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A turbulent dispersion model for particles or bubbles

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Abstract. A model for dispersed two-phase flow is derived based on a Boltzmann equation. This model is shown to be compatible with the two-fluid model, and includes the source of dispersion. In this model, dispersion is the result of the correlation of the liquid velocity fluctuations with the number density (perhaps more appropriately, with the trajectories of the individual dispersed units). Using this derived force, and a very simple assumption regarding the correlation of the presence of a dispersed unit and the carrier fluid velocity, a form for this force can be derived. This form gives a force which is proportional to the scalar (dot) product of the fluid Reynolds stress tensor with the gradient of bubble number density. For isotropic turbulence, the force is proportional to the gradient of number density. The constant of proportionality depends on the ratio of the dispersed unit relaxation time to the liquid turbulence time scale.

Key words: bubbly flows, diffusion, fluid-particle flows, turbulent dispersion

1. Introduction

A stream of bubbles or particles moving through a turbulent fluid will spread out. This spreading, or dispersion, is a collective result of the random motions of the fluid and dispersed material. The 'classical' model for this effect is to include a flux of dispersed material in a continuity equation (which is actually the number density equation) which is proportional to the gradient of number density.

The appropriateness of this assumption for the two-fluid approach is questionable, since the quantities affecting dispersed phase dynamics are coupled to a momentum equation, which is an equation for the dispersed phase (averaged) velocity. Moreover, it is unsettling that the diffusion model gives a flux of the dispersed phase, even when the velocity of the dispersed phase is zero. Classical motivations for the diffusion model derive diffusion as a flux of the dispersed material with respect to the CARRIER fluid velocity. This model therefore replaces the need for a momentum equation for the dispersed phase, and models the effect of the random fluid forces by a flux proportional to the gradient of the number density. Models which treat forces on the dispersed phase through a momentum balance are incompatible with the classical diffusion model, and models that use a diffusion term in the equation of conservation of mass, and a momentum equation for the forces on the dispersed phase have not been put on solid ground.

Derivations of the dispersed phase mass and momentum equations have not, to this point, led to a 'natural' model for dispersion. Models for motions of large numbers of particles include statistical mechanics, started by Maxwell and Boltzmann, reached a maturity in the 1950s (see [1]). This type of model assumes that the positions and velocities of the particles are random, and the randomization is due to collisions between the particles. All of these

approaches lead to equations of motion for a fluid via ensemble averaging. Models of this type are also used for plasmas and for quantum mechanics.

Statistical considerations are also important in turbulent flows, where the randomness arises from the growth and interaction of motions on scales smaller than the flow domain. Almost simultaneously to the development of turbulence models, the motion of small particles in turbulent flow was studied by Tchen [2]. Hinze's [3] book gives a good overview.

An approach that combines the derivation and solution of the probability density function (PDF) for the particle concentration and the statistics of velocity correlations has been developed by Reeks [4].

The motion of individual particles in a fluid was the subject of classical thinking by Archimedes, da Vinci and Michaelangelo. Quantitative progress was made by Stokes [5], and models for the motion of particles in a given fluid motion (sometimes referred to as the 'frozen' problem) include the BBO equation [6], and the model due to Maxey and Riley [7].

The motion of particles in fluids (but not necessarily in turbulent flow) stems from the work on fluidized beds [8], gas-liquid flows [9] and dusty gases [10]. General continuum equations, called two-fluid equations, have been derived by various methods (see [11–15]). Some of these models are derived by averaging, but all treat the particle motion and the fluid motion as two separate continuua. A systematic treatment is given by Drew and Passman [16].

A model for the motions of the particle continuum when the flow is turbulent has been derived by methods similar to that for the Reynolds averaged Navier-Stokes equations by Elghobashi and Abou-Arab [17]. In this model, they do not use Favre (*i.e.*, mass-weighted) averaging in the particle mass equation, but do not account for the difference thereby engendered between their aveage velocity and the average velocity that appears in the momentum equation.

In this paper, we wish to unify the two-fluid approach and the PDF approach. Specifically, we shall derive a version of the particle mass and momentum equations from the PDF for the particles, and use the expressions for the terms in the momentum equation, along with assumptions about the trajectories and randomness, to derive expressions for the terms resulting from the interactions of the particles with the fluid turbulence. This approach defines the particle velocity field in terms of the average mass flux. This very fundamental idea precludes the presence of a diffusion term in the particle mass balance equation. The essence of diffusion, *i.e.*, the net motion of particles from regions of high concentration to regions of low concentration, then must appear as a force in the particle momentum equation. This term is identified, and evaluated for different assumptions about the (microscopic, or individual) particle momentum equation.

2. Averaged balance equations

We can obtain averages of balance equations by taking the product of the balance equations with the phase indicator function, X_k , manipulating using the product rule for differentiation, and then performing the averaging process. For balance of mass, we have

$$\frac{\partial \overline{X_k \rho}}{\partial t} + \nabla \cdot \overline{X_k \rho \mathbf{v}} = \overline{\rho \left(\frac{\partial X_k}{\partial t} + \mathbf{v} \cdot \nabla X_k\right)}.$$
(1)

Here ρ is the density and **v** is the velocity, and the phase indicator function is defined by

$$X_k(\mathbf{x}, t) = \begin{cases} 1, & \text{if phase } k \text{ occupies } \mathbf{x}, \\ 0, & \text{otherwise.} \end{cases}$$
(2)

The probability of phase k occupying point **x** at time t is

$$\alpha_k = \overline{X_k}.\tag{3}$$

The vast majority of the literature in multiphase flow calls α_k the volume fraction. Although this is a misnomer, we shall also refer to it as such. The topological equation is

$$\frac{\partial X_k}{\partial t} + \mathbf{v}_i \cdot \nabla X_k = 0, \qquad (4)$$

where \mathbf{v}_i is the velocity of the interface. Substituting this in (1) we may reduce the right-hand side to

$$\Gamma_k = \overline{[\rho(\mathbf{v} - \mathbf{v}_i)] \cdot \nabla X_k} \,. \tag{5}$$

This is the interfacial source of mass due to phase change. Note that if $(\mathbf{v} - \mathbf{v}_i) \cdot \mathbf{n} = 0$, then $\Gamma_k = 0$. We also define the average density by

$$\alpha_k \overline{\rho}_k = \overline{X_k \rho}, \tag{6}$$

the average velocity of phase k by

$$\alpha_k \overline{\rho}_k \overline{\mathbf{v}}_k = \overline{X_k \rho \mathbf{v}}.\tag{7}$$

The average velocity defined by (7) is the mass flow velocity. If there is no mean flux of mass of phase k, then $\overline{\mathbf{v}}_k = 0$. If we use definition (7) in Equation (1), the equation of balance of mass for phase k becomes

$$\frac{\partial \alpha_k \overline{\rho}_k}{\partial t} + \nabla \cdot \alpha_k \overline{\rho}_k \overline{\mathbf{v}}_k = \Gamma_k \,. \tag{8}$$

The momentum equation for phase k is derived by multiplying the equation of balance of momentum by X_k and averaging. After some manipulation, the equation becomes

$$\frac{\partial \overline{X_k \rho \mathbf{v}}}{\partial t} + \nabla \cdot \overline{X_k \rho \mathbf{v} \mathbf{v}} = \nabla \cdot \overline{X_k \mathbf{T}} + \overline{X_k \rho \mathbf{g}} + \overline{\rho \mathbf{v} \left[(\mathbf{v} - \mathbf{v}_i) \cdot \nabla X_k \right] - \mathbf{T} \cdot \nabla X_k} \,. \tag{9}$$

where \mathbf{T} is the stress tensor, and \mathbf{g} is the external acceleration (due to gravity, for example). Defining the averaged stress by

$$\alpha_k \overline{\mathbf{T}}_k = \overline{X_k \mathbf{T}},\tag{10}$$

the Reynolds stress by

$$\alpha_k \mathbf{T}_k^{\text{Re}} = -\overline{X_k \rho \mathbf{v}_k' \mathbf{v}_k'}, \qquad (11)$$

the interfacial velocity by

$$\mathbf{v}_{ki}^{m}\Gamma_{k} = \rho \mathbf{v}(\mathbf{v} - \mathbf{v}_{i}) \cdot \nabla X_{k}$$
(12)

and the interfacial force by

$$\mathbf{M}_{k} = -\overline{\mathbf{T} \cdot \nabla X_{k}},\tag{13}$$

we arrive at the equation of balance of momentum in the form

$$\frac{\partial \alpha_k \overline{\rho}_k \overline{\mathbf{v}}_k}{\partial t} + \nabla \cdot \alpha_k \overline{\rho}_k \overline{\mathbf{v}}_k \overline{\mathbf{v}}_k = \nabla \cdot \alpha_k \left(\overline{\mathbf{T}}_k + \mathbf{T}_k^{\text{Re}} \right) + \alpha_k \overline{\rho}_k \mathbf{g} + \mathbf{M}_k + \mathbf{v}_{ki}^m \Gamma_k \,. \tag{14}$$

3. Kinetic-theory approach

In this section, we shall derive the balance equations for a dispersed phase consisting of spheres of a given size and mass, moving a fluid of constant density. We start from a Boltzmann equation. Comparison of the balance equations for mass and momentum with (8) and (14) results in a form for the interfacial force that is related to the random motions in the liquid and the dispersed phase units.

Let $f(\mathbf{z}, \mathbf{v}, t|\mathbf{u})$ be the number density of identical spheres in phase space, given that the liquid velocity field is assumed known for all \mathbf{x} in some flow domain, for all times previous to the instant t; that is, we assume that $\mathbf{u}(\mathbf{x}, t')$ is given for t' < t. Then in a small volume d \mathbf{z} , there are $f(\mathbf{z}, \mathbf{v}, t|\mathbf{u})$ d \mathbf{z} d \mathbf{v} spheres having velocity within d \mathbf{v} of velocity \mathbf{v} . The relation between the joint probability density for the dispersed unit statistics and the fluid statistics $f(\mathbf{z}, \mathbf{v}, \mathbf{u}, t)$ and the conditional probability density $f(\mathbf{z}, \mathbf{v}, t|\mathbf{u})$ is assumed to be

$$f(\mathbf{z}, \mathbf{v}, \mathbf{u}, t) = f(\mathbf{z}, \mathbf{v}, t | \mathbf{u}) P(\mathbf{u})$$

where $P(\mathbf{u})$ is the fluid velocity density function.

If the effects of collisions are neglected the equation becomes

$$\frac{\partial f}{\partial t} + \nabla \cdot (\mathbf{v}f) + \frac{\partial}{\partial \mathbf{v}} \cdot (f\mathbf{a}_d) = 0.$$
(15)

where \mathbf{a}_d is the acceleration of a dispersed unit. We assume that \mathbf{a}_d depends on the velocity of the dispersed unit and the velocity of the liquid. If we integrate Equation (15) over all dispersed unit velocities and fluid velocities, we have

$$\frac{\partial n_d}{\partial t} + \nabla \cdot n_d \overline{\mathbf{v}}_d = 0, \qquad (16)$$

where n_d is the dispersed unit number density,

$$n_d = \int f \, \mathrm{d}\mathbf{v} \, \mathrm{d}\mathbf{u},$$

and $\overline{\mathbf{v}}_d$ is the average dispersed unit velocity,

$$\overline{\mathbf{v}}_d = \frac{1}{n_d} \int \mathbf{v} f \, \mathrm{d} \mathbf{v} \, \mathrm{d} \mathbf{u} \, .$$

If we multiply Equation (15) by v, integrate over the velocities, and use the relation

$$\int \mathbf{v} \frac{\partial}{\partial \mathbf{v}} \cdot (f \mathbf{a}_d) \, \mathrm{d}\mathbf{v} = -\int f \mathbf{a}_d \, \mathrm{d}\mathbf{v} \,, \tag{17}$$

we have

$$\frac{\partial n_d \overline{\mathbf{v}}_d}{\partial t} + \nabla \cdot n_d \overline{\mathbf{v}} \overline{\mathbf{v}} = \overline{f} \mathbf{a}_d \,. \tag{18}$$

The term $n_d \overline{\mathbf{vv}}$ can be written as

$$n_d \overline{\mathbf{v}} \overline{\mathbf{v}} = n_d \overline{\mathbf{v}}_d \overline{\mathbf{v}}_d - n_d \mathbf{T}_d^{\operatorname{Re}},$$

where \mathbf{T}_d^{Re} is the dispersed phase stress, which corresponds to the Reynolds stress in the dispersed component. We shall also ignore dispersed unit contacts (collisions).

These equations are analogous to the dispersed component equations of balance of mass and momentum with $\Gamma_k = 0$ and $\overline{\mathbf{T}}_d = 0$. Specifically, if

$$\alpha_d = n_d \frac{4}{3} \pi r_d^3$$

then multiplying Equation (16) by $\frac{4}{3}\pi r_d^3$ gives Equation (8). The interpretation of Equation (18) is more complicated, since part of the acceleration appears in the virtual mass terms. However, we recognize that if **g** is the external force on the dispersed unit, and therefore if

 $\mathbf{a}_d = \mathbf{g} + \hat{\mathbf{a}}_d,$

then

$$\mathbf{F}_d = f \hat{\mathbf{a}}_d$$

is the average force on the dispersed phase due to interaction with the fluid. This force contains important interfacial forces, such as buoyancy, drag, lift and turbulent dispersion. If we assume that the force on the dispersed unit can be written as the force due to the average fields, plus a fluctuation, then we have

$$\hat{\mathbf{a}}_d(\mathbf{u},\mathbf{v}) = \hat{\mathbf{a}}_d(\overline{\mathbf{u}},\overline{\mathbf{v}}) + \mathbf{a}'_d.$$

Substituting this expression in the interfacial force density gives

$$\mathbf{F}_d = n_d \hat{\mathbf{a}}_d (\overline{\mathbf{u}}, \overline{\mathbf{v}}) + \mathbf{F}_d^{TD},$$

where

$$\mathbf{F}_d^{TD} = \overline{f \, \mathbf{a}_d'}$$

is the turbulent dispersion force.

3.1. TRAJECTORIES

If $\mathbf{u}(\mathbf{x}, t)$ is known, then the trajectory of any dispersed unit will be determined in terms of its initial position and velocity. If that trajectory is such that it arrives at point \mathbf{z} at time t with velocity \mathbf{v} , then its history is determined. Moreover, the acceleration of that unit is also known. The statistics of the trajectories, and therefore, of the acceleration of the dispersed unit at \mathbf{z} at time t are determined in terms of the statistics of the initial velocities and positions, and the carrier fluid statistics.



This reasoning leads to a net force, as indicated in Figure 1. If more particles arrive at the point indicated from above than from below, the net force is directed down.

Let us consider the trajectory of a dispersed unit that is at location z at time t, with velocity v. The position and velocity of that dispersed unit at any other time t' makes up its trajectory, and is denoted here as

$$\boldsymbol{\zeta}(t'; \boldsymbol{\omega}_e, \boldsymbol{\zeta}_e)$$

and

$$\boldsymbol{\omega}(t';\boldsymbol{\omega}_e,\boldsymbol{\zeta}_e) = \frac{\mathrm{d}\boldsymbol{\zeta}}{\mathrm{d}t'}(t';\boldsymbol{\omega}_e,\boldsymbol{\zeta}_e)$$

The trajectory is the solution of the initial value problem

$$\frac{\mathrm{d}^2\boldsymbol{\zeta}}{\mathrm{d}t'^2} = \mathbf{a}'_d, \qquad \boldsymbol{\zeta}(t_e, \boldsymbol{\omega}_e, \boldsymbol{\zeta}_e) = \boldsymbol{\zeta}_e, \qquad \frac{\mathrm{d}\boldsymbol{\zeta}}{\mathrm{d}t'}(t_e, \boldsymbol{\omega}_e, \boldsymbol{\zeta}_e) = \boldsymbol{\omega}_e$$

where t_e is the initial time, which is arbitrary thus far.

Given the liquid velocity field, the motion of an individual dispersed unit is given by

$$\left(\rho_d + C_{vm}\rho_l\right)\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = C_{vm}\rho_l\frac{\mathrm{D}\mathbf{u}}{\mathrm{D}t} - \nabla p + S(\mathbf{u} - \mathbf{v}) + C_L\rho_l(\mathbf{v} - \mathbf{u}) \times \nabla \times \mathbf{u} + \rho_d\mathbf{g},$$

where C_{vm} is the virtual mass coefficient, equal to $\frac{1}{2}$ for spherical units, C_L is the lift coefficient, also equal to $\frac{1}{2}$, and $S = \frac{3}{2r_d}C_D\rho_l|\mathbf{v} - \mathbf{u}|$ is the drag per unit velocity, with C_D the drag coefficient and r_d the particle radius. Here, D/Dt denotes the material derivative following the liquid. If we assume that the liquid momentum equation is unaffected by the dispersed units, we have

$$\rho_l \frac{\mathrm{D}\mathbf{u}}{\mathrm{D}\mathbf{t}} = -\nabla p + \rho_l \mathbf{g} \,.$$

If we use this equation to eliminate the pressure gradient, we have

$$(\rho_d + C_{vm}\rho_l)\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = (1 + C_{vm})\rho_l\frac{\mathrm{D}\mathbf{u}}{\mathrm{D}t} + S(\mathbf{u} - \mathbf{v}) + C_L\rho_l(\mathbf{v} - \mathbf{u}) \times \nabla \times \mathbf{u} + (\rho_d - \rho_l)\mathbf{g}.$$

It should be noted that this last substitution is inappropriate if there are coupling effects, that is, if the motion of the particles affect the fluid.

Note that \mathbf{a}_d is now given by

$$\mathbf{a}_{d} = \frac{(1+C_{vm})\,\rho_{l}}{\rho_{d}+C_{vm}\rho_{l}}\frac{\mathrm{D}\mathbf{u}}{\mathrm{D}\mathbf{t}} + \frac{1}{\tau_{d}}(\mathbf{u}-\mathbf{v}) + \frac{C_{L}\rho_{l}}{\rho_{d}+C_{vm}\rho_{l}}(\mathbf{v}-\mathbf{u})\times\nabla\times\mathbf{u}\,.$$
(19)

where the dispersed unit relaxation time is given by $\tau_d = \left(\rho_d + \frac{1}{2}\rho_l\right)/S$.

3.2. CORRELATION ASSUMPTIONS

We wish to use simple, yet reasonable assumptions about the interaction of the dispersed units with the fluid to calculate the Reynolds stress and the interfacial force density.

Thus, we assume that

$f(\mathbf{z}, \mathbf{v}, t | \mathbf{u}) \, \mathrm{d}\mathbf{z} \, \mathrm{d}\mathbf{v} = f(\boldsymbol{\zeta}, \boldsymbol{\omega}, t - \tau | \mathbf{u}) \, \mathrm{d}\boldsymbol{\zeta} \, \mathrm{d}\boldsymbol{\omega}.$

We denote $d\zeta d\omega/dz dv = J$. The randomness in the position and velocity of the dispersed unit is due to the randomness in the liquid velocity field, which is felt by the dispersed units through the various forces on the dispersed unit due to the liquid, and in the uncertainty in the initial position and velocity of the dispersed unit. In this work, we treat the randomness in the liquid velocity field by calculating trajectories, assuming that the liquid field is known, and then averaging over the liquid velocity field. Thus, the lack of predictability of the dispersed unit position ζ at time t_e , given that the dispersed unit is located at z at time t, is due to the lack of predictability in the *l*iquid velocity over the trajectory history. More specifically, we shall assume that the dispersed unit trajectory is highly correlated with liquid statistics for a short time, but is increasingly uncorrelated as the time between determination of the dispersed unit position increases.

Thus, we assume that dispersed units that reach z with velocity v at time t, come from position ζ_e with velocity ω_e , at time t_e .

We next make some assumptions about the trajectories of the dispersed units and how they are correlated with the forces that move them. Since we are interested in dispersion, we shall assume that the dispersed units have a spatial gradient in their average number density. We also assume that the dispersed unit trajectory and the velocity calculated along the trajectory are perfectly correlated for $t > t' > t - \tau_e$, and perfectly uncorrelated for $t' < t - \tau_e$. Thus, if a dispersed unit is at point \mathbf{z} , with velocity \mathbf{v} at time t, it was picked up by the fluid eddy at time $t_e = t - \tau_e$, at a position $\boldsymbol{\zeta}_e$ at random from the dispersed units that are at $\boldsymbol{\zeta}_e$. Thus, we assume that the conditional probability of having dispersed unit velocity \mathbf{v} , given that the fluid velocity is \mathbf{u} , and that the dispersed unit had velocity $\boldsymbol{\omega}_e$ at time t_e is

$$f(\mathbf{z}, \mathbf{v}, t | \mathbf{u}) = n_d(\boldsymbol{\zeta}_e) \delta(\mathbf{v} - \frac{\mathrm{d}\boldsymbol{\zeta}}{\mathrm{d}t}(t, \boldsymbol{\zeta}_e, \boldsymbol{\omega}_e, t_e)) \,\delta(\mathbf{z} - \boldsymbol{\zeta}(t, \boldsymbol{\zeta}_e, \boldsymbol{\omega}_e, t_e)), \tag{20}$$

where δ denotes the Dirac delta function, and $\zeta(t, \zeta_e, \omega_e, t_e)$ is the trajectory of a dispersed unit, given that it was entrained by a fluid eddy at time t_e at location ζ_e with velocity ω_e .

Next, we assume that the number density at ζ_e can be expressed as a Taylor series in the spatial coordinate. Thus, we have

$$n_d(\boldsymbol{\zeta}_e) = n_d(\mathbf{z}) + (\boldsymbol{\zeta}_e - \mathbf{z}) \cdot \nabla n_d(\mathbf{z}).$$
⁽²¹⁾

This assumption allows us to express the turbulent dispersion force density as

$$\mathbf{F}_{d}^{TD} = \overline{f} \, \mathbf{a}_{d}^{\prime} = \overline{\mathbf{a}_{d}^{\prime}(\boldsymbol{\zeta}_{e} - \mathbf{z})} \cdot \nabla n_{d} \,, \tag{22}$$

where we note that

 $\overline{n_d(\mathbf{z},t)\mathbf{a}_d'}=0.$

Equation (22) is a valid approximation when the particle trajectories are short 'rides' in the fluid eddies. The choice of scale of resolution for the problem attacked implies a spectrum of scales which are unresolved by the mean flow. The effect of these scales must be modelled. The underlying assumption here is that these scales are small compared to the length scales of the mean flow. The assumption of linearity in Equation (21) results in a turbulent dispersion force which is linear in the number density gradient, with the proportionality tensor given by the correlation between the fluctuating force and the change in position of a dispersed unit. We shall refer to the tensor $\mathbf{a}'_d(\boldsymbol{\zeta}_e - \mathbf{z})$ as the dispersion tensor.

4. Trajectories

The calculation of the correlation of the dispersed phase acceleration fluctuation with the dispersed phase presence is very different for particles and for gas bubbles. In the next few subsections we shall compute \mathbf{F}_d^{TD} when the dispersed units are particles or bubbles. We shall do this by considering trajectories of the dispersed units and making an assumption about the probability that the calculated trajectory occurs.

4.1. PARTICLE TRAJECTORIES

For small particles, where the density is of the same order of magnitude as the liquid, we see that the ratio of drag to inertia is of order St^{-1} where St is the Stokes number, which is the ratio of particle relaxation time to the fluid time scale. Thus, drag dominates the other forces on the particle.

That is,

$$\frac{1}{\tau_d} \left(\mathbf{u} - \mathbf{v} \right) \gg \frac{\mathrm{D}\mathbf{u}}{\mathrm{D}t}$$

and

$$\frac{1}{\tau_d} \left(\mathbf{u} - \mathbf{v} \right) \gg \left(\mathbf{v} - \mathbf{u} \right) \times \nabla \times \mathbf{u} \,.$$

Now we have

$$\hat{\mathbf{a}}_d(\overline{\mathbf{u}},\overline{\mathbf{v}}) = \frac{1}{\tau_d}(\overline{\mathbf{u}}-\overline{\mathbf{v}}),$$

and

$$\mathbf{a}_d' = \frac{1}{\tau_d} (\mathbf{u}' - \mathbf{v}').$$

We shall drop the primes. Thus, the equations of motion for a small particle in a liquid velocity field is

$$\frac{\mathrm{d}^2\boldsymbol{\zeta}}{\mathrm{d}t^2} = \frac{1}{\tau_d} \left(\mathbf{u} - \frac{\mathrm{d}\boldsymbol{\zeta}}{\mathrm{d}t} \right)$$

4.1.1. Turbulence model for particles

We assume that the turbulence is adequately modeled as a sequence of large-scale fluid eddies, each having a constant, uniform velocity [18]. From the Eulerian point of view, the fluid velocity field will be characterized by periods of constant velocity, separated by intervals of rapid change of velocity. In each eddy the particle trajectory is simple, starting from ζ with a particle velocity of ω at time t'. The force \mathbf{a}_d is then

$$\mathbf{a}_d = \frac{1}{\tau_d} (\mathbf{u} - \mathbf{v}), \qquad (23)$$

where τ_d is the particle relaxation time.

Using this model for turbulence suggests that the randomness of the particle velocity distribution is due to the mixing in the interval between uniform velocities. We shall refer to this model as the random flight model.

The trajectory that is at **z** with velocity **v** at time *t*, given that it started at $\boldsymbol{\zeta}$ with velocity $\boldsymbol{\omega}$ at time *t_e*, is given by

$$\mathbf{v}(t) = \mathbf{u} + e^{-\frac{(t-t_e)}{\tau_d}} (\boldsymbol{\omega} - \mathbf{u})$$

$$\mathbf{z}(t) = \mathbf{u}(t - t_e) + \tau_d e^{-\frac{(t-t_e)}{\tau_d}} (\mathbf{u} - \boldsymbol{\omega}) + \boldsymbol{\zeta} + \tau_d (\boldsymbol{\omega} - \mathbf{u}).$$

We assume that the particle has resided in the eddy for a constant (*i.e.*, non-random) time τ_e , the time of entrainment into the eddy is $t_e = t - \tau_e$.

4.1.1.1. Small eddy times

We wish to calculate the particle phase Reynolds stress

$$\mathbf{T}_{d}^{\text{Re}} = -m_{d} \overline{(\mathbf{v} - \overline{\mathbf{v}}_{d})(\mathbf{v} - \overline{\mathbf{v}}_{d})}.$$
(24)

Substituting the assumed and derived relations for the probability density functions, we obtain

$$\mathbf{T}_{d}^{\text{Re}}/\rho_{d} = -\int\!\!\!\int\!\!\!\int\!\!\int \left[(\boldsymbol{\omega}_{e} - \mathbf{u}) \mathrm{e}^{-(t-\tau_{e})/\tau_{d}} + \mathbf{u} \right] \left[(\boldsymbol{\omega}_{e} - \mathbf{u}) \mathrm{e}^{-(t-\tau_{e})/\tau_{e}} + \mathbf{u} \right] \\ \times \Pr(\boldsymbol{\omega}, \tau_{e}) \, \mathrm{d}\boldsymbol{\omega} \, \mathrm{d}\tau_{e} \Pr(\mathbf{u}) \, \mathrm{d}\mathbf{u} = -\overline{\boldsymbol{\omega}_{e}\boldsymbol{\omega}_{e}} \mathrm{e}^{-2\tau_{e}/\tau_{d}} - \overline{\mathbf{u}'\mathbf{u}'} \left(1 - \mathrm{e}^{-\tau_{e}/\tau_{d}} \right)^{2}, \tag{25}$$

where Pr denotes the probability density function for the given variables. Recognizing that

$$\mathbf{\Gamma}_d^{\mathrm{Re}}/\rho_d = -\overline{\mathbf{\omega}_e \mathbf{\omega}_e}$$

and

$$\overline{\mathbf{u}'\mathbf{u}'} = -\mathbf{T}_f^{\mathrm{Re}}/\rho_f$$

assuming homogeneity of the turbulence, and solving for $\mathbf{T}_{d}^{\text{Re}}$, we have

$$\mathbf{T}_{d}^{\text{Re}}/\rho_{d} = \mathbf{T}_{f}^{\text{Re}}/\rho_{f} \frac{(1 - e^{-\tau_{e}/\tau_{d}})^{2}}{1 - e^{-2\tau_{e}/\tau_{d}}}.$$
(26)

Note that as $\tau_e/\tau_d \to 0$, we have $\overline{\mathbf{T}}_d^{\text{Re}} \to 0$. Thus, if the particle relaxation time greatly exceeds the eddy time scale, the particle will not respond to the fluid motions, and the particle



Figure 2. Dispersion coefficient *D* vs. $s = \tau_e / \tau_p$

Reynolds stress will vanish. At the other extreme, as $\tau_e/\tau_d \rightarrow \infty$, the particles are able to follow the fluid velocity fluctuations relatively faithfully, and therefore,

$$\frac{\mathbf{T}_d^{\text{Re}}}{\rho_d} \to \frac{\mathbf{T}_f^{\text{Re}}}{\rho_f} \,. \tag{27}$$

Also, the dispersion tensor becomes

$$\frac{1}{\tau_d} \overline{\left(\mathbf{u} - \mathbf{v}\right)\left(\zeta - z\right)} = \left[-e^{-\frac{\tau_e}{\tau_d}} \left(\frac{\tau_e}{\tau_d} - \left(1 - e^{-\frac{\tau_e}{\tau_d}}\right)\right) \frac{1 - e^{-2\frac{\tau_e}{\tau_d}}}{\left(1 - e^{-\frac{\tau_e}{\tau_d}}\right)^2} + e^{-\frac{\tau_e}{\tau_d}} \left(1 - e^{-\frac{\tau_e}{\tau_d}}\right) \right] \overline{\mathbf{vv}} = -D(\tau_e/\tau_d) \overline{\mathbf{vv}} = D(\tau_e/\tau_d) \mathbf{T}_d^{\mathrm{Re}}/\rho_d,$$

The dispersion coefficient D is plotted in Figure 2.

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Note that the dispersion coefficient depends on the eddy residence time τ_e and the particle relaxation time τ_p , and is maximum when the two time scales are about equal. This seems sensible, because eddies in which the particles do not spend much time will not disperse the particles, and eddies in which the particles reside for long times will transport particles, but will not disperse them.

4.1.1.2. Large eddy times

In order to get the correct dispersion for turbulent flow containing a spectrum of time scales, and consequently a spectrum of eddy residence times, we consider the trajectories as shown in Figure 3.

In this case, we envision the fluid velocity fluctuation \mathbf{u} having a drift value and a smaller scale fluctuation. Clearly, the particle displacement is given by

$$\boldsymbol{\zeta} - \mathbf{z} \cong -(t - t_e) \mathbf{u}$$

Then if Equation (23) is used, the particle dispersion tensor is given by

$$\overline{\mathbf{a}_d(\boldsymbol{\zeta} - \mathbf{z})} \cong -\frac{1}{\tau_p} \overline{(t - t_e) (\mathbf{u} - \mathbf{v}) \mathbf{u}} \\ = -\frac{\tau_e}{\tau_p} \overline{\mathbf{u}} \overline{\mathbf{u}} = \frac{\tau_e}{\tau_p} \frac{1}{\rho_c} \mathbf{T}_c^{\text{Re}},$$



Figure 3. Long time trajectories.

where we again assume that the particle velocity and the fluid velocity are uncorrelated. If the particle relaxation time is large, we have

$$\mathbf{M}_{d}^{TD} = \frac{\tau_{e}}{\tau_{p}} \frac{\rho_{d}}{\rho_{c}} \mathbf{T}_{c}^{\mathrm{Re}} \cdot \nabla \alpha_{d}.$$

4.2. BUBBLE TRAJECTORIES

The equations of motion for a bubble in a fluid velocity field can be written as

$$\frac{\mathrm{d}^{2}\boldsymbol{\zeta}}{\mathrm{d}t^{2}} = \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u}\right) - 2\nabla p/\rho + \frac{1}{\tau} \left(\mathbf{u} - \frac{\mathrm{d}\boldsymbol{\zeta}}{\mathrm{d}t}\right) - 2\Omega \times \left(\mathbf{u} - \frac{\mathrm{d}\boldsymbol{\zeta}}{\mathrm{d}t}\right),$$

where τ_d is the bubble relaxation time, ∇p is the fluid pressure gradient, **u** is the fluid velocity field, and 2Ω is the vorticity. We assume that $\mathbf{u} = \mathbf{u}_0 + \Omega \times (\boldsymbol{\zeta} - \mathbf{z}_c)$, where \mathbf{z}_c is the center of the vortex line. Furthermore, we assume that $\nabla p = \nabla p_0 - \rho \mathbf{\Omega} \times \mathbf{\Omega} \times \boldsymbol{\zeta}$.

4.2.1. Turbulence model for bubbles

In order to describe the motion of a bubble in a liquid eddy, we assume that the effect of the eddy can be described at each spatial point for random times, by constant pressure gradient ∇p_0 , constant velocity \mathbf{u}_0 . We further assume that each eddy has no rotation, so that $\omega = 0$. Then the system of differential equations can be written as

$$\frac{\mathrm{d}\boldsymbol{\zeta}}{\mathrm{d}t} = \mathbf{v}, \quad \frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = \mathbf{f} - \frac{1}{\tau_b}\mathbf{v},$$

where $\mathbf{f} = -3\nabla p_0/\rho + \frac{1}{\tau_b}\mathbf{u}_0$.

The trajectory that is at z with velocity v at time t, given that it started at ζ with velocity ω at time t_e , is given by

$$\mathbf{v}(t) = \mathbf{f}\tau_d + e^{-\frac{(t-t_e)}{\tau_d}} \left(-\mathbf{f}\tau_d + \boldsymbol{\omega}\right),$$

$$\mathbf{z}(t) = \mathbf{f}\tau_d \left(t - t_e\right) + \tau_d e^{-\frac{(t-t_e)}{\tau_d}} \left(\mathbf{f}\tau_d - \boldsymbol{\omega}\right) + \zeta + \tau_d \left(\boldsymbol{\omega} - \mathbf{f}\tau_d\right).$$

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If we again assume that the bubble has resided in the eddy for a constant (*i.e.*, non-random) time τ_e , the time of entrainment into the eddy is $t_e = t - \tau_e$, and the velocity, position, and force statistics are related by

$$\mathbf{v} = \mathbf{f} \tau_d \left(1 - e^{-\frac{\tau_e}{\tau_d}} \right) + \mathbf{\omega} e^{-\frac{\tau_e}{\tau_d}},$$

$$\mathbf{z} = \boldsymbol{\zeta} + \mathbf{f} \tau_d \left(\tau_e + \tau_d \left(e^{-\frac{\tau_e}{\tau_d}} - 1 \right) \right) + \mathbf{\omega} \tau_d \left(1 - e^{-\frac{\tau_e}{\tau_d}} \right).$$

Then, if the force and the bubble velocity are uncorrelated, we have

$$\overline{\mathbf{vv}} = \overline{\mathbf{ff}} \tau_d^2 \left(1 - \mathrm{e}^{-\frac{\tau_e}{\tau_d}} \right)^2 + \overline{\mathbf{\omega}} \overline{\mathbf{\omega}} \mathrm{e}^{-2\frac{\tau_e}{\tau_d}}$$

If, further, the velocity statistics are homogeneous, we have $\overline{\mathbf{vv}} = \overline{\mathbf{\omega}\mathbf{\omega}}$, and

$$\overline{\mathbf{ff}} = \overline{\mathbf{vv}} \frac{1 - \mathrm{e}^{-2\frac{\tau_e}{\tau_d}}}{\tau_d^2 \left(1 - \mathrm{e}^{-\frac{\tau_e}{\tau_d}}\right)^2}.$$

Using this, the dispersion tensor becomes

$$\overline{\left(\mathbf{f} - \frac{1}{\tau_d}\mathbf{v}\right)(\mathbf{\zeta} - \mathbf{z})} = \left[-e^{-\frac{\tau_e}{\tau_d}} \left(\frac{\tau_e}{\tau_d} - \left(1 - e^{-\frac{\tau_e}{\tau_d}}\right)\right) \frac{1 - e^{-2\frac{\tau_e}{\tau_d}}}{\left(1 - e^{-\frac{\tau_e}{\tau_d}}\right)^2} - e^{-\frac{\tau_e}{\tau_d}} \left(1 - e^{-\frac{\tau_e}{\tau_d}}\right) \right] \overline{\mathbf{vv}}$$
$$= -D(\tau_e/\tau_d)\overline{\mathbf{vv}} = D(\tau_e/\tau_d)\mathbf{T}_d^{\mathrm{Re}}/\rho_d.$$

This is exactly the same dispersion tensor that was derived for small particles. However, in this case there is no relation between $\mathbf{T}_{d}^{\text{Re}}$ and $\mathbf{T}_{c}^{\text{Re}}$.

For eddy time scales that are large compared to the particle relaxation time, we have

$$\begin{aligned} \boldsymbol{\zeta} - \boldsymbol{z} &= -\mathbf{f} \boldsymbol{\tau}_d \left(\boldsymbol{\tau}_e + \boldsymbol{\tau}_d \left(e^{-\frac{\boldsymbol{\tau}_e}{\boldsymbol{\tau}_d}} - 1 \right) \right) - \boldsymbol{\omega} \boldsymbol{\tau}_d \left(1 - e^{-\frac{\boldsymbol{\tau}_e}{\boldsymbol{\tau}_d}} \right). \\ &\cong -\mathbf{f} \boldsymbol{\tau}_d \boldsymbol{\tau}_e \end{aligned}$$

Thus,

$$\overline{\mathbf{a}_d(\boldsymbol{\zeta}-\mathbf{z})} = \overline{\left(\mathbf{f}-\frac{1}{\tau_p}\mathbf{v}\right)(\boldsymbol{\zeta}-\mathbf{z})} \cong -\tau_e \tau_p \overline{\mathbf{f}} \overline{\mathbf{f}} \cong \frac{\tau_e}{\tau_p} \frac{1}{\rho_d} \mathbf{T}_d^{\mathrm{Re}},$$

so that the bubble dispersion force becomes

$$\mathbf{M}_{d}^{TD} = \frac{\tau_{e}}{\tau_{p}} \frac{C_{vm} \rho_{f}}{\rho_{d}} \mathbf{T}_{d}^{\text{Re}} \cdot \nabla \alpha,$$

where we have taken the effective density as the virtual density.

4.3. COMPARISON WITH A NUMERICAL EXPERIMENT

After some approximations have been made, the model has been implemented in a computer code to make bubbly-flow calculations by use of the two-fluid (ensemble averaged) approach suggested by Equations (8) and (14). This code has been used to predict the spreading of bubbles injected into a stream with decaying turbulence.



Figure 4. Volume fraction profiles for simulations. Symbols: DNS data. Lines: CFDShipM results. Present model with $C_{TD} = 0.108$.

First, we approximate the dispersed phase Reynolds stress by

$$\frac{\mathbf{T}_{d}^{\text{Re}}}{\rho_{d}} \approx -\frac{2}{3}k_{d}\mathbf{I} \approx -\frac{2}{3}k_{c}\mathbf{I}.$$
(28)

Furthermore, we assume that the particles are sufficiently small that the drag force is well approximated by Stokes drag, so that

$$\mathbf{r}_d = \frac{2}{9} \frac{a^2}{\mathbf{v}_c},\tag{29}$$

where *a* is the radius, and v_c is the fluid viscosity. Finally, consistent with the $k - \epsilon$ model, we assume that the fluid time scale is proportional to k_c/ϵ_c . Then, if τ_c/τ_d is small, we have

$$\mathbf{M}_{d}^{TD} = -C_{TD} \frac{\tau_{c}}{\tau_{d}} k_{c} \nabla \alpha_{d}, \tag{30}$$

where

$$\frac{\tau_c}{\tau_d} = \frac{9\nu_c k_c}{2a^2 \epsilon_c} \tag{31}$$

is the ratio of time scales, and the constant of proportionality is C_{TD} . This model agrees with that proposed by Lopez de Bertodano [19].

This model has been implemented in the code CFDShipM [20], and used to predict the dispersion of stream of particles released in decaying turbulence. The predictions were compared to 'data' generated by solving the Navier–Stokes equations with a dynamical model for bubble motions [21, 22]. Figure 4 shows the volume fraction predictions and data as a function of the transverse coordinate at several different downstream locations.

5. Discussion

The model presented here arrives naturally at a dispersion model even withstanding the fact that an oversimplified model for correlations is assumed. This dispersion model has several noteworthy features. We discuss each of these.

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The dispersed unit flux is given by number density times the (average) dispersed unit velocity. Thus, if there is a dispersed unit flux, there is a (non-zero) dispersed unit velocity. This makes sense. If the dispersed phase is not moving (on average), it has zero velocity. If there is a flux of dispersed units, then there is a non-zero velocity for the dispersed phase.

This means that the effect of dispersion is contained in a term in the dispersed unit *momentum* equation. The dispersion term is linear in the number density gradient to first approximation. The proportionality tensor is given by the dispersed phase Reynolds stress, times a scalar function of the ratio of the fluid eddy timescale and the dispersed unit relaxation time. Thus, the momentum flux of the dispersed phase is related to how much momentum flux the dispersed phase has, and also depends on a ratio of response time of an individual unit in an eddy.

Using simplified assumptions about the liquid turbulence structure allows us to obtain a closed form model. There are several physical effects that are omitted from this model. Note that the pressure gradient in the fluid phase is retained, but modeled in such a way that it will not have the local minimum lines that are evident in vortices. Thus, the particles will not migrate to centers of vortices in this model. Furthermore, the effect of lift is also left out by the same sort of assumption -i.e., the uniformity of an eddy precludes lift effects. These effects could be included by assuming that each eddy is a region of fluid velocity with a constant velocity, constant pressure gradient, and constant vorticity.

5.1. DIFFUSION MODEL

If we assume that the drag, turbulent dispersion, and the dispersed unit Reynolds stress dominate the gas phase momentum equation, we can write

$$0 = \alpha_d S(\mathbf{v}_l - \mathbf{v}_d) - D\mathbf{T}_d^{\text{Re}} \cdot \nabla \alpha_d + \nabla \cdot \alpha_d \mathbf{T}_d^{\text{Re}}$$

Then, we can solve for the gas velocity in terms of the liquid velocity

$$\mathbf{v}_d = \mathbf{v}_l - \frac{1}{\alpha_d S} D \mathbf{T}_d^{\text{Re}} \cdot \nabla \alpha_d + \frac{1}{\alpha_d S} \nabla \cdot \alpha_d \mathbf{T}_d^{\text{Re}}.$$
(32)

Substituting this in the equation of balance of mass for the dispersed unit phase gives

$$\frac{\partial \alpha_d}{\partial t} + \nabla \cdot \alpha_d \mathbf{v}_l = \nabla \cdot (\mathbf{D}_d \cdot \nabla \alpha_d) - \frac{1}{S} \nabla \cdot \left(\alpha_d \nabla \cdot \mathbf{T}_d^{\text{Re}} \right), \tag{33}$$

where the diffusivity tensor is defined as

$$\mathbf{D}_d = \frac{1}{S} \left(D - 1 \right) \mathbf{T}_d^{\text{Re}}.$$

Thus, we see that the turbulent dispersion term gives rise to a term that appears as diffusion of the dispersed units *relative to the liquid* in the equation of balance of dispersed unit mass. The effect of the carrier fluid turbulence giving rise to a drift velocity has been called *turbophoresis*. In this modeling approach, the second term on the right-hand side of (33) has this effect, and arises naturally from the equations.

This dispersion model reduces to a diffusion model by assuming that the inertial terms are negligible in the dispersed phase momentum equation. However, there are many situations involving bubbly fluids or particles in fluids where the inertia of the dispersed phase is not negligible – any curved or nozzle flow will exhibit acceleration and virtual mass effects that are not modeled by (33).

6. Conclusion

Note that the averaging used in the two-fluid model and the Boltzmann approach give an average particle velocity weighted by the presence of particles,

$$\alpha_d \mathbf{v}_d = \overline{X_d \mathbf{v}}$$

and

$$\overline{\mathbf{v}}_d = \frac{1}{n_d} \int \mathbf{v} f \, \mathrm{d} \mathbf{v} \, \mathrm{d} \mathbf{u},$$

where we assume constant density for the particle phase. Elghobashi and Abou-Arab [17] derive equations based on two separate averaging processes, first (tacitly assumed in their paper) over the particles to get a two-fluid (interpenetrating fluids) model, and then over the turbulence. When they (formally) apply the average over the turbulence, they do not weight the particle phase velocity by the concentration, and thereby obtain a conservation of mass equation for the particles of the form

$$\frac{\partial \overline{\alpha}_d}{\partial t} + \nabla \cdot \left(\overline{\alpha}_d \overline{\overline{\mathbf{v}}}_d + \overline{\alpha}_d \overline{\mathbf{v}}_d' \right) = 0$$

There are several problems with this approach. The first is esthetic, in that the quantity in the divergence term is the average flux of particles, and is

$$\overline{\alpha}_d \overline{\overline{\mathbf{v}}}_d + \overline{\alpha_d \mathbf{v}'_d} = \overline{\alpha_d} \overline{\overline{\mathbf{v}}}_d = \overline{\alpha}_d \overline{\overline{\mathbf{v}}}_d^T$$

where $\overline{\mathbf{v}}_d^F$ is the Favre averaged velocity. Here we have used the overbar symbol to denote two different averages; the proper notation would use two different symbols. The second problem is that the whole of the particle flux (*i.e.*, $\overline{\alpha}_d \overline{\mathbf{v}}_d + \alpha_d \mathbf{v}_d'$) is the term that appears in the momentum equation. Defining any velocity other than the Favre therefore requires the difference between that velocity and the defined (non-Favre) velocity to be accounted for in the derivation of the momentum equation. The third problem is the most crucial. Defining the velocity $\overline{\mathbf{v}}_d$ as indicated leads to situations where $\overline{\mathbf{v}}_d = 0$ but the particles still have a non-zero flux. This can be illustrated by considering a turbulent flow mixing layer with particles in one stream and none in the other. As the streams mix, particles move from the particle laden side to the non-particle laden side. If this motion is modeled as diffusion, then the flux of particles across the centerline of the mixing layer is non-zero, with the particle flux given by $\overline{\alpha}_d \mathbf{v}_d'$. Changes of inertia due to this flux is not accounted for in the non-Favre model.

The model for particle or bubble motion derived in this paper has the advantages that it (i) is based on the two-fluid model, so that all momentum effects are accounted for in the particle momentum equation; (ii) gives rise to a particle dispersion term that accounts for the tendency of random motions in the carrier fluid to spread the particles; and (iii) reduces to the diffusion model when particle inertia is small. Moreover, the full particle inertia model will give the correct inertia effects in flows where significant disequilibrium occurs.

We also note that another often overlooked disadvantage of the diffusion model is that information travels infinitely rapidly. That is, the effect of a localized disturbance, such as a spike in the concentration, is felt at $t = 0^+$ at all points in the domain, albeit at an exponentially small level. The full momentum model cannot give infinite dispersed phase velocities, and consequently, this feature of the diffusion model is not present in the full dispersed phase momentum model.

Those who purport to derive a diffusive model using the two-fluid approach essentially ignore definition (7), and define some other (sometimes reasonable) velocity for the dispersed units. Most of these derivations also ignore the fact that the same term appears in the time derivative in the momentum equation (14). This inconsistency is sometimes 'fixed' by using the other velocity, and ignoring the extra terms in the momentum equations.

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