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A COMPARISON OF STOCHASTIC SEPARATED FLOW MODELS FOR
PARTICLE DISPERSION IN TURBULENT FLOWS

by

Eleanor A. Hennick

A thesis submitted in conformity with the requirements
for the degree of Master of Applied Science
Graduate Department of Mechanical and Industrial Engineering
University of Toronto

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Abstract

A Comparison of Stochastic Separated Flow Models for Particle Dispersion in Turbulent Flows

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1998

This thesis investigates Stochastic Separated Flow (SSF) models for particle dispersion in turbulent flows. A new model is presented that incorporates a temporal and a spatial autocorrelation in the description of the fluctuating component of the turbulent gas-phase velocity. This model and four SSF models available in the literature are evaluated analytically and by comparing predictions with the grid-generated turbulence experiments of Snyder and Lumley (1971), and Wells and Stock (1983). Results are discussed and deficiencies in the models explored. The new model of Hennick and Lightstone compensates for the crossing trajectory effect with the inclusion of a spatial correlation based on the relative velocity of the particle and the timestep employed. Promising results are obtained using this model.

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Finally, I am grateful to my family for their unwavering belief in me. Their love gives me the strength that made this work possible.

Dedication

This thesis is dedicated to my family who believe I can do anything!

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Nomenclature

<i>Symbol</i>	<i>Definition</i>
<i>Greek</i>	
β	constant used in Zhou and Leschziner's model
δ_{ij}	Kronecker delta
δt	timestep
Δt	timestep
ϵ	turbulent diffusivity
μ	molecular dynamic viscosity
ν_t	turbulent kinematic viscosity
ρ	density
ρ_s	particulate phase loading
σ^2	variance
τ_p	particle relaxation time
τ_{LI}	Lagrangian integral timescale
θ	volume fraction of particles
<i>English</i>	
C_D	drag coefficient
C_μ	eddy viscosity model proportionality constant
d_p	particle diameter
D_p	turbulent particle diffusivity
f	ratio of the drag coefficient to Stokes drag
k	turbulent kinetic energy
l_e	characteristic eddy length
m_p	particle mass
P	pressure
$R(\delta t)$	Lagrangian temporal correlation
$R_t(\delta t)$	Lagrangian temporal correlation

Table 1: (continued)

<i>Symbol</i>	<i>Definition</i>
$R_x(\delta x)$	Lagrangian spatial correlation
Re_p	Reynolds number
t	time
t_e	eddy lifetime
t_{int}	particle interaction time
t_{tr}	transit time of a particle
u	instantaneous velocity
$\bar{U}$	mean velocity
u'	velocity fluctuation
u_{REL}	relative velocity of the particle
x_i	distance in i direction
<i>Subscripts</i>	
g	gas-phase
p	particle
t	time

Chapter 1

Introduction

1.1 Background

The dispersion of particulates in turbulent flows occurs in many engineering applications. Examples of particle laden industrial applications include the pneumatic transport of powder, droplet combustion systems, spray drying and cooling systems, and spray casting with molten liquid droplets. Understanding how particles disperse in turbulence can also give insight into environmental problems where particulate pollutants are released into the atmosphere.

This thesis is concerned with turbulent particle dispersion under dilute flow conditions. The focus of this work is the fundamental problem of predicting particle motion. The motion of a particle in a gas flow is governed by gravity and the particle's interaction with the turbulent fluid surrounding it. Other contributions to particle momentum such as chemical reactions or internal circulation in liquid particles are not considered in this investigation.

1.2 Objective and Scope

This work has two main objectives:

- To develop a model to predict the motion of particles in turbulent flows.
- To compare the predictions of the new model and existing Stochastic Separated Flow (SSF) models using analysis and the benchmark grid-turbulence experiments of Snyder and Lumley (1971) and Wells and Stock (1983).

The prediction of particle motion is implicitly linked to the problem of turbulence. The particle equation of motion is an expression for the acceleration of a particle as a balance of drag and gravity forces. There is an exact solution to the particle equation of motion, but, in order to predict particle velocity, the instantaneous gas-phase velocity must be known. The model of Hennick and Lightstone presented in this work derives an expression for the instantaneous gas-phase velocity experienced by a particle. This model is stochastic in nature; two particles with the same initial conditions will not see the same turbulent velocity fluctuations.

The new model and SSF models available in the literature are evaluated by considering the problem of dyed fluid particles released from a point source in homogeneous isotropic turbulence. Taylor (1921) derived an expression for the variance of the particles from mathematical considerations. The analysis of Taylor is extended to the models considered in this investigation for comparison with Taylor's result for long time dispersion.

Models are also evaluated by comparing predictions with experimental results. The grid-turbulence experiments of Snyder and Lumley (1971) and Wells and Stock (1983) are simulated using the TASCflow CFD code. Predictions of particle dispersion and velocity decay are compared with the experimental results.

1.3 Outline of the Thesis

Chapter 2 provides the background and a context for the current thesis. A general discussion of the behavior of particles released into a turbulent flow and the mathematical models used to describe that behavior are discussed. Particle dispersion models available in the literature are critically reviewed.

The model of Hennick and Lightstone is introduced in Chapter 3. The model is presented in detail and shown to exactly reproduce Taylor's results for the long time dispersion of dyed fluid particles in homogeneous isotropic turbulence.

An overview of the numerical methods used to obtain solutions to the governing equations is presented in Chapter 4. Implementation of the Stochastic Separated Flow (SSF) models described in Section 2.3.2 and Chapter 3 is outlined.

Chapter 5 extends the analysis of Lightstone and Raithby (1996) to each SSF model introduced in Section 2.3.2. Taylor's result (1921) for fluid particles at long times is reviewed and analysis is performed to determine if each model can reproduce Taylor's result.

Model predictions are compared to the experimental results of Snyder and Lumley (1971) and Wells and Stock (1983) in Chapters 6 and 7 respectively. In each chapter, the

design of the experiment is outlined and the numerical simulation described. Results are discussed in detail.

Chapter 8 presents a summary and conclusions of the thesis as well as recommendations for future work.

Chapter 2

Background

This chapter provides the background and a context for the current thesis. A general discussion of the behavior of particles released into a turbulent flow and the mathematical models used to describe that behavior are discussed.

The chapter begins with the governing equations for the flow. Conservation equations for the fluid phase are outlined focusing on the $k - \epsilon$ turbulence model presented by Launder and Spalding (1974). The particle equation of motion is presented and the underlying physics of the flow discussed. To gain further insight into the physics of particle dispersion, the analysis of Taylor forms the following section. Taylor examined the behavior of fluid particles dispersing in a homogeneous isotropic turbulent flow and derived an expression for the variance from mathematical considerations.

While the analysis of Taylor is useful for gaining an understanding of particle dispersion, the results are limited to idealized flows. To solve more complex problems, models that approximate the gas–solid interaction are required. The final section of this chapter is a critical review of models available in the literature that are capable of predicting the dispersion of a dilute concentration of particles in turbulent flows.

2.1 Governing Equations

In this section the governing equations for a particle–laden flow are presented. These equations include the conservation equations for mass and momentum of the flow field. Further, the $k - \epsilon$ model is outlined and the particle equation of motion is presented.

2.1.1 Conservation Equations for the Fluid Phase

Using a Cartesian coordinate system, the conservation equations for mass and momentum for an incompressible flow with constant viscosity may be expressed in tensor form (with the Einstein summation convention) as,

$$\frac{\partial}{\partial x_j}(\rho u_j) = 0 \quad (2.1)$$

$$\frac{\partial}{\partial t}(\rho u_i) + \frac{\partial}{\partial x_j}(\rho u_j u_i) = -\frac{\partial P}{\partial x_i} + \mu \frac{\partial^2 u_i}{\partial x_j \partial x_j} + F_i \quad (2.2)$$

where ρ is the density, u_i represents the velocities in the x_i coordinate directions. P is the pressure, μ is the dynamic viscosity of the fluid, and F_i represents all body forces.

Equations (2.1) and (2.2) involve the instantaneous values of fluid velocity and pressure. In considering a turbulent flow, the instantaneous value of any quantity may be expressed as a mean plus a fluctuating component through a process of Reynolds averaging. In order to solve the resulting equations, it is necessary to use a turbulence model to approximate the Reynolds stress terms.

In the present work the Reynolds stress terms are related to the mean flow variables using an eddy viscosity assumption, Hinze (1975).

$$-\overline{u_i' u_j'} = \nu_t \left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) - \frac{2}{3} k \delta_{ij} \quad (2.3)$$

where k is the turbulent kinetic energy, $\bar{u}$ is the mean velocity of the flow, u' is the fluctuating component of velocity, and ν_t is the turbulent kinematic viscosity.

$$\nu_t = C_\mu \frac{k^2}{\epsilon} \quad (2.4)$$

and C_μ is a constant and ϵ is the dissipation.

Thus, if k and ϵ can be determined, the Reynolds stresses can be computed and the time-averaged Navier-Stokes equations will be solved.

The turbulent kinetic energy equation (2.5) and the dissipation equation (2.6) form the basis for the $k - \epsilon$ model. The modeled forms of these equations, as presented by Launder and Spalding (1974) are:

$$\frac{Dk}{Dt} = \frac{1}{\rho} \frac{\partial}{\partial x_k} \left[\frac{\mu_t}{\sigma_k} \frac{\partial k}{\partial x_k} \right] + \frac{\mu_t}{\rho} \left(\frac{\partial \bar{u}_i}{\partial x_k} + \frac{\partial \bar{u}_k}{\partial x_i} \right) \frac{\partial \bar{u}_i}{\partial x_k} - \epsilon \quad (2.5)$$

$$\frac{D\epsilon}{Dt} = \frac{1}{\rho} \frac{\partial}{\partial x_k} \left[\frac{\mu_t}{\sigma_\epsilon} \frac{\partial \epsilon}{\partial x_k} \right] + \frac{C_1 \mu_t \epsilon}{\rho k} \left(\frac{\partial \bar{u}_i}{\partial x_k} + \frac{\partial \bar{u}_k}{\partial x_i} \right) \frac{\partial \bar{u}_i}{\partial x_k} - C_2 \frac{\epsilon^2}{k} \quad (2.6)$$

where $\sigma_k, \sigma_\epsilon, C_1$ and C_2 are constants. Suggested values for all of the constants used in the $k - \epsilon$ model are presented below:

C_μ	C_1	C_2	σ_k	σ_ϵ
0.09	1.44	1.92	1.0	1.3

2.1.2 Particle Equation of Motion

Consider a particle in a continuous fluid medium. The forces acting on a particle can be divided into four categories: (1) forces that act on a particle due to the motion of a particle; (2) forces that act on a particle due to the motion of a surrounding fluid; (3) forces that act on a particle irrespective of the fact that the particle is immersed in a fluid (body forces); and (4) forces that act on any object immersed in fluid regardless of the fluid or particle motion (for example, the buoyancy forces) (Shirolkar et al. (1996)). It should be noted that this analysis is concerned with dilute flows where particle motion is controlled by local aerodynamic forces rather than particle-particle collisions. The distinction between dilute and dense flow is quantitatively established by the ratio of aerodynamic response time, τ_A , to the time between collisions, τ_C . The aerodynamic response time is the time required for a particle, released from rest in a flowing stream, to achieve 63% of the free stream velocity. Thus if $\tau_A/\tau_C < 1$, a particle has time to respond to the local gas-phase velocity field before the next collision so its motion is dominated by aerodynamic forces and the flow is considered to be dilute (Crowe (1982)).

The particle momentum equation was first derived by Basset (1888), Boussinesq (1903), and Oseen (1927) for a fluid at rest but extended by Tchen (1947) to the case of a fluid moving with variable velocity, (Hinze (1975)).

$$\begin{aligned} m_p \frac{du_p}{dt} = & \underbrace{\rho_g \frac{1}{2} A_p C_D \|\vec{u}_g - \vec{u}_p\| (u_g - u_p)}_I + \underbrace{\frac{\pi}{6} d_p^3 \rho_g \frac{du_g}{dt}}_{II} + \underbrace{\frac{1}{2} \frac{\pi}{6} d_p^3 \rho_g \left(\frac{du_g}{dt} - \frac{du_p}{dt} \right)}_{III} \\ & + \underbrace{\frac{3}{2} d_p^2 \sqrt{\pi \rho_g \mu} \int_{t_0}^t \frac{\frac{d}{dt}(u_g - u_p)}{\sqrt{t - t'}} dt'}_{IV} + \underbrace{F_e}_V \end{aligned} \quad (2.7)$$

where t_0 is the starting time, the index g refers to the fluid, and the index p refers to the particle. The variables are defined as follows: m is the mass, u is the velocity, μ is the viscosity of the fluid, C_D is the drag coefficient, d is the diameter, and ρ is the density.

The terms in Equation (2.7) can be explained as follows: the term on the left side is the force required to accelerate the particle. The first term on the right side is the drag over the particle surface. The second term is due to the pressure gradient in the fluid surrounding the particle caused by acceleration of the fluid. The third term is the force required to accelerate the virtual mass of the fluid in half the volume occupied by the particle. The fourth term is the Basset force or history term which account for the deviation in flow pattern from steady state. The last term, F_e is an external potential force such as gravity or an electric field.

Dividing Equation (2.7) by the density of the particle indicates that the second, third, and fourth terms on the right hand side only become important when the density of the fluid becomes comparable or higher than the density of the particle. For the case of a gas-solid particle flow, the density of the particle is much greater than the density of the gas-phase. $\rho_g/\rho_p \ll 1$. If gravity is the only body force on the particle, Equation (2.7) reduces to

$$m_p \frac{du_p}{dt} = \frac{1}{2} \rho_g A_p C_d \|\vec{u}_g - \vec{u}_p\| (u_g - u_p) + m_p g \quad (2.8)$$

where C_d is the drag coefficient given by

$$C_d = \frac{24}{Re_p} f \quad (2.9)$$

Re_p is defined as

$$Re_p = \frac{\rho_g d_p \|\vec{u}_g - \vec{u}_p\|}{\mu} \quad (2.10)$$

and f is the ratio of the drag coefficient to the Stokes drag given by

$$f = 1 + 0.15 Re_p^{0.687} \quad (2.11)$$

The expression for the acceleration of a particle given in Equation (2.8) can be simplified even further by introducing a particle relaxation time, τ_p . Thus, Equation (2.8) becomes

$$\frac{du_p}{dt} = \frac{f}{\tau_p} (u_g - u_p) + g \quad (2.12)$$

where τ_p is given by

$$\tau_p = \frac{\rho_p d_p^2}{18\mu} \quad (2.13)$$

The particle relaxation time is a weighting factor that reflects the inertia and size of the particle. The inertia of a particle plays a significant role in its dispersion. If a particle is small and light, it can follow the high frequency fluctuations of the turbulence, essentially

Figure 2.1: Coordinate system and flow conditions for fluid particles dispersing in homogeneous isotropic turbulence

acting like a fluid tracer particle. If a particle is heavy, it has a reduced response to the turbulence and, therefore, reduced dispersion. This is called the inertia effect.

Not all researchers agree with this interpretation. Reeks (1977), Pismen and Nir (1978), Gouesbet et al. (1983), and Graham (1996), suggest that heavy particles disperse more rapidly in the long time and the dispersion coefficient for heavy particles should exceed that for fluid particles. The physical basis can be described by considering particle dispersion in a pipe: if a heavy particle is released with axial and radial velocity, the inertia of the particle will keep it on a path towards the pipe walls despite the effects of the eddies on the particle. The heavy particle will then experience a greater dispersion in comparison with a lighter particle that is captured by the eddies.

2.2 Taylor's Theorem

Understanding mathematical issues in describing fluid particle dispersion as developed by Taylor (1921) can aid in understanding particle dispersion models. Taylor mathematically described the dispersion of a fluid particle in stationary, homogeneous turbulence; this derivation is repeated here.

Consider a uniform flow where a single fluid particle is released from the origin as shown in Figure 2.1. The position and velocity of the fluid particle in a direction orthog-

onal to the main flow as a function of time are given by the expressions

$$v(t) = \frac{dy}{dt} \quad \text{and} \quad y(t) = \int_0^t v(t_1) dt_1 \quad (2.14)$$

Note that since this analysis is concerned with position and velocity in directions orthogonal to the main flow, $\overline{y(t)} = 0$ and $\overline{v(t)} = 0$.

Now consider a large number of fluid particles released from the origin, the ensemble-averaged fluid particle location as a function of time is given by

$$\overline{y(t)} = \int_0^t \overline{v(t_1)} dt_1 \quad (2.15)$$

The over-bar denotes an ensemble-average.

Using the definitions given in Equations (2.14) and (2.15), an expression for the variance of the fluid particle position as a function of time can be derived as follows

$$y = \bar{y} + y' \quad (2.16)$$

$$y'(t) = \int_0^t (v(t_1) - \overline{v(t_1)}) dt_1 = \int_0^t v'(t_1) dt_1 \quad (2.17)$$

$$\begin{aligned} \frac{dy'^2}{dt} &= 2y'(t) \frac{dy'}{dt} = 2 \left(\int_0^t v'(t_1) dt_1 \right) v'(t) \\ &= 2 \int_0^t v'(t) v'(t_1) dt_1 \end{aligned} \quad (2.18)$$

The variance of the particle position can be found by averaging Equation (2.18) and integrating

$$\frac{d\overline{y'^2}}{dt} = \frac{d\sigma_y^2}{dt} = 2 \int_0^t \overline{v'(t) v'(t_1)} dt_1 \quad (2.19)$$

$$\sigma_y^2(t) = 2 \int_0^t \int_0^{t_2} \overline{v'(t_2) v'(t_1)} dt_1 dt_2 \quad (2.20)$$

Thus, as shown in Equation (2.20), the variance of fluid particle position may be determined as a function of time given that the ensemble-averaged fluid particle velocity in Equation (2.15) and the correlation between the fluctuating fluid velocity at two different times appearing in Equation (2.20) are known for the given flow. It is important to note that the velocity correlation is for the *same* fluid particle at time t_2 . Hence the correlation is Lagrangian rather than Eulerian.

In a Lagrangian framework the autocorrelation function, $R(t_2, t_1)$, is defined as

$$R(t_2, t_1) = \frac{\overline{v'(t_2)v'(t_1)}}{\overline{v'^2(t_2)}} \quad (2.21)$$

Since the flow is stationary, the statistical properties of the fluid particle velocity are constant in time and, thus, the autocorrelation in Equation (2.21) depends only on the time difference, η . For stationary, homogeneous flows, Equation (2.21) becomes

$$R(\eta) = \frac{\overline{v'(t)v'(t+\eta)}}{\overline{v'^2}} \quad (2.22)$$

By replacing η with $\xi - t$. Equation (2.22) becomes

$$R(\xi - t) = \frac{\overline{v'(t)v'(\xi)}}{\overline{v'^2}} \quad (2.23)$$

Rearranging Equation (2.23) and integrating from $\xi = 0$ to $\xi = t$

$$\int_0^t \overline{v'(t)v'(\xi)} d\xi = \overline{v'^2} \int_0^t R(\xi - t) d\xi \quad (2.24)$$

Since averaging can be taken outside the integral and $v'(t)$ is independent of ξ , the left hand side of Equation (2.24) can be written as

$$\int_0^t \overline{v'(t)v'(\xi)} d\xi = \overline{\int_0^t v'(t)v'(\xi) d\xi} = \overline{v'(t) \int_0^t v'(\xi) d\xi} \quad (2.25)$$

Thus, Equation (2.24) becomes

$$\overline{v'(t) \int_0^t v'(\xi) d\xi} = \overline{v'^2} \int_0^t R(\xi - t) d\xi \quad (2.26)$$

Realizing that the integral of velocity is position

$$\int_0^t v'(\xi) d\xi = y'(t) - y'(0) = y'(t) \quad (2.27)$$

Substituting into Equation (2.26)

$$\overline{v'(t)y'(t)} = \overline{v'^2} \int_0^t R(\xi - t) d\xi \quad (2.28)$$

Looking at the left hand side of Equation (2.28)

$$\overline{v'(t)y(t)} = \overline{y(t)\frac{dy}{dt}} = \frac{1}{2} \frac{d\overline{y^2}}{dt} \quad (2.29)$$

Substituting Equation (2.29) into Equation (2.28) and rearranging gives

$$\frac{d\overline{y^2}}{dt} = 2\overline{v'^2} \int_0^t R(\xi - t) d\xi \quad (2.30)$$

Since the correlation is an even function such that

$$\int_0^t R(\xi - t) d\xi = \int_0^t R(\xi) d\xi \quad (2.31)$$

The final result of Taylor's work is

$$\frac{d\overline{y^2}}{dt} = 2\overline{v'^2} \int_0^t R(\xi) d\xi \quad (2.32)$$

Insight into the physics of dispersion can be obtained by considering the asymptotes of Equation (2.32). For very short times, the velocity correlation is approximately unity and Equation (2.32) becomes

$$\frac{d\overline{y^2}}{dt} = 2\overline{v'^2} t \quad (2.33)$$

so that Equation (2.32) becomes

$$\overline{y^2} = \overline{v'^2} t^2 \quad \text{for very short times} \quad (2.34)$$

The variance of particle position has a parabolic relationship to t when t is small so that the spread of the particles, $\sqrt{\overline{y^2}}$, is nearly linear. This is to be expected since

$$y \simeq v't \quad (2.35)$$

for short times.

The long time behavior of the dispersion is found by integrating Equation (2.32) from $t = 0$ to $t = \infty$. Noting that

$$\tau_{LI} = \int_0^\infty R(\eta) d\eta \quad (2.36)$$

an expression for the Lagrangian integral timescale, τ_{LI} , is obtained. This timescale is usually considered a measure of the longest time during which, on average, a particle persists in motion in a given direction, (Hinze (1975)). Thus, for long times, Equation (2.32)

becomes

$$\overline{y^2} = 2\overline{v'^2}\tau_{LI}t \quad \text{for very long times} \quad (2.37)$$

so that the variance of the particle position increases linearly with time for long times. hence the spread of the particles is proportional to $\sqrt{t}$.

2.3 Review of Existing Models

There are two approaches to modeling particle dispersion. One method is to treat the particulate phase as a continuum; particle diffusion is then obtained by solving a set of continuum conservation equations for both the fluid and the particulate phase. This method is referred to as Eulerian modeling since the fluid and particulate phases are solved using an Eulerian framework.

In contrast, the Lagrangian approach treats the particles as discrete entities within the fluid phase. Individual trajectories are predicted as a result of forces acting on a particle. Particle predictions are made after the solution of the fluid phase has been determined.

The following sections will explore both the Eulerian and Lagrangian approach, focusing on the Stochastic Separated Flow model.

2.3.1 Eulerian Models

There are two different types of Eulerian models: the Locally Homogeneous Flow model and the Two-Fluid Model. The main characteristic of Eulerian models is that the transport equations are solved in an Eulerian framework.

Locally Homogeneous Flow (LHF) Model

The LHF model is the simplest particle dispersion model. It assumes that the particle moves with the same velocity as the fluid surrounding it, ignoring slip between the particle and the gas. The particle concentration field is obtained by solving a partial differential equation for species conservation where mass transfer is assumed to be caused by advection and turbulent diffusion. Here the mass transfer diffusion coefficient is taken to be equal to the turbulent viscosity.

The assumption that every particle follows the high frequency fluctuations of the flow, regardless of its inertia, restricts the appropriate use of the model. The model is best suited to predict particle dispersion in cases where the particles are small and light

and particle inertia has little or no impact on dispersion. For more general cases where particle inertia may become important, the LHF model overpredicts particle dispersion. (Shuen et al. (1983a), Shuen et al. (1983b)).

Two-Fluid Models

The Two-Fluid model treats particles as a second fluid with a distinct velocity from the gas-phase, (Durst et al. (1984)). The particle phase is treated as a continuum without a pressure term in the equation of motion since the pressure gradient effects are already included in the drag coefficient, C_d , or assumed negligible. Reynolds decomposition and time-averaging is applied to the equations which result in correlations involving fluctuating particle concentrations, particle velocities and gas-phase velocities. The 'dusty gas' equations of Marble (as contained in Chen and Wood (1985)) form the governing equations for the dispersed phase.

$$\frac{\partial \rho_s}{\partial t} + \frac{\partial}{\partial x_j}(\rho_s u_j) = 0 \quad (2.38)$$

$$\frac{\partial}{\partial t}(\rho_s u_i) + \frac{\partial}{\partial x_j}(\rho_s u_i u_j) = 0 \quad (2.39)$$

where u_i is the instantaneous particle velocity, and ρ_s is the particulate phase loading. The particulate phase loading is given by

$$\rho_s = \rho_p \theta \quad (2.40)$$

where ρ_p is the material density of the particle, and θ is the volume fraction of particles.

For a steady, incompressible, dilute flow where triple correlations are considered negligible, Reynolds decomposition and time-averaging of Equations (2.38) and (2.39) yield expressions for particle mass and momentum respectively.

$$\frac{\partial \bar{\rho}_s U_j}{\partial x_j} = -\frac{\partial}{\partial x_j}(\overline{\rho'_s u'_j}) \quad (2.41)$$

$$\bar{\rho}_s U_j \frac{\partial U_i}{\partial x_j} = -\overline{\rho'_s u'_j} \frac{\partial U_i}{\partial x_j} - \frac{\partial}{\partial x_j}(\bar{\rho}_s \overline{u'_i u'_j}) - \frac{\partial}{\partial x_j}(U_j \overline{\rho'_s u'_i}) \quad (2.42)$$

The equations must be closed by expressing the unknown correlations in terms of known quantities. The simplest closure model parallels the eddy diffusion model by applying

the gradient diffusion hypothesis, Adeniji-Fashola and Chen (1990).

$$\overline{u_i' u_j'} = -\nu_p \frac{1}{2} \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) + \frac{2}{3} \delta_{ij} \left(-\frac{1}{2} \overline{u_i' u_i'} + \nu_p \frac{\partial U_i}{\partial x_i} \right) \quad (2.43)$$

$$\overline{\rho_s' u_i'} = -D_p \frac{\partial \bar{\rho}_s}{\partial x_i} \quad (2.44)$$

where ν_p is the ‘effective’ turbulent kinematic eddy viscosity, and D_p is the turbulent particle diffusivity.

To determine the dispersion of the particulate, the partial differential equations for the conservation of particle mass fraction and momentum are solved. Unfortunately there is uncertainty in the literature about appropriate values for the particle diffusivity.

Further, the Eulerian approach has some inherent difficulties. The inclusion of a diffusivity changes the nature of the equation from parabolic to elliptic, essentially failing to capture the physics of the problem (Crowe (1982)). There are also some restrictions on the appropriateness of the gradient diffusion approach when considering dilute particle flows, (Lightstone (1992)).

2.3.2 Lagrangian Models

Lagrangian models solve for the trajectories of individual particles by solving the particle equation of motion in a Lagrangian framework. The model is referred to as Lagrangian since the particle is tracked using a Lagrangian frame of reference. There are two types of Lagrangian models: the Deterministic Separated Flow model and the Stochastic Separated Flow model.

Deterministic Separated Flow (DSF) Model

The DSF model assumes that the particle trajectory has no randomness associated with it. Hence, in this model, the time-averaged fluid velocity (rather than instantaneous velocity) is used to determine the drag force on the particle. The model is referred to as deterministic since particles with the same physical properties and initial conditions will have identical trajectories.

The DSF model can be modified to account for turbulent dispersion by estimating a dispersive component of particle velocity.

$$u_i = u_i^c + u_i^d \quad (2.45)$$

where the superscript c refers to the convective component, and the superscript d refers to the dispersive component of the particle velocity. Here, u_i^d follows from the gradient diffusion approximation (Shirolkar et al. (1996)). As a result, this modified DSF model has the same problem as the Eulerian models because it requires an estimation of the turbulent diffusivity. These simplifications make it difficult to apply this model successfully for a wide range of flows.

Stochastic Separated Flow (SSF) Model

The SSF model is the most promising of the particle dispersion models studied and is the focus of the current thesis. In the following sections, the SSF Model is introduced using the conventional model of Gosman and Ioannides (1983). Fundamental considerations in particle dispersion models are explored. Model variations proposed by various researchers are presented.

The Conventional Model of Gosman and Ioannides, 1983

SSF models use a Lagrangian framework to solve the trajectory equations of a particle as it interacts with a succession of discrete turbulent eddies. While in an eddy the particle interacts with the instantaneous velocities of the gas-phase turbulence. The solution is stochastic since the model incorporates the turbulent fluctuations by random sampling to determine the instantaneous velocity of the continuous gas-phase.

In this approach, the instantaneous gas velocity is decomposed in a mean velocity plus a random fluctuation, $u_g = \overline{u_g} + u'_g$. Each particle is exposed to a new instantaneous velocity every time it enters an eddy. The fluctuating velocity is determined using a random number generator. In most models this velocity is kept constant during the particle-eddy interaction. The differences between particle dispersion models lie in the treatment of the gas-phase turbulence and the manner in which it is thought to interact with particle motion.

The conventional stochastic dispersion model of Gosman and Ioannides computes the gas-phase fluctuating components using random sampling of a Gaussian probability density function. The instantaneous velocity is assumed to be a random variable with a variance given by

$$\sigma^2 = \frac{2}{3}k \quad (2.46)$$

where k is the turbulent kinetic energy of the flow as determined by the $k-\epsilon$ model. Launder and Spalding (1974), for the turbulent gas-phase. Here, each orthogonal component of velocity is assumed to be statistically independent.

The time interval over which the particle interacts with the randomly sampled velocity field is determined by two time scales: the eddy lifetime, t_e , and the transit time, t_{tr} . The latter timescale is the time required for the particle to cross an eddy. If the particle is moving at nearly the same velocity as the fluid, it may be captured by the eddy and remain in the eddy for the entire eddy lifetime. However, if the particle has a velocity very different from that of the fluid, it can traverse the eddy before the eddy dies. This phenomenon is known as the ‘crossing trajectory’ effect, Csanady (1963). Thus the interaction time is determined by taking the minimum of the two scales, that is

$$t_{int} = \min(t_e, t_{tr}) \quad (2.47)$$

These times are estimated by assuming that the characteristic size of a randomly sampled eddy is the dissipation length scale, l_e , given by

$$l_e = C_\mu^{0.5} \frac{k^{1.5}}{\epsilon} \quad (2.48)$$

where C_μ is equal to 0.09 and ϵ is the dissipation rate of turbulence.

The eddy lifetime is given by

$$t_e = \frac{l_e}{|u'_g|} \quad (2.49)$$

where u'_g is the gas-phase velocity fluctuation.

The transit time of a particle, derived in Appendix A.1, is found from the solution of the linearized form of the equation of motion of a particle in uniform flow

$$t_{tr} = -\tau_p \ln \left(1 - \frac{l_e}{\tau_p |\vec{u}_g - \vec{u}_p|} \right) \quad (2.50)$$

where $\vec{u}_g - \vec{u}_p$ is the relative velocity at the beginning of the interaction time and τ_p is the particle relaxation time introduced in Section 2.1.2. When $l_e > \tau_p |\vec{u}_g - \vec{u}_p|$, Equation (2.50) has no solution. In this case, the particle is captured by the eddy, and the interaction time is the eddy lifetime.

While the SSF model of Gosman and Ioannides can account for both the inertia effect and the crossing trajectory effect, it does not account for the continuity effect proposed by Csanady in 1963. Consider a particle with a large drift velocity, where drift velocity refers to velocity of a particle resulting from a gravitational force. Stock (1996), explains that if the drift velocity is large, diffusivity is controlled by the particle transit time because the particle moves through the eddy before the eddy decays. Thus it is the turbulent length

scale, l_e , that determines the particle interaction time and not the eddy lifetime. In the free-fall direction, the turbulent length scale corresponds to the longitudinal spatial integral length scale, L_f and, in the two directions transverse to the fall direction, the turbulence length scale corresponds to the lateral spatial integral length scale, L_g . For isotropic turbulence, continuity constrains the turbulence and requires that $L_f = 2L_g$. Thus, for this limiting case, the dispersion in the fall direction is twice that in the two transverse directions.

Model Variations

Shuen, Chen, and Faeth (1983) proposed modifications to the expressions for characteristic eddy size and the eddy lifetime. Since the turbulent kinetic energy is related to the fluctuating turbulent velocity component, they defined the eddy lifetime as

$$t_e = \frac{l_e}{\sqrt{\frac{2}{3}k}} \quad (2.51)$$

In addition, the characteristic eddy size is defined similarly to that of Gosman and Ioannides but a different exponent is used, that is $C_\mu^{0.75}$. However, the value of the power that C_μ is raised to in Equation (2.48) is not agreed on by researchers. Analytical work by Lightstone and Raithby (1996) indicate an exponent of $C_\mu^{0.63}$. Their analysis is repeated in Section 5.2.

Using the Gosman and Ioannides methodology, the turbulent gas-phase velocity fluctuation in each orthogonal direction is sampled only once per eddy and the gas-phase velocity is held constant over the particle/eddy interaction time. With this approach, the particle interaction time is chosen to be large, such that the time correlation between fluctuating velocities in subsequent timesteps will be effectively zero. Zhou and Leschziner (1991a) argue that within an eddy, a particle will, in fact, see a series of time-correlated gas-phase velocities. The gas-phase velocity fluctuations in the Zhou and Leschziner model are therefore expressed as

$$u'_t = R(\delta t)u'_{t-\delta t} + e_t \quad (2.52)$$

where the first term on the right hand side includes all the effects from previous time steps while the second term represents effects arising from randomness during the time interval δt . It is important to note that δt is much smaller than the particle interaction times employed using the Gosman and Ioannides approach.

For any given δt , the expected value of e_t is given by

$$\bar{e}_t = \bar{u}_t' - R(\delta t)\overline{u_{t-\delta t}'} = 0 \quad (2.53)$$

and the variance is

$$\overline{e_t^2} = \overline{(u_t' - R(\delta t)u_{t-\delta t}')^2} = \overline{u_t'^2} - R^2(\delta t)\overline{u_{t-\delta t}'^2} \quad (2.54)$$

Hinze (1975) suggests that the time correlation may be approximated

$$R(\delta t) = \exp\left(-\frac{\delta t}{\tau_{LI}}\right) \quad (2.55)$$

The Lagrangian integral timescale, τ_{LI} , used in Zhou and Leschziner's model is given by

$$\tau_{LI} = \beta t_e = \beta(C_\mu^{0.75} \frac{k^{1.5}}{\epsilon}) / (\frac{2}{3}k)^{0.5} \quad (2.56)$$

Here, β is based on analytical and experimental considerations. Zhou and Leschziner report the optimum value of β to be 0.8.

Zhou and Leschziner (1991b) modified this model to include the spatial correlation as well. In this case a Reynolds Stress Transport (RST) model is used for the turbulent gas-phase to solve for the spatial correlations. Then temporal and spatial correlations are manipulated to yield a joint PDF describing the velocity fluctuations which are assumed to be Gaussian.

The SPEED model presented by Chen and Pereira (1996) introduces a similar idea. The variance of the PDF is a function of the variance at the previous timestep plus a function of eddy lifetime, the timestep, and the root mean square of the fluctuating velocity component of the carrier phase. Here an RST model is also used to describe the turbulent gas-phase.

2.4 Summary

This chapter began with the governing equations for the flow. For a dilute particle flow with the density of a particle much greater than the density of the gas, the particle equation of motion is reduced to a drag term plus gravitational forces. The physics of the flow were examined and phenomenon such as the inertia effect, continuity effect, and crossing trajectory effect were explained.

The behavior of particles in simple flows was examined by considering Taylor's ma-

nipulation of the correlation function. At short times, the variance of particles has a parabolic relationship so that the spread of particles is nearly linear. At long times, the variance of particle position increases linearly with time. Hence, the spread of the particles is proportional to $\sqrt{t}$ at long times.

A critical review of existing models was presented. The Eulerian LHF model assumes that every particle follows the high frequency fluctuations of the flow, regardless of its inertia. This assumption restricts the appropriateness of the model. The LHF model is best suited to predict particle dispersion in cases where particles are small and light, and overpredicts particle dispersion in cases where particle inertia may become important.

The Eulerian two-fluid model treats particles as a second fluid with a distinct velocity from the gas-phase. The model employs a gradient diffusion hypothesis by using a particle diffusivity and solving the partial differential equations for the conservation of particle mass fraction and momentum to determine the dispersion of the particulate. Unfortunately, there is uncertainty in the literature about appropriate values for the particle diffusivity. Further, the inclusion of a diffusivity changes the nature of the equation from parabolic to elliptic, essentially failing to capture the physics of the problem. There are also some restrictions on the appropriateness of the gradient diffusion approach when considering dilute flows.

Dilute flows are well-suited to Lagrangian models which solve for the trajectories of individual particles in a Lagrangian framework. The DSF model assumes that the particle trajectory has no randomness associated with it and ignores the gas-phase turbulence, therefore ignoring an important component to the physics of the flow. The DSF model can be modified to account for turbulent dispersion by estimating a dispersive component following the gradient diffusion approximation. As a result, this modified DSF model has the same problem as the Eulerian models because it requires an estimation of the turbulent diffusivity.

SSF models avoid the gradient diffusion hypothesis by incorporating the turbulent fluctuations using random sampling to determine the instantaneous velocity of the continuous gas-phase. In this approach, each particle interacts with a succession of discrete turbulent eddies; the instantaneous gas-phase velocity is selected at the beginning of the interaction time and, in most models, this velocity is kept constant until the particle enters a new eddy. The physics of the problem are preserved and the model is able to account for both the inertia and crossing trajectory effects. Zhou and Leschziner offer an alternative to this model by introducing a time-correlated gas-phase velocity fluctuation. Using Zhou and Leschziner's model, the timestep, δt , is selected *a priori* and it is important to note that the timestep is much smaller than the particle interaction times

employed by the conventional SSF model.

Chapter 3

The Model of Hennick and Lightstone

This chapter introduces the model of Hennick and Lightstone. A short summary of currently available particle dispersion models is included to outline the motivation for the new model. The model is presented in detail. The model is shown to exactly reproduce Taylor's result for the dispersion of dyed fluid particles in homogeneous, isotropic turbulence.

3.1 Motivation

Currently available models for particle dispersion in turbulent flows are presented in Section 2.3. There are two approaches to modeling the particulate phase: one is to treat the particles as a continuum; particle diffusion is then obtained by solving a set of continuum equations for both the fluid and particulate phases. This method is referred to as Eulerian modeling since the flow is computed entirely within an Eulerian framework.

Alternatively, the Lagrangian approach treats particles as discrete entities within the fluid phase. Individual trajectories are predicted as a result of forces acting on a particle. Particle predictions are made after the solution of the fluid phase has been determined.

Lagrangian models are physically superior to treating the particles as a continuum: disadvantages of Eulerian models are discussed in Section 2.3.1. However, while Lagrangian models sufficiently capture the physics of the flow, knowledge of the instantaneous velocity fluctuations of the fluid phase are required to obtain particle trajectories.

The conventional Stochastic Separated Flow (SSF) model of Gosman and Ioannides (1983) decomposes the instantaneous gas-phase velocity into a mean velocity plus a

random fluctuation, $u_g = \overline{u_g} + u'_g$. The flow field is modeled as a series of discrete eddies: each particle is exposed to a new instantaneous velocity every time it enters an eddy. The gas-phase fluctuating components are computed using random sampling of a Gaussian probability density function. The instantaneous velocity is assumed to be a random variable with variance given by

$$\sigma^2 = \frac{2}{3}k \quad (3.1)$$

where k is the turbulent kinetic energy of the flow as determined by the $k-\epsilon$ model, Launder and Spalding (1974), for the turbulent gas-phase. Here, each orthogonal component of velocity is assumed to be statistically independent.

Since the instantaneous gas-phase velocity is considered to be a random variable, the sampling rate of the gas-phase fluctuations must be limited to ensure that subsequent fluctuations are not correlated in time. Using the Gosman and Ioannides methodology, the turbulent gas-phase velocity fluctuation in each orthogonal direction is sampled only once per eddy and the gas-phase velocity is held constant over the particle/eddy interaction time.

Zhou and Leschziner (1991a) argue that a particle will see more than one turbulent velocity fluctuation within an eddy. The gas-phase velocity fluctuations are therefore expressed as

$$u'_t = R(\delta t)u'_{t-\delta t} + e_t \quad (3.2)$$

where u'_t is the gas-phase velocity fluctuation at the current time t , $R(\delta t)$ is the time correlation which accounts for all effects arising from previous timesteps, $u'_{t-\delta t}$ is the velocity fluctuation from the previous timestep, and e_t represents all effects arising from randomness during the time interval δt .

For any given δt , the expected value of e_t is zero and the variance is given by

$$\overline{e_t^2} = \overline{(u'_t - R(\delta t)u'_{t-\delta t})^2} = \overline{u_t'^2} - R^2(\delta t)\overline{u_{t-\delta t}'^2} \quad (3.3)$$

The time-correlation is approximated by the exponential function as suggested by Hinze (1975).

$$R(\delta t) = \exp\left(-\frac{\delta t}{\tau_{LI}}\right) \quad (3.4)$$

The Lagrangian integral timescale, τ_{LI} , used in Zhou and Leschziner's model is given by

$$\tau_{LI} = \beta t_e = \beta(C_\mu^{0.75} \frac{k^{1.5}}{\epsilon}) / (\frac{2}{3}k)^{0.5} \quad (3.5)$$

Here, β is based on analytical and experimental considerations. Zhou and Leschziner

report the optimum value of β to be 0.8.

Zhou and Leschziner's model improves the conventional SSF model by incorporating the temporal autocorrelation into the definition of the turbulent gas-phase velocity fluctuation. As a result, a particle may see more than one instantaneous velocity while in an eddy, closely modeling the physics of the flow. However, this methodology has two important weaknesses:

- (i) There is no clearcut method for prescribing the magnitude of the Lagrangian integral timescale, τ_{LI} .
- (ii) The model does not account for the crossing trajectory effect.

Zhou and Leschziner determine the magnitude of the Lagrangian integral timescale based on the performance of the model in comparison with particle dispersion measurements in grid-generated turbulence as reported by Wells and Stock (1983). The adequacy of the constant used to calculate τ_{LI} is discussed in Section 5.5.

The second weakness of the Zhou and Leschziner model has its basis in the physics of the flow. The crossing trajectory effect describes the migration of a particle from one eddy to another before the eddy dissipates. If a particle is moving at nearly the same velocity as the fluid, it may be captured by the eddy and remain in the eddy until the eddy dissipates. However, if the particle has a velocity very different from that of the fluid, it can traverse the eddy before the eddy dies. This phenomenon, known as the crossing trajectory effect, (Csanady (1963)), significantly affects the dispersion of the particles.

While Zhou and Leschziner's approach does not model the turbulence as a series of discrete eddies, the principle of the crossing trajectory effect may be applied to the model. Equation (3.2) describes the velocity fluctuation using a time-correlation coefficient $R(\delta t)$ derived for fluid particles. Unless a particle has a small particle relaxation time, it will not be able to follow the high frequency fluctuations of the turbulence, and in general, will not see the same velocity fluctuations as a fluid point. Thus, a particle falling through an eddy will see a velocity fluctuation at time t that should have a much lower correlation. However, using Zhou and Leschziner's model, a heavy particle sees velocity fluctuations that are highly correlated. Hence, the model is unable to capture the crossing trajectory effect.

3.2 The Model of Hennick and Lightstone

The model of Hennick and Lightstone compensates for the weaknesses outlined in the above section. The crossing trajectory effect is incorporated by introducing a spatial correlation coefficient based on the relative velocity of the particle and the timestep δt . In addition, the magnitude of the Lagrangian integral timescale is determined independent of the model's performance by relating the variance of particle position to Taylor's result for fluid particles.

Similar to conventional SSF models, the instantaneous gas-phase velocity is decomposed into a mean velocity plus a random fluctuation, $u_g = \overline{u_g} + u'_g$. Here, the subscript g is dropped for simplicity and the subscript employed refers to the velocity fluctuation with respect to time. The gas-phase velocity fluctuations are expressed as

$$u'_t = R(\delta t, \delta x)u'_{t-\delta t} + e_t \quad (3.6)$$

where u'_t is the gas-phase velocity fluctuation at the current time t , $R(\delta t, \delta x)$ is an autocorrelation based on time and position, $u'_{t-\delta t}$ is the velocity fluctuation at the previous timestep, and e_t is a random component incorporating all effects due to randomness during the current timestep, δt .

The autocorrelation is a function of the change in time and position experienced by a particle over a single timestep δt . As a simplification, the autocorrelation is decomposed into temporal and spatial components

$$R(\delta t, \delta x) \cong R_t(\delta t)R_x(\delta x) \quad (3.7)$$

This simplification allows for the independent estimation of each correlation function. The spatial correlation can be related to the temporal correlation by approximating the distance a particle travels in a single timestep using the relationship $\delta x = u_{REL}\delta t$ where u_{REL} is the relative velocity of the particle.

For any given δt , the expected value of e_t is zero and the variance is given by

$$\overline{e_t^2} = \overline{(u'_t - R_t(\delta t)R_x(u_{REL}\delta t)u'_{t-\delta t})^2} = \overline{u_t'^2} - R_t^2(\delta t)R_x^2(u_{REL}\delta t)\overline{u_{t-\delta t}'^2} \quad (3.8)$$

Hinze (1975) suggests that the time correlation may approximated by

$$R_t(\delta t) = \exp\left(-\frac{\delta t}{\tau_{LI}}\right) \quad (3.9)$$

where τ_{LI} is the Lagrangian integral timescale given by

$$\tau_{LI} = 0.135 \frac{k}{\epsilon} \quad (3.10)$$

Determination of the Lagrangian integral timescale follows from an extension of Taylor's work. Lightstone and Raithby (1996) relate the variance of particle position to Taylor's result for fluid particles released into a uniform flow of homogeneous isotropic turbulence. In contrast to Zhou and Leschziner's model, this result is obtained based solely on analytical considerations. The analysis of Lightstone and Raithby is repeated in Section 5.2.

The spatial autocorrelation is approximated by

$$R_x(u_{REL}\delta t) = \exp\left(-\frac{u_{REL}\delta t}{L_I}\right) \quad (3.11)$$

where $u_{REL} = |\vec{u}_g - \vec{u}_p|$, and L_I is the Lagrangian integral length scale given by

$$L_I = C_\mu^{0.63} \frac{k^{1.5}}{\epsilon} = 2\tau_{LI} \sqrt{\frac{2}{3}k} \quad (3.12)$$

This expression for L_I comes from the definition of the characteristic eddy length suggested by the analysis of Lightstone and Raithby outlined in Section 5.2. Similar to the expression for τ_{LI} , the Lagrangian integral length scale is determined based on analytical considerations.

Incorporating the approximations for the temporal and spatial autocorrelation, the gas-phase velocity fluctuation becomes

$$u'_t = \exp\left(-\left(\frac{\delta t}{\tau_{LI}} + \frac{u_{REL}\delta t}{L_I}\right)\right) u'_{t-\delta t} + e_t \quad (3.13)$$

The behaviour of the new model can be explored by considering the limiting cases of relative velocities.

Consider the gas-phase velocity fluctuation in the limit of dyed fluid particles. In the case of dyed fluid particles, there is no relative velocity and u_{REL} is zero. Thus the spatial correlation goes to unity and the velocity fluctuation is based solely on the temporal correlation as required. In contrast, if the relative velocity of the particle is large, then the spatial correlation becomes important and the correlation between old and new fluid velocities is reduced.

Now consider the dispersion of dyed fluid particles released from a point in homo-

geneous, isotropic turbulence as outlined in Chapter 5. The analysis of Lightstone and Raithby repeated in Section 5.2 leads to Equation (5.8) included here for completeness

$$\overline{y_p^2} = (\Delta t \overline{u_{g,i}^2}) t \quad (3.14)$$

At long times, the time correlation in Equation (3.13) goes to zero. Square Equation (3.13) and time average. Using the expression for the variance of e_t given by Equation (3.8) the result is

$$\overline{u_t'^2} = \overline{e_t^2} = \frac{2}{3} k \quad (3.15)$$

Substituting the expression for the turbulent gas-phase velocity fluctuation given in Equation (3.15) into Equation (3.14) yields

$$\overline{y_p^2} = \left(\frac{2}{3} k \Delta t \right) t \quad (3.16)$$

Taylor showed that for long times

$$\overline{y_p^2} = 2\tau_{LI} \overline{u_{g,i}^2} t \quad (3.17)$$

Combining Equation (3.16) with Equation (3.17) and substituting the expression for the Lagrangian integral timescale given by Equation (3.10) yields

$$\overline{y_p^2} = 0.135 \left(\frac{4}{3} \right) \frac{k^2}{\epsilon} = 2\nu_t t \quad (3.18)$$

This analysis shows that Hennick and Lightstone's model yields exactly Taylor's result for long times and exactly predicts the dispersion of dyed fluid particles in homogeneous isotropic turbulence when a timestep of $\Delta t = 2\tau_{LI}$ is chosen.

Consider the gas-phase velocity fluctuation in the limit of a particle with an infinitely large relative velocity. In this case, the value of the spatial correlation is zero, and the velocity fluctuation is based entirely on effects due to randomness, e_t . Thus the gas-phase velocity fluctuation can again be described by Equation (3.15) shown above. As required, the crossing trajectory effect is accounted for; the particle may travel a large distance in a very short time δt and will see uncorrelated velocity fluctuations.

3.3 Summary

Motivation for the model of Hennick and Lightstone is outlined. The model is presented in detail. The analysis of Taylor is extended to the model which is shown to exactly reproduce Taylor's result for the dispersion of dyed fluid particles in homogeneous isotropic turbulence.

Chapter 4

Solution of the Governing Equations

The governing equations for a particle-laden flow were presented in Section 2.1. These equations include the conservation equations for mass and momentum of the flow field, the turbulent kinetic energy and dissipation equations used in the $k - \epsilon$ model, and the particle equation of motion.

This chapter describes the numerical methods used to obtain solutions to the governing equations. The chapter begins with the numerical solution of the fluid flow equations. This section is designed to be a brief overview of the numerical solution method. Details are provided in the TASCflow Theory Manual, (1995). The following section outlines the numerical solution of the particulate phase. Implementation of the models described in Section 2.3.2 and Chapter 3 is outlined.

4.1 Numerical Solution of the Fluid Phase

The conservation equations for mass and momentum of the fluid phase were presented in Section 2.1.1. Consider the time-averaged form of the governing equations

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j}(\rho u_j) = 0 \quad (4.1)$$

$$\frac{\partial}{\partial t}(\rho u_i) + \frac{\partial}{\partial x_j}(\rho u_j u_i) = -\frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j} \left(\mu_{eff} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \right) + F_i \quad (4.2)$$

where ρ is the density, u_i represents the velocities in the x_i coordinate directions, P is the pressure, F_i represents all body forces, and μ_{eff} is the effective viscosity. The effective viscosity is a combination of the dynamic viscosity of the fluid plus the eddy viscosity. $\mu_{eff} = \mu + \mu_t$.

Using the finite volume approach, Equations (4.1) and (4.2) are integrated over a fixed control volume. Using Gauss' theorem the result is

$$\frac{\partial}{\partial t} \left(\int_v \rho dv \right) + \int_s \rho u_j dn_j = 0 \quad (4.3)$$

$$\frac{\partial}{\partial t} \left(\int_v \rho u_i dv \right) + \int_s \rho u_j u_i dn_j = - \int_s P dn_i + \int_s \mu_{eff} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) dn_j + \int_v F_i dv \quad (4.4)$$

where v and s denote volume and surface integrals respectively, and dn_i are the differential Cartesian components of the outward normal surface vector.

The cross-hatched region in Figure 4.1 indicates a control volume and its nodal point. The computational domain is discretized into elements which have nodal points in the corners. The control volume surfaces are defined by element mid-planes. Detailed information about control volume generation is provided in the TASCflow Theory Manual.

Figure 4.1: The definition of the control volume

Equations (4.3) and (4.4) are applied to each discrete control volume in the computational domain. The continuous volume integrations are straightforward as shown below. The continuous surface integrations are converted to a discrete form by integrating them at *integration points*. The location of the integrations points for one flux element is shown in Figure 4.2 for a 2-D quadrilateral element. In 3-D, the flux element consists of 8 octants and 12 integration point surfaces, each containing an integration point location.

The surface fluxes must be discretely represented at the integration points to complete the conversion of the continuous equations to their discrete counterparts. The details of this representation are provided in the TASCflow Theory Manual. The discrete form of the integral equations are written as

$$\rho V \left(\frac{\rho - \rho^o}{\Delta t} \right) + \sum_{ip} (\rho u_j \Delta n_j)_{ip} = 0 \quad (4.5)$$

$$\rho V \left(\frac{u - u^o}{\Delta t} \right) + \sum_{ip} \dot{m}_{ip} (u_j)_{ip} = \sum_{ip} (P \Delta n_i)_{ip} + \sum_{ip} \left(\mu_{eff} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \Delta n_j \right)_{ip} + F_i V \quad (4.6)$$

where

$$\dot{m}_{ip} = (\rho u_j \Delta n_j)_{ip}^o \quad (4.7)$$

and V is the volume of the control volume, the subscript ip denotes an integration point and the summation is over all the integration points of the surface, Δn_j is the surface area of the control volume face. Δt is the timestep, and the superscript o means "at the previous timestep."

Figure 4.2: Integration point definition for a 2-D quadrilateral element

Discretization of the boundary conditions is facilitated by the simple definition of control volumes along the boundaries. Figure 4.3 shows an example of a boundary control volume. Boundary control volumes touch the boundary on one or more faces: boundary conditions provide information necessary to evaluate the flow through the boundary surfaces of each boundary control volume.

The simulations created for this thesis employ very simple boundary conditions. Inlet

Figure 4.3: Example of a boundary control volume

conditions are described by a uniform mean velocity, and initial turbulent kinetic energy and dissipation. For a specified inlet velocity, u_i^{spec} , the inlet mass flow is calculated using the following

$$\dot{m}_{ip} = \rho_{ip} (A_i)_{ip} u_i^{spec} \quad (4.8)$$

Average static pressure is set over the outlet region. Thus the outlet pressure is constrained such that

$$\frac{1}{A} \int_s P dA = 0 \quad (4.9)$$

where the integral is over the entire outlet boundary surface and A is the total boundary surface area. A symmetry boundary condition is employed along the walls. The fluid velocity normal to the symmetry plane is zero and the mass flow is set to zero at each boundary integration points along the walls.

The control volume equations describe the flow of a conserved quantity through each face of a control volume. The flow is described in terms of the control volume values at each node where there is one value per node per dependent variable (TASCflow Theory Manual, (1995)).

TASCflow's treatment of advected quantities is not straightforward; the code employs a combination of different advection schemes based on the conservative finite volume ap-

proach with “special care taken to minimize the errors normally associated with upstream differencing schemes” (TASCflow Theory Manual, (1995)). TASCflow uses a Linear Profile Scheme (LPS) (Raw (1985)) and Mass Weighted Skewed (MWS) (Raithby (1976)) upstream differencing schemes with Physical Advection Correction (PAC) terms, (Raithby (1976), Lillington (1981), Huget (1985), Raw (1985)).

The PAC scheme provides a correction term to the Upwind Difference Scheme so that “the resulting algebraic equations ... correctly mimic the transport properties of the physical processes.” However, unphysical wiggles can arise when advection dominates. Thus, the MWS scheme is used to eliminate the need for the advective component of the PAC term (TASCflow Theory Manual, (1995)). The MWS scheme provides a mass weighted average of the advected quantity on the streamline upstream of the integration point. This is done by taking an average of the value of the scalar, ϕ , at the surrounding nodes and weighting it according to the mass flow passing through the control volume faces surrounding the streamline. The streamline value of ϕ is used to calculate the value of ϕ at the integration points. The LPS scheme is also used to determine the value of ϕ along the streamline by interpolating nodal values.

Pressure-velocity coupling is accomplished using a method involving colocated variables. An expression for integration point velocities is derived using the local pressure difference. The result is two expressions for velocity at a single integration point: one velocity is used to calculate the mass flux at that integration point, while the second velocity is the ‘advected velocity’ used to calculate the momentum flux. This method is outlined in greater detail in Section 5.3 of the TASCflow Theory Manual.

Simulating a turbulent flow is an important component to the current investigation. TASCflow uses the $k-\epsilon$ turbulence model of Launder and Spalding, (1974). The modeled forms of the turbulent kinetic energy equation and the dissipation equation were presented in Section 2.1.1. The discrete form of these equations are obtained in a manner analogous to any scalar transport equations.

Solution of the coupled equations is determined using a Gauss-Seidel solver. Gauss-Seidel solvers are able to reduce the total residual quickly by removing high-frequency error. However, when low-frequency error remains, the residual does not decrease as quickly and the solver stalls. To compensate for this problem, TASCflow uses an Additive Correction Multigrid (ACM) method, (Schlichting (1965)). Using this method, errors from a solution iteration are translated to a coarser grid. Therefore, low-frequency errors appear as high frequencies. The ACM method is described in detail in Chapter 7 of the TASCflow Theory Manual.

4.2 Numerical Solution of the Particle Equation of Motion

TASCflow performs the prediction of particle dispersion using a Lagrangian formulation. The Lagrangian approach treats particles as discrete entities within the fluid phase. Individual trajectories are predicted as a result of forces acting on a particle. Particle predictions are made after the solution of the fluid phase has been determined. Thus, the prediction of the particle motion is essentially post-processing.

This section begins with a review of the theoretical basis for Lagrangian particle tracking. The particle equation of motion is presented and the SSF model of Shuen, Chen and Faeth (1983) is outlined. The numerical solution of the particle equation of motion is discussed beginning with the integration of the equation of motion. The calculation of trajectories using local grid coordinates is explained with attention to the treatment of flux element boundaries and interfaces. The section is followed by a discussion of the implementation of various particle dispersion models considered in this thesis.

4.2.1 Particle Motion

The particle equation of motion was presented in Section 2.1.2. If the particle density is much greater than the fluid density and gravity is the only body force, the particle equation of motion reduces to

$$m_p \frac{du_p}{dt} = \frac{1}{2} \rho_g A_p C_d \|\vec{u}_g - \vec{u}_p\| (u_g - u_p) + m_p g \quad (4.10)$$

where the index g refers to the fluid, and the index p refers to the particle. The variables are defined as follows: m is the mass, u is the velocity, ρ_g is the density of the fluid, A_p is the cross-sectional area of the particle, and C_d is the drag coefficient given by

$$C_d = \frac{24}{Re_p} f \quad (4.11)$$

Re_p is defined as

$$Re_p = \frac{\rho_g d_p \|\vec{u}_g - \vec{u}_p\|}{\mu} \quad (4.12)$$

and f is introduced to account for experimental results on the viscous drag of a solid sphere. TASCflow uses two separate curves to account for a moderate Reynolds number

$0.01 < Re_p < 260$. The drag correction is

$$f = 1 + 0.1315(Re_p)^{0.82-0.05\alpha} \quad Re_p < 20 \quad (4.13)$$

$$= 1 + 0.1935(Re_p)^{0.6305} \quad Re_p > 20 \quad (4.14)$$

where $\alpha = \log Re_p$.

The analytical solution to the particle equation of motion requires the instantaneous turbulent velocity. Thus, the prediction of particle motion in turbulent flows is dependent on the accuracy of the flow field solution and the estimation of the turbulent velocity fluctuations. The Stochastic Separated Flow (SSF) particle dispersion models presented in Section 2.3.2 offer a variety of methods to determine the fluctuating gas-phase velocity component and a series of criterion that determine the sampling frequency of the turbulent flow field.

TASCFLOW employs the SSF model of Shuen, Chen and Faeth (1983). This model uses a Lagrangian framework to solve the trajectory equations of a particle as it interacts with a succession of discrete turbulent eddies. In this approach, the instantaneous gas-phase velocity is decomposed into a mean velocity plus a random fluctuation, $u_g = \overline{u_g} + u'_g$. The flow field is modeled as a series of discrete eddies; each particle is exposed to a new instantaneous velocity every time it enters an eddy. The gas-phase fluctuating components are determined using random sampling of a Gaussian probability density function. The instantaneous velocity is assumed to be a random variable with a variance given by

$$\sigma^2 = \frac{2}{3}k \quad (4.15)$$

where k is the turbulent kinetic energy of the flow. Here, each orthogonal component of velocity is assumed to be statistically independent.

The instantaneous gas-phase velocity is held constant while the particle remains in the eddy. There are two limits on the particle interaction time: the particle may be captured by the eddy and remain in the eddy for the lifetime of the eddy, or the particle may traverse the eddy before the eddy dies. Thus the interaction time is determined by taking a minimum of the two timescales.

These times are estimated by assuming that the characteristic size of a randomly sampled eddy is the dissipation length scale, l_e , given by

$$l_e = C_\mu^{0.75} \frac{k^{1.5}}{\epsilon} \quad (4.16)$$

where C_μ is equal to 0.09, k is the turbulent kinetic energy, and ϵ is the dissipation rate

of turbulence.

The eddy lifetime is given by

$$t_e = \frac{l_e}{\sqrt{\frac{2}{3}k}} \quad (4.17)$$

The transit time of a particle, derived in Appendix A.1, is found from the solution of the linearized form of the equation of motion of a particle in uniform flow

$$t_{tr} = -\tau_p \ln \left(1 - \frac{l_e}{\tau_p |\vec{u}_g - \vec{u}_p|} \right) \quad (4.18)$$

where $\vec{u}_g - \vec{u}_p$ is the relative velocity at the beginning of the interaction time and τ_p is the particle relaxation time introduced in Section 2.1.2. When $l_e > \tau_p |\vec{u}_g - \vec{u}_p|$, Equation (4.18) has no solution. In this case, the particle is captured by the eddy, and the interaction time is the eddy lifetime.

4.2.2 Lagrangian Tracking Implementation

Implementation of Lagrangian tracking in TASCflow involves the integration of particle paths through the discretized domain. Individual particles are tracked from their injection point until they escape the domain or some integration criterion has been met.

A distinction must be made between the particle interaction time and a sub-timestep that is employed for computational purposes. The particle interaction time is a physical timestep that is determined by taking the minimum of two timescales: the eddy lifetime and the particle transit time. The TASCflow CFD Code calculates a particle trajectory using computational sub-timesteps where a physical interaction time may be composed of many computational subimesteps.

Particle displacement is calculated using forward Euler integration of the particle velocity over the computational timestep, δt

$$x_i^n = x_i^o + \left. \frac{dx_i}{dt} \right|_o \delta t \quad (4.19)$$

where the superscripts n and o refers to the new and old values respectively, and the particle velocity is $u_{p,i} = dx_i/dt$. Note that using forward integration, the particle velocity is calculated at the start of the computational timestep and held constant over the computational timestep. At the end of the computational timestep, the new particle velocity is calculated using the analytical solution to the Equation (4.10). Note that for

the purpose of this investigation, gravity is the only body force acting on the particle.

$$u_p = u_g + (u_p^o - u_g) \exp\left(-\frac{\delta t}{\tau_p}\right) + g\tau_p \left(1 - \exp\left(-\frac{\delta t}{\tau_p}\right)\right) \quad (4.20)$$

where the subscripts p and g refer to the particle and gas-phase velocity respectively. u_p^o is the particle velocity at the start of the computational timestep, and τ_p is the particle relaxation time given by

$$\tau_p = \frac{\rho_p d_p^2}{18\mu} \quad (4.21)$$

where ρ_p is the particle density, d_p is the diameter of the particle, and μ is the fluid viscosity.

The actual calculation of particle trajectories is done using local grid coordinates. The use of local grid coordinates limits the progress of the particle to the flux element boundaries. Motivation for this limitation is two-fold: it is necessary to limit a particle to a single octant to accurately calculate its contribution to any mass, momentum and energy sources to a single control volume. This is required if the particle influences the fluid phase, a topic that is beyond the scope of this investigation. Secondly, this limitation allows the type of the adjoining element, such as a boundary element, to be checked before continuing with the track. The local fluid properties and fluid velocity are expressed in terms of the nodal values using shape functions, N_j . Shape functions and local grid coordinates are explained in detail in Section 4.3 of the TASCflow Theory Manual. (1995). As expected, the use of local grid coordinates does not affect particle tracking; particle velocity and position are returned to the user in Cartesian coordinates.

The computational timestep that may be taken by a particle is limited by one of three criteria:

1. The particle may not travel beyond an octant or flux element boundary in any timestep.
2. The particle may travel some user-specified fraction of the characteristic flux element length in any step. This allows the accuracy of the particle tracking integration to be separated from the grid resolution.
3. For a turbulent flow, the timestep may be limited by the lifetime of the eddy, given by Equation (4.17), or the time required by the particle to cross the eddy, the transit time given by Equation (4.18).

It is important to note that gas-phase velocity fluctuation remains constant during the physical timestep, the particle interaction time. A new velocity fluctuation is determined

if only if the cumulation of computational sub-timesteps is equal to the particle interaction time *or* if the particle interaction time is also the minimum computational timestep as outlined by the above criteria.

The implementation of these criteria is best explained by an example. For simplicity, consider tracking a single particle in 2-D as shown in Figure 4.4. A single particle enters the flux element at point 1 and moves to point 2 in a single step. The particle continues through the flux element where each movement from point to point is a single timestep. The time taken to travel from point 1 to point 2 and from point 4 to point 5 was limited either by criterion 2 or 3. Points 3, 4, and 6 are located on flux element or octant boundaries and in these case, the timestep was limited by criterion 1.

Figure 4.4: Example of a particle trajectory through a flux element

At point 6, the particle encounters a boundary and leaves the current flux element. At the boundary, a test is performed to determine the type of flux element the particle is about to enter. If the adjoining element is open to fluid flow, particle tracking continues. If the adjoining element is a boundary, one of two things may happen: (1) if the boundary is an inlet or an outlet, the particle escapes the domain; (2) if the boundary is a symmetry boundary or a wall, the particle is reflected.

4.2.3 Implementation of Particle Dispersion Models

TASCFLOW's Lagrangian particle tracking uses the SSF model of Shuen, Chen and Faeth (1983) described above. In addition to this model, four SSF models for particle dispersion are considered in this thesis. This section describes the implementation of these models in TASCFLOW.

The SSF models of Gosman and Ioannides (1983) and Lightstone and Raithby (1996) are similar to that of Shuen, Chen, and Faeth (1983). Analytical work by Lightstone and Raithby indicate an exponent of $C_\mu^{0.63}$ in the expression for the characteristic eddy length

$$l_e = C_\mu^{0.63} \frac{k^{1.5}}{\epsilon} \quad (4.22)$$

where C_μ is equal to 0.09, k is the turbulent kinetic energy, and ϵ is the dissipation rate of turbulence. The eddy lifetime is defined similar to Shuen, Chen, and Faeth given by

$$t_e = \frac{l_e}{\sqrt{\frac{2}{3}}k} \quad (4.23)$$

Thus, implementation of Lightstone and Raithby's model required that the exponent for C_μ was changed to 0.63.

Gosman and Ioannides model suggests that the exponent for C_μ is 0.5. The researchers also provide an alternative expression for the eddy lifetime. Implementation of the model of Gosman and Ioannides revealed ambiguity in the definition of eddy lifetime. This difficulty is discussed in greater detail in Section 6.3. It was found that using an eddy lifetime given by

$$t_e = \frac{l_e}{\sqrt{\frac{1}{3} \sum_{i=1}^3 v_{p,i}^2}} \quad (4.24)$$

produced results closest to those reported in the literature. Thus, the implementation of this model calculates the eddy lifetime using the fluctuating component of the turbulent gas-phase velocity at the beginning of the particle interaction time.

The model of Zhou and Leschziner, (1991a), modifies the conventional SSF model to introduce time-correlated gas-phase velocity fluctuations. The gas-phase velocity fluctuations are therefore expressed as

$$u'_t = R(\delta t)u'_{t-\delta t} + e_t \quad (4.25)$$

where u'_t is the gas-phase velocity fluctuation at the current time t , $R(\delta t)$ is the time

correlation which accounts for all effects arising from previous timesteps, $u'_{t-\delta t}$ is the velocity fluctuation from the previous timestep, and e_t represents all effects arising from randomness during the time interval δt . Note that the timestep δt is the *physical timestep* in the implementation of Zhou and Leschziner's model.

For any given δt , the expected value of e_t is zero and the variance is given by

$$\overline{e_t^2} = \overline{(u'_t - R(\delta t)u'_{t-\delta t})^2} = \overline{u_t'^2} - R^2(\delta t)\overline{u_{t-\delta t}'^2} \quad (4.26)$$

The time-correlation is approximated by the exponential function as suggested by Hinze (1975).

$$R(\delta t) = \exp\left(-\frac{\delta t}{\tau_{LI}}\right) \quad (4.27)$$

The Lagrangian integral timescale, τ_{LI} , used in Zhou and Leschziner's model is given by

$$\tau_{LI} = \beta t_e = \beta(C_\mu^{0.75} \frac{k^{1.5}}{\epsilon}) / (\frac{2}{3}k)^{0.5} \quad (4.28)$$

Here, β is based on analytical and experimental considerations. Zhou and Leschziner report the optimum value of β to be 0.8.

Implementation of Zhou and Leschziner's model requires a fixed timestep chosen *a priori*, denoted here as Δt . Calculation of e_t follows from Equation (4.26)

$$e_t = \Gamma \sqrt{\frac{2}{3}k_t - \exp\left(-\frac{2\Delta t}{\tau_{LI}}\right) \frac{2}{3}k_{t-\Delta t}} \quad (4.29)$$

where Γ is a random number selected from a Gaussian probability density function with a mean of zero and a standard deviation of unity. The subscript t refers to the current timestep, the subscript $t - \Delta t$ refers to the value at the previous timestep, and k is the turbulent kinetic energy.

Thus, the velocity fluctuation is given by

$$u'_t = \exp\left(-\frac{\Delta t}{\tau_{LI}}\right) u'_{t-\Delta t} + e_t \quad (4.30)$$

The new model introduced in Chapter 3 incorporates both a temporal and spatial autocorrelation in the definition of the fluctuating gas-phase velocity component. For simplicity, the autocorrelation is decomposed into temporal and spatial components to allow for independent estimation of each correlation function. The gas-phase velocity

fluctuation is therefore given by

$$u'_t = R_t(\delta t)R_x(\delta x)u'_{t-\delta t} + e_t \quad (4.31)$$

where u'_t is the gas-phase velocity fluctuation at the current time t , $R_t(\delta t)$ is the temporal autocorrelation, $R_x(\delta x)$ is the spatial autocorrelation, $u'_{t-\delta t}$ is the velocity fluctuation at the previous timestep, and e_t is a random component incorporating all effects due to randomness during the current timestep, δt . The spatial correlation can be related to the temporal correlation by approximating the distance a particle travels in a single timestep using the relationship $\delta x = u_{REL}\delta t$ where u_{REL} is the relative velocity of the particle at the beginning of the timestep. Similar to the implementation of Zhou and Leschziner's model, the timestep δt is the *physical timestep*.

For any given δt , the expected value of e_t is zero and the variance is given by

$$\overline{e_t^2} = \overline{(u'_t - R_t(\delta t)R_x(u_{REL}\delta t)u'_{t-\delta t})^2} = \overline{u_t'^2} - R_t^2(\delta t)R_x^2(u_{REL}\delta t)\overline{u_{t-\delta t}'^2} \quad (4.32)$$

Similar to Zhou and Leschziner's model, the temporal autocorrelation is approximated using the exponential function as suggested by Hinze (1975)

$$R_t(\delta t) = \exp\left(-\frac{\delta t}{\tau_{LI}}\right) \quad (4.33)$$

where τ_{LI} is the Lagrangian integral timescale given by

$$\tau_{LI} = 0.135 \frac{k}{\epsilon} \quad (4.34)$$

Here, the expression for τ_{LI} is based solely on analytical considerations. This expression follows from analytical work by Lightstone and Raithby (1996) repeated in Section 5.2.

The spatial autocorrelation is approximated by

$$R_x(u_{REL}\delta t) = \exp\left(-\frac{u_{REL}\delta t}{L_I}\right) \quad (4.35)$$

where $u_{REL} = |\vec{u}_g - \vec{u}_p|$, and L_I is the Lagrangian integral length scale given by

$$L_I = C_\mu^{0.63} \frac{k^{1.5}}{\epsilon} = 2\tau_{LI} \sqrt{\frac{2}{3}k} \quad (4.36)$$

This expression for L_I comes from the definition of the characteristic eddy length sug-

gested by the analysis of Lightstone and Raithby outlined in Section 5.2.

Implementation of the new model requires a fixed timestep denoted Δt . Calculation of e_t follows from Equation (4.32)

$$e_t = \Gamma \sqrt{\frac{2}{3}k_t - \exp\left(-2\left(\frac{\Delta t}{\tau_{LI}} + \frac{u_{REL}\Delta t}{L_I}\right)\right) \frac{2}{3}k_{t-\Delta t}} \quad (4.37)$$

where Γ is a random number selected from a Gaussian probability density function with a mean of zero and a standard deviation of unity. The subscript t refers to the current timestep, the subscript $t - \Delta t$ refers to the value at the previous timestep, and k is the turbulent kinetic energy.

Thus, the velocity fluctuation is given by

$$u'_t = \exp\left(-\left(\frac{\Delta t}{\tau_{LI}} + \frac{u_{REL}\Delta t}{L_I}\right)\right) u'_{t-\Delta t} + e_t \quad (4.38)$$

4.3 Summary

This chapter began with a description of the numerical methods used to obtain a solution of the fluid flow equations. The time-averaged form of the governing equations was presented and then integrated over a fixed control volume. Discretization of the integrated form of the equations was outlined with attention to the treatment of boundary conditions. The numerical solution procedure of the governing equations was briefly discussed.

The numerical solution of the particle equation of motion began with a review of the theoretical basis for Lagrangian particle tracking. Integration of the particle equation of motion was outlined and the calculation of particle trajectories was discussed. This section concluded with an outline of the implementation of various particle dispersion models considered in this thesis.

Chapter 5

An Extension of Taylor's Analysis

This chapter extends the analysis of Lightstone and Raithby (1996) to each model introduced in Section 2.3.2. Taylor's result (1921) for fluid particles at long times is reviewed and analysis is performed on each model to determine if each model can reproduce Taylor's result.

5.1 A Review of Taylor's Result

Taylor derived an analytical expression for the dispersion of dyed fluid particles released from a point source in homogeneous, isotropic turbulent flow. The variance of fluid particle position is given by

$$\frac{d\overline{y^2}}{dt} = 2\overline{v'^2} \int_0^t R(\xi) d\xi \quad (5.1)$$

where y is the fluid particle position, v' is the fluctuating velocity, and $R(\xi)$ is a Lagrangian time correlation given by

$$R(\xi) = \frac{\overline{v'(t)v'(\xi)}}{\overline{v'^2}} \quad (5.2)$$

The full derivation of Taylor's result is given in Section 2.2.

At long times, the integral in Equation (5.1) goes to a constant yielding

$$\overline{y^2} = 2\overline{v'^2}\tau_{LI}t \quad \text{for very long times} \quad (5.3)$$

where τ_{LI} is the Lagrangian integral timescale.

5.2 The Analysis of Lightstone and Raithby, 1996

Lightstone and Raithby develop an expression for the eddy lifetime, t_e , used in the SSF model by relating the variance of particle position to Taylor's result for fluid particles. Their analysis is repeated here.

Consider a particle undergoing a random walk in a uniform flow of homogeneous, isotropic turbulence. For a particle initially at $y = 0$ undergoing discrete steps, the y -position of the particle after N steps, $y_{p,N}$, is given by

$$y_{p,N} = \sum_{i=1}^N \Delta y_{p,i} = \sum_{i=1}^N v_{p,i} \Delta t_i \quad (5.4)$$

where $\Delta y_{p,i}$ is the size of the i th step, $v_{p,i}$ is the velocity of the particle, and Δt_i is the timestep. An equation for the variance of the particle position can be found by squaring both sides of Equation (5.4) and taking the expected value

$$\overline{y_{p,N}^2} = \overline{\left(\sum_{i=1}^N v_{p,i} \Delta t_i \right)^2} \quad (5.5)$$

Equation(5.5) can be simplified by making a number of assumptions. Assumption 1 follows from the analytical solution for homogeneous isotropic turbulence.

$$\text{Assumption \#1: } \frac{k^2}{\epsilon} = \text{constant} \quad (5.6)$$

$$\text{Assumption \#2: } \overline{v_{p,i} v_{p,j}} = 0 \quad \text{for } i \neq j \quad (5.7)$$

This assumes that Δt is sufficiently large so that particle velocity calculations at different steps are uncorrelated.

Simplify the timestep by allowing $\Delta t_i = \Delta t$ and consider fluid particles where $\overline{v_{p,i}^2} = \overline{v_{g,i}^2}$. Using the above assumptions and noting that $t = N\Delta t$, Equation (5.5) simplifies to

$$\overline{y_p^2} = (\Delta t \overline{v_{g,i}^2}) t \quad (5.8)$$

For fluid particles, Taylor showed (see Section 2.2) that

$$\overline{y_p^2} = (2\tau_{LI} \overline{v_g^2}) t \quad (5.9)$$

where τ_{LI} is the Lagrangian integral timescale.

Comparing Equations (5.8) and (5.9) yields the equality $\Delta t = 2\tau_{LI}$. An expression for τ_{LI} remains to be derived. This is done by considering the definition of the turbulent viscosity, ν_t , in terms of the rate of spread of fluid particles for a turbulent Schmidt number of unity (Csanady (1963))

$$\nu_t = \frac{1}{2} \frac{d\overline{y^2}}{dt} \quad (5.10)$$

Using the standard expression for the $k - \epsilon$ turbulence model (Launder and Spalding (1974))

$$\nu_t = C_\mu \frac{k^2}{\epsilon} \quad \text{with } C_\mu = 0.09 \quad (5.11)$$

with Equation (5.9) and the assumption of homogeneous, isotropic turbulence leads to an expression for τ_{LI}

$$\tau_{LI} = \frac{3}{2} C_\mu \frac{k}{\epsilon} = 0.135 \frac{k}{\epsilon} \quad (5.12)$$

Now consider modeling a fluid particle using the approach outlined by Shuen, Chen and Faeth (1982). A fluid particle experiences no relative velocity and, therefore, the particle interaction time is always the eddy lifetime. Thus, using Equation (5.9), $\Delta t = t_e$ and the result is

$$t_e = 2\tau_{LI} = 0.27 \frac{k}{\epsilon} \quad (5.13)$$

Combining Equation (5.13) with the expression for eddy lifetime seen in Equation (2.51) and the characteristic eddy size seen in Equation (2.48) yields an expression for the eddy lifetime.

$$t_e = C_\mu^\alpha \frac{k^{1.5}/\epsilon}{\sqrt{2k/3}} = C_\mu^\alpha \sqrt{\frac{3}{2}} \frac{k}{\epsilon} = 0.27 \frac{k}{\epsilon} \quad (5.14)$$

A value of $\alpha = 0.63$ for the exponent of C_μ is indicated.

Using the constant derived by Lightstone and Raithby yields a model capable of exactly reproducing Taylor's result for fluid particles at long times where $\overline{v_{p,i}^2} = \overline{v_{g,i}^2}$. The dissipation at long times is given by

$$\overline{y_p^2} = 2\nu_t t \quad (5.15)$$

5.3 The Model of Gosman and Ioannides, 1983

The model of Gosman and Ioannides (1983) introduced in Section 2.3.2 is evaluated for the problem of fluid particles released into a uniform flow of homogeneous, isotropic

turbulence. The analysis of Lightstone and Raithby repeated in Section 5.2 leads to Equation (5.8) shown here for completeness

$$\overline{y_p^2} = (\Delta t \overline{v_{g,i}^2})t \quad (5.16)$$

Recall that with SSF models, the timestep Δt is taken to be the minimum of the particle transit time and the eddy lifetime. For the case of fluid particles, a particle is captured by an eddy and remains in that eddy for the entire eddy lifetime. Thus, the physical interaction time is dominated by the eddy lifetime yielding $\Delta t = t_e$. It is important to note that the analysis leading to Equation (5.16) assumes that the timestep is deterministic.

Implementation of the model of Gosman and Ioannides revealed ambiguity in the definition of eddy lifetime. This difficulty is discussed in greater detail in Section 6.3. It was found that using an eddy lifetime given by

$$t_e = \frac{l_e}{\sqrt{\frac{1}{3} \sum_{i=1}^3 v_{p,i}^2}} \quad (5.17)$$

produced results closest to those reported in the literature. Substituting the expression for characteristic eddy length given by Equation (2.48) into Equation (5.17) yields

$$t_e = \sqrt{3C_\mu} \frac{k^{1.5}/\epsilon}{\sqrt{\sum_{i=1}^3 v_{p,i}^2}} \quad (5.18)$$

Consider fluid particles where $\overline{v_{p,i}^2} = \overline{v_{g,i}^2}$. Substitute the expression for eddy lifetime in Equation (5.18) into our initial expression for dispersion in Equation (5.16).

$$\overline{y_p^2} = \left(\sqrt{3C_\mu} \frac{k^{1.5}}{\epsilon} \frac{\overline{v_{g,i}^2}}{\sqrt{\sum_{i=1}^3 v_{g,i}^2}} \right) t \quad (5.19)$$

Note that the analysis of Lightstone and Raithby is not strictly employed; the definition of the eddy lifetime includes the random fluctuations of the gas-phase turbulence. Thus, the timestep, t_e is a random variable and this analysis is an approximation to the performance of the model.

Recognizing that timestep is not deterministic, the gas-phase fluctuations must be

approximated. Assuming

$$\sqrt{\sum_{i=1}^3 v_{g,i}^2} = \sqrt{\sum_{i=1}^3 \overline{v_{g,i}^2}} = \sqrt{2k} \quad (5.20)$$

Substituting Equation (5.20) into Equation (5.19) yields

$$\overline{y_p^2} = \left(\sqrt{\frac{2}{C_\mu}} \frac{k^2}{\epsilon} \right) t = 2.72 \nu_t t \quad (5.21)$$

This analysis shows that the model of Gosman and Ioannides cannot reproduce Taylor's result and overpredicts the long time dispersion of dyed fluid particles in homogeneous isotropic turbulence by just over 35%.

5.4 The Model of Shuen, Chen and Faeth, 1983

The analysis of Lightstone and Raithby is extended to compare the model of Shuen, Chen and Faeth (1983) introduced in Section 2.3.2 to Taylor's result.

Returning to fluid particles released into a uniform turbulent flow, the analysis of Lightstone and Raithby leads to an expression for the dissipation

$$\overline{y_p^2} = (\Delta t \overline{v_{g,i}^2}) t \quad (5.22)$$

Here, the physical interaction time is dominated by the eddy lifetime so $\Delta t = t_e$.

Shuen, Chen and Faeth use an expression for eddy lifetime given by

$$t_e = \frac{l_e}{\sqrt{2k/3}} = C_\mu^{.75} \frac{k^{1.5}/\epsilon}{\sqrt{2k/3}} = C_\mu^{.75} \sqrt{\frac{3}{2}} \frac{k}{\epsilon} \quad (5.23)$$

Substituting this expression into Equation (5.22) and, recognizing $\overline{u_{g,i}^2} = 2k/3$ for isotropic turbulence, yields

$$\overline{y_p^2} = C_\mu^{0.75} \sqrt{\frac{2}{3}} \frac{k^2}{\epsilon} t = 1.49 \nu_t t \quad (5.24)$$

This analysis shows that Shuen, Chen and Faeth's model underpredicts the long time dispersion of dyed fluid particles in homogeneous isotropic turbulence by just over 25%.

5.5 The Model of Zhou and Leschziner, 1991a

Zhou and Leschziner's model (1991a) presented in Section 2.3.2 modifies the conventional stochastic dispersion model to introduce time-correlated gas-phase velocity fluctuations. Considering particles undergoing a random walk in homogeneous isotropic turbulence, the analysis of Lightstone and Raithby repeated in Section 5.2 leads to Equation (5.8) shown here for completeness

$$\overline{y_p^2} = (\Delta t \overline{v_{g,i}^2}) t \quad (5.25)$$

In general, conventional SSF models hold the gas-phase velocity fluctuation constant over the particle/eddy interaction time. Zhou and Leschziner's model circumvents this assumption by defining a gas-phase velocity fluctuation that can be determined with greater frequency. The velocity fluctuations in the Zhou and Leschziner model are therefore expressed as

$$v'_t = R(\delta t) v'_{t-\delta t} + e_t \quad (5.26)$$

where $R(\delta t)$ is a Lagrangian time correlation, $v'_{t-\delta t}$ is the gas-phase velocity fluctuation at the previous timestep, and e_t represents all effects arising from randomness during the time interval δt . It is important to note that δt is much smaller than the particle interaction time used by conventional stochastic dispersion models.

At long times, the time correlation in Equation (5.26) goes to zero. Using the expression for e_t presented in Section 2.3.2, Equation (5.26) is

$$v'_t = e_t \quad (5.27)$$

hence

$$\overline{v_t'^2} = \overline{e_t^2} = \sqrt{\frac{2}{3}k} \quad (5.28)$$

for isotropic turbulence

Substituting the expression for the turbulent gas-phase velocity fluctuation given in Equation (5.27) into Equation (5.25) yields

$$\overline{y_p^2} = \left(\frac{2}{3} k \Delta t \right) t \quad (5.29)$$

Taylor showed that for long times $\Delta t = 2\tau_{LI}$, where τ_{LI} is the Lagrangian integral

timescale. Zhou and Leschziner define the Lagrangian integral timescale as

$$\tau_{LI} = \beta t_e = \beta C_\mu^{0.75} \left(\sqrt{\frac{3}{2}} \right) \left(\frac{k}{\epsilon} \right) \quad (5.30)$$

where t_e is the expression for the eddy lifetime given by Shuen, Chen and Faeth (1983). Here, β is based on analytical and experimental considerations. Zhou and Leschziner report the optimum value of β to be 0.8. Using Taylor's result and substituting the Zhou and Leschziner's expression for the Lagrangian integral timescale in Equation (5.30) into Equation (5.29) yields

$$\overline{y_p^2} = 2\beta C_\mu^{0.75} \left(\sqrt{\frac{2}{3}} \right) \frac{k^2}{\epsilon} t = 2.39\nu_t t \quad (5.31)$$

This analysis shows that Zhou and Leschziner's model cannot reproduce Taylor's result and overpredicts the dispersion of dyed fluid particles in homogeneous isotropic turbulence by almost 20%.

5.6 Summary

The analysis of Lightstone and Raithby (1996) has been extended to each model introduced in Section 2.3.2. A summary of the results is provided in the following table

Table 5.1: Summary: An Extension of Taylor's Analysis

Model	l_e	Δt	$\overline{y_p^2}^a$
Taylor	-	$2\tau_{LI}$	$2.0\nu_t t$
Lightstone & Raithby	$C_\mu^{0.63} \frac{k^{1.5}}{\epsilon}$	$\frac{l_e}{\sqrt{(\frac{2}{3}k)}}$	$2.0\nu_t t$
Gosman & Ioannides	$C_\mu^{0.5} \frac{k^{1.5}}{\epsilon}$	$\frac{l_e}{\sqrt{\frac{1}{3} \sum_{i=1}^3 u_{p,i}^2}}$	$2.72\nu_t t$
Shuen, Chen & Faeth	$C_\mu^{0.75} \frac{k^{1.5}}{\epsilon}$	$\frac{l_e}{\sqrt{(\frac{2}{3}k)}}$	$1.49\nu_t t$
Zhou & Leschziner	-	$0.8 \frac{l_e}{\sqrt{(\frac{2}{3}k)}}$	$2.39\nu_t t$
Hennick & Lightstone ^b	-	$0.27 \frac{k}{\epsilon}$	$2.0\nu_t t$

^a for fluid particles in homogeneous isotropic turbulence

^b analysis is included in Chapter 3

In summary, the SSF models of Gosman and Ioannides, Shuen, Chen and Faeth, and Zhou and Leschziner are not capable of reproducing Taylor's result. Gosman and Ioannides model overpredict the dispersion of fluid particles by just over 35%; Shuen, Chen and Faeth's model underpredicts by just over 25%; Zhou and Leschziner's model overpredicts the dispersion of fluid particles by almost 20%.

Lightstone and Raithby select a constant used in the SSF model formulation to maintain consistency with Taylor's result. The model of Hennick and Lightstone, introduced in Chapter 3 employs a Lagrangian integral timescale, τ_{LI} , indicated by the analysis of Lightstone and Raithby. Thus the model of Hennick and Lightstone exactly reproduces Taylor's result for the long time dispersion of dyed fluid particles released in homogeneous isotropic turbulence.

Chapter 6

The Experiment of Snyder and Lumley, 1971

The Stochastic Separated Flow (SSF) models described in Chapter 2 were evaluated by comparing model predictions to the experimental results of Snyder and Lumley (1971). These experiments considered the motion of single particles released from a point source into a uniform flow of grid-generated turbulence. The experiment was simulated using the TASCflow CFD code. Measurements of particle dispersion and velocity decay were compared to results generated by each model considered in this thesis.

This chapter presents the experiment of Snyder and Lumley. The design of the experiment is outlined and the numerical simulation described. The predictions of each model are presented. Results are discussed in detail.

6.1 The Design of the Experiment

In the experiment of Snyder and Lumley, single particles were released from a point source into a uniform flow of grid-generated turbulence. Figure 6.1 shows a diagram of Snyder and Lumley's experiment. The turbulence was generated using a grid with 2.54 cm spacing. Turbulence quantities were analyzed and the turbulence was shown to be homogeneous in planes parallel to the grid. Particles were injected individually at 20 grid spacings from the grid and with a mean velocity equal to that of the gas-phase. It was found that the turbulence quantities were unaffected by the particle injector downstream of $x/M = 41$ and that the turbulence was also unaffected by the presence of particles.

Single particles were tracked photographically from $x/M = 68$ to 168 allowing 48 mesh lengths to ensure that particle velocities were independent of the injected velocity.

Figure 6.1: Snyder and Lumley's grid turbulence experiment

Particle trajectories were photographed at ten locations, progressively farther apart. Photographs were digitized and particle velocity and displacement determined. Statistically significant results were obtained by tracking about 700 particles for each experiment.

Snyder and Lumley considered four particles types: hollow glass beads, solid glass beads, corn pollen, and copper beads. Details of the particles are given in Table 6.1. The particle relaxation time of the hollow glass beads was small allowing the particle to essentially follow the turbulent gas; the hollow glass beads therefore acted like 'fluid' or 'tracer' particles. Corn pollen had more inertia and therefore did not follow the turbulence exactly. The solid glass beads and the copper particles were the heaviest with similar relaxation times. Since the behaviour of the solid glass beads was nearly identical to the copper beads, the experiments involving the former were not considered and will not be included in further discussion.

Table 6.1: Particles and relevant parameters used in Snyder and Lumley's experiment

Particle Type	Diameter [μm]	Density [kg/m^3]	Time Constant [ms]	Reynolds Number*
hollow glass	46.5	260	1.7	0.05
corn pollen	87.0	1000	20.0	1.10
solid glass	87.0	2500	45.0	2.48
copper bead	46.5	8900	49.0	1.45

* based on mean relative velocity and particle diameter

6.2 Numerical Simulation

A simulation of Snyder and Lumley's experiment was performed using the TASCflow CFD code. In the experiment, turbulent quantities were reported from 41 mesh lengths and particles were injected at 20 mesh lengths. Since the particles were given almost 50 mesh lengths to fully develop an independent velocity from the injection velocity, the simulation required that particles were released as far upstream from the first camera as possible. However, it was also necessary to obtain the best possible fit to Snyder and Lumley's energy decay curves that are based on measured values 41 grid spacings from the inlet. Values of k and ϵ to be used at the inlet of the computational domain were calculated using the analytical solution for grid generated turbulence in conjunction with measured turbulent quantities further downstream at $x/M = 41$. The best placement of the inlet was determined to be $x/M = 30$.

The duct was simulated using rectangular control volumes. Nodes were spaced evenly throughout the domain with 100 nodes along the x-axis, and 25 nodes along the y- and z-axes. A symmetry boundary condition was employed at the wall to ensure that wall drag did not affect the particles. The numerical solution technique for the flow field is described in Section 4.1. Values for k and ϵ along the centerline were compared to Snyder and Lumley's energy decay curves and to the analytical solution for grid generated turbulence shown in Figures 6.2 and 6.3 respectively. Turbulent kinetic energy is well predicted at low x/M values, but both the analytical solution and reported values from Snyder and Lumley are underpredicted for high x/M . Dissipation is well predicted for all x/M values.

The procedure followed was to first determine the flow field solution: since the particles do not affect the flow field, the release of particles is essentially post-processing. Section 4.2 describes the numerical solution of the particle equation of motion. Single particles were released from a point at the inlet at their terminal velocity. The trajectory of each particle was recorded and written to a file. A single particle trajectory was verified for each model by comparing particle velocity and displacement to the analytical solution to the linearized particle equation of motion. The trajectories of 780 particles were recorded for each particle type for each model. The number of particle trajectories was doubled and produced identical results indicating statistical significance. Particle dispersion and velocity decay were determined by filtering the data and finding the variance of the quantities in question. The details of this process are available in Appendix B.

Figure 6.2: Turbulent kinetic energy along the centerline

6.3 The Model of Gosman and Ioannides, 1983

Figure 6.4 presents the particle dispersion of each particle type with respect to time using the model of Gosman and Ioannides (1983). Implementation of the model revealed ambiguity in the definition of the eddy lifetime. It was found that using an eddy lifetime described by Equation (6.1) produced results closest to those reported by the researchers as seen in Figure 6.5.

$$t_e = \frac{l_e}{\sqrt{\frac{u'^2 + v'^2 + w'^2}{3}}} \quad (6.1)$$

where the characteristic eddy length, l_e is given by

$$l_e = C_\mu^{0.5} \frac{k^{1.5}}{\epsilon} \quad (6.2)$$

where C_μ is equal to 0.09, k is the turbulent kinetic energy, and ϵ is the dissipation rate of turbulence.

It was not possible to exactly reproduce Gosman and Ioannides computed results for this flow. Researchers Shuen, Chen, and Faeth (1983), and Chen and Crowe (1984) reported the same difficulty. The reader is invited to compare the results of this work as seen in Figure 6.4 with the reported results of Gosman and Ioannides presented in Figure 6.5.

The model of Gosman and Ioannides underpredicts the dispersion of the hollow glass

Figure 6.3: Dissipation along the centerline

beads by 9%, overpredicts the dispersion of the copper beads by 2% and overpredicts the dispersion of the corn pollen by 4%. All reported errors are calculated using a root mean square method.

The underprediction of the hollow glass beads differs from the result obtained in Section 5.3 due to approximations used in the analysis. Section 5.3 extends the analysis of Taylor to the model of Gosman and Ioannides by considering the dispersion of dyed fluid particles from a point source in homogeneous isotropic turbulence. The model of Gosman and Ioannides is shown to overpredict fluid particle dispersion by just over 35%. The analysis assumes that the timestep for dyed fluid particles at long times is a deterministic quantity. Since dyed fluid particles follow the gas-phase turbulence exactly, the particles are captured by the eddies and the timestep is the eddy lifetime, t_e , given in Equation (6.1). The eddy lifetime incorporates the fluctuating gas-phase velocity which is a random variable and thus the timestep is not deterministic. Recognizing that the timestep is not deterministic, the gas-phase fluctuations are approximated by

$$\sqrt{\sum_{i=1}^3 v_{g,i}^2} = \sqrt{\sum_{i=1}^3 \overline{v_{g,i}^2}} = \sqrt{2k} \quad (6.3)$$

Further discussion of these assumptions is provided with the analysis in Section 5.3.

Figure 6.6 presents the particle velocity decay results of each particle type with respect to time using the model of Gosman and Ioannides. Note that Snyder and Lumley's reported results for the velocity decay of hollow glass beads is not included in Figure 6.6.

Figure 6.4: Predictions of Snyder and Lumley's experimental data for particle dispersion using the model of Gosman and Ioannides (1983)

Due to the low sampling rate of the experiment, Snyder and Lumley estimate that “as much as 40% of the energy of the hollow glass beads could have been lost....” (Snyder and Lumley (1973)). As a result, the hollow glass beads exhibit a lower velocity decay than the turbulent gas-phase though it is expected that “the hollow glass beads would follow even the highest frequency fluctuations of the turbulence,” (Snyder and Lumley (1973)). Thus, the velocity decay of the hollow glass beads is underpredicted by Gosman and Ioannides model as it does not follow the velocity decay of the turbulent gas-phase. The velocity decay of the corn pollen particles is overpredicted while the prediction of the copper beads is adequate.

The predicted dispersion of the corn pollen compared to the predicted dispersion of the hollow glass beads is interesting. From Figure 6.4 it is seen that the dispersion of the corn pollen is very close to that of the hollow glass beads. This can be explained as follows: since the hollow glass beads essentially follow the turbulent gas-phase, the particle interaction time for the hollow glass beads is dominated by the lifetime of the eddy as given in Equation (6.1). The hollow glass beads are considered to be captured by the eddies and follow the gas-phase turbulent fluctuations while traveling along the duct. The corn pollen particles are slightly heavier and therefore have a greater particle relaxation time; examination of the interaction time of the corn pollen revealed that the particle interaction time is dominated by the transit time of the particle for the initial physical timestep and then dominated by the eddy lifetime until the particle exits the

Figure 6.5: Gosman and Ioannides (1983) reported results for particle dispersion.

duct. Thus the corn pollen particles remain in the first eddy for the duration of the transit time and are then captured by the subsequent eddies similar to the hollow glass beads. This explains why the predicted dispersion of the corn pollen is so close to the hollow glass beads. The difference between the predictions is due to the increased particle relaxation time of the corn pollen particles. The greater particle relaxation time indicates that the corn pollen has more inertia than the hollow glass beads and therefore a reduced response to the turbulence.

Figure 6.5 shows Gosman and Ioannides reported dispersion results. While it was not possible to reproduce Gosman and Ioannides reported results for this flow, note that the dispersion of the corn pollen particles is very close to that of the hollow glass beads.

6.4 The Model of Shuen, Chen, and Faeth, 1983

The model of Shuen, Chen, and Faeth (1983) is a variation on the model of Gosman and Ioannides. Since the turbulent kinetic energy is related to the fluctuating turbulent velocity component, Shuen, Chen, and Faeth defined the eddy lifetime as

$$t_e = \frac{l_e}{\sqrt{\frac{2}{3}k}} \quad (6.4)$$

Figure 6.6: Predictions of Snyder and Lumley's experimental data for particle velocity decay using the model of Gosman and Ioannides (1983)

where l_e is the characteristic eddy length, and k is the turbulent kinetic energy. A key difference between the models of Shuen, Chen and Faeth and Gosman and Ioannides (1983) is the definition of the eddy lifetime. Gosman and Ioannides incorporate the fluctuation of the turbulent gas-phase velocity into the eddy lifetime, and thus, the eddy lifetime is a random variable. In contrast, Shuen, Chen and Faeth approximate the gas-phase velocity fluctuations using the turbulent kinetic energy. Thus the eddy lifetime defined in Equation (6.4) is a deterministic quantity. Shuen, Chen and Faeth use a characteristic eddy length that is defined similarly to that of Gosman and Ioannides but a different exponent is used, that is $C_\mu^{0.75}$.

Predicted results for particle dispersion using Shuen, Chen, and Faeth's model are shown in Figures 6.7. The model underpredicts the dispersion for all three particle types: hollow glass is underpredicted by 19%, corn pollen by 3%, copper beads by 19%. Note that the predicted dispersion of the corn pollen is close to the predicted dispersion of the hollow glass beads. The dispersion of the hollow glass beads exhibits the same trend as the result obtained by extending Taylor's analysis in Section 5.4 which showed that the model underpredicts the dispersion of dyed fluid particles in homogeneous, isotropic turbulence by just over 25%. Note that Figure 6.7 shows the prediction of the hollow glass particles as a 'wavy' line. This result is explained in Section 6.5.

Predicted dispersion results for all particle types do not agree with those reported in the literature. The computed results underpredict the reported results by as much as 20%

Figure 6.7: Predictions of Snyder and Lumley's experimental data for particle dispersion using the model of Shuen, Chen and Faeth (1983)

for the case of the hollow glass particles. However, it can be shown, using analysis similar to that of Lightstone and Raithby (1996) that these results are a correct implementation of the model for the case of hollow glass particles. This analysis is given below.

Consider a particle undergoing a random walk in a uniform flow of homogeneous, isotropic turbulence. For a particle initially at $y = 0$ undergoing discrete steps, the y -position of the particle after N steps, $y_{p,N}$, is given by

$$y_{p,N} = \sum_{i=1}^N \Delta y_{p,i} = \sum_{i=1}^N v_{p,i} \Delta t_i \quad (6.5)$$

where $\Delta y_{p,i}$ is the size of the i th step, $v_{p,i}$ is the velocity of the particle, and Δt_i is the timestep. An equation for the variance of the particle position can be found by squaring both sides of Equation (6.5) and taking the expected value

$$\overline{y_{p,N}^2} = \overline{\left(\sum_{i=1}^N v_{p,i} \Delta t_i \right)^2} \quad (6.6)$$

Equation (6.6) can be simplified by allowing $\Delta t_i = \Delta t$ where Δt is large enough that $\overline{v_{p,i} v_{p,j}} = 0$ for $i \neq j$. Consider fluid particles where $\overline{v_{p,i}^2} = \overline{v_{g,i}^2}$, and noting that $t = N \Delta t$. Equation (6.6) simplifies to

$$\overline{y_p^2} = (\Delta t \overline{v_g^2}) t \quad (6.7)$$

Now consider modeling a fluid particle using the approach outlined by Shuen, Chen, and Faeth. A fluid particle experiences no relative velocity and, therefore, the particle interaction time is always the eddy lifetime. Substituting the eddy lifetime given by Equation (6.4) into Equation (6.7) and, recognizing $\overline{v_{g,i}^2} = 2k/3$ for isotropic turbulence, yields

$$\overline{y_p^2} = C_\mu^{0.75} \sqrt{\frac{2}{3}} \frac{k^2}{\epsilon} t \quad (6.8)$$

The assumption

$$\frac{k^2}{\epsilon} = \text{constant} \quad (6.9)$$

follows from the analytical solution for grid-generated turbulence. Combining this assumption with Equation (6.8), the result is an equation for the line describing the dispersion of a fluid particle in homogeneous, isotropic turbulence. Values for k^2/ϵ were determined at four axial locations and the mean value was used to calculate the slope. Figure 6.8 shows the analytical solution given by Equation (6.8) plotted with the hollow glass dispersion curve computed using Shuen, Chen and Faeth's model, and a linear regression of the hollow glass prediction. The predicted dispersion of the hollow glass particles is seen, quantitatively, to have the same slope determined by Equation (6.8). This result provides confidence in the correct implementation of the model of Shuen, Chen, and Faeth. As mentioned in Section 6.2, a single particle trajectory was verified for this model; predictions for particle velocity and displacement were compared to the analytical solution for both physical and computational timesteps.

Predictions for particle velocity decay using the model of Shuen, Chen and Faeth are given in Figure 6.9 for all particle types. The velocity variance of the hollow glass beads is interesting; while the predictions follow the decay of the turbulent gas-phase as expected, the velocity variance exhibits distinct dips in the curve. This result is explained in detail in Section 6.5. Predictions for both the corn pollen and the copper beads are nearly straight lines and do not exhibit the trend of the experimental data. The velocity variance of the corn pollen is overpredicted and the variance of the copper beads is underpredicted.

6.5 The Model of Lightstone and Raithby, 1996

The model of Lightstone and Raithby is a variation on the models of Gosman and Ioannides and Shuen, Chen, and Faeth. Similar to Shuen et al. the eddy lifetime is given

Figure 6.8: Using the slope to show the correct implementation of the model of Shuen, Chen, and Faeth (1983)

by

$$t_e = \frac{l_e}{\sqrt{\frac{2}{3}k}} \quad (6.10)$$

where l_e is the characteristic eddy length, and k is the turbulent kinetic energy. The eddy length is described similar to Gosman and Ioannides but a different exponent is determined based on analytical considerations, that is $C_\mu^{0.63}$. Thus, the eddy length is

$$l_e = C_\mu^{0.63} \frac{k^{1.5}}{\epsilon} \quad (6.11)$$

where C_μ is equal to 0.09, k is the turbulent kinetic energy, and ϵ is the dissipation rate of turbulence.

Figure 6.10 and Figure 6.11 presents the particle dispersion and velocity decay of each particle type with respect to time using a conventional SSF model with constants suggested by Lightstone and Raithby (1996). The dispersion of the corn pollen is over-predicted by 4% and the dispersion of the copper beads is underpredicted by 0.5%. The dispersion of the hollow glass particles is more difficult to generalize; dispersion is over-predicted until 0.25 s and underpredicted beyond that time; root mean square error is 11%. It is interesting to note that the model of Lightstone and Raithby does not predict the dispersion of the hollow glass beads most accurately of all the conventional SSF models considered in this thesis. The model of Gosman and Ioannides underpredicts the

Figure 6.9: Predictions of Snyder and Lumley's experimental data for particle velocity decay using the model of Shuen, Chen and Faeth (1983)

dispersion of the hollow glass beads with an rms error of 9%, a result that differs from the result obtained in Section 5.3. As discussed in Section 6.3 above, the discrepancy is due to key assumptions made in applying Taylor's analysis to the model of Gosman and Ioannides.

Note that the prediction of the hollow glass particles is shown as a 'wavy' line: a similar trend is observed in the predicted dispersion of the hollow glass beads using the model of Shuen, Chen and Faeth shown in Figure 6.7. This can be accounted for as follows: a particle is injected into the flow where it enters a discrete eddy and sees an instantaneous turbulent velocity that is held constant for the lifetime of the eddy. The particle is captured by the eddy and quickly approaches the instantaneous velocity of the turbulence. When the eddy dies the particle enters a new eddy whose lifetime is determined once again by the turbulent kinetic energy and dissipation at the current axial position of the particle. When considering the statistics of many particles, it is seen that each particle will enter a new eddy at roughly the same axial position, corresponding to the valleys of the dispersion curve. The corn and copper particles do not exhibit this behaviour since the interaction time of each particle is not dominated by the eddy lifetime; the interaction time of the corn particle is distributed between the eddy lifetime and the transit time while the copper particle is dominated by the transit time.

The velocity decay of the hollow glass particles shown in Figure 6.11 displays even more prominent dips and is consistent with the prediction of the particle dispersion.

Figure 6.10: Predictions of Snyder and Lumley's experimental data for particle dispersion using the model of Lightstone and Raithby (1996)

This behaviour can be explained by considering the analytical solution to the equation of motion for Stokes flow. Consider the particle equation of motion for the y -direction. Note that the subscript p , indicating the particle velocity, is dropped for simplicity.

$$\frac{dv}{dt} = \frac{1}{\tau_p}(v_g - v) \quad (6.12)$$

Solving Equation (6.12) with initial condition $v(0) = v_o$ and $t \in [0, t_{int}]$, squaring the result and time averaging with $\overline{v_g v_o} = 0$ yields

$$\overline{v^2(t)} = \overline{v_g^2} - 2\overline{v_g^2}e^{\frac{-t}{\tau_p}} + (\overline{v_o^2} + \overline{v_g^2})e^{\frac{-2t}{\tau_p}} \quad (6.13)$$

Figure 6.12 was created using the analytical solution given in Equation (6.13). This curve was generated by setting $\overline{v_o^2} = 0.22$, $\overline{v_g^2} = 0.18$, and $\tau_p = 1.7 \times 10^{-3}$. This analytical result provides confidence in the predictions shown in Figure 6.11.

The waviness of the hollow glass curves shown in Figures 6.7 to 6.11 arise from the treatment of the turbulence as discrete eddies where the instantaneous gas-phase velocity is held constant for the duration of the particle interaction time. These 'waves' are an inherent flaw in an approach where the eddy lifetime and characteristic eddy size are essentially deterministic. These results provide motivation for an alternate method of describing the gas-phase turbulence.

Figure 6.11: Predictions of Snyder and Lumley's experimental data for particle velocity decay using the model of Lightstone and Raithby (1996)

6.6 The Model of Zhou and Leschziner, 1991a

The model of Zhou and Leschziner incorporates a time correlation in the definition of the gas-phase velocity fluctuation. The random fluctuation is described by

$$u'_t = R(\delta t)u'_{t-\delta t} + e_t \quad (6.14)$$

where $R(\delta t)$ is a Lagrangian time correlation, $u'_{t-\delta t}$ is the gas-phase velocity fluctuation at the previous timestep, and e_t represents all effects arising from randomness during the time interval δt . Using this description of the gas-phase velocity fluctuation, a particle may see more than one velocity fluctuation within an eddy depending on the selection of δt .

Zhou and Leschziner's model (1991a) was implemented using two different timesteps. $\delta t = 0.005$ and 0.01 s. These timesteps are between five and ten times smaller than a characteristic particle interaction time using the SSF model of Shuen, Chen, and Faeth. Predicted results for dispersion and velocity decay of the particles for the case of $\delta t = 0.005$ s are shown in Figures 6.13 and 6.14 respectively. For the case of $\delta t = 0.01$ s, predicted results for particle dispersion and velocity decay are shown in Figures 6.15 and 6.16 respectively.

For each timestep considered, the hollow glass particles, corn pollen, and copper particles are predicted to have roughly the same dispersion. The result can be explained

Figure 6.12: Velocity decay within an eddy predicted by theory

as follows. Consider a particle and a fluid point both originating at position $\bigcirc$ at $t - \delta t$ as seen in Figure 6.17. At time t , the fluid point will have moved to $\vec{x}_{f,t}$ while the particle will have moved to $\vec{x}_{p,t}$. The velocity fluctuation at time t seen by the fluid point may be related to the velocity fluctuation at the previous timestep by the expression given by Equation (6.14). However, unless the particle has a small particle relaxation time, it will not be able to follow the high frequency fluctuations of the turbulence and, in general, will not see the same velocity fluctuations as the fluid point. Thus the fluctuation that the particle will see at time t should have a much lower correlation. However, using Zhou and Leschziner's model, a heavy particle sees velocity fluctuations that are highly correlated. Thus the particle experiences a turbulent kinetic energy that is much greater than it should based on the current axial position of the particle. The particle experiences greater velocities and, therefore, greater dispersion. The poor predictions for the corn pollen and copper bead experiments are therefore attributed, at least in part, to the inability of Zhou and Leschziner's model to capture the 'crossing trajectory' effect.

The model of Zhou and Leschziner produces some interesting results. For a timestep of 0.005 s, the corn pollen has a higher predicted dispersion than the hollow glass beads while the copper beads have a lower predicted dispersion. For a timestep of 0.01 s, both the corn pollen and the copper beads have a higher predicted dispersion than the hollow glass beads. However, for all timesteps considered, both the corn pollen and copper beads have a lower particle velocity decay than the hollow glass. Further research is required to explain these results.

Figure 6.13: Predictions of Snyder and Lumley's experimental data for particle dispersion using the model of Zhou and Leschziner (1991a), $\delta t = 0.005$ s

6.7 The Model of Hennick and Lightstone, 1998

The model of Hennick and Lightstone incorporates both a temporal and spatial correlation in the definition of the gas-phase velocity fluctuation. Similar to the model of Zhou and Leschziner, this definition of the velocity fluctuation allows particles to see more than one velocity fluctuation within an eddy. The spatial correlation is introduced to compensate for the crossing trajectory effect. The gas-phase velocity fluctuations are expressed as

$$u'_t = R_t(\delta t)R_x(u_{REL}\delta t)u'_{t-\delta t} + e_t \quad (6.15)$$

where u'_t is the gas-phase velocity fluctuation at the current time t , $R_t(\delta t)$ is the temporal autocorrelation, $R_x(u_{REL}\delta t)$ is the spatial autocorrelation, $u'_{t-\delta t}$ is the velocity fluctuation at the previous timestep, and e_t is a random component incorporating all effects due to randomness during the current timestep, δt .

Hennick and Lightstone's model was implemented using two different timesteps. $\delta t = 0.005$ and 0.01 s. These timesteps were selected for two reasons: (1) the timesteps are between five and ten times smaller than a characteristic particle interaction time using the SSF model of Shuen, Chen, and Faeth, and (2) it was desirable to use the same δt as Zhou and Leschziner to compare the predictions of the two models.

Figures 6.18 and 6.19 present the particle dispersion and velocity decay respectively of each particle type for the timestep of $\delta t = 0.005$ s. The hollow glass is overpredicted by

Figure 6.14: Predictions of Snyder and Lumley's experimental data for particle velocity decay using the model of Zhou and Leschziner (1991a), $\delta t = 0.005$ s

6%, the copper beads are underpredicted by 0.1% and the corn pollen is underpredicted by 2%.

For a timestep of $\delta t = 0.01$ s, the particle dispersion and velocity decay are presented in Figures 6.20 and 6.21 respectively. The hollow glass is overpredicted by 10%, the copper beads are underpredicted by 0.3% and the corn pollen is underpredicted by 4%.

It is interesting to compare the predicted dispersion of the hollow glass beads using both Zhou and Leschziner's model and Hennick and Lightstone's model. The predictions for both models using timesteps of 0.005 and 0.01 s are presented in Figure 6.22. While Hennick and Lightstone's model incorporates a spatial correlation and a temporal correlation, the spatial correlation is based on the relative velocity of the particle. Since the hollow glass beads are small and light, the particles can follow the high frequency fluctuations of the turbulence and therefore have a negligible relative velocity. Thus the spatial correlation included in the model of Hennick and Lightstone will have a negligible effect on the predicted dispersion of the hollow glass beads; the correlation will be dominated by the temporal autocorrelation thus allowing a direct comparison with Zhou and Leschziner's model. The model of Zhou and Leschziner consistently overpredicts the dispersion of the hollow glass beads in comparison with Hennick and Lightstone's results and the experimental results of Snyder and Lumley. This result can be explained by examining the expression for the temporal autocorrelation directly. Each model employs a different value for the Lagrangian integral timescale; Zhou and Leschziner use

Figure 6.15: Predictions of Snyder and Lumley's experimental data for particle dispersion using the model of Zhou and Leschziner (1991a). $\delta t = 0.01$ s

$\tau_{LI} = 0.16k/\epsilon$ while Hennick and Lightstone use $\tau_{LI} = 0.135k/\epsilon$. Comparing the resulting autocorrelations at $x/M = 85$ where $k/\epsilon = 0.25$, the autocorrelations are shown in Figure 6.23. The autocorrelation used by Hennick and Lightstone is lower than Zhou and Leschziner's and thus the hollow glass particles will see fluctuations that are less highly correlated yielding a more accurate prediction of the hollow glass particles. This result is consistent with the extension of Taylor's analysis to each model; Section 5.5 shows that Zhou and Leschziner's model will overpredict the dispersion of dyed fluid particles in homogeneous isotropic turbulence by almost 20% for large timesteps. Hennick and Lightstone's model introduced in Chapter 3 employs a Lagrangian integral timescale that exactly reproduces Taylor's result for the particle dispersion at long times.

Figure 6.16: Predictions of Snyder and Lumley's experimental data for particle velocity decay using the model of Zhou and Leschziner (1991a), $\delta t = 0.01$ s

Figure 6.17: Motion of a particle, x_p , and a fluid point, x_f , in time interval δt

Figure 6.18: Predictions of Snyder and Lumley's experimental data for particle dispersion using the model of Hennick and Lightstone, $\delta t = 0.005$ s

Figure 6.19: Predictions of Snyder and Lumley's experimental data for particle velocity decay using the model of Hennick and Lightstone, $\delta t = 0.005$ s

Figure 6.20: Predictions of Snyder and Lumley's experimental data for particle dispersion using the model of Hennick and Lightstone, $\delta t = 0.01$ s

Figure 6.21: Predictions of Snyder and Lumley's experimental data for particle velocity decay using the model of Hennick and Lightstone, $\delta t = 0.01$ s

Figure 6.22: A comparison for the dispersion predictions of hollow glass beads using the models of Zhou & Leschziner and Hennick & Lightstone

Figure 6.23: Temporal autocorrelations used by Zhou & Leschziner and Hennick & Lightstone

6.8 Summary

The experimental results of Snyder and Lumley were used to evaluate four Stochastic Separated Flow (SSF) models described in Chapter 2 and the new model presented in Chapter 3. These experiments involved the release of single particles into a uniform flow of grid-generated turbulence. Measurements of particle dispersion and velocity decay were compared to results generated by each model considered in this thesis.

The chapter began with an outline of the design of Snyder and Lumley's experiment. The numerical simulation was described. The results of each model were presented beginning with a review of the model considered and continued with a detailed discussion of results.

The conventional SSF model of Gosman and Ioannides was the first model considered. Variations on this model as suggested by Shuen, Chen, and Faeth, and Lightstone and Raithby were also evaluated. Of these conventional models, the model of Lightstone and Raithby produced results closest to those reported by Snyder and Lumley. However, the predicted dispersion of the hollow glass beads exhibited waves; this was shown to be an inherent flaw in an approach where the eddy lifetime and characteristic eddy size are essentially deterministic.

Alternative methods of describing the gas-phase turbulence were explored by considering the models of Zhou and Leschziner and Hennick and Lightstone. Zhou and Leschziner incorporate a time correlation in the definition of the gas-phase velocity fluctuation. This model produced satisfactory results for small, light particles that were able to follow the high frequency fluctuations of the turbulence. However, heavier particles saw highly correlated velocity fluctuations and the dispersion is greatly overpredicted. This result is attributed in part to the inability of Zhou and Leschziner's model to capture the 'crossing trajectory' effect.

Hennick and Lightstone compensates for the crossing trajectory effect by introducing a spatial correlation in the description of the gas-phase velocity fluctuation. The model of Hennick and Lightstone predicted the dispersion of all particle types with the greatest accuracy of all models considered in this thesis.

Chapter 7

The Experiment of Wells and Stock, 1983

The performance of the Stochastic Separated Flow (SSF) models described in Chapter 2 was examined by comparing predictions of particle velocity and dispersion with the experimental results of Wells and Stock (1983). These experiments focused on the effects of ‘crossing trajectories’ and inertia on the dispersion of single particles from a point source in grid-generated turbulence. The experiment was simulated using the TASCflow CFD code. Measurements of particle dispersion and velocity decay were compared to results generated by each model considered in this thesis.

The chapter begins with a description of the experiment of Wells and Stock. The numerical simulation is described and the predictions of each model are presented. Results are discussed in detail.

7.1 The Design of the Experiment

The experiment of Wells and Stock investigated the effects of ‘crossing trajectories’ and inertia on particles dispersed from a point source in grid-generated turbulence. The crossing trajectory effect refers to the “effect of particle trajectories crossing fluid trajectories under the influence of a potential force (usually gravity) [forcing] the particles from one region of highly correlated flow to another. In this manner, particles lose velocity correlation more rapidly than the corresponding fluid points and as a result disperse less.” (Wells and Stock (1983)). The inertia effect refers to particle sensitivity to turbulent fluctuations; if a particle is small and light, it can follow the high frequency fluctuations of the turbulence. However, if a particle is heavy, it has a reduced response to the tur-

Figure 7.1: Wells and Stock's grid turbulence experiment

bulence and, therefore, reduced dispersion. Thus, a heavy particle experiences reduced dispersion as a result of the coupled effects of crossing trajectories and inertia.

The purpose of Wells and Stock's investigation was to separate experimentally the effects of inertia from that of crossing trajectories. This section describes the design of the experiment.

Wells and Stock used an identical grid system to Snyder and Lumley (1971) to produce a turbulent flow. In contrast to Snyder and Lumley, Wells and Stock's experiment was oriented with the main axis of the flow along the x-axis and gravity along the negative y-axis. Figure 7.1 shows a diagram of Wells and Stock's experiment. The turbulence was generated using a grid with 2.54 cm spacing. Mean turbulent velocity was held constant at 6.55 m/s. Turbulence quantities were analyzed and the turbulence was shown to be homogeneous in planes parallel to the grid. Single particles were injected 15 grid spacings from the grid.

Two different sizes of solid glass beads were used in the experiment: 5 and 57 μm in diameter. Details of the particles are given in Table 7.1.

Table 7.1: Particles and relevant parameters used in Wells and Stock's experiment

Particle Type	Diameter [μm]	Density [kg/m^3]	Time Constant [ms]	Reynolds Number*
glass sphere	5	2475	0.192	6.3e-4
glass sphere	57	2420	24.4	0.887

* based on mean relative terminal velocity and particle diameter

To separate the crossing trajectories and inertia effects, particles were exposed to a potential field where the strength of field could be varied. Particles were charged and a uniform electric field was set up between two parallel plates in the wind tunnel. The electric field strength was sufficient to counter gravitational effects and to intensify the potential force. Details on the strength of the potential field and the resulting drift velocities experienced by the particles are provided in Table 7.2.

Table 7.2: Potential field strength and resulting particle drift velocities used in Wells and Stock's experiment

Particle Diameter [μm]	Potential Field Strength* [m/s^2]	Drift Velocity [cm/s]
57	0	0
	6.1	13.5
	12.1	25.8
	19.5	39.7
	27.8	54.5
	44.4	81.5
	67.9	108.0
5	0	0
	143.0	2.73
	308.3	5.86
	705.5	13.31
	907.2	17.06
	1115.4	20.91
	1264.2	23.65

* potential field strength values include gravity

Single particles were tracked using a Laser Doppler Anemometer (LDA) mounted on a mechanism that traversed the length of the wind tunnel. Measurements of particle velocity variance were taken at intervals of ten grid spacings from $x/M = 20$ to 90. Mean and rms measurements of particle velocity were based on averages from 6000 sample points. Mean square displacement was determined at intervals of ten grid spacings from $x/M = 20$ to 70 by the measurement of the relative number density. Relative number density is defined as the number of particles per unit time per unit linear displacement. Displacement measurements were based on 6000 data points or until 65 s elapsed, whichever occurred first. Dispersion measurements were reported from $x/M = 20$ to 70 to restrict results to a quasi-stationary turbulent region. Wells and Stock states that dispersion measurements “were found to be very nearly linear with distance from the grid suggesting further evidence of the validity of the quasi-stationary assumption.” (Wells and Stock (1983)).

7.2 Numerical Simulation

A simulation of Wells and Stock’s experiment was performed using the TASCflow CFD code. The simulation of the duct began 15 mesh lengths from the grid so that the inlet coincided with the injection point for the particles. Values for k and ϵ at $x/M = 15$ were calculated using the analytical solution for grid generated turbulence in conjunction with energy decay curves provided by Wells and Stock.

The duct was simulated using rectangular control volumes. Nodes were spaced evenly throughout the domain with 100 nodes along the x-axis, and 25 nodes along the y- and z-axes. A symmetry boundary condition was employed at the wall to ensure that wall drag did not affect the particles. The numerical solution technique for the flow field is described in Section 4.1. Values for k and ϵ along the centerline were compared to Wells and Stock’s energy decay curves and to the analytical solution for grid generated turbulence shown in Figures 7.2 and 7.3 respectively.

Simulations of the experiment required a separate flow field solution for each potential field strength investigated. Potential field strengths of 0, 6, 12, 19 and 27 m/s^2 were simulated for the large particle; potential field strengths of 0, 143, 308 and 907 m/s^2 were simulated for the small particle all along the negative y-axis. For the large particle, field strengths were selected to encompass a variety of gravitational values from zero to almost three times gravity. Selection was also limited by the experimental data: complete dispersion measurements were not available for field strengths greater than 27 m/s^2 . For the small particle, field strengths were selected to provide a wide range of gravitational

Figure 7.2: Turbulent kinetic energy along the centerline

values. Particle trajectories for each particle type were predicted by each model for all gravities simulated.

Since the particles do not affect the flow field, the release of particles is essentially post-processing. Section 4.2 describes the solution of the particle equation of motion. The trajectory of each particle was recorded and written to a file. A single particle trajectory was verified for each model by comparing particle velocity and displacement to the analytical solution of the linearized particle equation of motion. The trajectories of 780 particles were recorded for each particle type for each model. The number of particle trajectories was doubled and produced identical results indicating statistical significance. Particle dispersion and velocity decay were determined by filtering the data and finding the variance of the quantities in question. The details of this process are available in Appendix C.

Details about the initial conditions of the particles were not available. To compensate for the lack of information on particle initial conditions, the small and large particles were treated separately.

In the simulation of the small particles, single particles were released from the inlet at their drift velocity. Since the particles are small and light, they were able to follow the high frequency fluctuations of the turbulence and exhibit the appropriate velocity variance at the position of the first measurement, $x/M = 20$.

In the simulation of the large particles, single particles were released as close as possible to the position of the first measurement. At the injection point, particles were released

Figure 7.3: Dissipation along the centerline

with an instantaneous velocity comprised of a mean plus a fluctuating component. The fluctuating component was determined by random sampling of a Gaussian probability density function with zero mean and variance equal to the reported experimental value at the position of the first measurement.

To further compensate for the lack of information on particle initial conditions, dispersion results for both the small and large particles were adjusted to reflect the dispersion reported at $x/M = 20$ for each gravity case. The results were modified as follows: the difference in the reported and predicted dispersion was calculated at $x/M = 20$. This difference was added to the predicted dispersion results for the length of the duct. Appendix D shows that the addition of a constant to the variance of position is mathematically equivalent to releasing particles with a Gaussian distribution of zero mean and specified variance.

7.3 Results

The performance of the Stochastic Separated Flow (SSF) models described in Chapter 2 was examined by comparing predictions of particle velocity and dispersion with the experimental results of Wells and Stock (1983). The results of this investigation are presented in two sections: the first section presents model predictions of the small particles, the second presents models predictions of the large particles.

7.3.1 Results: Small Particles

Wells and Stock investigated the dispersion of small particles with a low particle relaxation time of $\tau_p = 0.194$ ms. These particles were small and light and could follow the high frequency fluctuations of the turbulent gas-phase. This section presents the predictions of the models and the experimental results of Wells and Stock for the small particles.

The results are divided into two groups: the predictions of the SSF models of Gosman and Ioannides (1983), Shuen, Chen and Faeth (1983), and Lightstone and Raithby (1996) are grouped together; the predictions of the models of Zhou and Leschziner (1991a), and Hennick and Lightstone are presented together. In each of the figures, the points correspond to the experimental measurements of Wells and Stock, and the lines represent the model predictions.

The following figures present predictions obtained using the SSF models. Figures 7.4 and 7.5 present the predictions for particle dispersion and velocity decay respectively. The models of Gosman and Ioannides and Lightstone and Raithby overpredict particle velocity variance while the model of Shuen, Chen and Faeth underpredicts velocity variance. The models of Gosman and Ioannides and Lightstone and Raithby yield almost identical predictions of particle dispersion. Both models underpredict dispersion by 16%. The model of Shuen, Chen and Faeth underpredicts particle dispersion by 31%. All reported errors are calculated using a root mean square method.

Figure 7.4: Predictions of Wells and Stock's experimental data for the dispersion of small particles in zero gravity using SSF models

Figure 7.5: Predictions of Wells and Stock's experimental data for the velocity of small particles in zero gravity using SSF models

The underprediction of Gosman and Ioannides model differs from the results obtained in Section 5.3. Section 5.3 extends the analysis of Taylor to this model by considering the dispersion of dyed fluid particles from a point source in homogeneous isotropic turbulence. The model of Gosman and Ioannides is shown to overpredict fluid particle dispersion by just over 35% at long times. The discrepancy is due to key assumptions made in extending the analysis of Taylor to the model of Gosman and Ioannides. The analysis assumes that the timestep for dyed fluid particles at long times is a deterministic quantity. Since dyed fluid particles follow the gas-phase turbulence exactly, the particles are captured by the eddies and the timestep is the eddy lifetime, t_e , given by

$$t_e = \frac{l_e}{\sqrt{\frac{u'^2 + v'^2 + w'^2}{3}}} \quad (7.1)$$

where u' , v' and w' are the fluctuating components of the instantaneous gas-phase velocity, and l_e is the characteristic eddy length given by

$$l_e = C_\mu^{0.5} \frac{k^{1.5}}{\epsilon} \quad (7.2)$$

where C_μ is equal to 0.09, k is the turbulent kinetic energy, and ϵ is the dissipation rate of turbulence.

The eddy lifetime incorporates the fluctuating gas-phase velocity which is a random

variable and thus the timestep is not deterministic. An additional assumption is the approximation of the gas-phase fluctuations to complete the analysis. Further discussion of these assumptions are provided with the analysis in Section 5.3.

The model of Lightstone and Raithby is similar to that of Gosman and Ioannides but uses a different expression for the eddy lifetime, that is

$$t_e = \frac{l_e}{\sqrt{\frac{2}{3}k}} \quad (7.3)$$

where k is the turbulent kinetic energy. The eddy length is described similar to Gosman and Ioannides but a different exponent is used, that is $C_\mu^{0.63}$. The value for the exponent follows from an extension of Taylor's analysis repeated in Section 5.2. This constant is derived to yield a model capable of exactly reproducing Taylor's result for the long time dispersion of dyed fluid particles in homogeneous, isotropic turbulence at long times. Thus, the underprediction of the dispersion of the small glass beads is surprising. Further research is required to explain these results.

Shuen, Chen and Faeth's model greatly underpredicts the particle dispersion. This is consistent with the result obtained by extending Taylor's analysis to this model in Section 5.4. The model is shown to underpredict the dispersion of dyed fluid particles in homogeneous, isotropic turbulence by just over 25% for long times.

Figures 7.6 and 7.7 present the particle dispersion and velocity decay results using the SSF models for the case of gravity = 143 m/s². Gosman and Ioannides' model underpredicts particle dispersion by 12%, Lightstone and Raithby's model underpredicts by 14%, and Shuen, Chen and Faeth's model underpredicts by 25%. Predictions of particle velocity variance are nearly identical to the zero gravity case: the models of Gosman and Ioannides overpredicts particle velocity variance, and the model of Shuen, Chen and Faeth underpredicts velocity variance.

Particle dispersion and velocity decay results for the case of gravity = 308 m/s² are presented in Figures 7.8 and 7.9. Gosman and Ioannides' model underpredicts particle dispersion by 55%, Lightstone and Raithby's model underpredicts dispersion by 60% and Shuen, Chen and Faeth's model underpredicts dispersion by 81%. It should be noted that these values are high due to the difference in experimental results and predictions at $x/M = 60$.

In comparison with model predictions for the zero gravity case and gravity = 143 m/s², predictions for velocity variance drop slightly for the case of gravity = 308 m/s². However, the trend of the predictions remains the same: Gosman and Ioannides and Lightstone and Raithby's models overpredict velocity variance while Shuen, Chen and Faeth's model

Figure 7.6: Predictions of Wells and Stock's experimental data for the dispersion of small particles in gravity = 143 m/s^2 using SSF models

underpredicts velocity variance.

Figures 7.10 and 7.11 present the particle dispersion and velocity decay results respectively for the case of gravity = 907 m/s^2 . Gosman and Ioannides' model underpredicts particle dispersion by 11%, Lightstone and Raithby's model underpredicts dispersion by 16% and Shuen, Chen and Faeth's model underpredicts dispersion by 29%. Predicted velocity variance decreases with increasing gravity: the models of Gosman and Ioannides and Lightstone and Raithby overpredict velocity variance while the model of Shuen, Chen and Faeth underpredicts velocity variance.

Notice that all small particle dispersion predictions from the models of Shuen, Chen and Faeth and Lightstone and Raithby are shown as a 'wavy' line. This result is similar to results obtained in the simulation of Snyder and Lumley's experiment for the case of the hollow glass particles. The waviness of the small particle dispersion curves results from the treatment of the turbulence as a series of discrete eddies where the instantaneous velocity is held constant for the lifetime of the eddy. These waves are an inherent flaw in an approach where the eddy lifetime and eddy length are essentially deterministic.

The waves seen in the particle dispersion predictions for Shuen, Chen and Faeth and Lightstone and Raithby's models also indicate that the particle interaction time of the small particles is dominated by the eddy lifetime. While the gravitational force increases, thus increasing the terminal velocity of the particle, these models fail to capture the crossing trajectory effect. This can be explained by considering the transit time equation.

Figure 7.7: Predictions of Wells and Stock's experimental data for the velocity of small particles in gravity = 143 m/s^2 using SSF models

The transit time, derived in Appendix A.1 is given by

$$t_{tr} = -\tau_p \ln \left(1 - \frac{l_e}{\tau_p |\vec{u}_g - \vec{u}_p|} \right) \quad (7.4)$$

where $\vec{u}_g - \vec{u}_p$ is the relative velocity at the beginning of the interaction time and τ_p is the particle relaxation time introduced in Section 2.1.2. When $l_e > \tau_p |\vec{u}_g - \vec{u}_p|$, Equation (7.4) has no solution. In this case, the particle is captured by the eddy, and the interaction time is the eddy lifetime.

Consider the model of Shuen, Chen and Faeth where the characteristic eddy length is described by

$$l_e = C_\mu^{0.75} \frac{k^{1.5}}{\epsilon} \quad (7.5)$$

Using this expression for the characteristic eddy length in Equation (7.4), and values for turbulent kinetic energy and dissipation from the analytical solution for grid-generated turbulence along the length of the duct, the relative velocity of the small particle must be at least 30 m/s for the particle interaction time to be dominated by the transit time along the length of the duct. For the model of Lightstone and Raithby, where the characteristic eddy length is described similar to Equation (7.5) but C_μ is raised to the power of 0.63, the relative velocity of the particle must be at least 40 m/s . The greatest drift velocity of the particle considered in the Wells and Stock simulations is 17.06 cm/s for the case

Figure 7.8: Predictions of Wells and Stock's experimental data for the dispersion of small particles in gravity = 308 m/s^2 using SSF models

of gravity = 907 m/s^2 . Thus, the transit time never dominates the particle interaction time for the case of the small particle. As a result, the particle dispersion is predicted to be similar for all gravity cases for the small particle.

The experimental results of Wells and Stock can be summarized and compared to the predicted dispersion results using a gradient diffusion approach. The gradient diffusion equation for particles released from a point source is given by

$$\frac{DC}{Dt} = \Gamma_p \left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2} \right) \quad (7.6)$$

where C is the particle concentration, DC/Dt is the total convective derivative based on mean velocities, and Γ_p is the particle turbulent diffusivity. The analytical solution to Equation (7.6) is given by

$$\frac{d\bar{y}^2}{dt} = 2\Gamma_p \quad (7.7)$$

Particle dispersion coefficients for each drift velocity are presented in Figure 7.12 for the SSF models. Linear curves were fit through the $\bar{y}^2$ data and the slope was then used to calculate the dispersion coefficients as given in Equation (7.7). Dispersion coefficients for the SSF models are plotted with a 95% confidence interval. The dispersion coefficients for the experimental data were digitized from Wells and Stock's results.

The dispersion coefficients for the small particles indicate that the SSF models are

Figure 7.9: Predictions of Wells and Stock's experimental data for the velocity of small particles in gravity = 308 m/s^2 using SSF models

not sensitive to the increase in gravity, however, this result is supported by Wells and Stock's experimental data. Wells and Stock report that "the crossing trajectory effect appears to be negligible when the drift velocity is less than the rms fluid velocity;" (Wells and Stock (1983)). Additionally, the scatter of the dispersion measurements for each gravity case is less than the 10% reported experimental error.

Predictions using the models of Zhou and Leschziner and Hennick and Lightstone are presented in the following figures. Figures 7.13 and 7.14 present the particle dispersion and velocity decay respectively. The predictions are made using two different timesteps chosen *a priori*, that is $\delta t = 0.005$ and 0.01 s . The model of Zhou and Leschziner produces the best results with an rms error of 2% for both the timesteps employed. The model of Hennick and Lightstone underpredicts particle dispersion by 4 and 5% for timesteps of 0.005 and 0.01 s respectively.

The prediction of particle dispersion using Zhou and Leschziner's model is consistent with results reported by the researchers. This model is well suited to small, light particles that essentially follow the high frequency fluctuations of the turbulence. Zhou and Leschziner's model incorporates a time correlation into the definition of the gas-phase velocity fluctuation. The velocity fluctuation is expressed as

$$u'_t = R(\delta t)u'_{t-\delta t} + e_t \quad (7.8)$$

Figure 7.10: Predictions of Wells and Stock's experimental data for the dispersion of small particles in gravity = 907 m/s^2 using SSF models

where $R(\delta t)$ is a Lagrangian time correlation, $u'_{t-\delta t}$ is the gas-phase velocity fluctuation at the previous timestep, and e_t represents all effects arising from randomness during the time interval δt . Zhou and Leschziner's model is outlined in detail in Section 2.3.2.

The time-correlation is approximated by the exponential function as suggested by Hinze (1975).

$$R(\delta t) = \exp\left(-\frac{\delta t}{\tau_{LI}}\right) \quad (7.9)$$

The Lagrangian integral timescale, τ_{LI} , used in Zhou and Leschziner's model is given by

$$\tau_{LI} = \beta t_e = \beta (C_\mu^{0.75} \frac{k^{1.5}}{\epsilon}) / (\frac{2}{3} k)^{0.5} \quad (7.10)$$

Here, β is based on analytical and experimental considerations. Zhou and Leschziner report the optimum value of β to be 0.8 based on their simulation of the experiment of Wells and Stock.

The accurate prediction of Zhou and Leschziner's model seen in Figure 7.13 differs from results obtained by extending Taylor's analysis to this model. In Section 5.5, the model is shown to overpredict the dispersion of dyed fluid particles in homogeneous isotropic turbulence by almost 20% for large Δt . Lightstone and Raithby's analysis, provided in Section 5.2 of the same Chapter, indicates $\Delta t = 2\tau_{LI} = 0.27k/\epsilon$. The largest timestep used in the Zhou and Leschziner simulation was $\delta t = 0.01 \text{ s}$. Calculations show that, at minimum, $\Delta t \approx 2.5\delta t$ for the largest timestep employed. Thus, the analysis may

Figure 7.11: Predictions of Wells and Stock's experimental data for the velocity of small particles in gravity = 907 m/s^2 using SSF models

not be applied to this simulation.

The model of Hennick and Lightstone incorporates a temporal and spatial correlation in the definition of the gas-phase velocity fluctuation. The spatial correlation is introduced to account for the crossing trajectory effect. The velocity fluctuation is defined as

$$u'_t = R_t(\delta t) R_x(\delta x) u'_{t-\delta t} + e_t \quad (7.11)$$

where u'_t is the gas-phase velocity fluctuation at the current time t , $R_t(\delta t)$ is the temporal autocorrelation, $R_x(\delta x)$ is the spatial autocorrelation, $u'_{t-\delta t}$ is the velocity fluctuation at the previous timestep, and e_t is a random component incorporating all effects due to randomness during the current timestep, δt . The spatial correlation can be related to the temporal correlation by approximating the distance a particle travels in a single timestep using the relationship $\delta x = u_{REL} \delta t$ where u_{REL} is the relative velocity of the particle at the beginning of the timestep. The model of Hennick and Lightstone is presented in detail in Chapter 3.

Similar to Zhou and Leschziner's model, the temporal autocorrelation is approximated using the exponential function as suggested by Hinze (1975)

$$R_t(\delta t) = \exp\left(-\frac{\delta t}{\tau_{LI}}\right) \quad (7.12)$$

Figure 7.12: Particle dispersion coefficients for the small particles from $\overline{Y}^2$ predictions using SSF models

where τ_{LI} is the Lagrangian integral timescale given by

$$\tau_{LI} = 0.135 \frac{k}{\epsilon} \quad (7.13)$$

Here, the expression for τ_{LI} is based solely on analytical considerations. This expression follows from analytical work by Lightstone and Raithby (1996) repeated in Section 5.2.

The spatial autocorrelation is approximated by

$$R_x(u_{REL}\delta t) = \exp\left(-\frac{u_{REL}\delta t}{L_I}\right) \quad (7.14)$$

where $u_{REL} = |\vec{u}_g - \vec{u}_p|$, and L_I is the Lagrangian integral length scale given by

$$L_I = C_\mu^{0.63} \frac{k^{1.5}}{\epsilon} = 2\tau_{LI} \sqrt{\frac{2}{3}k} \quad (7.15)$$

This expression for L_I comes from the definition of the characteristic eddy length suggested by the analysis of Lightstone and Raithby outlined in Section 5.2.

It is interesting to note that the model of Hennick and Lightstone underpredicts particle dispersion by 4 and 5% for timesteps of 0.005 and 0.01 s respectively for the case of small particles in zero gravity. Values for the Lagrangian integral timescale and length-scale were selected based on the analysis of Lightstone and Raithby to exactly reproduce

Figure 7.13: Predictions of Wells and Stock's experimental data for the dispersion of small particles in zero gravity using models involving correlations

Taylor's result for the dispersion of dyed fluid particles in homogeneous, isotropic turbulence for large Δt . As outlined for the small particle predictions of Zhou and Leschziner, the analysis provided in Section 3.2 does not apply to this simulation since the largest timestep employed does not constitute a large Δt . That is, at minimum, $\Delta t \approx 2.5\delta t$ where $\delta t = 0.01$ s, the largest timestep employed in this simulation.

For the case of gravity = 143 m/s^2 , predictions of small particle dispersion and velocity decay using the models of Zhou and Leschziner and Hennick and Lightstone are presented in Figures 7.15 and 7.16 respectively. Zhou and Leschziner's model overpredicts particle dispersion by 7 and 6% using a timestep of 0.005 and 0.01 s respectively. Hennick and Lightstone's model underpredicts particle dispersion by 4 and 3% for a timestep of 0.005 and 0.01 s respectively.

Figures 7.17 and 7.18 present the particle dispersion and velocity predictions respectively for the case of gravity = 308 m/s^2 . Zhou and Leschziner's model exhibits errors of 14 and 12% for timesteps of 0.005 and 0.01 s respectively. Hennick and Lightstone's model underpredicts particle dispersion by 27 and 26% for timesteps of 0.005 and 0.01 s respectively.

Predictions using the models of Zhou and Leschziner and Hennick and Lightstone for the case of gravity = 907 m/s^2 are presented in Figures 7.19 and 7.20. Zhou and Leschziner's model overpredicts particle dispersion by 5 and 6% for timesteps of 0.005 and 0.01 s respectively. Hennick and Lightstone's model underpredicts particle dispersion

Figure 7.14: Predictions of Wells and Stock's experimental data for the velocity of small particles in zero gravity using models that involve correlations

by 13 and 11% for timesteps of 0.005 and 0.01 s respectively.

The predicted results using the models of Zhou and Leschziner and Hennick and Lightstone are summarized using a gradient diffusion approach. Figure 7.21 presents particle dispersion coefficients for each drift velocity with a 95% confidence interval. Dispersion coefficients are calculated for each model for each timestep employed.

The dispersion coefficients for the small particles indicate that the model of Zhou and Leschziner is not sensitive to the increase in gravity. However, this result is supported by Wells and Stock's experimental data. Wells and Stock report that "the crossing trajectory effect appears to be negligible when the drift velocity is less than the rms fluid velocity." (Wells and Stock (1983)). Additionally, the scatter of the dispersion measurements for each gravity case is less than the 10% reported experimental error for a timestep of 0.005 s.

Dispersion coefficients for the model of Hennick and Lightstone shows that dispersion is predicted to decrease with increasing gravitational force. The physical basis is the principle of the crossing trajectory effect: with increasing gravity, the particle experiences an increased terminal velocity. As a result of this terminal velocity, the particle falls from one eddy to another faster than the average eddy decay rate. The particle tends to "lose velocity correlation more rapidly than the corresponding fluid points and as a result, disperse[s] less," (Wells and Stock (1983)). Hennick and Lightstone's model captures this effect with the inclusion of a spatial correlation that is based on the relative

Figure 7.15: Predictions of Wells and Stock's experimental data for the dispersion of small particles in gravity = 143 m/s^2 using models that involve correlations

velocity of the particle. The spatial correlation is employed even when the drift velocity is less than the rms fluid velocity, accounting for the difference between model predictions and experimental results. Due to the experimental error of the measurements of Wells and Stock, further research is required to determine if the crossing trajectory effect is negligible under these conditions.

Figure 7.16: Predictions of Wells and Stock's experimental data for the velocity of small particles in gravity = 143 m/s^2 using models that involve correlations

Figure 7.17: Predictions of Wells and Stock's experimental data for the dispersion of small particles in gravity = 308 m/s^2 using models that involve correlations

Figure 7.18: Predictions of Wells and Stock's experimental data for the velocity of small particles in gravity = 308 m/s^2 using models that involve correlations

Figure 7.19: Predictions of Wells and Stock's experimental data for the dispersion of small particles in gravity = 907 m/s^2 using models that involve correlations

Figure 7.20: Predictions of Wells and Stock's experimental data for the velocity of small particles in gravity = 907 m/s^2 using models that involve correlations

Figure 7.21: Particle dispersion coefficients for the small particles from $\overline{Y}^{-2}$ predictions using models involving correlations

Figure 7.22: Predictions of Wells and Stock's experimental data for the dispersion of large particles in zero gravity using SSF models

7.3.2 Results: Large Particles

Wells and Stock investigated the dispersion of particles with a particle relaxation time of $\tau_p = 24.4$ ms. These particles had significant inertia and could not follow the high frequency fluctuations of the flow exhibiting a reduced response to the turbulence. This section presents the predictions of the models and the experimental results of Wells and Stock for the large particles.

Similar to the previous section, the results are divided into two groups: the predictions of the SSF models of Gosman and Ioannides (1983), Shuen, Chen and Faeth (1983), and Lightstone and Raithby (1996) are grouped together; the predictions of the models of Zhou and Leschziner (1991a), and Hennick and Lightstone are presented together. In each of the figures, the points correspond to the experimental measurements of Wells and Stock, and the lines represent the model predictions.

Figures 7.22 and 7.23 present the predictions for particle dispersion and velocity decay using the SSF models for the zero gravity case. The model of Gosman and Ioannides predicts particle dispersion with an rms error of 7%, Lightstone and Raithby's model underpredicts dispersion by 17% and the model of Shuen, Chen and Faeth underpredicts dispersion by 27%. All reported errors are calculated using a root mean square method.

Particle velocity variance is well predicted by both Gosman and Ioannides' and Lightstone and Raithby's model. Shuen, Chen and Faeth's model underpredicts velocity variance.

Figure 7.23: Predictions of Wells and Stock's experimental data for the velocity of large particles in zero gravity using SSF models

Particle dispersion and velocity decay results for the case of gravity $= 6 \text{ m/s}^2$ are presented in Figures 7.24 and 7.25. Gosman and Ioannides' model underpredicts particle dispersion by 5%, Lightstone and Raithby's model underpredicts dispersion by 12% and Shuen, Chen and Faeth's model underpredicts dispersion by 19%. Similar to the zero gravity case, the models of Gosman and Ioannides and Lightstone and Raithby yield accurate predictions of particle velocity variance while Shuen, Chen and Faeth's model underpredicts velocity variance.

Dispersion results improve for the case of gravity $= 12 \text{ m/s}^2$. Figures 7.26 and 7.27 present the particle dispersion and velocity decay results using the SSF models. Gosman and Ioannides' model overpredicts particle dispersion by 7%, Lightstone and Raithby's model predicts dispersion with an rms error of 5%, and Shuen, Chen and Faeth's model predicts dispersion with an rms error of 11%. Particle velocity variance results weaken with the underprediction of velocity variance by all three SSF models.

Predictions using the SSF models for the case of gravity $= 19 \text{ m/s}^2$ are presented in Figures 7.28 and 7.29. The model of Gosman and Ioannides overpredicts dispersion by 6%, Lightstone and Raithby's model predicts dispersion with an rms error of 4% and Shuen, Chen and Faeth's model predicts dispersion with an rms error of 11%. Velocity variance predictions improve from the case of gravity $= 12 \text{ m/s}^2$, however, velocity variance is still underpredicted by all three models.

The final simulation was computed with a gravitational force of 27 m/s^2 . Figures 7.30

Figure 7.24: Predictions of Wells and Stock's experimental data for the dispersion of large particles in gravity = 6 m/s^2 using SSF models

and 7.31 present the particle dispersion and velocity decay results respectively. Gosman and Ioannides model overpredicts particle dispersion by 14%. Lightstone and Raithby's model overpredicts dispersion by 6%, and Shuen, Chen and Faeth's model overpredicts particle dispersion by 9%. Particle velocity variance predictions improve from the case of gravity = 19 m/s^2 , however, velocity variance is still underpredicted by all three models.

Particle dispersion predictions are summarized using a gradient diffusion approach. Figure 7.32 presents particle dispersion coefficients for each of the SSF models. Linear curves were fitted through the $\overline{y^2}$ data and the slope was then used to calculate the dispersion coefficients as given in Equation (7.7). Dispersion coefficients for the SSF models are plotted with a 95% confidence interval. The dispersion coefficients for the experimental data were digitized from Wells and Stock's results.

Dispersion coefficients calculated from predictions using the SSF models indicate that dispersion decreases with increasing drift velocity. This result is consistent with the physical premise for the crossing trajectory effect: with increasing gravity, the particle experiences an increasing terminal velocity and may traverse each eddy faster than the eddy decay rate. By crossing the eddy, the particle is exposed to the instantaneous turbulent velocity for less time than if it had been captured by the eddy, and, as a result, dispersion decreases. Wells and Stock report that "the dispersion coefficient was found to decrease approximately as the drift velocity squared within the range of velocities

Figure 7.25: Predictions of Wells and Stock's experimental data for the velocity of large particles in gravity = 6 m/s^2 using SSF models

tested.” (Wells and Stock (1983)).

The following figures present predictions using the models of Zhou and Leschziner and Hennick and Lightstone outlined in the previous section. Figures 7.33 and 7.34 present the particle dispersion and velocity decay respectively for the zero gravity case. The predictions are made using two different timestep chosen *a priori*, that is $\delta t = 0.005$ and 0.01 s . The model of Zhou and Leschziner produces results with an rms error of 7 and 16% for timesteps of 0.005 and 0.01 s respectively. The model of Hennick and Lightstone underpredicts particle dispersion by 27 and 23% for timesteps of 0.005 and 0.01 s respectively. Velocity variance is overpredicted by the model of Zhou and Leschziner for both timesteps considered. Hennick and Lightstone's model adequately predicts particle velocity variance using a timestep of 0.01 s; velocity variance is underpredicted for a timestep of 0.05 s.

For the case of gravity = 6 m/s^2 , predictions of large particle dispersion and velocity decay are presented in Figures 7.35 and 7.36 respectively. Zhou and Leschziner's model predicts particle dispersion with an rms error of 4 and 3% using a timestep of 0.005 and 0.01 s respectively. Hennick and Lightstone's model underpredicts particle dispersion by 20 and 17% for a timestep of 0.005 and 0.01 s respectively. The model of Zhou and Leschziner overpredicts velocity variance using both timesteps considered; Hennick and Lightstone's model underpredicts velocity variance for both timesteps considered.

Hennick and Lightstone's dispersion results improve for the case of gravity = 12 m/s^2 .

Figure 7.26: Predictions of Wells and Stock's experimental data for the dispersion of large particles in gravity = 12 m/s^2 using SSF models

Figures 7.37 and 7.38 present the particle dispersion and velocity decay results respectively. Hennick and Lightstone's model underpredicts particle dispersion by 7 and 5% for timesteps of 0.005 and 0.01 s respectively. Zhou and Leschziner's model overpredicts particle dispersion by 8 and 10% for timesteps of 0.005 and 0.01 s respectively. Predictions of velocity variance using Zhou and Leschziner's model improve to yield adequate predictions for both timesteps considered. The model of Hennick and Lightstone continues to underpredict velocity variance for the case of gravity = 12 m/s^2 .

Hennick and Lightstone's dispersion results improve further for the case of gravity = 19 m/s^2 . Figures 7.39 and 7.40 present the particle dispersion and velocity decay results respectively. Hennick and Lightstone's model predicts particle dispersion with an rms error of 6 and 4% for timesteps of 0.005 and 0.01 s respectively. Zhou and Leschziner's model overpredicts particle dispersion by 13 and 14% for timesteps of 0.005 and 0.01 s respectively. Particle velocity variance results are poorly predicted: the model of Zhou and Leschziner overpredicts velocity variance for both timesteps considered while the model of Hennick and Lightstone underpredicts particle velocity variance for both timesteps considered.

The final simulation was computed with a gravitational force of 27 m/s^2 . Figures 7.41 and 7.42 present the particle dispersion and velocity decay results respectively. Hennick and Lightstone's results continue to improve with particle dispersion overpredicted by 2 and 3% for timesteps of 0.005 and 0.01 s respectively. Zhou and Leschziner's model

Figure 7.27: Predictions of Wells and Stock's experimental data for the velocity of large particles in gravity = 12 m/s^2 using SSF models

overpredicts dispersion by 13 and 15% for timesteps of 0.005 and 0.01 s respectively. Zhou and Leschziner's model overpredicts particle velocity variance for each timestep considered. The model of Hennick and Lightstone underpredicts particle velocity variance for both timesteps considered.

The predicted results using the models of Zhou and Leschziner and Hennick and Lightstone are summarized using a gradient diffusion approach. Figure 7.43 presents particle dispersion coefficients for each drift velocity with a 95% confidence interval. Dispersion coefficients are calculated for each model for each timestep employed.

Particle dispersion was not well predicted by Zhou and Leschziner's model for any of the five gravities considered in this simulation. Dispersion coefficients show that the predictions of this model did not decrease with increasing gravitational force. The similar predictions of Zhou and Leschziner's model for all gravity cases may be explained as follows. Zhou and Leschziner's model uses an expression for the gas-phase velocity fluctuation given by

$$u'_t = R(\delta t)u'_{t-\delta t} + e_t \quad (7.16)$$

where $R(\delta t)$ is a Lagrangian time correlation, $u'_{t-\delta t}$ is the gas-phase velocity fluctuation at the previous timestep, and e_t represents all effects arising from randomness during the time interval δt .

The correlation included in Equation (7.16) is the temporal autocorrelation for a dyed fluid particle. Thus, the correlation term assumes that the particle is a dyed fluid

Figure 7.28: Predictions of Wells and Stock's experimental data for the dispersion of large particles in gravity $= 19 \text{ m/s}^2$ using SSF models

particle carried along by the flow. The large particle considered in this simulation has significant inertia and cannot follow the high frequency fluctuations of the flow. Thus the fluctuation that the large particle sees at time t should have a much lower correlation. However, using Zhou and Leschziner's model, a heavy particle sees velocities that are highly correlated. The poor predictions are therefore attributed, at least in part, to the inability of Zhou and Leschziner's model to capture the crossing trajectory effect.

Hennick and Lightstone's model incorporates the crossing trajectory effect by introducing a spatial correlation coefficient in the description of the fluctuating component of the instantaneous turbulent velocity. The spatial correlation coefficient is based on the relative velocity of the particle and the timestep δt . As the gravitational force increases, therefore increasing the relative velocity of the particle, the predictions of the model improve. Dispersion coefficients for the model of Hennick and Lightstone decrease with increasing drift velocity capturing the crossing trajectory effect as expected.

Figure 7.29: Predictions of Wells and Stock's experimental data for the velocity of large particles in gravity = 19 m/s^2 using SSF models

Figure 7.30: Predictions of Wells and Stock's experimental data for the dispersion of large particles in gravity = 27 m/s^2 using SSF models

Figure 7.31: Predictions of Wells and Stock's experimental data for the velocity of large particles in gravity = 27 m/s^2 using SSF models

Figure 7.32: Particle dispersion coefficients for the large particles from $\bar{\gamma}^{-2}$ predictions using SSF models

Figure 7.33: Predictions of Wells and Stock's experimental data for the dispersion of large particles in zero gravity using models involving correlations

Figure 7.34: Predictions of Wells and Stock's experimental data for the velocity of large particles in zero gravity using models that involve correlations

Figure 7.35: Predictions of Wells and Stock's experimental data for the dispersion of large particles in gravity = 6 m/s^2 using models that involve correlations

Figure 7.36: Predictions of Wells and Stock's experimental data for the velocity of large particles in gravity = 6 m/s^2 using models that involve correlations

Figure 7.37: Predictions of Wells and Stock's experimental data for the dispersion of large particles in gravity $= 12 \text{ m/s}^2$ using models that involve correlations

Figure 7.38: Predictions of Wells and Stock's experimental data for the velocity of large particles in gravity $= 12 \text{ m/s}^2$ using models that involve correlations

Figure 7.39: Predictions of Wells and Stock's experimental data for the dispersion of large particles in gravity = 19 m/s^2 using models that involve correlations

Figure 7.40: Predictions of Wells and Stock's experimental data for the velocity of large particles in gravity = 19 m/s^2 using models that involve correlations

Figure 7.41: Predictions of Wells and Stock's experimental data for the dispersion of large particles in gravity = 27 m/s^2 using models that involve correlations

Figure 7.42: Predictions of Wells and Stock's experimental data for the velocity of large particles in gravity = 27 m/s^2 using models that involve correlations

Figure 7.43: Particle dispersion coefficients for the large particles from $\overline{\gamma}^2$ predictions using models involving correlations

7.4 Summary

The experiments of Wells and Stock were used to evaluate Stochastic Separated Flow (SSF) models described in Chapter 2 and the new model presented in Chapter 3. These experiments focused on the effects of ‘crossing trajectories’ and inertia on the dispersion of single particles from a point source in grid-generated turbulence. Measurements of particle dispersion and velocity decay were compared to results generated by each model considered in this thesis.

The chapter began with an outline of the design of Wells and Stock’s experiment. The numerical simulation was described. The results were presented in two sections: predictions for the small particles were grouped together and predictions for the large particles were grouped together.

Predicted dispersion of the the small particles using the SSF models indicate that the models are not sensitive to increasing gravitational force. Similarly, the time-correlated model of Zhou and Leschziner does not show sensitivity to increasing gravitational force for the small particle dispersion predictions. This result is supported by Wells and Stock who report that “the crossing trajectory effect appears to be negligible when the drift velocity is less than the rms fluid velocity,” (Wells and Stock (1983)). Additionally, the scatter of the dispersion measurements is less than the 10% reported experimental error.

The model of Hennick and Lightstone predicts decreased dispersion with increasing gravitational force for the small particle case. The model employs both a temporal and a spatial correlation in the description of the fluctuating velocity component of the instantaneous turbulent velocity. The spatial correlation is based on the relative velocity of the particle and is employed even when the drift velocity is less than the rms fluid velocity. Due to the experimental error of the measurements of Wells and Stock, further research is required to determine if the crossing trajectory effect is negligible under these conditions.

Predicted dispersion of the large particles using the SSF models show a distinct decrease in dispersion with increasing gravitational force. Similarly, the model of Hennick and Lightstone shows sensitivity to increasing gravitational force for the large particle predictions. This result is consistent with the physical premise for the crossing trajectory effect: with increasing gravity, the particle experiences an increasing terminal velocity and may traverse each eddy faster than the eddy decay rate. By crossing the eddy, the particle is exposed to the instantaneous turbulent velocity for less time than if it had been captured by the eddy, and, as a result, dispersion decreases. Wells and Stock report that “the dispersion coefficient was found to decrease approximately as the drift velocity

squared within the range of velocities tested,” (Wells and Stock (1983)).

Dispersion coefficients for the predictions of Zhou and Leschziner’s model for the large particle case indicate that the model is insensitive to increasing gravitational force. The model produces similar dispersion predictions for all gravity cases. The similarity arises from the description of the gas-phase velocity fluctuation used in the model. The model uses a temporal autocorrelation to describe the fluctuating gas-phase component. The correlation term depends only in the timestep employed and assumes that the particle is a dyed fluid particle. The large particle considered in this simulation has significant inertia and cannot follow the high frequency fluctuations of the flow. As a result, the sole use of the temporal correlation leads to velocity fluctuations that are highly correlated. The poor predictions are therefore attributed, at least in part, to the inability of Zhou and Leschziner’s model to capture the crossing trajectory effect.

Particle velocity variance was very well predicted for the small particles by all models considered in this investigation. Velocity variance for the large particles was reasonably well predicted by all models considered.

Chapter 8

Closure

8.1 Summary and Conclusions

This thesis has been concerned with modeling the dispersion of particles in turbulent flow. The prediction of particle motion is implicitly linked to the problem of turbulence. The particle equation of motion is an expression for the acceleration of a particle due to drag and gravity forces. There is an exact solution to the particle equation of motion for the case of linear drag, but, in order to predict particle velocity, the instantaneous gas-phase velocity must be known.

Estimating the instantaneous gas-phase velocity is the major challenge in modeling particle motion. The new model of Hennick and Lightstone presented in this work derives an expression for the instantaneous gas-phase velocity experienced by a particle. This model is stochastic in nature: two particles with the same initial conditions will not see the same turbulent velocity fluctuations and will therefore experience different trajectories through the fluid.

The new model and Stochastic Separated Flow (SSF) models available in the literature were evaluated by considering the problem of dyed fluid particles released from a point source in homogeneous isotropic turbulence. Taylor (1921) derived an expression for the variance of particle position from mathematical considerations. Models were evaluated by extending the analysis of Taylor to each model. Long time dispersion results for each model were compared to Taylor's result for long time particle dispersion.

The new model was shown to exactly reproduce Taylor's result for the long time dispersion of dyed fluid particles in homogeneous isotropic turbulence. Each of the SSF models considered in this investigation could not reproduce Taylor's long time dispersion result with the exception of the model of Lightstone and Raithby (1996). This result is

not surprising since the derivation of the model of Lightstone and Raithby is based on the analytical work of Taylor for the problem of long time particle dispersion.

Models were also evaluated by comparing predictions with experimental results. The grid-turbulence experiments of Snyder and Lumley (1971) and Wells and Stock (1983) were simulated using the TASCflow CFD code. Predictions of particle dispersion and velocity decay were compared to experimental results.

The grid-turbulence experiments of Snyder and Lumley involved the release of single particles into a uniform flow of grid-generated turbulence. Three types of particles were considered in the simulation: small, light hollow glass beads that essentially acted like ‘fluid’ or ‘tracer’ particles, corn pollen particles which had more inertia and therefore did not follow the turbulence exactly, and copper beads which were the heaviest of the particles considered.

In the simulation of Snyder and Lumley’s experiment, the conventional SSF model of Gosman and Ioannides was the first model considered. Variations on this model as suggested by Shuen, Chen, and Faeth, and Lightstone and Raithby were also evaluated. Of these conventional models, the model of Lightstone and Raithby produced results closest to those reported by Snyder and Lumley. However, the predicted dispersion of the hollow glass beads exhibited waves; this was shown to be an inherent flaw in an approach where the eddy lifetime and characteristic eddy size are essentially deterministic.

Alternative methods of describing the gas-phase turbulence were explored by considering the models of Zhou and Leschziner and Hennick and Lightstone. While the model of Zhou and Leschziner produced satisfactory results for the hollow glass beads, the dispersion of heavier particles was greatly overpredicted. This result was partly attributed to the inability of Zhou and Leschziner’s model to capture the ‘crossing trajectory’ effect.

The model of Hennick and Lightstone compensates for the crossing trajectory effect by introducing a spatial correlation in the description of the gas-phase velocity fluctuation. This model predicted the dispersion of all particle types with the greatest accuracy of all models considered in this thesis in the simulation of Snyder and Lumley’s experiment.

The purpose of Wells and Stock’s investigation was to separate experimentally the effects of inertia from that of crossing trajectories. Particles were exposed to a potential field where the strength of field could be varied. Particles were charged and a uniform electric field was set up between two parallel plates in a wind tunnel. The electric field strength was sufficient to counter gravitational effects and to intensify the potential force. Single charged particles were released from a point source in grid-generated turbulence similar to Snyder and Lumley’s experiment. Wells and Stock examined the dispersion of solid glass beads of two different sizes: 5 and 57 μm in diameter.

Predicted dispersion of the the small particles using the SSF models indicated that the models are not sensitive to increasing gravitational force. Similarly, the time-correlated model of Zhou and Leschziner did not show sensitivity to increasing gravitational force for the small particle dispersion predictions. This result is supported by Wells and Stock who report that “the crossing trajectory effect appears to be negligible when the drift velocity is less than the rms fluid velocity,” (Wells and Stock (1983)). Additionally, the scatter of the dispersion measurements was less than the 10% reported experimental error.

The model of Hennick and Lightstone predicted decreased dispersion with increasing gravitational force for the small particle case. The model employs both a temporal and a spatial correlation in the description of the fluctuating velocity component of the instantaneous turbulent velocity. The spatial correlation is based on the relative velocity of the particle and is employed even when the drift velocity is less than the rms fluid velocity. Due to the experimental error of the measurements of Wells and Stock, further research is required to determine if the crossing trajectory effect is negligible under these conditions.

Predicted dispersion of the large particles using the SSF models showed a distinct decrease in dispersion with increasing gravitational force. Similarly, the model of Hennick and Lightstone showed sensitivity to increasing gravitational force for the large particle predictions. This result is consistent with the physical premise for the crossing trajectory effect: with increasing gravity, the particle experiences an increasing terminal velocity and may traverse each eddy faster than the eddy decay rate. By crossing the eddy, the particle is exposed to the instantaneous turbulent velocity for less time than if it had been captured by the eddy, and, as a result, dispersion decreases. Wells and Stock report that “the dispersion coefficient was found to decrease approximately as the drift velocity squared within the range of velocities tested,” (Wells and Stock (1983)).

Dispersion coefficients for the predictions of Zhou and Leschziner’s model for the large particle case indicated that the model is insensitive to increasing gravitational force. The model produced similar dispersion predictions for all gravity cases. The similarity arises from the description of the gas-phase velocity fluctuation used in the model. The model uses a temporal autocorrelation to describe the fluctuating gas-phase component. The correlation term depends only in the timestep employed and assumes that the particle is a dyed fluid particle. The large particle considered in Wells and Stock simulation had significant inertia and could not follow the high frequency fluctuations of the flow. As a result, the sole use of the temporal correlation led to velocity fluctuations that were highly correlated. The poor predictions were therefore attributed, at least in part, to the

inability of Zhou and Leschziner's model to capture the crossing trajectory effect.

This thesis has satisfied two main objectives:

- A new model has been developed to predict particle motion in turbulent flows.
- The predictions of the new model and existing SSF models have been compared using analysis and the benchmark grid-turbulence experiments of Snyder and Lumley (1971) and Wells and Stock (1983).

8.2 Recommendations for Future Work

While the model of Hennick and Lightstone produced promising results in this research, much work remains to be done. Recommendations for future work are as follows:

- Methods to account for the continuity effect in the new model should be studied. Continuity constrains the turbulence and requires that the longitudinal spatial integral length scale is two times the lateral spatial length scale, $L_f = 2L_g$. It is recommended that description of the gas-phase velocity fluctuation is modified to produce two distinct expressions for the velocity fluctuation: one for the free-fall direction, and one for the transverse direction, where the Lagrangian integral length scale used in the spatial correlation in each direction is required to satisfy continuity.
- Further research is required to determine the effect of crossing trajectories where the drift velocity is lower than the rms fluid velocity.
- The autocorrelation function is approximated using the exponential function. Further research is required to determine the impact of this approximation.
- Methods to account for the modulation of the gas-phase turbulence by the particles should be investigated.
- Finally, the model of Hennick and Lightstone should be validated over a wide range of flows such as pipes, jets, boundary layers and wakes.

Appendix A

Derivation of the Transit Time Equation

A.1 Derivation of the Transit Time Equation

Consider the particle equation of motion for low Reynolds number flow.

$$\frac{du_p}{dt} = \frac{u_g - u_p}{\tau_p} \quad (\text{A.1})$$

where u_g is the velocity of the gas-phase, u_p is the velocity of the particle, and τ_p is the particle relaxation time. Assuming u_g is constant and $u_p(0) = u_{p,o}$, solving Equation (A.1) yields

$$u_p(t) = u_g + (u_{p,o} - u_g)e^{-t/\tau_p} \quad (\text{A.2})$$

Integrating Equation (A.2) over a time period t gives

$$\int_0^t \frac{dx}{dt_1} dt_1 = \int_0^t \{u_g + (u_{p,o} - u_g)e^{-t_1/\tau_p}\} dt_1 \quad (\text{A.3})$$

where $x(t)$ is the position of the particle at time t .

$$\begin{aligned} x(t) - x(0) &= u_g t - \tau_p (u_{p,o} - u_g) e^{-t_1/\tau_p} \Big|_0^t \\ \underbrace{x(t) - x(0)}_I - \underbrace{u_g t}_{II} &= -\tau_p (u_{p,o} - u_g) (e^{-t/\tau_p} - 1) \end{aligned} \quad (\text{A.4})$$

The left hand side of Equation (A.4) can be explained as follows: term I is the distance that the particle travels during time t , and term II is the distance that the eddy travels during time t . The difference between term I and term II, denoted L , is then the distance

traveled by the particle relative to the eddy.

$$L = x(t) - x(0) - u_g t \quad (\text{A.5})$$

Thus Equation (A.4) becomes

$$L = -\tau_p(u_{p,o} - u_g)(e^{-t/\tau_p} - 1) \quad (\text{A.6})$$

If a particle crosses an eddy, than the distance L that the particle travels is equal to the characteristic eddy length, l_e , and the time is the time required for the particle to cross the eddy. That time interval is referred to as the particle transit time, t_{tr} . Solving Equation (A.6) for the particle transit time yields

$$t_{tr} = -\tau_p \ln \left(1 - \frac{l_e}{\tau_p(u_{p,o} - u_g)} \right) \quad (\text{A.7})$$

Appendix B

Post Processing of the Snyder and Lumley Simulation

The experiments of Snyder and Lumley (1971) were simulated using the TASCflow CFD Code. Measurements of particle dispersion and velocity decay were compared to results generated by each model considered in this thesis. This appendix outlines how particle trajectories generated by TASCflow are processed in order to compare predictions of particle velocity and displacement to the experimental results of Snyder and Lumley.

A series of filters are performed on each particle trajectory to produce trajectories with values for position and velocity at each instant in time. The mean and variance of particle position and velocity are calculated.

B.1 Filtering

Figure 6.1 shows a diagram of Snyder and Lumley's experiment. Turbulence was generated using a grid with $M = 2.54$ cm spacing. Single particles were injected at $x/M = 20$ and tracked photographically from $x/M = 68$ to 168 allowing 48 mesh lengths to ensure that particle velocities were independent of the injected velocity. Photographs were digitized and particle velocity and displacement determined with respect to time. Section 6.1 outlines the experiment of Snyder and Lumley in detail.

The simulation requires that particles are released from $x/M = 30$. Particles are tracked using a Lagrangian formulation; the numerical solution of the particle equation of motion is outlined in Section 4.2. As described in Section 4.2, a computational timestep is selected based on particle position within a control volume; a particle cannot exit an octant and enter an adjacent octant during a single computational timestep. This

method of calculation results in information on the position and velocity of each particle to be written to a file at each computational timestep. As a result, the time series of a particle trajectory is unique. The objective of the following filters is to standardize particle information with a single time series beginning at $t = 0$ at the position of the first camera. The position and velocity information for each particle is linearly interpolated to yield information from $t = 0$ in increments of 0.005 s until the particle exits the duct.

The following filter linearly interpolates particle information for each trajectory to ensure that values for time, particle position, and velocity are available at the axial location of the first camera, $x/M = 68$, a physical location of $x = 0.97536$. It is important to note that particle trajectories are written as follows: time, x, y, z, u, v, w. All filters use awk, a pattern scanning and processing language that executes commands on each line of a file.

```
BEGIN {wanted_x=.97536; switch=0; old_time=0; old_x=0;\
old_y=0; old_z=0; old_u=0; old_v=0; old_w=0} {\
current_time=$1;\
current_x=$2;\
current_y=$3;\
current_z=$4;\
current_u=$5;\
current_v=$6;\
current_w=$7;\
if (($2 > wanted_x)&&(switch==0)){\
switch=1;\
next}\
if (($2 > wanted_x)&&(switch==1)) {\
wanted_time=(wanted_x-old_x)*(current_time-old_time)/\
    (current_x-old_x)+old_time;\
wanted_y=(wanted_x-old_x)*(current_y-old_y)/(current_x-old_x)+old_y;\
wanted_z=(wanted_x-old_x)*(current_z-old_z)/(current_x-old_x)+old_z;\
wanted_u=(wanted_x-old_x)*(current_u-old_u)/(current_x-old_x)+old_u;\
wanted_v=(wanted_x-old_x)*(current_v-old_v)/(current_x-old_x)+old_v;\
wanted_w=(wanted_x-old_x)*(current_w-old_w)/(current_x-old_x)+old_w;\
printf("%12.8f %12.8f %12.8f %12.8f %12.8f %12.8f %12.8f\n",\
    wanted_time, wanted_x, wanted_y, wanted_z, wanted_u,\
    wanted_v, wanted_w);\
}
```

```

old_time=current_time;\
old_x=current_x;\
old_y=current_y;\
old_z=current_z;\
old_u=current_u;\
old_v=current_v;\
old_w=current_w;\
switch=2;\
}\
else {\
old_time=current_time;\
old_x=current_x;\
old_y=current_y;\
old_z=current_z;\
old_u=current_u;\
old_v=current_v;\
old_w=current_w;\
printf("%12.8f %12.8f %12.8f %12.8f %12.8f %12.8f %12.8f\n",
        current_time, current_x, current_y, current_z, current_u,
        current_v, current_w);\
}\
if ($2 == wanted_x){\
wanted_time=current_time;\
wanted_x=current_x;\
wanted_y=current_y;\
wanted_z=current_z;\
wanted_u=current_u;\
wanted_v=current_v;\
wanted_w=current_w;\
printf("%12.8f %12.8f %12.8f %12.8f %12.8f %12.8f %12.8f\n",
        wanted_time, wanted_x, wanted_y, wanted_z, wanted_u,
        wanted_v, wanted_w);\
old_time=current_time;\
old_x=current_x;\
old_y=current_y;\
old_z=current_z;\

```

```

old_u=current_u;\
old_v=current_v;\
old_w=current_w;\
}\
}

```

Snyder and Lumley set particle displacement to zero at $t = 0$ at the position of the first camera. The following filters the data by removing particle information before the first camera position. It also adjusts the particle information so that particles are released from a point at the position of the first camera; the filter stores the time, x , y , and z at $t = 0$ and subtracts these values from particle information for $t > 0$.

```

BEGIN {wanted_x=.97536}{\
current_time=$1;\
current_x=$2;\
current_y=$3;\
current_z=$4;\
current_u=$5;\
current_v=$6;\
current_w=$7;\
if (current_x == wanted_x) {\
time=$1;\
x=$2;\
y=$3;\
z=$4;\
current_time=0.0
current_x=0.0
current_y=0.0
current_z=0.0
printf("%12.8f %12.8f %12.8f %12.8f %12.8f %12.8f %12.8f\n",
        current_time, current_x, current_y, current_z, current_u,
        current_v, current_w);\
}\
if (current_x > wanted_x) {\
current_time=current_time - time;\
current_x=current_x - x;\
current_y=current_y - y;\

```

```

current_z=current_z - z;\
printf("%12.8f %12.8f %12.8f %12.8f %12.8f %12.8f %12.8f\n",
      current_time, current_x, current_y, current_z, current_u,
      current_v, current_w);\
}\
}

```

The following filter standardizes particle information with a single time series. The position and velocity are interpolated to yield information from $t = 0$ in increments of 0.005 s until the particle exits the duct. A typical particle will remain in the duct for approximately 0.5 s. Linear interpolation is justified: particle trajectories are reduced from approximately 595 lines of information to 98 lines.

```

BEGIN {wanted_time=0.005; increment=0.005; old_time=0; old_x=0;\
old_y=0; old_z=0; old_u=0; old_v=0; old_w=0} {\
current_time=$1;\
current_x=$2;\
current_y=$3;\
current_z=$4;\
current_u=$5;\
current_v=$6;\
current_w=$7;\
if ($1 > wanted_time) {\
wanted_x=(wanted_time-old_time)*(current_x-old_x)/
      (current_time-old_time)+old_x;\
wanted_y=(wanted_time-old_time)*(current_y-old_y)/
      (current_time-old_time)+old_y;\
wanted_z=(wanted_time-old_time)*(current_z-old_z)/
      (current_time-old_time)+old_z;\
wanted_u=(wanted_time-old_time)*(current_u-old_u)/
      (current_time-old_time)+old_u;\
wanted_v=(wanted_time-old_time)*(current_v-old_v)/
      (current_time-old_time)+old_v;\
wanted_w=(wanted_time-old_time)*(current_w-old_w)/
      (current_time-old_time)+old_w;\
printf("%12.8f %12.8f %12.8f %12.8f %12.8f %12.8f %12.8f\n",
      wanted_time, wanted_x, wanted_y, wanted_z, wanted_u,

```

```

        wanted_v, wanted_w);\
old_time=current_time;\
old_x=current_x;\
old_y=current_y;\
old_z=current_z;\
old_u=current_u;\
old_v=current_v;\
old_w=current_w;\
wanted_time=wanted_time+increment;\
}\
else {\
old_time=current_time;\
old_x=current_x;\
old_y=current_y;\
old_z=current_z;\
old_u=current_u;\
old_v=current_v;\
old_w=current_w;\
}\
if ($1 == wanted_time){\
wanted_time=current_time;\
wanted_x=current_x;\
wanted_y=current_y;\
wanted_z=current_z;\
wanted_u=current_u;\
wanted_v=current_v;\
wanted_w=current_w;\
printf("%12.8f %12.8f %12.8f %12.8f %12.8f %12.8f %12.8f\n",
        wanted_time, wanted_x, wanted_y, wanted_z, wanted_u,
        wanted_v, wanted_w);\
wanted_time=wanted_time+increment;\
old_time=current_time;\
old_x=current_x;\
old_y=current_y;\
old_z=current_z;\
old_u=current_u;\

```



```

old_v=current_v;\
old_w=current_w;\
}\
}

```

B.2 Calculations

This section provides the programs that calculate the mean and variance of particle position and velocity. These calculations can only be performed after the data has been filtered as described in the previous section. In the following programs, filtered particle files are named `part_filt.#` where `#` is the particle number. Programs are written in Fortran.

The following program calculates the mean of particle position and velocity at each instance in time. Mean values are written to the file `mean.dat`.

```

*      file mean.f
*****
*
*
*      OPENS FILTERED PARTICLE FILES TO AVERAGE COLUMN VALUES AT EACH
*      INSTANCE IN TIME
*
*****
*
*
      IMPLICIT NONE
*
      INTEGER ID,JD,I,J,NP
      PARAMETER(ID=102)
      PARAMETER(NP=780)
      REAL TIME(ID),X(ID),Y(ID),Z(ID),U(ID),V(ID),W(ID)
      REAL OLDX(ID),OLDY(ID),OLDZ(ID),OLDU(ID),OLDV(ID),
&      OLDW(ID)

      INTEGER IFILE,PART,NOL,L
      CHARACTER *16 NAMES(NP)

```

```

*
* -----
*   Start program main
*
      NOL=98
*   IFILE=11
*
      OPEN(55, FILE='part_names')
      DO 20 J=1,NP
        IF ( J .LE. 9) THEN
          WRITE(55,100) 'part_filt.',J
        ENDIF
        IF (J .LT. 100) THEN
          IF (J .GE. 10) THEN
            WRITE(55,105) 'part_filt.',J
          ENDIF
        ENDIF
        IF (J .LT. 1000) THEN
          IF (J .GE. 100) THEN
            WRITE(55,110) 'part_filt.',J
          ENDIF
        ENDIF
        IF (J .GE. 1000) THEN
          WRITE(55,115) 'part_filt.',J
        ENDIF
20      CONTINUE

      close(55)

      OPEN(55, FILE='part_names')

      DO 22 J=1,NP
        IF ( J .LE. 9) THEN
          READ(55,101) NAMES(J)
        ENDIF
        IF (J .LT. 100) THEN

```

```

        IF (J .GE. 10) THEN
            READ(55,106) NAMES(J)
        ENDIF
    ENDIF
    IF (J .LT. 1000) THEN
        IF (J .GE. 100) THEN
            READ(55,111) NAMES(J)
        ENDIF
    ENDIF
    IF (J .GE. 1000) THEN
        READ(55, 116) NAMES(J)
    ENDIF
22  CONTINUE

    close(55)

100  FORMAT(1X,A10,I1)
101  FORMAT(1X,A12)
105  FORMAT(1X,A10,I2)
106  FORMAT(1X,A13)
110  FORMAT(1X,A10,I3)
111  FORMAT(1X,A14)
115  FORMAT(1X,A10,I4)
116  FORMAT(1X,A15)

*    Begins a loop to open all particle files.
    DO 167 L=1,N01
        oldx(1)=0.0
        oldy(1)=0.0
        oldz(1)=0.0
        oldu(1)=0.0
        oldv(1)=0.0
        oldw(1)=0.0
167  CONTINUE
    DO 10 PART=1,NP
        IFILE=16

```

```

      OPEN(IFILE,FILE=NAMES(PART))
      DO 30 L=1,NOL
      READ(IFILE,200)TIME(L),X(L),Y(L),Z(L),U(L),V(L),W(L)
          OLDX(L)=X(L)+OLDX(L)
          OLDY(L)=Y(L)+OLDY(L)
          OLDZ(L)=Z(L)+OLDZ(L)
          OLDU(L)=U(L)+OLDU(L)
          OLDDV(L)=V(L)+OLDDV(L)
          OLDW(L)=W(L) + OLDW(L)
30      CONTINUE
          CLOSE(IFILE)
10      CONTINUE
200      FORMAT(7f13.8)
201      FORMAT(7e14.6)
202      format(3e14.6)

      OPEN(75, FILE='mean.dat')
      DO 40 L=1,NOL
      OLDX(L)=OLDX(L)/NP
      OLDY(L)=OLDY(L)/NP
      OLDZ(L)=OLDZ(L)/NP
      OLDU(L)=OLDU(L)/NP
      OLDDV(L)=OLDDV(L)/NP
      OLDW(L)=OLDW(L)/NP
      WRITE(75,201) TIME(L),OLDX(L),OLDY(L),OLDZ(L),
C  OLDU(L),OLDDV(L),OLDW(L)
40      CONTINUE

      CLOSE(75)

      STOP
      END

```

The following program calculates the variance of particle position and velocity at each instance in time. Values for time, $\overline{y^2}$ and $\overline{v^2}$ are written to the file **final.dat**; values for the variance of particle position and velocity are written to the file **stddev.dat**.

```

*      file final.f
*****
*
*
*      OPENS FILTERED PARTICLE FILES TO AVERAGE COLUMN VALUES AT EACH
*      INSTANCE IN TIME
*
*****
*
*
*
      IMPLICIT NONE
*
      INTEGER ID,J,NP
      PARAMETER(ID=102)
      PARAMETER(NP=780)
      REAL TIME(ID),X(ID),Y(ID),Z(ID),U(ID),V(ID),W(ID)
      REAL TB(ID),XB(ID),YB(ID),ZB(ID),UB(ID),VB(ID),WB(ID)
      REAL OLDX(ID),OLDY(ID),OLDZ(ID),OLDU(ID),OLDV(ID),OLDW(ID)
      REAL PLOTV(ID), PLOTY(ID)

      INTEGER IFILE,PART,NOL,L
      CHARACTER *16 NAMES(NP)
*
*
*      -----
*      Start program main
*
      NOL=98
*      IFILE=11
*

      OPEN(55, FILE='part_names')
      DO 20 J=1,NP
        IF ( J .LE. 9) THEN
          WRITE(55,100) 'part_filt.',J

```

```

ENDIF
IF (J .LT. 100) THEN
  IF (J .GE. 10) THEN
    WRITE(55,105) 'part_filt.',J
  ENDIF
ENDIF
IF (J .LT. 1000) THEN
  IF (J .GE. 100) THEN
    WRITE(55,110) 'part_filt.',J
  ENDIF
ENDIF
IF (J .GE. 1000) THEN
  WRITE(55,115) 'part_filt.',J
ENDIF
20 CONTINUE

close(55)

OPEN(55, FILE='part_names')

DO 22 J=1,NP
  IF ( J .LE. 9) THEN
    READ(55,101) NAMES(J)
  ENDIF
  IF (J .LT. 100) THEN
    IF (J .GE. 10) THEN
      READ(55,106) NAMES(J)
    ENDIF
  ENDIF
  IF (J .LT. 1000) THEN
    IF (J .GE. 100) THEN
      READ(55,111) NAMES(J)
    ENDIF
  ENDIF
  IF (J .GE. 1000) THEN
    READ(55, 116) NAMES(J)

```

```

                ENDIF
22      CONTINUE

100      FORMAT(1X,A10,I1)
101      FORMAT(1X,A12)
105      FORMAT(1X,A10,I2)
106      FORMAT(1X,A13)
110      FORMAT(1X,A10,I3)
111      FORMAT(1X,A14)
115      FORMAT(1X,A10,I4)
116      FORMAT(1X,A15)

        DO 167 L=1,N01
            oldx(1)=0.0
            oldy(1)=0.0
            oldz(1)=0.0
            oldu(1)=0.0
            oldv(1)=0.0
            oldw(1)=0.0
167      CONTINUE
*      Begins a loop to open all particle files.
        DO 10 PART=1,NP
            IFILE=16
            OPEN(75, FILE='mean.dat')
            OPEN(IFILE,FILE=NAMES(PART))
            DO 30 L=1,N0L
                READ(75,201)TB(L),XB(L),YB(L),ZB(L),UB(L),VB(L),WB(L)
                READ(IFILE,200)TIME(L),X(L),Y(L),Z(L),U(L),V(L),W(L)
                    OLDX(L)=(X(L)-XB(L))**2.0+OLDX(L)
                    OLDY(L)=(Y(L)-YB(L))**2.0+OLDY(L)
                    OLDZ(L)=(Z(L)-ZB(L))**2.0+OLDZ(L)
                    OLDU(L)=(U(L)-UB(L))**2.0+OLDU(L)
                    OLDV(L)=(V(L)-VB(L))**2.0+OLDV(L)
                    OLDW(L)=(W(L)-WB(L))**2.0+OLDW(L)
30          CONTINUE

```

```

        CLOSE(IFILE)
        CLOSE(75)
10      CONTINUE
200     FORMAT(7f13.8)
201     FORMAT(7e14.6)
202     FORMAT(3e14.6)

        OPEN(65, FILE='stddev.dat')
        OPEN(67, FILE='final.dat')
        DO 40 L=1,NOL
            OLDX(L)=OLDX(L)/(NP-1)
            OLDY(L)=OLDY(L)/(NP-1)
            OLDZ(L)=OLDZ(L)/(NP-1)
            OLDU(L)=OLDU(L)/(NP-1)
            OLDDV(L)=OLDDV(L)/(NP-1)
            OLDW(L)=OLDW(L)/(NP-1)
            PLOTY(L)=OLDY(L)
            PLOTV(L)=(6.55)**2/(OLDDV(L))
            WRITE(65,201) TIME(L),OLDX(L),OLDY(L),OLDZ(L),
C      OLDU(L),OLDDV(L),OLDW(L)
            WRITE(67,202) TIME(L),PLOTY(L),PLOTV(L)
40      CONTINUE

        CLOSE(65)
        CLOSE(67)

        STOP
        END

```


Appendix C

Post Processing of the Wells and Stock Simulation

The experiments of Wells and Stock (1983) were simulated using the TASCflow CFD Code. Measurements of particle dispersion and velocity decay were compared to results generated by each model considered in this thesis. This appendix outlines how particle trajectories generated by TASCflow are processed in order to compare predictions of particle velocity and displacement to the experimental results of Wells and Stock.

A series of filters are performed on each particle trajectory to produce trajectories with values for position and velocity at each instant in time. The mean and variance of particle position and velocity are calculated.

C.1 Filtering

Figure 7.1 shows a diagram of Wells and Stock's experiment. Turbulence was generated using a grid with $M = 2.54$ cm spacing. Single particles were injected at $x/M = 15$ and tracked using a Laser Doppler Anemometer from $x/M = 20$ to 90. Particle velocity and displacement determined with respect to position. Section 7.1 outlines the experiment of Wells and Stock in detail.

The simulation requires that particles are released from $x/M = 15$. Particles are tracked using a Lagrangian formulation; the numerical solution of the particle equation of motion is outlined in Section 4.2. As described in Section 4.2, a computational timestep is selected based on particle position within a control volume; a particle cannot exit an octant and enter an adjacent octant during a single computational timestep. This method of calculation results in information on the position and velocity of each particle

to be written to a file at each computational timestep. As a result, the time series of a particle trajectory is unique. The objective of the following filters is to standardize particle information with a single series based on position in normalized coordinates of x/M beginning at $x/M = 20$, the position of the first measurement. The position and velocity information for each particle is linearly interpolated to yield information from $x/M = 20$ in increments of 1 until the particle exits the duct.

The following filter linearly interpolates particle information for each trajectory to ensure that values for time, particle position, and velocity are available at the axial location of the first measurement, $x/M = 20$, a physical location of $x = 0.127$. It is important to note that particle trajectories are written as follows: time, x, y, z, u, v, w. All filters use awk, a pattern scanning and processing language that executes commands on each line of a file.

```
BEGIN {wanted_x=.127; switch=0; old_time=0; old_x=0;\
old_y=0; old_z=0; old_u=0; old_v=0; old_w=0} {\
current_time=$1;\
current_x=$2;\
current_y=$3;\
current_z=$4;\
current_u=$5;\
current_v=$6;\
current_w=$7;\
if (($2 > wanted_x)&&(switch==0)){\
switch=1;\
next}\
if (($2 > wanted_x)&&(switch==1)) {\
wanted_time=(wanted_x-old_x)*(current_time-old_time)/\
    (current_x-old_x)+old_time;\
wanted_y=(wanted_x-old_x)*(current_y-old_y)/(current_x-old_x)+old_y;\
wanted_z=(wanted_x-old_x)*(current_z-old_z)/(current_x-old_x)+old_z;\
wanted_u=(wanted_x-old_x)*(current_u-old_u)/(current_x-old_x)+old_u;\
wanted_v=(wanted_x-old_x)*(current_v-old_v)/(current_x-old_x)+old_v;\
wanted_w=(wanted_x-old_x)*(current_w-old_w)/(current_x-old_x)+old_w;\
printf("%12.8f %12.8f %12.8f %12.8f %12.8f %12.8f %12.8f\n",\
    wanted_time, wanted_x, wanted_y, wanted_z, wanted_u,\
    wanted_v, wanted_w);\
}
```

```
old_time=current_time;\
old_x=current_x;\
old_y=current_y;\
old_z=current_z;\
old_u=current_u;\
old_v=current_v;\
old_w=current_w;\
switch=2;\
}\
else {\
old_time=current_time;\
old_x=current_x;\
old_y=current_y;\
old_z=current_z;\
old_u=current_u;\
old_v=current_v;\
old_w=current_w;\
printf("%12.8f %12.8f %12.8f %12.8f %12.8f %12.8f %12.8f\n",
      current_time, current_x, current_y, current_z, current_u,
      current_v, current_w);\
}\
if ($2 == wanted_x){\
wanted_time=current_time;\
wanted_x=current_x;\
wanted_y=current_y;\
wanted_z=current_z;\
wanted_u=current_u;\
wanted_v=current_v;\
wanted_w=current_w;\
printf("%12.8f %12.8f %12.8f %12.8f %12.8f %12.8f %12.8f\n",
      wanted_time, wanted_x, wanted_y, wanted_z, wanted_u,
      wanted_v, wanted_w);\
old_time=current_time;\
old_x=current_x;\
old_y=current_y;\
old_z=current_z;\
```

```

old_u=current_u;\
old_v=current_v;\
old_w=current_w;\
}\
}

```

The following filters the data by removing particle information before the first measurement, $x/M = 20$. It also sets time equal to zero at the position of the first measurement.

```

BEGIN {wanted_x=.127}{\
current_time=$1;\
current_x=$2;\
current_y=$3;\
current_z=$4;\
current_u=$5;\
current_v=$6;\
current_w=$7;\
if (current_x == wanted_x) {\
time=$1;\
x=$2;\
current_time=0.0
current_x=wanted_x
printf("%12.8f %12.8f %12.8f %12.8f %12.8f %12.8f %12.8f\n",
        current_time, current_x, current_y, current_z, current_u,
        current_v, current_w);\
}\
if (current_x > wanted_x) {\
current_time=current_time - time;\
current_x=current_x;\
printf("%12.8f %12.8f %12.8f %12.8f %12.8f %12.8f %12.8f\n",
        current_time, current_x, current_y, current_z, current_u,
        current_v, current_w);\
}\
}

```

The following filter standardizes particle information with a series based on position. The position and velocity are interpolated to yield information from $t = 0$ at the normal-

ized position of the first measurement at $x/M = 20$ in increments of normalized position $x/M = 1$ until the particle exits the duct. A typical particle will remain in the duct for approximately 0.5 s. Linear interpolation is justified; particle trajectories are reduced from approximately 595 lines of information to 73 lines.

```
BEGIN {wanted_x=.127; increment=.0254; old_time=0; old_x=0;\
old_y=0; old_z=0; old_u=0; old_v=0; old_w=0; old_xoverm=0} {\
current_time=$1;\
current_x=$2;\
current_y=$3;\
current_z=$4;\
current_u=$5;\
current_v=$6;\
current_w=$7;\
current_xoverm=$2/.0254+15;\
if ($2 > wanted_x) {\
wanted_time=(wanted_x-old_x)*(current_time-old_time)/\
    (current_x-old_x)+old_time;\
wanted_y=(wanted_x-old_x)*(current_y-old_y)/(current_x-old_x)+old_y;\
wanted_z=(wanted_x-old_x)*(current_z-old_z)/(current_x-old_x)+old_z;\
wanted_u=(wanted_x-old_x)*(current_u-old_u)/(current_x-old_x)+old_u;\
wanted_v=(wanted_x-old_x)*(current_v-old_v)/(current_x-old_x)+old_v;\
wanted_w=(wanted_x-old_x)*(current_w-old_w)/(current_x-old_x)+old_w;\
wanted_xoverm=(wanted_x-old_x)*(current_xoverm-old_xoverm)/\
    (current_x-old_x)+old_xoverm;\
printf("%12.8f %12.8f %12.8f %12.8f %12.8f %12.8f %12.8f %12.8f\n",\
    wanted_time, wanted_x, wanted_y, wanted_z, wanted_u, wanted_v,\
    wanted_w, wanted_xoverm);\
old_time=current_time;\
old_x=current_x;\
old_y=current_y;\
old_z=current_z;\
old_u=current_u;\
old_v=current_v;\
old_w=current_w;\
old_xoverm=current_xoverm;\
```

```
wanted_x=wanted_x+increment;\
}\
else {\
old_time=current_time;\
old_x=current_x;\
old_y=current_y;\
old_z=current_z;\
old_u=current_u;\
old_v=current_v;\
old_w=current_w;\
old_xoverm=current_xoverm;\
}\
if ($2 == wanted_x){\
wanted_time=current_time;\
wanted_x=current_x;\
wanted_y=current_y;\
wanted_z=current_z;\
wanted_u=current_u;\
wanted_v=current_v;\
wanted_w=current_w;\
wanted_xoverm=current_xoverm;\
printf("%12.8f %12.8f %12.8f %12.8f %12.8f %12.8f %12.8f %12.8f\n",
        wanted_time, wanted_x, wanted_y, wanted_z, wanted_u, wanted_v,
        wanted_w, wanted_xoverm);\
wanted_x=wanted_x+increment;\
old_time=current_time;\
old_x=current_x;\
old_y=current_y;\
old_z=current_z;\
old_u=current_u;\
old_v=current_v;\
old_w=current_w;\
old_xoverm=current_xoverm;\
}\
}
```

C.2 Calculations

This section provides the programs that calculate the mean and variance of particle position and velocity. These calculations can only be performed after the data has been filtered as described in the previous section. In the following programs, filtered particle files are named `part_filt.#` where `#` is the particle number. Programs are written in Fortran.

The following program calculates the mean of particle position and velocity at each normalized x/M position. Mean values are written to the file `mean.dat`.

```
*      file mean.f
*****
*
*
*      OPENS FILTERED PARTICLE FILES TO AVERAGE COLUMN VALUES AT EACH
*      X/M POSITION
*
*****
*
*
      IMPLICIT NONE
*
      INTEGER ID,JD,I,J,NP
      PARAMETER(ID=102)
      PARAMETER(NP=780)
      REAL TIME(ID),X(ID),Y(ID),Z(ID),U(ID),V(ID),W(ID),XOVERM(ID)
      REAL OLDTIME(ID),OLDY(ID),OLDZ(ID),OLDU(ID),OLDV(ID),
&      OLDW(ID)

      INTEGER IFILE,PART,NOL,L
      CHARACTER *16 NAMES(NP)
*
*
*      -----
*      Start program main
*
      NOL=74
```

*

```
OPEN(55, FILE='part_names')
DO 20 J=1,NP
  IF ( J .LE. 9) THEN
    WRITE(55,100) 'part_filt.',J
  ENDIF
  IF (J .LT. 100) THEN
    IF (J .GE. 10) THEN
      WRITE(55,105) 'part_filt.',J
    ENDIF
  ENDIF
  IF (J .LT. 1000) THEN
    IF (J .GE. 100) THEN
      WRITE(55,110) 'part_filt.',J
    ENDIF
  ENDIF
  IF (J .GE. 1000) THEN
    WRITE(55,115) 'part_filt.',J
  ENDIF
20 CONTINUE

close(55)

OPEN(55, FILE='part_names')

DO 22 J=1,NP
  IF ( J .LE. 9) THEN
    READ(55,101) NAMES(J)
  ENDIF
  IF (J .LT. 100) THEN
    IF (J .GE. 10) THEN
      READ(55,106) NAMES(J)
    ENDIF
  ENDIF
  IF (J .LT. 1000) THEN
```



```
        IF (J .GE. 100) THEN
          READ(55,111) NAMES(J)
        ENDIF
      ENDIF
      IF (J .GE. 1000) THEN
        READ(55, 116) NAMES(J)
      ENDIF
22    CONTINUE

      close(55)

100    FORMAT(1X,A10,I1)
101    FORMAT(1X,A12)
105    FORMAT(1X,A10,I2)
106    FORMAT(1X,A13)
110    FORMAT(1X,A10,I3)
111    FORMAT(1X,A14)
115    FORMAT(1X,A10,I4)
116    FORMAT(1X,A15)

*      Begins a loop to open all particle files.
      DO 167 L=1,N01
        oldTIME(1)=0.0
        oldy(1)=0.0
        oldz(1)=0.0
        oldu(1)=0.0
        oldv(1)=0.0
        oldw(1)=0.0
167    CONTINUE
      DO 10 PART=1,NP
        IFILE=16
        OPEN(IFILE,FILE=NAMES(PART))
        DO 30 L=1,NOL
          READ(IFILE,200)TIME(L),X(L),Y(L),Z(L),U(L),V(L),W(L),XOVERM(L)
          OLDTIME(L)=TIME(L)+OLDTIME(L)
```

```

        OLDY(L)=Y(L)+OLDY(L)
        OLDZ(L)=Z(L)+OLDZ(L)
        OLDU(L)=U(L)+OLDU(L)
        OLDV(L)=V(L)+OLDV(L)
        OLDW(L)=W(L) + OLDW(L)
30      CONTINUE
        CLOSE(IFILE)
10      CONTINUE

200     FORMAT(8f13.8)
201     FORMAT(8e14.6)
202     FORMAT(3e14.6)

        OPEN(75, FILE='mean.dat')
        DO 40 L=1,NOL
        OLDTIME(L)=OLDTIME(L)/NP
        OLDY(L)=OLDY(L)/NP
        OLDZ(L)=OLDZ(L)/NP
        OLDU(L)=OLDU(L)/NP
        OLDV(L)=OLDV(L)/NP
        OLDW(L)=OLDW(L)/NP
        WRITE(75,201) OLDTIME(L),X(L),OLDY(L),OLDZ(L),
C  OLDU(L),OLDV(L),OLDW(L),XOVERM(L)
40      CONTINUE

        CLOSE(75)

        STOP
        END

```

The following program calculates the variance of particle position and velocity at each x/M position. Values for time, $\overline{y^2}$, $\overline{v^2}$ and x/M are written to the file `final.dat`; values for the variance of particle position and velocity are written to the file `stddev.dat`.

```

*      file final.f
*****

```

```
*
*
*   OPENS FILTERED PARTICLE FILES TO AVERAGE COLUMN VALUES AT EACH
*   X/M POSITION
*
*****
*
*
*   IMPLICIT NONE
*
*   INTEGER ID,J,NP
*   PARAMETER(ID=102)
*   PARAMETER(NP=780)
*   REAL TIME(ID),X(ID),Y(ID),Z(ID),U(ID),V(ID),W(ID),XOVERM(ID)
*   REAL TB(ID),XB(ID),YB(ID),ZB(ID),UB(ID),VB(ID),WB(ID)
*   REAL OLDTIME(ID),OLDY(ID),OLDZ(ID),OLDU(ID),OLDV(ID),OLDW(ID)
*   REAL PLOTV(ID), PLOTY(ID)
*
*   INTEGER IFILE,PART,NOL,L
*   CHARACTER *16 NAMES(NP)
*
*
*   -----
*   Start program main
*
*   NOL=74
*
*
*   OPEN(55, FILE='part_names')
*   DO 20 J=1,NP
*     IF ( J .LE. 9) THEN
*       WRITE(55,100) 'part_filt.',J
*     ENDIF
*     IF (J .LT. 100) THEN
*       IF (J .GE. 10) THEN
*         WRITE(55,105) 'part_filt.',J
```

```
ENDIF
ENDIF
IF (J .LT. 1000) THEN
    IF (J .GE. 100) THEN
        WRITE(55,110) 'part_filt.',J
    ENDIF
ENDIF
IF (J .GE. 1000) THEN
    WRITE(55,115) 'part_filt.',J
ENDIF
20 CONTINUE

close(55)

OPEN(55, FILE='part_names')

DO 22 J=1,NP
    IF ( J .LE. 9) THEN
        READ(55,101) NAMES(J)
    ENDIF
    IF (J .LT. 100) THEN
        IF (J .GE. 10) THEN
            READ(55,106) NAMES(J)
        ENDIF
    ENDIF
    IF (J .LT. 1000) THEN
        IF (J .GE. 100) THEN
            READ(55,111) NAMES(J)
        ENDIF
    ENDIF
    IF (J .GE. 1000) THEN
        READ(55, 116) NAMES(J)
    ENDIF
22 CONTINUE
```

```
100    FORMAT(1X,A10,I1)
101    FORMAT(1X,A12)
105    FORMAT(1X,A10,I2)
106    FORMAT(1X,A13)
110    FORMAT(1X,A10,I3)
111    FORMAT(1X,A14)
115    FORMAT(1X,A10,I4)
116    FORMAT(1X,A15)

      DO 167 L=1,N01
        oldTIME(1)=0.0
        oldy(1)=0.0
        oldz(1)=0.0
        oldu(1)=0.0
        oldv(1)=0.0
        oldw(1)=0.0
167    CONTINUE
      DO 10 PART=1,NP
        IFILE=16
        OPEN(75, FILE='mean.dat')
        OPEN(IFILE,FILE=NAMES(PART))
        DO 30 L=1,NOL
          READ(75,201)TB(L),XB(L),YB(L),ZB(L),UB(L),VB(L),WB(L),XOVERM(L)
          READ(IFILE,200)TIME(L),X(L),Y(L),Z(L),U(L),V(L),W(L)
            OLDTIME(L)=(TIME(L)-TB(L))*2.0+OLDTIME(L)
            OLDY(L)=(Y(L)-YB(L))*2.0+OLDY(L)
            OLDZ(L)=(Z(L)-ZB(L))*2.0+OLDZ(L)
            OLDU(L)=(U(L)-UB(L))*2.0+OLDU(L)
            OLDV(L)=(V(L)-VB(L))*2.0+OLDV(L)
            OLDW(L)=(W(L)-WB(L))*2.0+OLDW(L)
30      CONTINUE
        CLOSE(IFILE)
        CLOSE(75)
10    CONTINUE
```

```

200    FORMAT(8f13.8)
201    FORMAT(8e14.6)
202    FORMAT(4e14.6)

      OPEN(65, FILE='stddev.dat')
      OPEN(67, FILE='final.dat')
      DO 40 L=1,NOL
      OLDTIME(L)=OLDTIME(L)/(NP-1)
      OLDY(L)=OLDY(L)/(NP-1)
      OLDZ(L)=OLDZ(L)/(NP-1)
      OLDU(L)=OLDU(L)/(NP-1)
      OLDDV(L)=OLDDV(L)/(NP-1)
      OLDW(L)=OLDW(L)/(NP-1)
      PLOTY(L)=OLDY(L)
      PLOTV(L)=(6.55)**2/(OLDDV(L))
      WRITE(65,201) OLDTIME(L),X(L),OLDY(L),OLDZ(L),
C     OLDU(L),OLDDV(L),OLDW(L),XOVERM(L)
      WRITE(67,202) OLDTIME(L),PLOTY(L),PLOTV(L),XOVERM(L)
40    CONTINUE

      CLOSE(65)
      CLOSE(67)

      STOP
      END

```

C.3 Adjustment of Particle Dispersion Results

Due to a lack information about particle initial conditions, particle dispersion results were adjusted to reflect the dispersion reported by Wells and Stock (1983) at the position of the first camera. Appendix D shows that the addition of a constant to the variance of position is mathematically equivalent to releasing particles with a Gaussian distribution of zero mean and specified variance.

The following program calculates the difference between the predicted and reported variance at $x/M = 20$ and adds the difference to the predicted variance along the length of

the duct. Note that the initial variance is specific to the particle type and gravitational force applied. This program was written to adjust results for the big particle under zero gravity conditions. This program was written using awk, a pattern scanning and processing language that executes commands on each line of a file.

```
BEGIN {value=.8125e-4; switch=0; increment = 0} {\
current_time=$1;\
current_y=$3;\
current_v=$6;\
current_xoverm=$8;\
if (switch == 0) {\
increment = value - current_y;\
new_y=current_y+increment;\
switch = 1;\
}\
else {\
new_y=current_y+increment;\
}\
printf("%12.8f %12.8f %12.8f %12.8f %12.8f\n", current_time,
        current_y, current_v, current_xoverm, new_y);\
}
```

Appendix D

Variance of Particle Dispersion

This appendix shows that the addition of a constant to the variance of position is mathematically equivalent to releasing particles with a Gaussian distribution of zero mean and specified variance.

D.1 Proof

Consider particles released from a point x_o . Let $y(x)$ be the y-position of particles with variance $\sigma_{y(x)}^2$.

Now consider releasing particles with an initial distribution $f(y^*)$. Let $f(y^*)$ be a Gaussian probability density function with a zero mean and a variance of σ_o^2 . Thus, y^* is a random variable for the initial distribution and the new position is described by

$$\hat{y}(x) = y(x) + y^* \quad (\text{D.1})$$

where $\hat{y}(x)$ is the new particle position, and $y(x)$ is the particle position when released from point x_o .

Now calculate the variance for the new position, $\hat{y}(x)$.

$$\begin{aligned} \sigma_{\hat{y}}^2 &= E[(\hat{y}(x) - \overline{\hat{y}(x)})^2] \\ &= E[(y(x) + y^* - (\overline{y(x)} + \overline{y^*}))^2] \end{aligned} \quad (\text{D.2})$$

Since the expected value of y^* is zero, Equation (D.2) can be reduced and rearranged

$$\sigma_{\hat{y}}^2 = E[((y(x) - \overline{y(x)}) + y^*)^2] \quad (\text{D.3})$$

Equation (D.3) can be expanded

$$\sigma_y^2 = E[(y(x) - \overline{y(x)})^2 + y^{*2} + 2y^*(y(x) - \overline{y(x)})] \quad (D.4)$$

Expected value is additive thus Equation (D.4) may be simplified to

$$\sigma_y^2 = E[(y(x) - \overline{y(x)})^2] + E[y^{*2}] + 2E[y^*(y(x) - \overline{y(x)})] \quad (D.5)$$

Since y^* and $y(x)$ are independent variables, Equation (D.5) may be further simplified to

$$\sigma_y^2 = \sigma_{y(x)}^2 + \sigma_o^2 + 2E[y^*]E[(y(x) - \overline{y(x)})] \quad (D.6)$$

Since the expected value of y^* is zero, the end result is

$$\sigma_y^2 = \sigma_{y(x)}^2 + \sigma_o^2 \quad (D.7)$$

where the term on the left side is the variance of particles released with an initial distribution $f(y^*)$, the first term on the right side is the variance predicted by TASCflow for particles released from a point source, and the second term on the right side is the variance of the distribution $f(y^*)$.

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