1}^*) + c_3 \frac{dW}{dt} \right] \exp(c_1 \Delta t) + \exp(c_1 \Delta t) a_n \]  

(3.9)

\[ u_{n+1} = \frac{1}{2} \Delta t [a_n + a_{n+1}^*] + u_n. \]  

(3.10)

The SLM equations are solved on Lagrangian fluid elements; however, if the spatial fields are of interest, such as for making contour plots, then fluid values will be needed on a grid. The interpolation of data from randomly distributed particles to a fixed grid poses various challenges. A number of methods exist, and an overview of popular methods are discussed by (Marshall & Sala, 2012), including the particle counting method, standard blob method, conservative blob method, moment preserving \( M_4' \) method, and a moment preserving method using a Gaussian weighing function. Of these methods we use the so-called \( M4' \) method introduced by Monaghan (1985). This method works well for this application because it has limited smearing effects compared with the other methods that use weighted averages. The \( M_4' \) method yields an interpolation function of the form

\[
M_4'(x) = \begin{cases} 
0 & \text{if } x > 2 \\
\frac{1}{2} (2-x)^2(1-x) & \text{if } 1 \leq x \leq 2 \\
1 - \frac{5}{2} x^2 + \frac{3}{2} x^3 & \text{if } x < 1 
\end{cases}
\]  

(3.11)

If \( h \) denotes the grid increment size, the turbulent kinetic energy is set on the grid

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nodes by

\[ q_i(x_g, y_g, z_g) = \sum_{n=1}^{N} \frac{u_{i,n}'}{2} h^{3} M_i' \left( \frac{x_{i,g} - \hat{x}_{i,n}}{h} \right) \]  

(3.12)

where \( u_{i,n}' \) is the rms velocity on the Lagrangian fluid elements, \( x_{i,g} \) is the grid location of the \( i^{th} \) direction (\( x, y, \) or \( z \)) and \( (x_g, y_g, z_g) \) are the grid node locations. The velocity is then computed by

\[ u_i(x_g, y_g, z_g) = S_i(x_g, y_g, z_g) \sqrt{\frac{2q_i(x_g, y_g, z_g)}{h^3}} \]  

(3.13)

where \( S_i \) is a coefficient to keep track of the sign and is defined by

\[ S_i(x_g, y_g, z_g) = \begin{cases} 
+1 & \text{if } \sum_{n=1}^{P} u_i' \geq 0 \\
-1 & \text{if } \sum_{n=1}^{P} u_i' < 0 
\end{cases} \]  

(3.14)

where \( P \) is the number of particles contributing to \( q_i(x_g, y_g, z_g) \).

### 3.2 Stochastic vortex structure method

We propose here a new stochastic vortex structure (SVS) model that approximates the fluctuating vorticity field of the turbulent flow by a set of three-dimensional vortex structures, which have certain features based on scaling analysis and other features selected as random variables from a prescribed probability distribution function. The method is designed to mimic turbulence with a specified kinetic energy and length scale, but to do so using a structure-based vorticity field rather than the randomly-forced vorticity field that is typical of stochastic Lagrangian methods. The emphasis on vortex structures in the SVS approach is based on the understanding that coherent
vortex structures are primarily responsible for the small-scale dispersion of particles which leads to local concentration heterogeneity in turbulent particulate flows.

The current study employs a scaling approach based on the energy-containing motion of a homogeneous turbulent fluid flow. Specifically, the total number of vortex structures in the computational domain, \( N_v \), is set so that the average distance between the vortex centers, \( L_v \), is proportional to the Lagrangian integral length scale, \( L = u_0^3/(2\epsilon) \), where \( u_0 \) is a characteristic velocity scale of the energy-containing motion, \( q = 3u_0^2/2 \) is the turbulent kinetic energy and \( \epsilon \) is the turbulent dissipation rate. The length of the vortex structures is set equal to \( L_v \), and is hence also proportional to the integral length scale, while the vortex core radius, \( r \), is proportional to the Kolmogorov length scale \( \eta = (\nu^3/\epsilon)^{1/4} \), where \( \nu \) is the fluid kinematic viscosity. Each vortex structure has a finite life, \( T_v \), that is set equal to the integral time scale, \( T_L = q/3\epsilon \). The maximum vortex strength, \( \Gamma_{\text{max}} \), is set to be proportional to the ratio of \( L^2/T_L \). Based on this energy-containing scaling and denoting the computational domain volume by \( V \), these scaling relationships can be summarized as follows:

\[
N_v = \alpha_1 V/L_v^3, \quad L_v = \alpha_1 L, \quad r = \alpha_2 \eta, \quad T_v = T_L, \quad \Gamma_{\text{max}} = \alpha_3 L^2/T_L, \quad (3.15)
\]

where \( \alpha_1, \alpha_2, \) and \( \alpha_3 \) are adjustable coefficients.

The scaling (3.15) is typical of what one might use in a RANS based simulation study, in which only the mean flow is directly simulated and the turbulence is characterized by measures such as the turbulent kinetic energy and dissipation rate. An alternative scaling might be used for coupling the SVS method to LES, where here the energy-containing scales are directly simulated and the SVS structures are meant to approximate the smaller, sub-grid eddy structures. It is also noted that the current
work demonstrates the SVS approach using homogeneous turbulence, which provides for a simple description of the SVS method and also simplifies the DNS comparison study.

The flow field is initiated by placing $N_v$ vortex structures in the computational domain, which in the current computations was selected to be a triply-periodic cube with side length $2\pi$. The centroid position and orientation of each vortex structure are selected randomly using a uniform probability distribution, and the position of each vortex structure is fixed in time. Each vortex structure has the form of a straight line segment of length $L_v$. The initial set of vortex structures are each assigned an initial age $\tau_{0n}$, chosen as a random variable for which the ratio $\tau_{0n}/T_v$ has a uniform distribution between 0 and 1. The age $\tau_n(t)$ of the $n^{th}$ vortex structure increases with time as

$$\tau_n = \tau_{0n} + t - t_{0n}$$

where the time $t_{0n}$ at which the vortex structure is introduced is set equal to zero for the initial set of vortex structures. When $\tau_n \geq T_v$, the $n^{th}$ vortex structure is removed from the flow field and a new vortex structure is introduced with $t_{0n} = t$ and $\tau_{0n} = 0$. This new vortex structure is located with centroid position and vortex orientation selected as random variables with uniform probability distribution, as was done for the initial vortex structures.

The vortex strength $\Gamma_n(t)$ is specified as

$$\Gamma_n(t) = \Gamma_{max} A_n \begin{cases} 5\tau_n/T_v & \text{for } 0 \leq \tau_n/T_v < 0.2 \\ 1 & \text{for } 0.2 \leq \tau_n/T_v \leq 0.8 \\ 1 - 5(\tau_n/T_v - 0.8) + 1 & \text{for } 0.8 < \tau_n/T_v \leq 1 \end{cases}$$

(3.17)
so that it ramps up gradually near the beginning of the vortex life, remains constant throughout the middle part of the vortex life, and ramps back down near the end of the vortex life. The parameter $A_n$ in (3.17) is a normally-distributed random variable with zero mean and unit variance, which is set once for each vortex at the time that the vortex is initialized.

The induced velocity from each vortex structure is obtained using a Gaussian vortex blob formation (Marshall & Grant, 1996). The number of blobs per vortex structure, $N_b$, is a constant determined by

$$N_b = \frac{\beta L_v}{r}, \quad (3.18)$$

where the blob radius is set equal to the vortex ring radius $a$ and $\beta$ is a blob “overlap” coefficient that is usually set equal to 2. For each vortex blob with blob centroid $x_m$, $m = 1, ..., N_b$, there is an associated vorticity field of the form

$$\omega_m(x, t) = \frac{\Omega_m}{\pi^{3/2}r^3} \exp \left( -\frac{|x - x_m|^2}{r^2} \right), \quad (3.19)$$

where the blob amplitude $\Omega_m$, given by

$$\Omega_m = (\Gamma_n L / N_b) \lambda_b, \quad (3.20)$$

is the same for all blobs in a given vortex structure $n$ with strength $\Gamma_n$. Here $\lambda_b$ is a unit vector oriented along the axis of the $n^{th}$ vortex structure. Substituting (3.19) in the Biot-Savart integral yields the velocity field induced by the $m^{th}$ vortex blob as

$$u_m(x, t) = P \left( \frac{3}{2}, \frac{|x - x_m|^2}{a^2} \right) \frac{\Omega_m}{4\pi|x - x_m|^3} \times (x - x_m), \quad (3.21)$$
where \( P(r, z) \) is the incomplete gamma function with limit \( P(r, 0) = 0 \) and \( P(r, \infty) = 1 \). When \( r = 3/2 \) and \( z = x^2 \) for some real variable \( x \), a convenient expression for the incomplete gamma function in terms of the error function \( \text{erf}(x) \) can be written as (Abramowitz & Stegun, 1965)

\[
P\left(\frac{3}{2}, x^2\right) = \text{erf}(x) - \frac{2x \exp(-x^2)}{\sqrt{\pi}}.
\]

(3.22)

The induced velocity from all vortex blobs are added to obtain the total velocity field.

At the start of the computation, the induced velocity from a single vortex structure that has unit strength (\( \Gamma_n = 1 \)), centroid at the origin, and orientation in the positive \( x \)-direction is computed and stored on a grid covering the \( x-y \) plane. At all subsequent times, the induced velocity from a vortex structure \( n \) at grid point \( x \) is obtained by orienting a plane centered at the vortex centroid \( x_n \) and passing through \( x \) that is tangent to the vortex axis unit vector \( \lambda_n \). The position of the grid point \( x \) is obtained in this plane by integer division and the velocity induced by the vortex is interpolated onto the grid point and reoriented to lie in the global coordinate system.

In order to enforce the periodic boundary condition, the velocity induced by vortex structures in one period on each side of the computational domain are included in the computation, resulting in a total of \( 27N_v \) vortex structures to be accounted for in determining the total velocity at each grid point.

### 3.3 Direct Numerical Simulation

A direct numerical simulation (DNS) is employed to compute forced homogeneous turbulence. The fluid flow computations are performed using a pseudo-spectral method.
with second-order Adams-Bashforth time stepping and exact integration of the viscous term (Vincent & Meneguzzi, 1991). In this approach, the spectral Navier-Stokes equations are evolved in time after having been projected onto a divergence-free space using the operation \( P_{ij} = k_i k_h / k^2 - \delta_{ij} \) according to the expression

\[
\hat{u}^{n+1} = \hat{u}^n \exp(-\nu k^2 \Delta t) + \Delta t P \cdot \left[ \frac{3}{2} (\hat{u} \times \hat{\omega})^n \exp(-\nu k^2 \Delta t) \right. \\
- \left. \frac{1}{2} (\hat{u} \times \hat{\omega})^{n-1} \exp(-2\nu k^2 \Delta t) \right] + \hat{f}(k) \Delta t
\]

(3.23)

where \( \mathbf{u} \) and \( \mathbf{\omega} \) are the velocity and vorticity vectors, a top-hat denotes Fourier transform in three space dimensions, a superscript indicates the time step, \( \nu \) is the fluid kinematic viscosity, and \( \mathbf{f} \) is a small-wavenumber forcing vector. The velocity field is made divergence-free at each time step by taking its Fourier transform and using the spectral form of the continuity equation. Results with and without dealiasing are found to exhibit no significant differences at the large scales, so dealiasing is not used in the current computations in order to consider the broadest possible spectral range.

The DNS computations are performed on a periodic \( 128^3 \) cubic grid with domain side length \( 2\pi \) and dimensionless kinematic viscosity \( \nu = 1/1000 \). The flow is initiated by a randomly perturbed velocity field with uniform probability distribution for wavenumbers spanning the interval \( 1 \leq k \leq 64 \). A preliminary computation is run as a decaying turbulent flow field until time \( t = 10 \) in order to allow the turbulence to develop a range of length scales characteristic of homogeneous turbulence. The computation is then restarted with particles and forcing. The forcing vector is assumed to be proportional to the fluid velocity (Lundgren, 2003; Rosales & Meneveau, 2005).
such that

\[ \hat{f} = \begin{cases} C\hat{u} & \text{for } k < k_{\text{crit}} \\ 0 & \text{for } k > k_{\text{crit}} \end{cases} \]  

(3.24)

where the coefficient \( C \) is adjusted at each time step so as to maintain approximately constant turbulence kinetic energy. The current computations are performed with \( k_{\text{crit}} = 5 \), so that the forcing acts only on the large-scale eddies.

### 3.4 Discrete-element model

A discrete-element method (DEM) is used to examine particle transport at finite Stokes number (Marshall, 2009). The computational method is performed using three distinct time steps: the fluid time step \( \Delta t = f_1T_F \), the particle time step \( \Delta t_p = f_2T_P \), and the collision time step \( \Delta t_c = f_3T_C \) where \( f_1 \), \( f_2 \), and \( f_3 \) are constants with values much less than unity. The time steps satisfy \( \Delta t > \Delta t_p > \Delta t_c \). The method follows the motion of individual particles in the three-dimensional fluid flow by solution of the particle momentum and angular momentum equations

\[
m \frac{dv}{dt} = F_F + F_A, \quad I \frac{d\Omega}{dt} = M_F + M_A,
\]

(3.25)

under forces and torques induced by the fluid flow (\( F_F \) and \( M_F \)) and by the particle collision (\( F_A \) and \( M_A \)). In these equations, the fluid forces on the particle is denoted by \( F_F \), and the elastic collision force and van der Waals adhesion force together are denoted \( F_A \). In the angular momentum equation, \( M_F \) and \( M_A \) denote the corresponding fluid torque and the sum of the collision and van der Waals adhesion torques on the particle. \( m \) is the particle mass and \( I \) is the moment of inertia. The
dominant fluid force is the drag force, approximated by a modified form of the Stokes drag law

$$ F_d = -3\pi \mu d (v - u)f, $$  \hspace{1cm} (3.26)

where \( v \) and \( u \) are the particle and local fluid velocities, respectively, \( f \) is a friction factor that accounts for the effect of local particle crowding, which takes the value \( f = 1 \) for an isolated sphere. We use a correlation of DiFelice (1994) for \( f \) as a function of local particle concentration \( c \) and particle Reynolds number \( Re_p = |v - u|d/\nu \). The associated fluid torque arises from a difference in rotation rate of the particle and the local fluid region and is given by

$$ M_F = -\pi \mu d^3 (\Omega - \frac{1}{2} \omega), $$  \hspace{1cm} (3.27)

where \( \Omega \) is the particle rotation rate and \( \omega \) is the local fluid vorticity vector. The force due to lift is given by (Saffman, 1965, 1968)

$$ F_l = -2.18m^2 \rho f \frac{(v - u) \times \omega}{\rho_p Re_p^{1/2} \alpha_L^{1/2}} $$  \hspace{1cm} (3.28)

where \( \alpha_L \equiv |\omega|d/(2|v - u|) \). When a particle has different rotation rate than the surrounding fluid, there is an associated force known as the Magnus force (Rubinow & Keller, 1961). This force is particularly important in the case of particle-particle collisions. The expression is given by

$$ F_m = -\frac{3}{4} \rho f m \left( \frac{1}{2} \omega - \Omega \right) \times (v - u). $$  \hspace{1cm} (3.29)
The ratio of the particle density to the fluid density is sufficiently large, \( \rho_p/\rho_f \geq 10 \), such that the added mass and pressure gradient forces can be ignored.

Particle collisions are simulated by employing a soft-sphere collision model, where each collision includes a normal force \( F_n \) along the line of collision and frictional resistances for sliding and twisting motions of the particles. Presented here is the theory for adhesive forces, while the case without adhesive forces is a limiting case. For the details on this limiting case we direct the reader to the theory by Marshall (2006). The total collision and adhesion force and torque for a particle of radius \( r_i \) are given by

\[
F_A = F_n n + F_s t_S \quad M_A = r_i F_s (n \times t_S) + M_t n. \tag{3.30}
\]

The normal vector \( n \) is written in terms of the centroids \( x_i \) and \( x_j \) of two colliding particles as

\[
n = (x_j - x_i)/|x_j - x_i|. \tag{3.31}
\]

The unit vector \( t_S \equiv v_S/|v_S| \) indicates the direction of sliding between two particles, where the slip velocity \( v_S \) is defined by \( v_S = v_R - (v_R \cdot n)n + r_i \Omega_i \times n + r_j \Omega_j \times n \) and \( v_R = v_i - v_j \) is the particle relative velocity. The sliding resistance also imposes a torque on the particles in the \( n \times t_s \) direction. The rolling resistance applies a torque on the particle in the \( t_R \times n \) direction, where \( t_R \) is the direction of the rolling velocity.

The normal elastic force of two colliding particles can be expressed in terms of the particle effective radius \( R \) and the elastic and shear moduli, \( E \) and \( G \), are defined by

\[
\frac{1}{R} \equiv \frac{1}{r_i} + \frac{1}{r_j}, \quad \frac{1}{E} \equiv \frac{1 - \sigma_i^2}{E_i} + \frac{1 - \sigma_j^2}{E_j} \quad \frac{1}{G} \equiv \frac{2 - \sigma_i}{G_i} + \frac{2 - \sigma_j}{G_j}, \tag{3.32}
\]

where \( \sigma_i \) are the Poisson ratios, \( r_i \) are the individual particle radii and \( E_i \) and \( G_i \) are
the elastic and shear moduli of the individual particles. The adhesive forces between
the two particles depends on the surface potential \( \gamma \), where the work required to
separate two spheres colliding over a contact region of radius \( a(t) \) is given by \( 2\pi \gamma a^2 \)
in the absence of further elastic deformation. The normal force is further decomposed
into an elastic and dissipative part, \( F_{ne} \) and \( F_{nd} \) respectively. The elastic part of the
normal force can be expressed in terms of the contact region radius \( a(t) \) and the
particle overlap \( \delta_N \) by (Chokshi et al., 1993)

\[
\frac{\delta_N}{\delta_C} = 6^{1/3} \left[ 2 \left( \frac{a}{a_0} \right)^2 - \frac{4}{3} \left( \frac{a}{a_0} \right)^{1/2} \right], \quad \frac{F_{ne}}{F_C} = 4 \left( \frac{a}{a_0} \right)^3 - 4 \left( \frac{a}{a_0} \right)^{3/2}
\]

where the particle overlap \( d_N \) is defined by

\[
\delta_N = r_i + r_j - |x_i - x_j|.
\]

The critical overlap \( \delta_C \), the critical normal force \( F_C \), and the equilibrium contact
radius \( a_0 \) are given by (Johnson et al., 1971)

\[
F_C = 3\pi \gamma R, \quad \delta_C = \frac{a_0^2}{2(6)^{1/3}R}, \quad a_0 = \left( \frac{9\pi \gamma R^2}{E} \right)^{1/3}.
\]

As two particles move away from each other, they remain in contact until \( F_{ne} = -F_C \)
and \( \delta_N = \delta_C \) due to the necking within the contact region caused by particle adhesive
forces. Beyond this state any further separation leads the two particles to break
apart. In the limit of no adhesive force, (3.33) reduces to the particle repulsion force
formula of Hertz (1882).

In addition to the normal adhesive force, the normal dissipation force \( F_{nd} \) is given
by

$$F_{nd} = -\eta_N \mathbf{v}_R \cdot \mathbf{n},$$  \hspace{1cm} (3.36)$$

where $\eta_N$ is the normal friction coefficient. Tsuji et al. (1992) propose an expression for $\eta_N$ of the form

$$\eta_N = \bar{\alpha} (mk_N)^{1/2},$$ \hspace{1cm} (3.37)$$

where the coefficient $\bar{\alpha}$ is written as a function of the coefficient of restitution $e$ and $k_N = F_{ne}/\delta_N$ is the normal stiffness coefficient. In the current work the Stokes number is sufficiently small, less than $St = 10$, so that we set $e = 0$, in accordance with the experimental results of Joseph et al. (2001)

Sliding resistance between two particles is relatively rare for adhesive particles due to their relatively small momenta. It is predominantly important in situations where an aggregate of particles is torn apart by fluid shear forces. We use a spring-dashpot-slider model for the sliding resistance proposed by Cundall & Strack (1979), in which the tangential sliding force $F_s$ is first absorbed by the spring and dashpot until its magnitude reaches a critical value $F_{crit}$. The expression for the sliding resistance of the form Cleary et al. (1998)

$$F_s = -k_T \left( \int_{t_0}^{t} v_s(\zeta) d\zeta \right) \cdot \mathbf{t}_S$$ \hspace{1cm} (3.38)$$

is used for the subcritical case when $|F_s| < F_{crit}$. The slip velocity $v_S(t)$ is the tangent projection of $\mathbf{v}_R$ to the particle surface at the contact point, or $v_S = \mathbf{v}_R - (\mathbf{v}_R \cdot \mathbf{n})\mathbf{n}$ and the slip direction is $\mathbf{t}_S = \mathbf{v}_S/|\mathbf{v}_S|$. The tangential stiffness coefficient $k_T$ is derived by Mindlin (1949). In terms of the radius of the contact region $a(t)$ the coefficient...
can be written as $k_T = 8Ga(t)$. The critical sliding force is approximated by

$$F_{crit} = \mu_f|F_{ne} + 2F_C|,$$  \hspace{1cm} (3.39)

where the addition of the $2F_C$ term is to make sure the force is applied only as the particles are separating. In the limiting case of no adhesion, this term would be given by $F_{crit} = \mu_f|F_n|$.

Twisting resistance occurs when particles collide that have different rotations in the direction normal to the contact region, $n$. The relative twisting rate $\Omega_T$ is defined by

$$\Omega_T = (\Omega_i - \Omega_j) \cdot n.$$  \hspace{1cm} (3.40)

The torque due to twisting can be derived analogously to the case for frictional sliding. The details of the this derivation, including the derivation of the coefficients, is done by Marshall (2009). The resulting expression for twisting resistance is

$$M_t = -k_\Omega \int_{t_0}^{t} \Omega(\tau) d\tau - \eta_Q \Omega_T,$$  \hspace{1cm} (3.41)

where $k_\Omega = k_t a^2/2$ is the torsional stiffness and $\eta_Q = \eta_T a^2/2$ is the friction coefficient. Particles will spin relative to one another when the torque exceeds a critical value

$$M_{t, crit} = 2/3 \mu_f a|F_n + 2F_C|.$$  \hspace{1cm} (3.42)

In the limiting case of no adhesion this is given by $M_{t, crit} = 2aF_{crit}/3$. When the torque between the particles exceeds this critical value, such that $|M_t| > M_{t, crit}$ the twisting resistance is given by $M_t = -M_{t, crit} \Omega_T/|\Omega_T|$. 

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Chapter 4

Computational Results

4.1 Measures

A set of measures to categorize the fluid characteristics that lead to particle dispersion are described. These measures were designed to isolate specific features of a flow field and allow both a qualitative and quantitative comparison between the models and DNS.

4.1.1 Particle dispersion measure

Particle dispersion occurs when particles drift across fluid streamlines as the particles are carried by the flow. In order to derive a variable that characterizes the potential of a flow for dispersion of particles, it is necessary to examine the dominant terms in the particle momentum equation that govern dispersion. While there are a variety of effects that influence particle motion, the two dominant terms in the particle momentum equation will always be particle inertia and drag force (Zhao & Marshall, 2008). Assuming drag is the dominant force on the particle and fairly dilute particulate flow,
the momentum equation for particle velocity $\mathbf{v}$ becomes

$$
m \frac{d\mathbf{v}}{dt} = -3\pi \mu d (\mathbf{v} - \mathbf{u}),
$$

(4.1)

where $m$ is the particle mass, $d$ is the particle diameter, $\mu$ is the fluid viscosity, $\mathbf{u}$ is the fluid velocity at the location of the particle centroid, and $d/dt$ is the time derivative following the moving particles. The velocity and time variables in (4.1) can be non-dimensionalized using a characteristic fluid velocity scale $u_0$ and length scale $\ell$ as

$$
\mathbf{u}^\ast = \mathbf{u}/u_0 \quad \mathbf{v}^\ast = \mathbf{v}/u_0 \quad t^\ast = tu_0/\ell,
$$

(4.2)

to write (4.1) as

$$
\frac{d\mathbf{v}^\ast}{dt^\ast} = - \frac{1}{St} (\mathbf{v}^\ast - \mathbf{u}^\ast)
$$

(4.3)

where $St = mu_0/(3\pi \mu d \ell)$ is the Stokes number.

For small values of the Stokes number, the particle nearly follows the fluid streamlines, with a drift velocity $\mathbf{v}_d \equiv \mathbf{v} - \mathbf{u}$ that scales as $O(St u_0)$ (Crowe et al., 1998). The particle acceleration can thus be written as (see Appendix C.1)

$$
\frac{d\mathbf{v}^\ast}{dt^\ast} = \frac{D\mathbf{u}^\ast}{Dt^\ast} + \frac{d\mathbf{v}^\ast_d}{dt^\ast} + \mathbf{v}^\ast_d \cdot \nabla \mathbf{u}^\ast,
$$

(4.4)

where $D/Dt$ denotes material derivative following a Lagrangian fluid element. The first term on the right-hand side of (4.4) is $O(1)$, and the second and third terms are $O(St)$. Substituting (4.4) into (4.3) and retaining only leading order terms in the Stokes number, an approximate equation for particle drift velocity is obtained as (Ferry et al., 2003)

$$
\mathbf{v}^\ast_d = -St \mathbf{a}^\ast + O(St^2),
$$

(4.5)
where \( \mathbf{a}^* \equiv D\mathbf{u}^*/Dt^* \) is the dimensionless fluid acceleration following the fluid element. The result (4.5) illustrates the importance of accurately modeling the fluid acceleration field for simulation of particle dispersion.

Particle sampling bias occurs when particles drift across the fluid streamlines, leading to formation of flow regions in which the particle concentration is both significantly greater and significantly less than the mean concentration. In such a case, the probability of finding a given particle is higher in high concentration regions of the flow, and so the particle does not sample regions of the flow field with equal probability as it moves about.

The particle sampling bias is related to the component of the particle drift velocity that carries the particles normal to the fluid streamlines. If \( \hat{n} \equiv \mathbf{u}/||\mathbf{u}|| \) denotes a unit vector oriented along the fluid streamline, the magnitude of the cross-stream particle diffusion is given by \( ||\mathbf{v}_d \times \hat{n}|| \). A dimensionless measure of particle sampling bias can be formed by dividing this quantity by the fluid velocity magnitude to yield

\[
\phi_s(x, t) = \frac{||\mathbf{v}_d \times \mathbf{u}||}{||\mathbf{u}||^2} \quad (4.6)
\]

Substituting the approximation (4.4) for the particle drift velocity into (4.6), the sampling bias measure can be written as

\[
\phi_s(x, t) = St \frac{||\mathbf{a}^* \times \mathbf{u}^*||}{||\mathbf{u}^*||^2}. \quad (4.7)
\]

### 4.1.2 Fluid length scale measure

Given that the spatial structure of turbulence is important in determining the degree of particle dispersion, a measure characterizing the length scales of the flow was
employed. A method for computing an effective diameter of a non-spherical droplet, called Sauter’s diameter, was used. Sauter’s diameter of a droplet is defined as the diameter of a sphere having the same ratio of external surface area to volume as the droplet (Fan & Zhu, 1998). The concept of the Sauter’s diameter is applied here in two dimensions.

Instead of droplet sizing, we use the method to find the area of a fluid property, \( p_f \), in a two-dimensional slice of the domain that exceeds a certain threshold, \( p_{th} \). The perimeter and area of the 2D slice with \( p_f \geq p_{th} \) are denoted \( \ell_t \) and \( A_t \), respectively. The length scale is then derived by assuming a circular geometry of each region above the threshold. Thus the area and perimeter are \( A_t = \pi a^2 N_r \) and \( \ell_t = 2\pi a N_r \), where \( a \) is the radius and \( N_r \) is the total number of regions. Solving for the radius gives \( a = 2(A_t / \ell_t) \). The two-dimensional equivalent of Sauter’s diameter \( \lambda_d \) is then given by

\[
\lambda_d = 4 \frac{A_t}{\ell_t}. \tag{4.8}
\]

### 4.2 Simulation parameters

The fluid simulations are performed on a periodic cube with a domain length of \( 2\pi \). The value of the turbulent kinetic energy was chosen to match the average value of the energy from DNS results. The time was nondimensionalized by \( t' = t/T \) where \( T = q/(3\langle \epsilon \rangle) \) is the integral time scale, \( q \) is the turbulent kinetic energy and \( \langle \epsilon \rangle \) is the mean dissipation rate and the simulations were carried out such that \( t'_{final} = 10 \). The time step was chosen to satisfy the CFL condition such that the CFL number, \( C \), satisfies

\[
C = \frac{u \Delta t}{\Delta x} < 1 \tag{4.9}
\]
for the time stepping methods. The CFL condition ensures that the ratio of the
time step to the grid spacing is small enough that a particle moving through the
flow would not pass through more than one grid cell per time step. The Reynolds
number is \( Re = UL/\nu \approx 240 \) where \( U = \sqrt{3q/2} \) is the integral velocity scale,
\( L = 1/(2\epsilon)(2q/3)^{3/2} \) is the integral length scale and \( \nu = \mu/\rho \) is the kinematic fluid
viscosity. Simulation parameters are shown in Table 4.1.

<table>
<thead>
<tr>
<th>Simulation Parameters</th>
<th>Turbulence Parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>Time step</td>
<td>0.002</td>
</tr>
<tr>
<td>Cycles</td>
<td>15000</td>
</tr>
<tr>
<td>Grid</td>
<td>128^3</td>
</tr>
<tr>
<td>Turbulent kinetic energy, ( q )</td>
<td>0.12 ( m^2/s^2 )</td>
</tr>
<tr>
<td>Mean dissipation rate, ( \langle \epsilon \rangle )</td>
<td>0.0161 ( m^2/s^3 )</td>
</tr>
<tr>
<td>Kinematic viscosity, ( \nu )</td>
<td>0.001 ( m^2/s )</td>
</tr>
</tbody>
</table>

Table 4.1: Simulation parameters

Three different cases were examined for particles in this study, corresponding to
\( St \approx 0.5, 1.0, 1.5 \). The parameter values are given in Table 4.2. The particle radius,
\( r_p \), and the number of particles are varied. The particle-fluid density ratio, \( \rho_p/\rho_f \),
the particle field concentration \( C_p \), and fluid viscosity are fixed. The parameter
values were determined by an algorithm that satisfies the restraints for the various
dimensionless parameters in this specific problem.

The one-way coupling assumption, in which the fluid affects the particles but the
particles don’t affect the fluid, can be validated by the momentum coupling parameter,
\( \Pi_{mom} \) (Crowe et al., 1998). This dimensionless parameter compares the drag force of
the dispersed phase with the momentum flux of the continuous phase. The parameter
can be written as

\[
\Pi_{mom} = \frac{C_m}{1 + St}
\]  

(4.10)

where \( C_m \) is a mass concentration which in this case is \( C_m = C_p \cdot (\rho_p/\rho_f) \). The
Stokes number defined earlier can be written as \( St = (\rho_p d^2 U)/(18 \mu_c L) \), where \( d \) is
the particle diameter, \( L \) is the integral length scale, \( U \) is the integral velocity scale and \( \mu_c \) is the density of the continuous phase. The limit of \( \Pi_{mom} \) for the one-way coupling validation is 10%. The values for the current work are given in Table 4.2.

<table>
<thead>
<tr>
<th>Case</th>
<th>( N_p )</th>
<th>( r_p )</th>
<th>( C_p )</th>
<th>( \rho_p/\rho_f )</th>
<th>( St )</th>
<th>( \Pi_{mom} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case 1</td>
<td>17576</td>
<td>0.00897</td>
<td>1.5034%</td>
<td>10.0</td>
<td>1.05</td>
<td>0.073</td>
</tr>
<tr>
<td>Case 2</td>
<td>46656</td>
<td>0.00540</td>
<td>1.5013%</td>
<td>10.0</td>
<td>0.55</td>
<td>0.097</td>
</tr>
<tr>
<td>Case 3</td>
<td>9261</td>
<td>0.00850</td>
<td>1.5025%</td>
<td>10.0</td>
<td>1.61</td>
<td>0.058</td>
</tr>
</tbody>
</table>

Table 4.2: Three different cases for particle parameters.

### 4.3 Validation for homogeneous turbulence

A desirable attribute of a mathematical model of a physical system is that it obeys conservation laws. The three SLMs described in Section 3.1 are prescribed an initial turbulent kinetic energy and were observed to preserve the energy, consistent with DNS results, shown in Figure 4.1. The PDF of the velocity and acceleration fields produced by SLMs has been widely studied and there is agreement upon the results each model yields. Presented in Figure 4.2 are results for the PDFs of velocity and acceleration. Consistent with previous research, all the models yield good agreement with the velocity PDF when compared to DNS. Of the three SLMs considered, the Reynolds model is the only one that predicts the non-Gaussian acceleration statistics observed in DNS and experiments. Also shown is DNS data from Lee (2005) who performed a DNS study on a 128\(^3\) grid.

Similarly, the SVS model described in Section 3.2 should conserve kinetic energy, as shown in Figure 4.3a. The SVS model is also observed to closely approximate the acceleration PDF of the flow field, as shown in Figure 4.3b.
Figure 4.1: Turbulent kinetic energy $q$ plotted against the dimensionless time $t'$ for the various SLMs; Thompson (red), Sawford (green), Reynolds (blue), and DNS (black).

Figure 4.2: (a) $x$-direction of the normalized velocity PDF and (b) $x$-direction of the normalized acceleration PDF for Thompson (red), Sawford (green), Reynolds (blue) and DNS (black). In plot (a) all the lines fall on top of each other. In plot (b) the results from the Thompson and Sawford models produce Gaussian acceleration statistics, the lines fall on top of each other. The circles are data from Lee (2005).
Figure 4.3: Left: Comparison of (a) the turbulent kinetic energy, $q$ and (b) the PDF of the $x$-direction acceleration for DNS (black), SVS (blue) and DNS data from Lee (2005) from FIG 3 (circles).
4.4 Analysis of fluid flow field

The characteristics of the fluid flow that lead to particle dispersion are examined. DNS is used as a baseline for comparing the results produced by the SVS method and the SLMs. When examining real turbulence, such as with DNS, it is often difficult to extract the certain features of the flow pertaining to a specific problem. Here that problem is particle dispersion and we use two different models to isolate some of the fluid flow features that lead to particle dispersion.

It is known that particles drift across fluid streamlines in regions of high vorticity and acceleration. Furthermore, particles have been observed to selectively sample the flow domain such that the probability of particle location is a function of the flow characteristics. Thus, the spatial structure of the turbulence is important.

The velocity field is easily plotted for DNS and SVS because these methods solve velocity on a grid. The SLMs however, are solved on Lagrangian fluid elements, thus requiring an interpolation to a grid in order to plot contours. The $M'_4$ method was used to interpolate the velocity from the Lagrangian elements to the grid nodes.

The velocity field produced by DNS is shown in 4.4d. The flow seen in this figure is fully developed turbulence that has reached quasi-equilibrium. The DNS field contains a large spectrum of length scales, which is characteristic of turbulence. The Thompson and Reynolds model are shown in Figures 4.4a and 4.4b. The velocity field generated by these models are similar to each other, and both are dominated by structures that are on the order of the grid spacing. Put differently, there are no large scale flow features observed with this method. Lastly, the SVS method, shown in Figure 4.4c, is seen to contain spatial structures similar to DNS. This method, by design, incorporates vortex structures into the flow to reproduce the large length
scales characteristic of turbulence. The SVS method does not, however, contain the small scale structures seen with DNS.

This initial finding is not surprising. The SLM equations are derived in such a way that certain fluid statistics, namely the PDFs of velocity and acceleration, are accurate. They accomplish this by adding a normalized random variable to the mean flow. When averaged over time and space, these methods produce reasonable results for bulk flow characteristics of turbulence. In contrast, the SVS inputs vortex structures into the flow which inherently builds a structural velocity field.

Since the SVS model is based on a scaling analysis, the model parameters can be adjusted within a reasonable limit. The scaling term for the core radius was chosen such that the radius is at least twice the grid spacing, in order to resolve the flow across the core. The other scaling parameters for core length and circulation are more flexible. It is required that the parameters be chosen such that the average kinetic energy is equal to that observed by DNS. Table 4.3 gives a list of different scaling configurations that produce a similar average kinetic energy. Sensitivity to model parameters is not a desirable trait of a model, which is why many different cases were examined.

<table>
<thead>
<tr>
<th>Configuration</th>
<th>$\alpha_1$</th>
<th>$\alpha_2$</th>
<th>$\alpha_3$</th>
<th>$N_v$</th>
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<tbody>
<tr>
<td>1</td>
<td>1.2</td>
<td>6.3</td>
<td>3.15</td>
<td>399</td>
</tr>
<tr>
<td>2</td>
<td>0.9</td>
<td>6.3</td>
<td>6.4</td>
<td>945</td>
</tr>
<tr>
<td>3</td>
<td>1.2</td>
<td>8.0</td>
<td>3.7</td>
<td>399</td>
</tr>
<tr>
<td>4</td>
<td>0.9</td>
<td>8.0</td>
<td>6.7</td>
<td>945</td>
</tr>
<tr>
<td>5</td>
<td>1.0</td>
<td>6.3</td>
<td>4.65</td>
<td>689</td>
</tr>
<tr>
<td>6</td>
<td>1.4</td>
<td>6.3</td>
<td>2.7</td>
<td>251</td>
</tr>
<tr>
<td>7</td>
<td>0.8</td>
<td>6.3</td>
<td>8.6</td>
<td>1345</td>
</tr>
</tbody>
</table>

Table 4.3: SVS scaling configurations that give a similar total turbulent kinetic energy.

To quantify the observations made from Figure 4.4, the length scale measure de-
scribed in Section 4.1.2 was used. The results for the SLM, shown in Figure 4.5, are consistent with previous observations (Ayyalasomayajula et al., 2008) that SLM over-produce small scale structures and under-produce large scale structures. A logarithmic y-axis was used to fit the data points onto one plot. SLM does not have values for $p_{th}(0.8)$ or $p_{th}(0.9)$ because those are above the maximum value of velocity observed in the slice. The bulk velocity measures observed in the slice of the flow used in the length scale computation are displayed in Table 4.4.

<table>
<thead>
<tr>
<th></th>
<th>DNS</th>
<th>Thompson</th>
<th>Sawford</th>
<th>Reynolds</th>
<th>SVS</th>
</tr>
</thead>
<tbody>
<tr>
<td>Max</td>
<td>1.0032</td>
<td>0.7147</td>
<td>0.7163</td>
<td>0.7036</td>
<td>1.7368</td>
</tr>
<tr>
<td>Min</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0037</td>
</tr>
<tr>
<td>Mean</td>
<td>0.4181</td>
<td>0.3566</td>
<td>0.3554</td>
<td>0.3536</td>
<td>0.3750</td>
</tr>
<tr>
<td>RMS</td>
<td>0.1722</td>
<td>0.0956</td>
<td>0.0956</td>
<td>0.0946</td>
<td>0.2240</td>
</tr>
</tbody>
</table>

Table 4.4: Bulk flow measures for velocity magnitude for the slice taken to compute $\lambda_d$.

Length scale results for SVS are presented in Figure 4.6. Shown first is a length scale plot for the different SVS scaling configurations presented in Table 4.3. There is some degree of sensitivity in $\lambda_d$ for $p_{th}(0.1)$, but the rest of the threshold values have limited sensitivity. A ‘best case’ scaling configuration was picked and compared with DNS.

One reason it is important to match the spatial structure of a flow is that coherent structures exhibit certain behaviors. For instance it is known that there is large fluid accelerations surrounding vortex structures. This plays a key role in particle dispersion. This characteristic is examined first qualitatively by contour plots. Figure 4.7 shows a $x$-slice of the acceleration magnitude field with iso-surfaces of vorticity magnitude from the Reynolds model. The observed size of the vorticity iso-surfaces are on the order of the grid spacing. There is no spatial structure associated with the
iso-surfaces. This is to be expected, given that the average length scale of the flow produced by this method is on the order of the grid spacing.

The structural design of the SVS model is clearly seen in Figure 4.8. Surrounding each vortex structure is a region of large fluid acceleration. The magnitude of the acceleration is proportional to the random variable that scales the vortex strength. Contours of the acceleration measure $\phi_s$ derived in Section 4.1.1 are shown in Figure 4.9. Similar to acceleration, regions of large $\phi_s$ are found surrounding vortex structures. This result is consistent with theoretical implications of (4.7), which states that particles will disperse in fluid regions in which the acceleration vector is in a different direction than the fluid streamline at that point.

It is known that particles tend to cluster in regions between vortices. The centrifugal force acts to throw particles out of the vortex structures, and inertia effects cause the particle to drift across fluid streamlines. The SVS model was constructed to replicate this effect and the qualitative findings observed in Figure 4.9 are consistent with these findings.

Next we examine the $\phi_s$ contour field for DNS results. Figure 4.10 shows iso-surfaces of negative $\lambda_2$, a vortex identification method introduced by Jeong & Hussain (1995) with contours of $\phi_s$. The $\phi_s$ field is notably more complex than that observed by SVS. This result is not surprising, as SVS imitates the large scales of the flow and is less representative of the small scales. In the zoomed view in Figure 4.10, it is observed that large $\phi_s$ is associated with the vortex structures.

There are some regions of large $\phi_s$ in the DNS field that are not passing through a vortex structure. In these cases, the fluid streamlines have strong curvature which is consistent with what (4.7) predicts.

Contour plots for $\phi_s$ are not shown for the SLMs for the reasons seen in Figure 56.
4.7. The contours and iso-surfaces are too noisy to see anything useful. To compare \( \phi_s \) between DNS, SVS, and SLM in a quantitative manner, we look at the PDF of \( \phi_s \) over the entire flow domain. Figure 4.11a plots the PDF of \( \phi_s \) for DNS and SVS at two different times. It was found that the PDF is not very sensitive to time. While there are some differences, the PDFs are reasonably close.

Conversely, the PDF of \( \phi_s \) produced by the SLMs are quite different than DNS, shown in Figure 4.11b. The presence of much larger \( \phi_s \) with SLM could be attributed to the lack of relationship between velocity and acceleration in these equations. Somewhat surprisingly, the velocity based method has the same PDF as the acceleration based methods. This further confirms that the type of random forcing in these equations does not produce physically accurate results.

Lastly, the power spectrum for each of the methods is computed and is shown in Figure 4.12. SVS matches with DNS at the large scales, but is lacking energy at the small scales. The power spectrum seen by SLM does not have a similar shape to the DNS power spectrum, and it is seen to hold the majority of its energy at the small scales.
Figure 4.4: Comparison of velocity fields at $t' = 10$ for the Thompson (a) and Reynolds models (b), SVS (c) and DNS (d).
Figure 4.5: Length scale of velocity plot comparing DNS (black squares) and the Thompson (red circles), Sawford (green triangles) and Reynolds (blue gradients) SLMs. The logarithmic $y$-axis was used to fit all the points onto one plot without skewing the data too much.

Figure 4.6: (a) SVS scaling parameters for the seven cases presented in Table 4.3. (b) SVS scaling for case 3 (blue diamonds) and DNS (black squares).
Figure 4.7: $x$-slice of acceleration magnitude with iso-surfaces of vorticity magnitude from Reynolds SLM.

Figure 4.8: (a) $x$-slice of contours of acceleration magnitude with iso-surfaces of vorticity magnitude from the SVS method. Plot (b) shows a zoomed view showing large acceleration surrounding a vortex surface.
Figure 4.9: (a) $x$-slice of contours of $\phi_s$ with iso-surfaces of vorticity magnitude from the SVS method. Plot (b) shows a zoomed view. Vortex structures are surrounded by regions of high $\phi_s$ as well as acceleration which is shown in Figure 4.8.

Figure 4.10: $x$-slice of contours of $\phi_s$ with iso-surfaces of negative $\lambda_2$ from DNS. Plot (b) is a zoomed view showing large $\phi_s$ surrounding vortex surfaces.
Figure 4.11: PDF of $\phi_s$ over the entire flow domain for (a) DNS (black, red) and SVS (green, blue) at two different times and (b) DNS (black) and the Thompon (red), Sawford (green), and Reynolds (blue) SLMs.

Figure 4.12: Velocity power spectrum for DNS (black), SVS (red) and Reynolds model (blue).
4.5 Particle collisions with no adhesion forces

In this section results are presented for particles with no adhesion using the DEM. For both of the grid based methods, SVS and DNS, the velocity field is passed to the DEM via a grid and the velocity is interpolated to the solid particles. With SLM however, velocity is not known on a grid therefore a different approach is needed.

One option would be to use an interpolation scheme to get the velocity on a grid, like what was done using the $M'_4$ method in Section 4.4 to make contour plots. This approach has a number of drawbacks. Firstly, given the the number of grid points and fluid elements, the $M'_4$ interpolation vastly increases the computational time. While this is not a concern when performing post processing operations, such as contour plots, performing this interpolation at every time step is not favorable. Second, there is the potential to introduce error due to the interpolation. This error would not grow in time, however, because the Lagrangian elements are independent of the interpolation. A second interpolation would be needed to go from the grid to the inertial particles. With two interpolation processes it brings into question whether the velocity seen by the particles is accurate.

Another option is that the fluid velocity be computed by the SLM equations at the solid particle locations. This method requires no interpolation which is favorable in terms of no interpolation error and it is computationally quicker. This approach has been used by various researchers (Iliopoulos & Hanratty, 2004; Vegendla et al., 2011). Since SLMs don’t require any knowledge of the fluid element location or surrounding fluid elements the argument can be made that because the fluid elements are spatially independent; it doesn’t matter where they are solved since they are only influenced by their velocity at the previous time step. During collisions however, the velocity
seen by the particle is recomputed by the SLM on the time scale of the collision rather than the fluid time scale. The particle field is dilute and thus collision time is small enough that this can be reasonably ignored. The approach of solving the SLM equations at the solid particle locations is used in the current work.

Particle collision rate is known to be enhanced by preferential concentration of particles. Here we use collision rate as an indirect measure of how each method predicts particle dispersion. It also offers another opportunity to exam the parameter sensitivity of the SVS model. Figure 4.13 shows the the total number of collisions $N_c$ for $St \approx 1.5$ (Case 3). The number of collisions predicted by SVS is reasonably close between the different scaling configurations. A comparison between SVS and DNS in this case shows a better prediction of collisions than SLM.

![Figure 4.13: Total number of collisions for DNS (black), the Thompson (red, dashed), Sawford (green, dashed), Reynolds (blue, dashed) models and SVS (colored, solid) for the various scalings presented in Table 4.3 for $St \approx 1.5$ (Case 3).](image)

The initial transient behavior is due to initialization of the particles in an array.
After a short period of time the particles have dispersed from the array and reach a quasi-equilibrium with the flow, depicted by the region of curve with a constant slope. The SLM and DNS appear to have a similar time frame for dispersing particles from their initial condition. The SVS method, however, takes longer to disperse particles into a quasi-equilibrium with the flow. This could be attributed to the lack of small scale velocity fluctuations in the flow. The acceleration field is only large in regions immediately surrounding vortex structures, as seen in Figure 4.8. It was observed during the beginning of the run that particles near vortex structures dispersed very rapidly, while those that were far away took much longer to move. After a few eddy turn over times there has been sufficient cycling of the velocity field to have dispersed the particles. If this is poses a problem, it would be possible to initialize the particles with a random velocity on the order of the average fluid velocity. There would still be a transient period in which the particles equalize with the flow.

At this point we have observed that different SLMs produced almost identical results for all measures used in the current work. In subsequent discussion we only present results for the Reynolds SLM to aid in the clarity of both the discussion and figures. Relatedly the different SVS scaling configurations produce similar results and further results are only presented for Configuration 3 which is shown in Figure 4.6. A comparison of total collision rate between SVS, DNS, and Reynolds SLM for $St \approx 0.5, 1$ are shown in Figure 4.14. These findings are similar to what is seen with Figure 4.13.

Of the three particle cases considered, the SVS matches the collision of DNS best for $St \approx 0.5$. This case has the most number of particles and the particles are more susceptible to small velocity fluctuations. One possible conclusion is that at large Stokes numbers the SVS will over-predict the collision rate, because it holds all it’s
Figure 4.14: Total number of collisions for DNS (black), SVS (red), and Reynolds model (blue) for (a) $St \approx 1$ (Case 1) and (b) $St \approx 0.5$ (Case 2).

energy in large scales, versus DNS which has energy in a range of length scales. The DNS field has a reduced spectrum of velocities that can influence particles motion, thus decreasing the total dispersion. At lower Stokes number more of the velocity fluctuations impact the particles, thus increasing total dispersion.

### 4.6 Particles with adhesive forces

Here we consider particles with adhesive forces for the parameters given by Case 2 from Table 4.2. The particle collision results did not take into account where the collisions were taking place, which is important for the formation of large aggregates. Aggregation statistics provide further metrics for comparison between the models. In Figure 4.15 the average number of particles per aggregate is plotted as a function of time. Both models under-predict what is seen with DNS. The initial transient spike is
the time taken for the first aggregate to form. For SLMs this can be explained by the high shear of the flow which is more likely to break agglomerates apart. SVS however was expected to give a similar results, especially because the number of collisions was similar. What this plot suggests is that while there are a similar number of collisions, the distribution of aggregate size is incorrect due to some flow features. The flat slope of SVS can be attributed to lack of energy at the small scales. As seen with the particle collision plots the SVS model is initially slower at advecting the particles than DNS or SLM.

![Average number of particles per aggregates as a function of time for DNS (black), SVS (red), and Reynolds SLM (blue).](image)

**Figure 4.15:** Average number of particles per aggregates as a function of time for DNS (black), SVS (red), and Reynolds SLM (blue).

To consider this further, the number of particles in each aggregate is determined and used to compute an aggregate size distribution. The aggregate sizes are grouped into logarithmic bins of base 2 where the value of the aggregate size is the nominal bin value. The first bin (aggregate size 2) contains aggregates of 2 particles, the second bin (aggregate size 3) contains aggregates of 3-4 particles, the third bin (aggregate size 4) contains aggregates of 5-6 particles, and so on. This distribution provides insight into the growth dynamics of the aggregates over time.
size 6) contains aggregates of 5-8 particles, etc. The number of aggregates of a certain size is indicated by the percent of aggregating particles contained in an aggregate of that size. Figure 4.16 shows the distribution of aggregate sizes.

![Aggregate size distribution](image)

Figure 4.16: Aggregate size distribution showing percent of aggregating particles contained in aggregates of the given size range at $t' = 10$ for DNS (black), SVS (red), and Reynolds SLM (blue).

Again, neither model compares well with DNS results. The Reynolds model overestimates the number of aggregates at a given size up to aggregate size 48. For aggregate bin number 96 it underestimates the number of particles in aggregates of this size, and predicts 0 particles in aggregates of bin size 192. This can be attributed to the spatial structure of the model. The small structures move the particles such that they collide frequently, seen in Figure 4.14, however, the particle never preferentially cluster due to lack of large length scales, so large aggregates never form. The SVS also over predicts the aggregates of small particles but in a different manner than the SLM. The large number of particles in aggregates of small numbers could arise
from the lack of small scales in SVS. When particles are away from vortex structures, they are unlikely to collide with other particles as there is limited velocity in these regions. The lack of velocity in these regions also reduces the probability that a small aggregate will break up.

The fact that SVS predicted the total number of collisions reasonably well but does not have the correct distribution of aggregate sizes aligns with what exists in the literature. Preferential clustering of particles is known to increase particle collision rate (Section 2.2.1, Sundaram & Collins (1997)). The SVS model forces this preferentially clustering due to the implicit placement of vortex structures. In regions between vortices particles collide at a high frequency, and particles away from vortices collide infrequently, which is qualitatively shown in Figure 4.9. This disparity is not seen in the total collisions plots because the location of the collision is irrelevant. Thus, the large number of collisions in regions between vortices balances with the small number of collisions in regions away from vortices to produces an average that is similar to what is seen in DNS.
Chapter 5

Conclusions and Future Work

The fluid features that are characteristic of particle dispersion were examined. A stochastic vortex structure model was introduced that replicates large scale vortex structures. The motivation for the model was two-fold. First, no well-established metrics exist for predicting if a fluid flow model has the correct length scales and will accurately predict particle dispersion. Second, a model was needed to test the developed metrics in a way that isolates the fluid features of interest.

Furthermore, there has been a significant amount of work done involving stochastic Lagrangian methods but less work involving inertial particles, even less that include particles that collide, and none to our knowledge that examine adhesive particles. The spatial characteristics of these models have not been fully examined, although a few researchers have mentioned the lack of spatial structure in the velocity field (Ayyalasomayajula et al., 2008).

The conclusion that the spatial structure of the fluid fields produced by SLMs is unphysical was easily hypothesized. The location of the Lagrangian fluid elements is irrelevant, because the equations do not consider surrounding particles in the velocity
computation. This is easily seen in Figure 4.4. It was quantitatively shown via the length scale measure $\lambda_d$ and the acceleration measure $\phi_s$.

Much work has gone into developing SLMs that have the correct PDF of velocity and acceleration. It was shown here that this is in no way an indication that the spatial structure of the flow will be accurate. The Reynolds model accurately captures the velocity and acceleration PDFs observed in DNS results, but produces an inaccurate flow field.

By comparison the SVS model faired reasonably well in comparison between DNS in this analysis. It conserves total kinetic energy, and even produces an acceleration PDF that matches with DNS. The model was shown to be relatively insensitive to model parameters, so long as the computed kinetic energy was the same. Comparison of the length scales showed that SVS model produces the large scales of the flow.

The SVS was seen to over-predict the collision rate of particles with no adhesion force. This could be due to the fact the SVS model holds the majority of its energy at the large scales. The particle Stokes numbers also impact which scales of the velocity field will be effectively filtered out, which suggests more cases should be considered.

In simulations with adhesive forces, neither of the models performed particularly well. This can generally be attributed to the incorrect spectrum of scales. The variation of length scales matters spatially, as a function of surrounding scales, which the SVS model does not account for.

It is concluded that spatial structure is important for predicting particle dispersion. Preferential clustering of particles is directly related to the large, coherent scales of the flow, which SVS is designed to replicate. It was seen however, that the small scales play a role in advecting particles as well, especially in regions away from structures. The SLMs were seen to over-produce the small scales.
5.1 Future work

The results suggest that SVS is a feasible method for simulating turbulence and particle dispersion. Future applications of the SVS method could extend the approach to more general flow fields by allowing the scaling parameters used for specifying vortex structures to be space and/or time dependent. The structures could be allowed to move through the flow to account for advection.

SVS was seen to produce large scale fluid structures that are present in DNS and experiments but lacked the small scale structures. A hybridized version could include a modeling feature that simulates small scale fluctuations, something SLM has shown to be good at. This would allow the SVS method to hold energy at all scales of the flow, rather than just at the large scale.

This research here considered a small range of cases for particle configurations. A more comprehensive study of particle configurations would provide a more complete analysis. Of particular interest would be cases with smaller but substantially more particles. Such a case would allow for more metrics of dispersion to be used, such as the particle number density distribution function (Squires & Eaton, 1991). Bounded domains should also be considered to test the boundary effects on the flow results.

A next step from this research could examine the effects of particle filtering, in which agglomerate of particles have a different effective Stokes number than a single particle. A broader range of Stokes numbers could require two-way coupling between the fluid and the particles.

Measures such as particle collision rate and the average number of aggregates do not give enough details about particle dispersion. The total number of collisions tells little about the local particle concentration field. More advanced spatial and temporal
measures that characterize local heterogeneity are needed.

The simulations for particle aggregation could be run longer, to a time of $t_{\text{final}}'$ = 30 or greater. This would allow for the long time effects to be better understood for each model. The computational time for a simulation of this length would be over 30 days on the current hardware.
References


Appendix A

Nomenclature

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a_0$</td>
<td>Lagrangian velocity structure constant, fit from DNS $= 0.13 \cdot Re_{\lambda}^{0.64}$</td>
</tr>
<tr>
<td>$a'_0$</td>
<td>Universal structure constant, fit from DNS</td>
</tr>
<tr>
<td>$a_i$</td>
<td>Acceleration vector</td>
</tr>
<tr>
<td>$a'^2_i$</td>
<td>root-mean-squared acceleration</td>
</tr>
<tr>
<td>$A_n$</td>
<td>Scaling factor for $\Gamma_n(t)$ that is a normally-distributed random variable</td>
</tr>
<tr>
<td>$C_0$</td>
<td>Kolmogorov constant for Lagrangian velocity structure, fit from DNS</td>
</tr>
<tr>
<td>$E$</td>
<td>Elastic modulus</td>
</tr>
<tr>
<td>$F_A$</td>
<td>Collision and adhesive force on a particle</td>
</tr>
<tr>
<td>$F_C$</td>
<td>Maximum particle adhesive force</td>
</tr>
<tr>
<td>$F_d$</td>
<td>Fluid drag force on a particle</td>
</tr>
<tr>
<td>$F_F$</td>
<td>Fluid force on a particle</td>
</tr>
<tr>
<td>$F_l$</td>
<td>Fluid lift force on a particle</td>
</tr>
<tr>
<td>$F_m$</td>
<td>Magnus force</td>
</tr>
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<td>$F_n$</td>
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<td>$F_{ne}$</td>
<td>Elastic part of normal collision/adhesion force</td>
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<td>$F_s$</td>
<td>Sliding force</td>
</tr>
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<td>$G$</td>
<td>Effective shear modulus of colliding particles</td>
</tr>
<tr>
<td>$h$</td>
<td>Grid step size</td>
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<tr>
<td>$I$</td>
<td>Moment of inertia</td>
</tr>
<tr>
<td>$k$</td>
<td>Wavenumber</td>
</tr>
<tr>
<td>$k_n$</td>
<td>Normal stiffness coefficient, $= F_{ne}/\delta_N$</td>
</tr>
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<td>$L$</td>
<td>Integral length scale, $L = 1/(2\epsilon)(2q/3)^{3/2}$</td>
</tr>
<tr>
<td>$L_v$</td>
<td>Average distance between vortex centers, SVS model</td>
</tr>
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<td>$m$</td>
<td>Mass of a particle</td>
</tr>
<tr>
<td>Symbol</td>
<td>Description</td>
</tr>
<tr>
<td>--------</td>
<td>-------------</td>
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<tr>
<td>$M_A$</td>
<td>Collision and adhesive moment on a particle</td>
</tr>
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<td>Fluid moment on a particle</td>
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<td>$M_t$</td>
<td>Twisting torque on particle</td>
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<tr>
<td>$N_b$</td>
<td>Number of blobs per vortex structure</td>
</tr>
<tr>
<td>$N_c$</td>
<td>Total number of collisions, function of time</td>
</tr>
<tr>
<td>$N_v$</td>
<td>Total number of vortex structures in SVS model</td>
</tr>
<tr>
<td>$P(r,z)$</td>
<td>Incomplete gamma function</td>
</tr>
<tr>
<td>$p_{th}$</td>
<td>Threshold value for length scale measure $\lambda_d$</td>
</tr>
<tr>
<td>$q$</td>
<td>Turbulent kinetic energy, $q = \frac{3}{2} u'^2$</td>
</tr>
<tr>
<td>$R$</td>
<td>Effective radius of colliding particles</td>
</tr>
<tr>
<td>$Re_\lambda$</td>
<td>Taylor microscale Reynolds number</td>
</tr>
<tr>
<td>$Re_p$</td>
<td>Particle Reynolds number, $\equiv</td>
</tr>
<tr>
<td>$S_i$</td>
<td>Sign constant for $M'_4$ interpolation</td>
</tr>
<tr>
<td>$St$</td>
<td>Stokes number</td>
</tr>
<tr>
<td>$t'$</td>
<td>Nondimensional time, $\equiv t/T$</td>
</tr>
<tr>
<td>$T$</td>
<td>Lagrangian integral time scale, $T = q/3\langle \epsilon \rangle$</td>
</tr>
<tr>
<td>$T_L$</td>
<td>Lagrangian integral length scale, $\frac{1}{2\epsilon_7} \sqrt{\frac{2q^3}{3}}$</td>
</tr>
<tr>
<td>$T_v$</td>
<td>Vortex life for SVS model</td>
</tr>
<tr>
<td>$T_\chi$</td>
<td>Time scale associated with local dissipation rate, $\equiv 2\sigma_u^2/C_0\langle \epsilon \rangle$</td>
</tr>
<tr>
<td>$U$</td>
<td>Integral velocity scale, $U = \sqrt{3k/2}$</td>
</tr>
<tr>
<td>$u_i$</td>
<td>Fluid velocity vector</td>
</tr>
<tr>
<td>$u'_i^2$</td>
<td>Root-mean-squared velocity</td>
</tr>
<tr>
<td>$v$</td>
<td>Particle velocity vector</td>
</tr>
<tr>
<td>$v_d$</td>
<td>Drift velocity vector</td>
</tr>
<tr>
<td>$V$</td>
<td>Computational domain</td>
</tr>
<tr>
<td>$dW$</td>
<td>Gaussian distributed random variable, independent of $d\xi$</td>
</tr>
<tr>
<td>$x$</td>
<td>Position vector</td>
</tr>
</tbody>
</table>

Table A.1: Roman letters
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\bar{\alpha}$</td>
<td>Coefficient of friction</td>
</tr>
<tr>
<td>$\alpha_1$</td>
<td>SVS scaling parameter for core length</td>
</tr>
<tr>
<td>$\alpha_2$</td>
<td>SVS scaling parameter for core radius</td>
</tr>
<tr>
<td>$\alpha_3$</td>
<td>SVS scaling parameter for vortex strength</td>
</tr>
<tr>
<td>$\beta$</td>
<td>Blob overlap factor</td>
</tr>
<tr>
<td>$\chi$</td>
<td>Logarithm or normalized dissipation rate, $\equiv \ln(\epsilon/\langle \epsilon \rangle)$</td>
</tr>
<tr>
<td>$\delta_C$</td>
<td>Overlap at critical adhesive force</td>
</tr>
<tr>
<td>$\delta_N$</td>
<td>Normal overlap of particles</td>
</tr>
<tr>
<td>$\epsilon$</td>
<td>Local dissipation rate</td>
</tr>
<tr>
<td>$\langle \epsilon \rangle$</td>
<td>Mean dissipation rate</td>
</tr>
<tr>
<td>$\phi_s$</td>
<td>Fluid dispersion measure</td>
</tr>
<tr>
<td>$\Gamma_{\text{max}}$</td>
<td>Max vortex strength in SVS model</td>
</tr>
<tr>
<td>$\Gamma_n(t)$</td>
<td>Individual vortex strength in SVS model</td>
</tr>
<tr>
<td>$\lambda_b$</td>
<td>Unit vector along the axis of a vortex structure from SVS model</td>
</tr>
<tr>
<td>$\lambda_d$</td>
<td>Effective diameter</td>
</tr>
<tr>
<td>$\mu$</td>
<td>Dynamic fluid viscosity</td>
</tr>
<tr>
<td>$\Pi_{\text{mom}}$</td>
<td>Momentum coupling parameter</td>
</tr>
<tr>
<td>$\sigma_u^2$</td>
<td>Velocity variance</td>
</tr>
<tr>
<td>$\sigma_{a</td>
<td>\epsilon}$</td>
</tr>
<tr>
<td>$\sigma_\chi^2$</td>
<td>Variance of $\chi$</td>
</tr>
<tr>
<td>$\tau_c$</td>
<td>SLM time scale, $\equiv 4T/C_0$</td>
</tr>
<tr>
<td>$\tau_n$</td>
<td>Age of vortex structure in SVS model</td>
</tr>
<tr>
<td>$\tau_\eta$</td>
<td>Kolmogorov time scale, $\equiv \sqrt{\nu/\epsilon}$</td>
</tr>
<tr>
<td>$\eta$</td>
<td>Kolmogorov length scale, $(\nu^3/\langle \epsilon \rangle)^{1/4}$</td>
</tr>
<tr>
<td>$\eta_c$</td>
<td>SLM length scale, $\equiv C_0\tau_\eta/2a_0$</td>
</tr>
<tr>
<td>$\eta_n$</td>
<td>Normal friction coefficient</td>
</tr>
<tr>
<td>$\rho_f$</td>
<td>Fluid density</td>
</tr>
<tr>
<td>$\rho_p$</td>
<td>Particle density</td>
</tr>
<tr>
<td>$\nu$</td>
<td>Fluid kinematic viscosity, $m^2/s$</td>
</tr>
<tr>
<td>$\omega$</td>
<td>Vorticity vector</td>
</tr>
<tr>
<td>$\Omega$</td>
<td>Angular rotation rate of particle</td>
</tr>
<tr>
<td>$\Omega_m$</td>
<td>Vortex blob amplitude</td>
</tr>
<tr>
<td>$\Omega_T$</td>
<td>Relative twisting rate</td>
</tr>
<tr>
<td>$d\xi$</td>
<td>Gaussian distributed random variable, independent of $dW$</td>
</tr>
</tbody>
</table>

Table A.2: Greek letters
Appendix B

SLM numerical formulations

In this section the numerical formulations of the various SLMs is shown. The solution is presented in one dimension, but is identical in all dimensions.

B.1 The Thompson model

Equation 3.1 is integrated using an implicit numerical formulation. Starting with Equation 3.1

\[ du + \frac{u}{T} dt = cd\xi \]  \hspace{1cm} (B.1)

where \( c = (4q/T)^{1/2} \) we multiply by an integration factor of \( \exp(t/T) \) and use the chain rule to define the differential

\[ d[\exp(t/T)u] = \exp(t/T) \left[ \frac{du}{dt} + \frac{u}{T} \right] dt. \]  \hspace{1cm} (B.2)
After plugging in the differential and reducing we have

\[ d [\exp(t/T)u] = \exp(t/T)cd\xi \]  \hspace{1cm} (B.3)

and then divide both sides by \( dt \) and integrate

\[
\int_{t_n}^{t_{n+1}} d [\exp \left( \frac{t}{T} u \right)] = \int_{t_n}^{t_{n+1}} \exp \left( \frac{t}{T} \right) \frac{d\xi}{dt},
\]  \hspace{1cm} (B.4)

resulting in

\[
\exp(t_{n+1}/T)u_{n+1} - \exp(t_n/T)u_n = Tc \left[ \exp(t_{n+1}/T) - \exp(t_n/T) \right] \frac{d\xi}{dt} .
\]  \hspace{1cm} (B.5)

To solve for \( u_{n+1} \) first divide by \( \exp(t_n/T) \)

\[
\exp(\Delta t/T)u_{n+1} - u_n = Tc(\exp(\Delta t/T) - 1) \frac{d\xi}{dt}
\]  \hspace{1cm} (B.6)

and then solve for \( u_{n+1} \) and plug back in for \( c \)

\[
u_{i}^{n+1} = u_{i}^{n}\exp(-\Delta t/T) + (4q_{i}T)^{1/2}[1 - \exp(-\Delta t/T)] \frac{\Delta\xi}{\Delta t}.
\]  \hspace{1cm} (B.7)

**B.2 The Reynolds model**

We seek to solve the system of equations defined by

\[
d\chi = -(\chi - \langle \chi \rangle)\frac{dt}{T_\chi} + \left(\frac{2\sigma^2}{T_\chi} \right)^{\frac{1}{2}} dW
\]  \hspace{1cm} (B.8)
\[ da = - \left( \frac{1}{\tau_c} + \frac{1}{\eta_c} - \frac{1}{a} \frac{d\sigma_a}{dt} \right) adt - \frac{u}{\tau_c\eta_c} dt + \sqrt{2\sigma_a^2 \left( \frac{1}{\tau_c} + \frac{1}{\eta_c} \right)} \frac{1}{\tau_c\eta_c} d\xi \]  
\quad (B.9)

\[ du = adt. \]  
\quad (B.10)

First we examine (B.8). To simplify the analysis we define the following constants, 
\[ c_1 = \langle \chi \rangle T^{-1}_\chi \] and \[ c_2 = \sqrt{2\sigma^2 \chi T^{-1}_\chi} \] to result in

\[ d\chi = -\chi T \chi dt + c_1 dt + c_2 dW. \]  
\quad (B.11)

Next multiply by an integration factor of \( \exp(T_\chi t) \) and integrate

\[ \int_{t_n}^{t_{n+1}} \frac{d}{dt} \left[ \exp(T_\chi t) \chi \right] dt = \int_{t_n}^{t_{n+1}} c_1 \exp(T_\chi t) dt + c_2 \exp(T_\chi t) \frac{dW}{dt} dt \]  
\quad (B.12)

we can integrate the left hand side and the first term of the right hand side analytically,

\[ \exp(T_\chi t_{n+1})\chi_{n+1} - \exp(T_\chi t_n)\chi_n = \]  
\quad \frac{c_1}{T_\chi} (\exp(T_\chi t_{n+1}) - \exp(T_\chi t_n)) \] + \int_{t_n}^{t_{n+1}} c_2 \exp(T_\chi t) \frac{dW}{dt} dt  
\quad (B.13)

divide both sides by \( \exp(T_\chi t_{n+1}) \) and simplify,

\[ \chi_{n+1} = \]  
\quad \exp(-T_\chi \Delta t)\chi_n + \frac{c_1}{T_\chi} (1 - \exp(-T_\chi \Delta t)) + \exp(-T_\chi t_{n+1} c_2) \int_{t_n}^{t_{n+1}} \exp(T_\chi t) \frac{dW}{dt} dt. \]  
\quad (B.14)
The last term in the right hand side is a random variable, so it suffices to use the first order Forward Euler method

\[
\chi_{n+1} = \exp(-T\chi \Delta t) \chi_n + \frac{c_1}{T\chi} (1 - \exp(-T\chi \Delta t)) + c_2 \Delta t \exp(-T\chi \Delta t) \frac{dW}{dt}.
\] (B.15)

From this result we can now solve for the instantaneous dissipation rate \( \epsilon = \epsilon(x, t), \)

\[
\epsilon = \langle \epsilon \rangle \exp(\chi)
\] (B.16)

To solve (B.9) and (B.10) we proceed by defining some parameters for the equations that change in time, \( c_3 = -\left(\frac{1}{\tau_c} + \frac{1}{\eta_c} - \frac{1}{\sigma_u} \frac{d\sigma_a}{dt}\right), \) \( c_4 = -\frac{1}{\tau_c \eta_c}, \) and \( c_5 = \sqrt{2\sigma_u^2 \left(\frac{1}{\tau_c} + \frac{1}{\eta_c}\right) \frac{1}{\tau_c \eta_c}}. \) Equation (B.9) reduces to

\[
da = c_3 a + c_4 u dt + c_5 dW.
\] (B.17)

Multiply by an integration factor of \( \exp(-c_3 t) \) the equations simplify to

\[
\frac{d}{dt} [\exp(-c_3 t)a] = \exp(-c_3 t) \left[ c_4 u + c_5 \frac{d\xi}{dt} \right]
\] (B.18)

\[
\frac{du}{dt} = a.
\] (B.19)

A predictor-corrector method is used to solve equations (B.18) and (B.19). The predictor steps are

\[
a_{n+1}^* = \exp(c_3 \Delta t) a_n + \Delta t \exp(-c_3 t) \left[ c_4 u_n + c_5 \frac{d\xi}{dt} \right]
\] (B.20)
\[ u_{n+1}^* = u_n + \Delta t a_n, \]  
(B.21)

and the corrector steps are

\[
a_{n+1} = \exp(c_3 \Delta t) a_n + \Delta t \exp(-c_3 t) \left[ \frac{c_4}{2} (u_n + u_{n+1}^*) + c_5 \frac{d \xi}{dt} \right]
\]  
(B.22)

\[
u_{n+1} = u_n + \frac{\Delta t}{2} (a_n + a_{n+1}^*).
\]  
(B.23)
Appendix C

Derivations

C.1 Derivation of (4.4)

The material derivative of some function $f$ with respect to the fluid velocity at a fixed point in space is given by

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + v \cdot \nabla f$$  \hspace{1cm} (C.1)

while the material derivative of $f$ following a Lagrangian fluid element is given by

$$\frac{Df}{Dt} = \frac{\partial f}{\partial t} + u \cdot \nabla f.$$  \hspace{1cm} (C.2)

Subtracting (C.2) from (C.1) yields

$$\frac{df}{dt} = \frac{Df}{Dt} + (v - u) \cdot \nabla f.$$  \hspace{1cm} (C.3)
If we take the function $f$ to be the fluid velocity $\mathbf{v}$ then (C.3) becomes

$$\frac{d\mathbf{v}}{dt} = \frac{D\mathbf{v}}{Dt} + \mathbf{v}_d \cdot \nabla \mathbf{v}. \quad (C.4)$$

If we plug the fluid velocity $\mathbf{v} = \mathbf{u} + \mathbf{v}_d$ into the right hand side of (C.4) we get

$$\frac{d\mathbf{v}}{dt} = \frac{D\mathbf{u}}{Dt} + \frac{D\mathbf{v}_d}{Dt} + \mathbf{v}_d \cdot \nabla \mathbf{u} + \mathbf{v}_d \cdot \nabla \mathbf{v}_d \quad (C.5)$$

and then using (C.3) simplifies to

$$\frac{d\mathbf{v}}{dt} = \frac{D\mathbf{u}}{Dt} + \frac{d\mathbf{v}_d}{dt} + \mathbf{v}_d \cdot \nabla \mathbf{u}. \quad (C.6)$$