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MATHEMATICAL MODELING OF TWO-PHASE FLOW

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UNIVERSITY OF WISCONSIN - MADISON
MATHEMATICS RESEARCH CENTER

MATHEMATICAL MODELING OF TWO-PHASE FLOW

D. A. Drew

Technical Summary Report # 2343

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ABSTRACT

A continuum mechanics approach to two-phase flow is reviewed. An averaging procedure is discussed and applied to the exact equations of motion. Constitutive equations are supplied and discussed for the stresses, pressure differences and the interfacial force. The nature of the resulting equations is studied.

AMS (MOS) Subject Classification: 76T05

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SIGNIFICANCE AND EXPLANATION

Equations describing the motions of two materials, one dispersed throughout the other, are derived. There is some controversy over the ability of certain simplified forms of these equations to predict meaningful flows. Consequently, evidence is presented to verify the forms of various terms appearing in the equations. The consequences of the assumed forms are discussed.

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MATHEMATICAL MODELING OF TWO-PHASE FLOW

D. A. Drew

INTRODUCTION

Dispersed two-phase flows occur in many natural and technological situations. For example, dust in air and sediment in water contribute to erosion and silting, and can cause problems for machinery such as helicopters and power plants operating in such an environment. Also, many energy conversion and chemical processes involve two-phase flows. Boiling a fluid such as water or sodium and extracting the heat by condensation at a different location provides a practical energy flow process. Many kinds of chemical reactants and catalysts are mixed in a dispersion of fine particles to expose as much interfacial area as possible.

In such a large class of problems, many diverse mechanisms are important in different situations. The models used for these different situations have many common features, such as interfacial drag.

This paper examines the common features of dispersed two phase flows from a continuum mechanical approach. Since it is not universally accepted that such an approach is valid, we shall discuss some philosophical reasons for taking such an approach. The approach is based on the view that it is sufficient to describe each material as a continuum, occupying the same region in space. This new "material" consists of two interacting materials (called phases, even though they often are not different phases of the same material). The two phase material is often called the mixture. In analogy with continuum mechanics, we shall have to specify how the mixture interacts with itself. In ordinary continuum mechanics (ignoring thermodynamic

considerations) that requires a constitutive equation expressing the stress as a function of various fields. In two-phase flow mechanics, it requires specification of stresses for each phase, plus a relation for the interaction of the two materials.

Researchers who do not subscribe to this view treat the mechanics of the two materials, plus the dynamics of the interface as fundamental, and use derived results and/or measurements to gain the understanding needed for their particular application. It is instructive to consider the approaches to gas dynamics. Most scientists believe that a gas is a collection of many molecules which move, vibrate, and interact in a complex, but describable way. Indeed, with the aid of large computers, molecular dynamics has made great strides in understanding such phenomena as shocks and phase transition, among others. In spite of the knowledge of the "correctness" of this model, many scientists and engineers use a continuum model for gas dynamics. Indeed, anyone wishing to describe, for example, the flow around an airfoil, would be hard pressed to find a computer big enough to do it as a problem in molecular dynamics. As a problem in continuum gas dynamics, it is still a large problem; however, it is done quite routinely numerically, including shocks. In addition, certain solutions to the continuum equations can be obtained analytically. While these are not always of direct technical interest, they often suggest phenomena or techniques which do have direct bearing on problems of interest. Experiments in

gas dynamics can be useful. Without a model for comparison or scaling, however, one is limited to understanding only the particular geometry and scale of the experiment. The ability to infer is lost.

While these points seem obvious for gas dynamics, they nevertheless should be discussed and understood for the analogous situation of two-phase flow mechanics. For a particular flow with only a few particles which interact only slightly, it is best (and perhaps even necessary) to describe them "molecularly", that is, by predicting the trajectories of each one. If many particles are involved, it is better to use a continuum description. As in gas dynamics, both descriptions have their place. Furthermore, it is often instructive to try to ascertain what one model implies about the other, as in using the Boltzmann description of a gas to get continuum properties.

The analogy is apt for a continuum description of two-phase flows. This paper will review the connection with the exact, or microscopic description through the application of an averaging process to the continuum mechanical equations describing the exact motion of each material at each point. If the exact flows were known, the averaged equations would be completely determined, and therefore unnecessary, since desired averaged information (such as the average concentration of particles) could be determined without using the averaged equations. The solutions are not known, nor is it necessary to the continuum approach that they be known. The resulting averaged equations are assumed to describe a material (the mixture) for which the

interactions must be specified. This specification is then done according to certain rules which are reasonable and not too limiting. We shall discuss these rules and their implications.

The forms of the resulting equations are determined by the choice of a list of variables which are assumed to influence the interactions. The resulting equations have several unknown coefficients. These coefficients are assumed to be determinable by experiments. For the model we propose, we examine the experimental data and their implications on the coefficients. The result is, in essence, a recommendation for a model which has many known features of two-phase flow dynamics. An enlightened investigator can use the model to make predictions in a situation which falls within the range of assumptions made. The model can also be a starting point to obtain generalizations (such as the inclusion of electromagnetic effects). As with all models, it should never be used blindly, but with caution and careful examination of the results and implications.

Historically, geophysical flows involving sediment and clouds were among the first two-phase flows observed from a scientific point of view. Sediment meant erosion and loss of property, or deposition and loss of navigability. Clouds signalled possible rainfall. The amounts could mean drought, bountiful harvests or devastating floods. An analytical description awaited the development of the calculus, fluid mechanics and partial differential equation theory. The industrial revolution spurred the need for understanding of all of basic science, including two phase flows, although the correlation between progress and

the acquisition of fundamental knowledge is not exact. For example, automobiles have worked reasonably well without a detailed knowledge of the flow and evaporation of fuel droplets; on the other hand, efficient design of fluidized beds have been reliant on the understanding and stabilizing effects obtained from analytical models.

Early work on the form taken by beds of particles subject to forces due to flowing fluid (DuBuat 1786, Helmholtz 1888, Blasius 1912 and Exner 1920) lead to interesting fundamental results such as the stability of the interface between two fluids and a practical understanding of the macroscopic properties of sedimentation and bed form evolution. A more microscopic look (Bagnold 1941) dealt with the mechanics of the interactions between the particles and the fluid, and the particles and the bed. A recent perspective is given by Engelund and Fredsøe (1982).

Developments in cloud physics occurred in physical chemistry of nucleation and formation. The need for detailed mechanical considerations was low due to the fact that the vapor, nucleation sites and the formed droplets all flow with the surrounding air (until raindrops form).

Porous medium theory, a two phase flow where the solid phase does not move appreciably, developed with some different concerns (Darcy 1856), but Biot (1955) was instrumental in putting the empirical knowledge on a sound continuum basis. The desire to extract

hydrocarbons from deep inside the earth's crust has given a great impetus to the study of flow in porous media. See Scheidegger's (1974) book for a discussion of porous bed modeling concerns.

The next important milestone in the development of two-phase flow continuum mechanics theory was the development and use of equations of dusty gases in the 1950's. Models for dusty gases are summarized by Marble (1970).

Chemical processing in fluidized beds gave an urgency to the development of the theory of particle-fluid systems. Early theoretical papers include those of Jackson (1963), Murray (1965a,b), and Anderson and Jackson (1967, 1968). The flow regime involved in fluidization is one of the most difficult for particle-fluid flows. The particle concentrations are high, the dispersed phase is relatively dense, the dispersed phase undergoes a random micromotion, and often it is desirable to have chemical reactions occur in the flow.

In the early 1960's the emergence of commercial atomic energy spurred the study of flows of steam and water. The work of Zuber (1964) was a pioneering landmark. Fluid-fluid flows have a difficulty not encountered in particle-fluid flows, namely that the shape of the dispersed-phase can change, resulting in changing interfacial area and consequent interactions between the fluids. In spite of much progress (Lahey & Moody 1977), two phase flow studies in nuclear reactors are still a concern.

The parallel development of mixture theory had some small influence on the progress of two-phase flows. Indeed, the concept of interpenetrating continuum is natural in mixtures where the dispersion occurs on the molecular level. The development of the ideas of diffusion by Fick (1855), the thermodynamic concepts in mixtures by Duhem (1893), Meixner (1943), Prigogine and Mazur (1951) lead naturally to the theory of mixtures expounded by Truesdell and Toupin (1960). The theory of mixtures, as applied to the specific mixtures where the two constituents remain unmixed, is the basis of the present work, and (whether explicitly recognized or not) much of the more specific previous work. Kenyon (1976) applies the mixture theory to multiphase flows. See also the review by Bedford and Drumheller (1982).

By the 1960's enough of the common features of the diverse two-phase flows were evident. Several influential books of a general nature appeared, including Fluid Dynamics of Multiphase Systems by Soo (1967), One-dimensional Two-Phase Flow, by Wallis (1969), and Flowing Gas-Solid Suspensions, by Boothroyd (1971). Wallis' approach was strongly influenced by gas-liquid flows, and dealt with the basic concept of interpenetrability by considering cross-sectionally averaged equations, and introduced constitutive assumption by quoting appropriate experiments. Soo's work was largely based on particle-fluid flows. He assumed interpenetrability from the start, and included forces in the particular momentum equation known from experiments or inferred from calculations. Boothroyd was interested in particle-gas flows, and contributed ideas on turbulence and drag reduction.

A different, but somewhat related approach to the problem of a mechanical description of two-phase flows uses the single-particle or several interacting particle flow fields, along with an averaging approach to yield rheological or transport properties. The celebrated result in this area is the effective viscosity result due to Einstein (1906), which shows that in slow flow the mixture behaves like a fluid with viscosity increased by a factor of $1 + \frac{5}{2} \alpha$, where α is the volumetric concentration of particles. An approach outlined by Brinkman (1947) has been influential. The philosophical roots of this approach are elegantly discussed in the book Low Reynolds Number Hydrodynamics, by Happel and Brenner (1965). The idea is to use solutions of the flow equations in special cases (such as Stoke's flow around an array of spheres) to infer information about the flow (such as the total force on the particulate phase). Several aspects of this work have been discussed in this Review; see the papers by Brenner (1970), Batchelor (1974), Herczyński and Piénkowska (1980), Leal (1980) and Russel (1981).

Several authors (Bedford & Drumheller 1978, Drumheller & Bedford 1980) have pursued a variational approach to two-phase flows, generalizing the work of Biot (1977). The variational formulation starts with Hamilton's principle, given by

$$\delta \int_{t_2}^{t_1} (T-V)dt + \int_{t_1}^{t_2} \delta W dt = 0$$

where δ represents the variation over an appropriate space of functions, T and V are the kinetic and potential energies, δW is the virtual work and t_1 and t_2 are two arbitrary times. A

variational formulation has an advantage in that if it is desired to include a certain effect (for example, the virtual work), that effect would be included consistently in the mass, momentum, and kinetic energy equations. A more concrete and immediate advantage is in formulating numerical techniques, and specifically, finite element techniques, where variational formulation eases the translation of the partial differential equations into discrete equations.

In order to use a variational formulation, it is necessary to define the variation δ , the kinetic and potential energies T and V and the virtual work δW . Constraints must be included with Lagrange multipliers. Bedford & Drumheller (1982) note that Hamilton's principle is usually formulated with a "control mass", that is, for material volumes. The problem of having two materials moving at different velocities is dealt with by assuming a control volume which coincides with a rigid surface through which no material of either phase passes.

They use the technique to show how the effect of oscillations in bubble diameter can be included by including the kinetic energy of the liquid due to a change in bubble diameter. They similarly include virtual mass by arguing that relative accelerations increase the kinetic energy. A conceptual difficulty with the approach is that the user must decide which fluctuations contribute to the total kinetic energy, and which contribute to virtual work. For example, viscous drag is due to "fluctuations" of the fluid velocity near a particle, but is included as a virtual work term. A rule of thumb might be to consider whether the energy is recoverable or not. Virtual work is associated with

unrecoverable energy, kinetic and potential energy with recoverable energy. Variational formulations (in general) do not mention the effect of Reynolds stresses, which are one manifestation of fluctuations. We conclude that while variational formulations are useful, it is not always straightforward to formulate them.

EQUATIONS OF MOTION

We start by assuming that each material involved can be described as a continuum, governed by the partial differential equations of continuum mechanics. The materials are separated by an interface, which we assume to be a surface. At the interface, jump conditions express the conditions of conservation of mass and momentum.

The equations of motion for each phase are (Truesdell and Toupin 1960)

- (1) conservation of mass

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{v} = 0 \quad (1)$$

- (2) conservation of linear momentum

$$\frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \cdot \rho \mathbf{v} \mathbf{v} = \nabla \cdot \mathbf{T} + \rho \mathbf{f} \quad (2)$$

valid in the interior of each phase. Here ρ denotes the density, \mathbf{v} the velocity, \mathbf{T} the stress tensor, and \mathbf{f} the body force density. Conservation of angular momentum becomes $\mathbf{T} = \mathbf{T}^t$, where t denotes the transpose. At the interface, the jump conditions are

- (1) jump condition for mass

$$[[\rho(\mathbf{v} - \mathbf{v}_i) \cdot \mathbf{n}]] = 0 \quad (3)$$

- (2) jump condition for momentum

$$[[\rho \mathbf{v}(\mathbf{v} - \mathbf{v}_i) \cdot \mathbf{n} - \mathbf{T} \cdot \mathbf{n}]] = \sigma \kappa \mathbf{n} \quad (4)$$

Here $[[\]]$ denotes the jump across the interface, \mathbf{v}_i is that velocity of the interface, σ is the surface tension, assumed to be a constant, κ is the mean curvature of the interface, and \mathbf{n} is the unit normal (Aris 1962). We shall assume that \mathbf{n} points out of phase k , and that the jump between f in phase k and f in phase l is

defined by $[[f]] = f^l - f^k$, where a superscript k denotes the limiting value from the phase k side. As a sign convention for the curvature, we assume that κ is positive (concave) toward $-n$. The mass of the interface has been neglected, and the surface stresses have been assumed to be in the form of classic surface tension.

We do not discuss any thermodynamic relations in this paper. Thermodynamic considerations are important for many multiphase flows. Our discussion focuses on the mechanics of two-phase flows, hence we elect to forego a discussion of thermodynamics for the sake of simplicity.

Constitutive equations must be supplied to describe the behavior of each material involved. For example, if one material is an incompressible liquid, then specifying the value of ρ , and assuming $\mathbf{T} = -p\mathbf{I} + \mu(\nabla\mathbf{v} + (\nabla\mathbf{v})^t)$ determines the nature of the behavior of the fluid in that phase. Similar considerations are possible for solid particles or a gas. The resulting differential equations, along with the jump conditions, provide a fundamental description of the detailed or exact flow.

Usually, however, the details of the flow are not required. For most purposes of equipment or process design, averaged, or macroscopic flow information is sufficient. Fluctuations, or details in the flow must be resolved only to the extent that they effect the mean flow (like the Reynolds stresses effect the mean flow in a turbulent flow).

Averaging

In order to obtain equations which do not contain the details of the flow, it has become customary to apply some sort of averaging process. It is not essential to do so; indeed, some researchers prefer to postulate macroscopic equations without reference to any microscopic equations. Certainly, the necessary terms in the macroscopic equations can be deduced without using an averaging process. One advantage of a postulational approach is obvious - not having to deal with the worries of the averaging process. The advantages of averaging are less obvious. First, the various terms appearing in the macroscopic equations are shown to arise from appropriate microscopic considerations. For example, stress terms arise from microscopic stresses (pressure, for example) and also from velocity fluctuations (Reynolds stresses). Knowledge of this fact does give a modicum of insight into the formulation of constitutive equations. If a term appeared in the averaging which was not expected in the postulational approach, then it would be obligatory to include it in the postulated model, or else explain why it is superfluous.

An additional advantage of averaging is that the resulting macroscopic variables are related to microscopic variables. If the microscopic problem can be solved for some special situation, the solution can then be used to get values of the macroscopic variables. This cannot replace the need to postulate constitutive equations, but it can give insights into the types of terms expected to be important in the constitutive relations. The philosophy taken here is that whatever

information can be gained from averaging is worthwhile, and therefore we present a generic averaging method, and its results. If the reader feels that averaging is unnecessary, he can skip this section, and assume the equations (40) - (43) have been postulated, along with the interpretations given at the end of this Section.

Averaging the equations of motion is suggested by the averaging approach to turbulence (see Hinze 1959). Time and space averages were the first to appear (Frankl 1953, Teletov 1958). These averages have been refined by weighting, by multiple application, and by judicious choice of averaging region. The highlights can be found in the work of Anderson and Jackson (1967), Vernier and Delhaye (1968), Drew (1971), Whitaker (1973), Ishii (1975), Nigmatulin (1979), and Gough (1980). Statistical averages are most convenient for the rheology work; see Batchelor (1974) for a summary. The application of statistical averages to the equations of motion is straightforward; the paper of Buyevich and Shchelchkova (1978) summarizes the approach nicely.

Let $\langle \rangle$ denote an averaging process so that if $f(\mathbf{x},t)$ is an exact microscopic field, then $\langle f \rangle(\mathbf{x},t)$ is the corresponding averaged field. We shall specify shortly the requirements which an average should possess, however, for now we merely suggest that it should be smoothing in the sense that no details appear in the averaged variables. Some examples of commonly used averages in multiphase flow are the time average:

$$\langle f \rangle_1(\mathbf{x},t) = \frac{1}{T} \int_{t-T}^t f(\mathbf{x},t') dt' \quad (5)$$

where T is an averaging time scale; the space average:

$$\langle f \rangle_2(\mathbf{x}, t) = \frac{1}{L^3} \int_{x_1 - \frac{1}{2}L}^{x_1 + \frac{1}{2}L} \int_{x_2 - \frac{1}{2}L}^{x_2 + \frac{1}{2}L} \int_{x_3 - \frac{1}{2}L}^{x_3 + \frac{1}{2}L} f(\mathbf{x}', t) dx'_3 dx'_2 dx'_1 \quad (6)$$

where L is an averaging length scale; a weighted space average

$$\langle f \rangle_3(\mathbf{x}, t) = \iiint_{R^3} g(\mathbf{x} - \mathbf{x}') f(\mathbf{x}', t) d\mathbf{x}' \quad (7)$$

where $\iiint_{R^3} g(\mathbf{s}) d\mathbf{s} = 1$, and various combinations of averages and/or specific R^3 types of weightings. Also mentioned in the literature are ensemble averages:

$$\langle f \rangle_4(\mathbf{x}, t) = \frac{1}{N} \sum_{n=1}^N f_n(\mathbf{x}, t) \quad (8)$$

or

$$\langle f \rangle_5(\mathbf{x}, t) = \int_{\Omega} f(\mathbf{x}, t; \omega) d\mu(\omega) \quad (9)$$

where $f_n(\mathbf{x}, t)$ or $f(\mathbf{x}, t; \omega)$ denote a realization of the quantity f over a set of possible "equivalent" realizations Ω . One way in which randomness might be introduced in a particular flow situation is by allowing the particles to have random initial positions.

The averaging process is assumed to satisfy

$$\langle f+g \rangle = \langle f \rangle + \langle g \rangle \quad (10)$$

$$\langle \langle f \rangle g \rangle = \langle f \rangle \langle g \rangle \quad (11)$$

$$\langle c \rangle = c$$

$$\left\langle \frac{\partial f}{\partial t} \right\rangle = \frac{\partial}{\partial t} \langle f \rangle \quad (12)$$

$$\left\langle \frac{\partial f}{\partial x_i} \right\rangle = \frac{\partial}{\partial x_i} \langle f \rangle \quad (13)$$

The first three of these relations are called Reynolds rules, the fourth is called Liebnitz' rule, and the fifth is called Gauss' rule.

Some difficulty is encountered when trying to apply the average to the equations of motion for each phase. In order to do this, we introduce the phase function $X_k(\mathbf{x}, t)$ which is defined to be

$$X_k(\mathbf{x}, t) = \begin{cases} 1 & \text{if } \mathbf{x} \text{ is in phase } k \text{ at time } t \\ 0 & \text{otherwise} \end{cases} \quad (14)$$

We shall deal with X_k as a generalized function, in particular in regard to differentiating it. Recall that a derivative of a generalized function can be defined in terms of a set of "test functions" ϕ , which are "sufficiently smooth" and have compact support. Then $\frac{\partial X_k}{\partial t}$ and $\frac{\partial X_k}{\partial x_i}$ are defined by

$$\int_{R^3 \times R} \frac{\partial X_k}{\partial t}(\mathbf{x}, t) \phi(\mathbf{x}, t) d\mathbf{x} dt = - \int_{R^3 \times R} X_k(\mathbf{x}, t) \frac{\partial \phi}{\partial t}(\mathbf{x}, t) d\mathbf{x} dt \quad , \quad (15)$$

$$\int_{R^3 \times R} \frac{\partial X_k}{\partial x_i}(\mathbf{x}, t) \phi(\mathbf{x}, t) d\mathbf{x} dt = - \int_{R^3 \times R} X_k(\mathbf{x}, t) \frac{\partial \phi}{\partial x_i}(\mathbf{x}, t) d\mathbf{x} dt \quad . \quad (16)$$

It can be shown that

$$\frac{\partial X_k}{\partial t} + \mathbf{v}_i \cdot \nabla X_k = 0 \quad (17)$$

in the sense of generalized functions. To see this, consider

$$\begin{aligned} & \int_{R^3 \times R} \left(\frac{\partial X_k}{\partial t} + \mathbf{v}_i \cdot \nabla X_k \right) \phi d\mathbf{x} dt \\ &= \int_{R^3 \times R} X_k \left(\frac{\partial \phi}{\partial t} + \nabla \cdot \phi \mathbf{v}_i \right) d\mathbf{x} dt \end{aligned}$$

$$\begin{aligned}
 &= - \int_{-\infty}^{\infty} \left(\int_{R_k} \left(\frac{\partial \phi}{\partial t} + \nabla \cdot \phi \mathbf{v}_i \right) d\mathbf{x} \right) dt \\
 &= - \int_{-\infty}^{\infty} \left(\frac{d}{dt} \int_{R_k(t)} \phi d\mathbf{x} \right) dt \\
 &= \int_{R_k} \phi d\mathbf{x} \Big|_{-\infty}^{\infty} = 0 \quad , \quad (18)
 \end{aligned}$$

since ϕ has compact support in t . Here $R_k(t)$ is the region occupied by phase k at time t , and we assume that \mathbf{v}_i is extended smoothly through phase k (in order that the second line makes sense).

If f is smooth except at S , then $f \nabla X_k$ is defined via

$$\begin{aligned}
 \int_{R^3 \times R} f \nabla X_k \phi d\mathbf{x} dt &= - \int_{R^3 \times R} X_k \nabla(f\phi) d\mathbf{x} dt \\
 &= \int_{-\infty}^{\infty} \int_{R_k(t)} \nabla(f\phi) d\mathbf{x} dt \\
 &= \int_{-\infty}^{\infty} \int_S \mathbf{n}_k f^k \phi dS dt \quad , \quad (19)
 \end{aligned}$$

where \mathbf{n}_k is the unit normal exterior to phase k , and f^k denotes the limiting value of f on the phase- k side of S .

It is also clear that ∇X_k is zero, except at the interface. Equation (19) describes the behavior of ∇X_k at the interface. Note that it behaves as a "delta-function", picking out the interface S , and has the direction of the normal interior to phase k .

This motivates writing

$$\nabla X_k = \mathbf{n}_k \frac{\partial X}{\partial n} \quad (20)$$

where $\partial X/\partial n$ is a scalar valued generalized function which has the property that

$$\int_{R^3 \times R} \left[\frac{\partial X}{\partial n}(\mathbf{x}, t) \right] \phi(\mathbf{x}, t) d\mathbf{x} dt = - \int_{-\infty}^{\infty} \int_S \phi(\mathbf{x}, t) dS dt \quad (21)$$

The quantity $\partial X/\partial n$ then picks out the interface S . We write

$$\left\langle \frac{\partial X}{\partial n} \right\rangle = s \quad (22)$$

where s is the average interfacial area per unit volume.

Averaged Equations

In order to derive averaged equations for the motion of each phase, we multiply the equation of conservation of mass valid in phase k (1) by X_k and average. Noting that

$$X_k \frac{\partial \rho}{\partial t} = \frac{\partial}{\partial t} X_k \rho - \rho \frac{\partial X_k}{\partial t} = \frac{\partial}{\partial t} X_k \rho + \rho \mathbf{v}_i \cdot \nabla X_k \quad (23)$$

and

$$X_k \nabla \cdot \rho \mathbf{v} = \nabla \cdot X_k \rho \mathbf{v} - \rho \mathbf{v} \cdot \nabla X_k \quad (24)$$

we have

$$\frac{\partial}{\partial t} \langle X_k \rho \rangle + \nabla \cdot \langle X_k \rho \mathbf{v} \rangle = \langle [\rho(\mathbf{v} - \mathbf{v}_i)]^k \cdot \nabla X_k \rangle \quad (25)$$

Similar considerations for the momentum equations yield

$$\begin{aligned} \frac{\partial}{\partial t} \langle X_k \rho \mathbf{v} \rangle + \nabla \cdot \langle X_k \rho \mathbf{v} \mathbf{v} \rangle &= \nabla \cdot \langle X_k \mathbf{T} \rangle + \langle X_k \rho \mathbf{f} \rangle \\ &+ \langle [\rho \mathbf{v}(\mathbf{v} - \mathbf{v}_i) - \mathbf{T}]^k \cdot \nabla X_k \rangle \quad (26) \end{aligned}$$

The terms

$$\langle [\rho(\mathbf{v} - \mathbf{v}_i)]^k \cdot \nabla X_k \rangle = \Gamma_k \quad (27)$$

and

$$\langle [\rho \mathbf{v}(\mathbf{v} - \mathbf{v}_i) - \mathbf{T}]^k \cdot \nabla X_k \rangle = M_k \quad (28)$$

are the interfacial source terms. As noted, ∇X_k picks out the interface, and causes discontinuous quantities multiplying it to be evaluated on the phase-k side of the interface.

The jump conditions are derived by multiplying equations (2.3) and (2.4) by $\partial X/\partial n$, and recognizing that $n_1 = -n_2$. We obtain

$$\sum_{k=1}^2 \langle [\rho(\mathbf{v}-\mathbf{v}_i)]^k \cdot \nabla X_k \rangle = \sum_{k=1}^2 \Gamma_k = 0 \quad (29)$$

$$\sum_{k=1}^2 \langle [\rho\mathbf{v}(\mathbf{v}-\mathbf{v}_i) - \mathbf{T}]^k \cdot \nabla X_k \rangle = \sigma \langle \kappa \nabla X_1 \rangle \quad (30)$$

$$= \mathbf{M}_m .$$

The term \mathbf{M}_m is the contribution to the total force on the mixture due to the interface, and specifically due to surface tension.

Applying a different averaging process requires a different set of machinations regarding the interfacial source terms (Anderson & Jackson 1967, Drew 1971, Ishii 1975, Delhaye and Achard 1979). Almost all of the derivations for specific averaging processes seem to be more complicated than the above; however, the trade-off for the simple derivation is that all manipulations now involve generalized functions.

The volumetric concentration (or volume fraction, or relative residence time) of phase k is defined by

$$\alpha_k = \langle X_k \rangle . \quad (31)$$

We note that

$$\frac{\partial \alpha_k}{\partial t} = \left\langle \frac{\partial X_k}{\partial t} \right\rangle \quad (32)$$

and

$$\nabla \alpha_k = \langle \nabla X_k \rangle . \quad (33)$$

There are two types of averaged variables which are useful in two-phase mechanics, namely the phasic, or X_k -weighted average, and the mass-weighted average. Which is appropriate is suggested by the appearance of the quantity in the equation of motion. The phasic average of the variable ϕ is defined by

$$\bar{\phi}_k = \langle X_k \phi \rangle / \alpha_k \quad (34)$$

and the mass weighted average of the variable ψ is defined by

$$\hat{\psi}_k = \langle X_k \rho \psi \rangle / \alpha_k \bar{\rho}_k \quad (35)$$

It is convenient to write the stresses $\bar{\mathbf{T}}_k$ in terms of pressures plus extra stresses. Thus,

$$\bar{\mathbf{T}}_k = -\bar{p}_k \mathbf{I} + \bar{\mathbf{T}}_k \quad (36)$$

It is expected that readers familiar with fluid dynamical concepts are familiar with the concept of pressure in fluids; in this case, \bar{p}_k can be thought of as the average of the microscopic pressure. If one of the phases consists of solid particles, the concept is less familiar. In this case, the microscopic stress (involving small elastic deformations, for example) is thought of being made up of a spherical part (acting equally in all directions) plus an extra stress. The spherical part, when averaged, yields the pressure \bar{p}_k in equation (36).

It has further become customary to separate various parts of the interfacial momentum transfer term. This is done by defining the interfacial velocity of the k^{th} phase by

$$\Gamma_{k,i} \mathbf{v}_{k,i} = \langle [\rho \mathbf{v}(\mathbf{v} - \mathbf{v}_i)]^k \cdot \nabla X_k \rangle \quad (37)$$

and the interfacial pressure on the k^{th} phase by

$$p_{k,i} |\nabla \alpha_k|^2 = \langle p^k \nabla X_k \rangle \cdot \nabla \alpha_k \quad (38)$$

Equation (38) is the dot product of $\nabla\alpha_k$ of the "standard" definition (Ishii 1975) of the interfacial pressure. The standard definition uses three equations to define one scalar quantity, and cannot be a generally valid definition. Here the remaining part of the contribution of the pressure at the interface is lumped with the viscous stress contribution at the interface, and is treated through the use of a constitutive equation. Thus, we write

$$\mathbf{M}^k = \Gamma_k \mathbf{v}_{k,i} - p_{k,i} \nabla\alpha_k + \mathbf{M}_k^d, \quad (39)$$

where $\mathbf{M}_k^d = \langle (p - p_{k,i})^k \nabla X_k - \tau_k^k \cdot \nabla X_k \rangle$ is referred to as the interfacial force density, although it does not contain the effect of the average force on the interface due to the average interfacial pressure. The term $-p_{k,i} \nabla\alpha_k$, which does contain the force due to the average interfacial pressure, is sometimes referred to as the buoyant force. The reason for this terminology is, of course, that the buoyant force on an object is due to the distribution of the pressure of the surrounding fluid on its boundary.

With equations (31) and (34) - (39), the equations of motion (25) and (26) become

$$\frac{\partial \alpha_k \tilde{\rho}_k}{\partial t} + \nabla \cdot \alpha_k \tilde{\rho}_k \hat{\mathbf{v}}_k = \Gamma_k \quad (40)$$

$$\begin{aligned} \frac{\partial \alpha_k \tilde{\rho}_k \hat{\mathbf{v}}_k}{\partial t} + \nabla \cdot \alpha_k \tilde{\rho}_k \hat{\mathbf{v}}_k \hat{\mathbf{v}}_k &= -\alpha_k \tilde{\nabla} p_k + \nabla \cdot \alpha_k (\tilde{\tau}_k + \tilde{\sigma}_k) \\ &+ \Gamma_k \mathbf{v}_{k,i} + (p_{k,i} - p_k) \nabla\alpha_k \\ &+ \mathbf{M}_k^d. \end{aligned} \quad (41)$$

The jump conditions (29) and (30) are

$$\sum_{k=1}^2 \Gamma_k = 0 \quad (42)$$

$$\sum_{k=1}^2 [\Gamma_k \mathbf{v}_{k,i} + p_{k,i} \nabla \alpha_k + \mathbf{M}_k^d] = \mathbf{M}_m \quad (43)$$

Adequate models for compressibility and phase change require consideration of thermodynamic processes. These are beyond the scope of this paper; therefore we shall restrict our attention to incompressible materials where no phase change occurs. Thus we assume that

$$\bar{\rho}_k = \text{constant} \quad (44)$$

and

$$\Gamma_k = 0 \quad (45)$$

In order to simplify the notation, we shall drop all symbols denoting averaging.

CONSTITUTIVE EQUATIONS

In order to have a useable model for an ordinary single-phase material, relations must be given which specify how the material interacts with itself. These relations specify how the material transmits forces from one part of the body to another. For single-phase materials a relation between the stress and other field variables is usually required. For two-phase materials, where we desire to track both phases, we must specify the stresses for both phases and the way in which the materials interact across the interface. Thus, we require constitutive equations for the stresses $(\tau + \sigma_k)$, the interfacial force density M_k^d , and the pressure differences $p_k - p_{k,i}$, consistent with the equations of motion and the jump conditions.

The fundamental process consists of proposing forms for the necessary terms within the framework of the principles of constitutive equations, finding solutions of the resulting equations, and verifying against experiments. The process can be iterative, with some experiment indicating that a more involved form is needed for some constituted variable. The ideal end result of the process is a set of equations which could be used to predict the behavior of the two-phase flow, for example with a computer code. With the equations should come a set of conditions for the validity of the values of the constants and other functions used in the constitutive equations.

The stresses $\tau_k + \sigma_k$, the interfacial force density M_k^d and the pressure differences $p_k - p_{k,i}$ are assumed to be functions of α_k , $\partial\alpha_k/\partial t$, $\nabla\alpha_k$, \mathbf{v}_k , $\nabla\mathbf{v}_k$, $\partial\mathbf{v}_k/\partial t$, ... , where ... represents the material

properties, such as the viscosities and densities of the two materials, and other geometric parameters such as the average particle size, or the interfacial area density.

For concreteness, we shall refer to phase one as the particulate, or dispersed phase and include in that description solid particles, droplets, or bubbles. Phase two is then the continuous, or carrier phase, and can be liquid or gas. We shall denote

$$\alpha = \alpha_1 \tag{46}$$

so that

$$1-\alpha = \alpha_2 \tag{47}$$

It is evident that both α and $1-\alpha$ need not be included as independent variables in forming constitutive equations.

Drew and Lahey (1979) consider the general process of constructing constitutive equations. The principle of consequence is that of material frame indifference, or objectivity. This principle requires that constitutive equations be appropriately invariant under a change of reference frame. The motivation behind this assumption is that we expect the way in which a two-phase material distributes forces to be independent of the coordinate system used to express it. Those who doubt this principle often argue that the momentum equation is not frame indifferent, needing Coriolis forces and centrifugal forces to correct it in non-inertial frames. This argument is incorrect, since the appropriate formulation of the momentum equation deals not with "acceleration" but with "acceleration relative to an inertial frame". When formulated with the "acceleration relative to an inertial frame",

the momentum equations are frame indifferent (Truesdell 1977). This introduces an interesting question: Can the mixture know whether or not it is being referred to a inertial frame? That is, can the interfacial force and the Reynolds stresses depend on the reference frame? The principle of material frame indifference, as used here, claims that they cannot. Others claim that they must (Ryskin and Rallison 1981).

The principle of objectivity is now examined (Drew & Lahey 1979). The approach we take deals with coordinate changes, but is equivalent to more abstract approaches (Truesdell 1977). Consider a coordinate change from system \mathbf{x} to system \mathbf{x}^* , given by

$$\mathbf{x}^* = \mathbf{Q}(t) \cdot \mathbf{x} + \mathbf{b}(t) \quad , \quad (48)$$

where $\mathbf{Q}(t)$ is an orthonormal tensor and \mathbf{b} is a vector. A scalar is objective if its value is the same in both the starred and unstarred systems, that is, if

$$\phi^*(\mathbf{x}^*, t) = \phi(\mathbf{x}, t) \quad . \quad (49)$$

A vector is objective if it transforms coordinates correctly, that is, if

$$\mathbf{v}^* = \mathbf{Q} \cdot \mathbf{v} \quad . \quad (50)$$

A tensor is objective if

$$\mathbf{T}^* = \mathbf{Q} \cdot \mathbf{T} \cdot \mathbf{Q}^t \quad . \quad (51)$$

The scalar α is objective; however $\partial\alpha/\partial t$ is not. It is straightforward to show that $D_k \alpha / Dt = \partial\alpha/\partial t + \mathbf{v}_k \cdot \nabla \alpha$ is objective.

Let us next consider objective vectors. The volume fraction gradient $\nabla \alpha$ is objective. If we differentiate (48) with respect to t following a material particle of phase k , we see that

$$\mathbf{v}_k^* = Q(t) \cdot \mathbf{v}_k + (\dot{Q} \cdot \mathbf{x} + \dot{\mathbf{b}}) \quad (52)$$

Hence velocities are not objective. This is obvious physically, since the velocity of a point depends on the coordinate system. If we take equation (2.53), for $k = 1$ and 2 , and subtract, we have

$$\mathbf{v}_1^* - \mathbf{v}_2^* = Q \cdot (\mathbf{v}_1 - \mathbf{v}_2) \quad (53)$$

Thus, the relative velocity between the phases is objective.

For accelerations, differentiating (52) following a material particle of phase j yields

$$\frac{D_j \mathbf{v}_k^*}{Dt} = Q \cdot \frac{D_j \mathbf{v}_k}{Dt} + \ddot{Q} \cdot \mathbf{x} + \dot{Q} \cdot \mathbf{v}_j + \dot{Q} \cdot \mathbf{v}_k + \ddot{\mathbf{b}} \quad (54)$$

Thus, subtracting the value for $j = 1, k = 1$ from the value for $j = 2, k = 1$ yields the result that

$$\mathbf{a}_{12} = \frac{D_1 \mathbf{v}_2}{Dt} - \frac{D_2 \mathbf{v}_1}{Dt} \quad (55)$$

is objective.

The list of tensors which we consider is motivated by the desire to model two-phase flows. Thus, velocity gradients (expressing rate of deformation) are included, but displacement gradients (expressing deformation) are not. It is well known (Truesdell and Toupin 1960) that

$$\mathbf{D}_{k,b} = \frac{1}{2} (\nabla \mathbf{v}_k + (\nabla \mathbf{v}_k)^t) \quad (56)$$

are objective. We further note that $\nabla(\mathbf{v}_1 - \mathbf{v}_2)$ is an objective tensor.

Thus, the problem of forming constitutive equations reduces to expressing

$$\tau_k + \sigma_k, p_k - p_{k,i}, M_k^d \quad (57)$$

in terms of

$$\alpha, D_k \alpha / Dt, \nabla \alpha, \mathbf{v}_1 - \mathbf{v}_2, D_2 \mathbf{v}_1 / Dt - D_1 \mathbf{v}_2 / Dt, \\ D_{1,b}, D_{2,b}, \nabla(\mathbf{v}_1 - \mathbf{v}_2) \quad (58)$$

We shall assume that the materials are isotropic. This means that no direction is preferred in either material or in the way they interact. Note that a particular flow may occur in such a way that a preferred direction (down, for example) might emerge. In that case, the flow is anisotropic, but the materials and the mixture are isotropic.

If f is a scalar, then f can depend on the scalars and the scalar invariants formed from the vectors and tensors in the list (58). The length of a vector is a scalar invariant, as are the trace, determinant and Euclidean norm of a tensor.

If \mathbf{F} is a vector, then \mathbf{F} must be linear in all the vector in the list (58), plus any vectors which can be formed in an invariant way from the vectors and tensors in that list. Thus

$$\mathbf{F} = \sum a_i \mathbf{V}_i \quad (59)$$

where \mathbf{V}_i are the objective vectors so formed. Each scalar coefficient a_i can be a function of all the scalars and scalar invariants.

If F is a second order tensor, then

$$F = \sum B_j \mathbf{Y}_j \quad (60)$$

where \mathbf{Y}_j are the objective tensors which can be formed from the list (58). The scalars B_j can be functions of all the scalars. If F is symmetric, we need only consider symmetric \mathbf{Y}_j .

The general approach (Drew and Lahey 1979) gives a problem too big to be practical or meaningful. Thus, we shall consider here forms for the stresses, etc., which we expect to be important in two-phase flows. Obviously, we shall have the constant worry that something has been forgotten; however, the alternative of stopping at this point, awaiting evaluation of over two-thousand scalar coefficients seems less attractive.

Stresses

Let us now discuss specific considerations for the specific constitutive equations needed. Let us begin with the stresses. The extra stress (viscous or elastic) and turbulent stresses are combined as $\tau_k + \sigma_k$. Macroscopically, at least in the context of this model, one sees no way to separate them. Microscopically, one is due to the actual stresses, and the other is due to velocity fluctuations from the mean. In many cases of interest the extra stress is smaller than the turbulent stress, one reason being that any appreciable slip between the phases generates velocity fluctuations, which appear in this model in the turbulent stresses. These fluctuations can transport momentum. The conceptual situation is analogous to that for single-phase turbulent momentum transport, with "eddies" carrying momentum across planes parallel to the shearing direction and losing it into the mean flow. The fluctuations in single-phase turbulent flow are there because of instabilities in the laminar shear flow; in two-phase flow they also come from fluctuations generated due to the flow around individual particles.

Drew and Lahey (1981) have generated a model for the turbulent stresses in bubbly air-water flow. The model they deduce in this case has the form

$$\sigma_2 = 2\mu_2^T D_{2,b} + a_2 I + b_2 (\mathbf{v}_1 - \mathbf{v}_2)(\mathbf{v}_1 - \mathbf{v}_2) \quad (61)$$

for the liquid phases. Here μ_2^T is the eddy viscosity, a_2 is an induced eddy "pressure", and b_2 is associated with bubble passages. The parameters μ_2^T , a_2 and b_2 depend on α , the bubble radius r , the relative velocity $|\mathbf{v}_1 - \mathbf{v}_2|$ and the Euclidean norm of $D_{2,b}$. Nigmatulin (1979) uses a cell model, assuming inviscid flow around a spherical particle in each cell, to calculate values of a_2 and b_2 .

He obtains

$$b_2 = -\frac{1}{2} \rho_2 \quad (62)$$

$$a_2 = \frac{1}{6} \rho_2 |\mathbf{v}_1 - \mathbf{v}_2|^2 \quad (63)$$

He does not obtain a term involving the eddy viscosity because the cell model is unsuited to obtaining shear flow results. His results are valid for dilute flows. Other effects are present in most turbulent flows.

Drew and Lahey (1981) used mixing lengths to evaluate the coefficients in eq. (61). The data available thus far (Serizawa 1975) allows only evaluation of the ratios of various Karman constants, nonetheless, the importance of the problem in nuclear reactor technology has spurred the acquisition of more direct data in special cases (Lance 1981). This data should be available shortly, and should allow the evaluation of a_2 and b_2 for bubbly flows.

Evidence (Serizawa 1975) also indicates that

$$\sigma_1 = O\left(\frac{\rho_1}{\rho_2} \sigma_2\right) \quad (64)$$

and is negligible in dispersed bubbly flows. A model for σ_1 analogous to eq. (61) is

$$\sigma_1 = 2\mu_1^T D_{1,b} + a_1 I + b_1 (\nabla_1 - \nabla_2)(\nabla_1 - \nabla_2) \quad (65)$$

If the particulate phase follows the fluid phase closely, the quantities in equations (61) and (65) representing both velocity scales and mixing lengths of large eddy processes should be approximately equal. If this is the case, then

$$\mu_1^T \cong \frac{\rho_1}{\rho_2} \mu_2^T \quad (66)$$

The remaining terms in eq. (65) arise at least in part due to the motion of the particles through the fluid. No constraints are placed on these coefficients.

Ishii (1975) argues that for the viscous fluid phase, the average of the microscopic viscous stress lead to

$$\tau_2 = 2\mu_2 D_{2,b} + \mu_2 \frac{b(1-\alpha)}{1-\alpha} [\nabla\alpha(\nabla_1 - \nabla_2) + (\nabla_1 - \nabla_2)\nabla\alpha] \quad (67)$$

where μ_2 is the exact viscosity of the fluid, and b is called the mobility of phase two. He argues that $b(1-\alpha) \geq 1$ for α near zero. No experimental evidence has been offered to verify (67).

In the case when the particulate phase consists of solid particles, it is usually assumed that $\tau_1 = 0$. If the particulate phase is also a viscous fluid, then it is sometimes assumed that

$$\tau_1 = 2\mu_1 D_{1,b} \quad (68)$$

This corresponds to Ishii's result (see eq. 67)) with $b = 0$.

Murray (1965a) offers a model for a particle-fluid flow in which he assumes that the particles experience a viscous stress with a viscosity coefficient proportional to the fluid viscosity. His argument indicates that the force he is calculating is not a stress, but an interfacial force.

Pressure Relations

The pressure differences $p_k - p_{k,i}$ are discussed next. First, we note that with the assumption of local incompressibility of each phase, we must constitute all but one of $p_1, p_2, p_{1,i}$ and $p_{2,i}$. The other will then be a solution of the equations of motion.

The simplest assumption for pressure differences, is to assume none. That is, assume $p_k = p_{k,i}$ for $k = 1, 2$. This assumes that there is "instantaneous" microscopic pressure equilibration which will be the case if the speed of sound in each phase is large compared with velocities of interest. In applications which do not deal with acoustic effects or bubble expansion/contraction, this assumption is adequate. For a discussion of bubble oscillation effects, see the article by van Wijngaarden (1972). Cheng (1982) studies the consequences of several modeling assumptions on wave propagation in a bubble mixture.

In situations where surface tension is important and no contacts occur between the particles, we assume that the jump condition (4) becomes

$$p^1 - p^2 = \sigma \kappa' \quad (69)$$

where κ' is the exact curvature of the interface. Multiplying by ∇x_1 and averaging gives

$$(p_{1,i} - p_{2,i})\nabla\alpha = \sigma\kappa \nabla\alpha, \quad (70)$$

where κ is the average mean curvature. Since this equation holds for all $\nabla\alpha$, we have

$$p_{1,i} - p_{2,i} = \sigma\kappa. \quad (71)$$

If the surface tension is negligible, equation (2.72) gives $p_{1,i} = p_{2,i}$.

When contacts occur between particles, these considerations are not always simple. The contacts provide mechanisms for causing the average pressure at the interface in one phase to be higher than the other. Consider solid particles submerged in fluid, with no motion, and with the particles under a compressive force (supporting their own weight, or the weight of an object, for example). The resulting stress will be transmitted from particle to particle through the areas of particle-particle contact. Just on the particle side of the interface where the contact occurs, the stress (pressure) level will be large. At places where no contact occurs, the stress will be equal to the pressure in the surrounding fluid. Under normal circumstances, the contact areas will be a small fraction of the total interfacial area. Thus, the approximation $p_{1,i} \approx p_{2,i} = p_i$ is usually valid. In the more general situation, these contacts may be intermittent, when the particles are bumping together, or may be constant, as when the particles are at rest. In this case, also, we expect $p_{1,i} = p_{2,i} = p_i$.

Stuhmiller (1977) argues that

$$p_2 - p_{2,i} = \xi \rho_2 |\mathbf{v}_2 - \mathbf{v}_1|^2 \quad (72)$$

where ξ is taken to be a constant. The argument leading to (72) is exactly the calculation of form drag, which is usually part of the interfacial drag. It is not clear whether using (72) and a drag law (79) includes the form drag consistently.

We shall assume that for the fluid phase, $p_2 = p_i$. To allow for the possibility of the extra stress due to contacts, in the particulate phase when it consists of solid particles, we shall write

$$p_1 = p_{1,i} + p_c = p_2 + p_c \quad (73)$$

where p_c is the pressure in the particles due to contacts. A model is needed for p_c . Several modelers (Gough 1980, Kuo et al. 1976) have used a model with $p_c = p_c(\alpha)$, with $p_c(\alpha) = 0$ for $\alpha < \alpha_c$, where α_c is the packing concentration of the particles, and $p_c(\alpha)$ rapidly increasing for $\alpha > \alpha_c$. This further suggests an "incompressible" model, with $p_c = 0$ for $\alpha < \alpha_c$, and $\alpha = \alpha_c$, and p_c unspecified, otherwise. In this latter region, the particle momentum equation is meaningless. Such a model has not been exploited.

Interfacial Momentum Transfer

Let us now consider the interfacial momentum transfer terms. In a sense, the crucial modeling for two-phase flow is done with these terms, since they are the terms which couple the two phases together.

Let us consider M_m . In analogy with Ishii (1975), we write

$$M_m = \sigma \kappa \nabla \alpha \quad (74)$$

where κ is the average mean curvature of the interface. In this case,

the momentum jump condition becomes

$$\mathbf{M}_1^d + p_{1,i} \nabla \alpha + \mathbf{M}_2^d - p_{2,i} \nabla \alpha = \sigma \kappa \nabla \alpha \quad (75)$$

Using condition (71), we have

$$\mathbf{M}_1^d + \mathbf{M}_2^d = 0 \quad (76)$$

Therefore, we need only provide a model for \mathbf{M}_1^d . \mathbf{M}_2^d then is determined by the jump condition (76).

The interfacial momentum transfer \mathbf{M}_1^d contains the forces on the particulate phase due to viscous drag, wake and boundary layer formation, and unbalanced pressure distributions leading to lift or virtual mass effects, except for the mean interfacial pressure. The model which we discuss here should contain, as much as possible, the above forces. Indeed, this motivates the inclusion of certain quantities in the list of variables (58).

We postulate

$$\begin{aligned} \mathbf{M}_1^d = & A_1 (\mathbf{v}_2 - \mathbf{v}_1) + A_2 \left[\left(\frac{\partial \mathbf{v}_2}{\partial t} + \mathbf{v}_1 \cdot \nabla \mathbf{v}_2 \right) - \left(\frac{\partial \mathbf{v}_1}{\partial t} + \mathbf{v}_2 \cdot \nabla \mathbf{v}_1 \right) \right] \\ & + A_3 (\mathbf{v}_2 - \mathbf{v}_1) \cdot \mathbf{D}_{1,b} + A_4 (\mathbf{v}_2 - \mathbf{v}_1) \cdot \mathbf{D}_{2,b} + A_5 (\mathbf{v}_2 - \mathbf{v}_1) \cdot \nabla (\mathbf{v}_2 - \mathbf{v}_1) \\ & + A_6 (\mathbf{v}_1 - \mathbf{v}_2) \cdot [\nabla (\mathbf{v}_1 - \mathbf{v}_2)]^t \end{aligned} \quad (77)$$

where $A_1 - A_6$ are scalar functions of the invariants.

The first term represents the classical drag forces. To conform with customary useage, we write

$$A_1 = \frac{3}{8} \alpha \rho_2 \frac{C_D}{r} |\mathbf{v}_1 - \mathbf{v}_2| \quad (78)$$

where r is the effective particle radius, and C_D is the drag coefficient. It is usually assumed that $C_D = C_D(\alpha, Re)$, where

$Re = 2\rho_2 |\mathbf{v}_1 - \mathbf{v}_2| r / \mu_2$ is the particle Reynolds number. A careful study, including extensive comparisons with data, is given by Ishii and Zuber (1979). Their conclusions for the drag coefficient are summarized in Table 1, which is adapted from their paper.

The combination

$$A_2 \left[\left(\frac{\partial \mathbf{v}_2}{\partial t} + \mathbf{v}_1 \cdot \nabla \mathbf{v}_2 \right) - \left(\frac{\partial \mathbf{v}_1}{\partial t} + \mathbf{v}_2 \cdot \nabla \mathbf{v}_1 \right) \right] + A_5 (\mathbf{v}_2 - \mathbf{v}_1) \cdot \nabla (\mathbf{v}_2 - \mathbf{v}_1) \quad (79)$$

is an acceleration term. Drew, Cheng and Lahey (1979) write

$$A_2 = \alpha \rho_1 C_{VM}(\alpha) \quad , \quad (80)$$

$$A_5 = A_2 (1 - \lambda(\alpha)) \quad , \quad (81)$$

where C_{VM} is referred to as the virtual volume. If $C_{VM} = \frac{1}{2}$, and no spatial velocity gradients are present, then (79) reduces to the classically accepted virtual mass force. It is less easy to obtain correlations for C_{VM} than for C_D , since the ratio of virtual mass forces to drag forces is of order $V t^* / r$, where V is a velocity scale and t^* is a time scale. In order for the virtual mass force to be appreciable, the time scale must be of the order r/V . For most multiphase flow applications, r is small, and V is not. Thus, we see virtual mass effects only at relatively high frequencies.

Zuber (1964) considered finite concentration effects on virtual mass by considering a sphere moving inside a spherical "cell". He obtained

$$C_{VM}(\alpha) \simeq \frac{1}{2} \frac{1+2\alpha}{1-\alpha} \simeq \frac{1}{2} + \frac{3}{2} \alpha \quad (82)$$

for small α . Nigmatulin (1976) also calculates the virtual mass coefficient from a cell model. He obtained $C_{VM}(\alpha) \simeq \frac{1}{2}$ to $O(\alpha)$. The form of the acceleration which he derives is not objective. It is

possible that this is due to the inability of cell models to adequately deal with velocity gradient terms. The value of the virtual mass coefficient derived by van Wijngaarden (1976) is

$$C_{VM}(\alpha) = 0.5 + 1.39\alpha \quad (83)$$

Moheyev (1977) obtained an empirical correlation

$$C_{VM}(\alpha) = 0.5 + 2.1\alpha \quad (84)$$

by using an electrodynamic analog. Thus, there seems to be a consensus that $C_{VM} \rightarrow \frac{1}{2}$ as $\alpha \rightarrow 0$. There is less agreement on the $O(\alpha)$ correction. In addition, there are several models in the literature (Wallis 1969, Hinze 1972) which use non-objective forms of the virtual mass. There is no compelling evidence at this point as to whether the objective or non-objective forms conform more closely to reality.

Cheng (1982) has done extensive predictions using virtual mass models for accelerating air-water bubbly flows. For low frequency small disturbances in a one-dimensional flow, he found that the value of C_{VM} had a significant effect on the propagation speed, but that the data were scattered so that a particular value could not be estimated. For higher frequency waves (sound waves) and for critical flow, compressibility effects were important. For nozzle flow, the virtual mass effects were insignificant. None of the calculations showed any effect of different values of λ .

The term

$$A_4(\nabla_2 - \mathbf{v}_1) \cdot \mathbf{D}_{2,b} \quad (85)$$

contains the effect of the lift. We write $A_4 = \alpha L$. On the other hand, the forces represented by $A_3(\nabla_2 - \mathbf{v}_1) \cdot \mathbf{D}_1$ and

$A_6(\mathbf{v}_1 - \mathbf{v}_2) \cdot [\nabla(\mathbf{v}_1 - \mathbf{v}_2)]^T$ have no analogs in single particle calculations, and, no observations confirm their presence. Thus we assume $A_3 = A_6 = 0$. Very little experimental evidence for A_4 exists.

Interfacial Geometry Models

It is evident from eqs. (71) and (78) that a relation is needed for expressing the geometry of the interface. Several such relations have been used; however, none is so compelling as to be called general. The one which comes closest is due to Ishii (1975) (derived for the time average; the generalization is obvious). We shall discuss this later. First, we present the simplest models. If the particles are solid spheres each of the same radius r , we have

$$\alpha = \frac{4}{3} \pi r^3 n, \quad (86)$$

where n is the number density. Other quantities of interest are immediately obtainable from α and r , for example, the average interfacial area per unit volume is $\frac{3\alpha}{r}$. Note that n is conserved since α is; specifically, we have

$$\frac{\partial n}{\partial t} + \nabla \cdot n \mathbf{v}_1 = 0. \quad (87)$$

If the particles are not monodisperse, it may be necessary to derive a model where each size of particle is treated separately. Some recent efforts along these lines show great promise (Greenspan 1982). Particle breaking, agglomeration, or accretion/erosion also necessitates a more complicated model. An effort (without macroscopic mechanical considerations) is given by Seinfeld (1980). Both approaches are essential geared to an equation analogous to (87) for a number density.

A more general approach is suggested by Ishii (1975) (for time averaged equations), where he writes

$$\frac{\partial s}{\partial t} + \nabla \cdot \mathbf{v}_i s = \phi_i \quad , \quad (88)$$

where s is the interfacial area per unit volume, which in the present notation is $\langle \partial X / \partial n \rangle$, \mathbf{v}_i is the averaged interfacial velocity, and ϕ_i is a source of interfacial area, due to "bulging" of the interface. This approach is probably best suited to flows where the particulate phase (bubbles or drops) can coalesce or break up. It has not been investigated to any degree.

MODEL CONSIDERATIONS

The main aspect of two-phase flows which makes them fundamentally different from a single-phase flow is the interfacial interaction terms, and, thus, in the absence of interfacial mass transfer the difference is contained in the interfacial force M_k^d . The modeling of this term must proceed carefully, with attention paid to any possible inconsistencies or untoward predictions. A canonical problem involving simplified two-phase flow models has surfaced in the literature; namely, that the one-dimensional, incompressible, inviscid flow equations without virtual mass effects are ill-posed as an initial value problem (Ramshaw & Trapp 1978).

To see this, consider the equations with $C_{VM} = 0$ and $L = 0$.

(This represents the model used in most practical calculations.)

$$\frac{\partial \alpha}{\partial t} + \frac{\partial \alpha v_1}{\partial x} = 0 \quad (89)$$

$$-\frac{\partial \alpha}{\partial t} + \frac{\partial (1-\alpha)v_2}{\partial x} = 0 \quad (90)$$

$$\alpha \rho_1 \left(\frac{\partial v_1}{\partial t} + v_1 \frac{\partial v_1}{\partial x} \right) = -\alpha \frac{\partial p}{\partial x} + A_1 (v_2 - v_1) \quad (91)$$

$$(1-\alpha) \rho_2 \left(\frac{\partial v_2}{\partial t} + v_2 \frac{\partial v_2}{\partial x} \right) = -(1-\alpha) \frac{\partial p}{\partial x} + A_1 (v_1 - v_2) \quad (92)$$

If the pressure is eliminated from system (89) - (92) and the resulting equations are expressed in the form $A \frac{\partial u}{\partial t} + B \frac{\partial u}{\partial x} = C$, where $u = [\alpha, v_1, v_2]^T$, A and B are 3×3 matrices and C is a 3-vector, then the characteristics of the system are given by $\frac{dz_i}{dt} = v_i$, $i = 1, 2, 3$,

where v_i are the three characteristic values of $\det[AV-B] = 0$. Note that since C contains no derivative terms, it is not involved in determining the characteristics. The characteristic values v_i for the system as given are a pair of complex conjugate roots $v_{1,2} = \alpha \pm i\beta$ (with $\beta \neq 0$), and $v_3 = \infty$ (resulting from the assumption of incompressibility). This implies (Garabedian 1964) that the initial value problem is ill-posed.

One implication of the ill-posed nature of the system can be seen as follows. Consider the linear stability of a constant solution. The solution of the linearized equations has the form $u(x,t) = u_0 + u_1 e^{vt+ikx}$, where k is real. Substitution into the linearized system results in the eigenvalue problem

$$[A(u_0)v + B(u_0)ik - C(u_0)]u_1 = 0 \quad (93)$$

for v . The eigenvalue equation is

$$\det[A(u_0) \frac{iv}{k} - B(u_0) - \frac{C(u_0)}{k} - i] = 0 \quad (94)$$

For k large, two roots of (94) are

$$\frac{vi}{k} = \alpha \pm i\beta \quad (95)$$

Thus,

$$v_{1,2} = k(\pm\beta - \alpha i) \quad (96)$$

As long as $\beta \neq 0$, one of the v 's will have positive real part, indicating linear instability. Note, too, that as k increases, the growth rate $|\beta k|$ increases. This shows that finer disturbances grow faster. This implies that at any $t > 0$, $\max|u_1 e^{vt+ikx}|$ can be made as large as desired by taking k sufficiently small. Contrast this with the behavior of an instability of a well-posed system, where the

solution $u_1 e^{vt+ikx}$ can be made as small as desired at a finite t by making u_1 small, for any k . The instability in the well posed system has some realistic physical meaning, while the instability always present in the ill-posed system suggests that the model is not treating small scale phenomena correctly.

The extension of the argument to three space dimensions is straightforward, and shows that the system is ill-posed in three dimensions also.

The ill-posed nature of the model makes it desirable to seek physical modifications of that simple model to find a well posed model. An effort has been made to determine whether and/or to what extent virtual mass makes the inviscid model well posed. Lahey, et al. (1980) have shown that the model becomes well-posed for certain values of C_{VM} . The value of C_{VM} which makes the system well-posed is usually large unless α is extremely small, or other somewhat non-physical assumptions are made. Thus, even though it is a possible "fix" to the question of the well vs. ill-posed nature of the model, virtual mass does not seem to be the total answer.

We note here that if the viscous and Reynolds stresses are included in the equation, and they are assumed to depend on ∇v_k , the equations become parabolic, and hence are well-posed if enough boundary conditions are used. Also Prosperetti and van Wijngaarden (1976) have shown that using certain compressibility assumptions in gas-liquid systems gives

real characteristics. Stuhmiller (1977) shows that his model including the form drag (see eq. 72) gives real characteristics for sufficiently large ξ .

The question of the role of the inviscid model remains. In single-phase fluid mechanics, the inviscid model is extremely important, and governs the flow outside of boundary layers, shear layers and other singular structures. In two-phase flows, the inviscid equations are ill-posed, possessing the unrealistic feature that small scale phenomena grow rapidly. This seems to imply that an inviscid model is nowhere valid for two-phase flows, that is, viscous or eddy stresses are important everywhere. An important unanswered question is whether the inviscid limit of the two-phase flow equations is meaningful.

Let us examine another possible hypothesis about the interfacial force which leads to an interesting form of the virtual mass and lift terms. The hypothesis is that the interfacial force must be dissipative for all conceivable flows. This requirement can be derived from considerations involving an entropy inequality. The argument is complicated (Drew and Lahey 1981), and will not be presented here. It depends on the correct grouping of several terms in the energy and entropy equations.

If we form the total kinetic energy equation by dotting (42) with \mathbf{v}_k , and adding for $k = 1, 2$, we obtain

$$\frac{\partial}{\partial t} \sum_{k=1}^2 \alpha_k \rho_k \frac{v_k^2}{2} + \nabla \cdot \sum_{k=1}^2 \alpha_k \rho_k \mathbf{v}_k \frac{v_k^2}{2} = - \sum_{k=1}^2 \alpha_k \mathbf{v}_k \cdot \nabla p_k$$

$$\begin{aligned}
 & + \nabla \cdot \sum_{k=1}^2 [\alpha_k (\tau_k + \sigma_k) \cdot \mathbf{v}_k] + \sum_{k=1}^2 (p_{k,i} - p_k) \mathbf{v}_k \cdot \nabla \alpha_k \\
 & + \sum_{k=1}^2 \alpha_k (\tau_k + \sigma_k) : \nabla \mathbf{v}_k + \mathbf{M}_1^d \cdot (\mathbf{v}_1 - \mathbf{v}_2) \quad . \quad (97)
 \end{aligned}$$

The terms on the left represent the rate of change total (mean flow) kinetic energy. The pressure terms contribute to the stored internal energy. The term $\sum_{k=1}^2 \alpha_k (\tau_k + \sigma_k) \cdot \mathbf{v}_k$ is the working of the stresses. The two terms $-\sum_{k=1}^2 \alpha_k (\tau_k + \sigma_k) : \nabla \mathbf{v}_k$ and $-\mathbf{M}_1^d \cdot (\mathbf{v}_1 - \mathbf{v}_2)$ are the (bulk) dissipation and the interfacial dissipation, respectively. We require the total dissipation to be expressible as

$$\frac{\partial A}{\partial t} + \nabla \cdot \mathbf{B} + C \quad , \quad (98)$$

where $A > 0$ and $C > 0$ for all possible flows. The term A represents the extra kinetic energy attributable to interactions, \mathbf{B} represents the extra kinetic energy flux, and C is the (actual) total dissipation.

We shall present the results of the dissipativity requirement for $\tau_k = 0$ and $\sigma_k = 0$. If we then take eq (78) for \mathbf{M}_1^d , and assume that C_{VM} , λ and L are constants, we have

$$\begin{aligned}
 -\mathbf{M}_1^d \cdot (\mathbf{v}_1 - \mathbf{v}_2) &= A_1 (v_1 - v_2)^2 \\
 &+ \frac{\partial}{\partial t} \left[\alpha C_{VM} \rho_2 \frac{(v_1 - v_2)^2}{2} \right] \\
 &+ \nabla \cdot \left\{ \alpha C_{VM} \rho_2 \left[\mathbf{v}_2 + (1-\lambda)(\mathbf{v}_1 - \mathbf{v}_2) \right] \frac{(v_1 - v_2)^2}{2} \right\} \\
 &- \frac{(v_1 - v_2)^2}{2} \left[\alpha C_{VM} \rho_2 (\lambda-2) \nabla \cdot (\mathbf{v}_1 - \mathbf{v}_2) \right]
 \end{aligned}$$

$$- (\alpha C_{VM} \rho_2 + \alpha L) (\mathbf{v}_1 - \mathbf{v}_2) \cdot \nabla \mathbf{v}_2 \cdot (\mathbf{v}_1 - \mathbf{v}_2) \quad (99)$$

If we examine (99) for uniform fields, we obtain the first result of the dissipativity requirement, namely that $A_1 > 0$. Furthermore, we note that since the other terms depend on spatial gradients, and we can impose them at will, we have

$$\lambda = 2 \quad (100)$$

$$L = -C_{VM} \rho_2 \quad (101)$$

Note also that the requirement that $A > 0$ results in $C_{VM} > 0$. The resulting form for M_1^d is

$$\begin{aligned} M_1^d = & A_1 (\mathbf{v}_2 - \mathbf{v}_1) + \frac{\partial}{\partial t} \alpha C_{VM} \rho_2 (\mathbf{v}_2 - \mathbf{v}_1) \\ & + \nabla \cdot [\alpha C_{VM} \rho_2 \mathbf{v}_1 (\mathbf{v}_2 - \mathbf{v}_1)] \\ & + \alpha C_{VM} \rho_2 (\mathbf{v}_1 - \mathbf{v}_2) \cdot \frac{1}{2} [\nabla \mathbf{v}_2 - (\nabla \mathbf{v}_2)^t] \quad (102) \end{aligned}$$

In this form, the virtual mass terms are in conservation form, with the convective velocity \mathbf{v}_1 . The non-objective nature of these terms must be compensated for by the lift term, resulting in the last term in (102). Note that if $\boldsymbol{\omega}_2 = \nabla \times \mathbf{v}_2$ is the fluid vorticity, the last term becomes $\alpha C_{VM} \rho_2 (\mathbf{v}_1 - \mathbf{v}_2) \times \boldsymbol{\omega}_2$. Thus, the remaining part of the lift is always perpendicular to the slip and the fluid vorticity.

TABLE I. Local Drag Coefficients in Multiparticle System

	Fluid Particle System		Solid Particle System	
	Bubble in Liquid	Drop in Liquid	Drop in Gas	
Viscosity Model	$\frac{\mu_m}{\mu_2} = (1 - \frac{\alpha}{\alpha_m})^{-2.5\alpha} \mu_m^*$ $\mu_m^* = \frac{\mu_1 + 0.4\mu_2}{\mu_1 + \mu_2}$			
Max. Packing α_m	~ 1	~ 1	$0.62 \sim 1$	~ 0.62
μ^*	0.4	~ 0.7	1	1
$\frac{\mu_m}{\mu_2}$	$(1-\alpha)^{-1}$	$(1-\alpha)^{-1.75}$	$\sim (1-\alpha)^{-2.5}$	$(1 - \frac{\alpha}{0.62})^{-1.55}$
Stokes Regime C_D	$C_D = 24/N_{Re} \text{ where } N_{Re} = 2r\rho_2 \nabla_2 - \nabla_1 /\mu_m$			
Viscous Regime C_D	$C_D = 24 (1 + 0.1 N_{Re}^{3/4})/N_{Re}$			
Newton's Regime C_D	$C_D = 0.45 \left\{ \frac{1 + 17.67[f(\alpha)]^{6/7}}{18.67 f(\alpha)} \right\}^2$			
$\frac{\rho_2 g \Delta p}{\mu_2} \geq 34.65, \Delta p = \rho_2 - \rho_1 $ $\frac{\rho_2 g \Delta p}{\mu_2} \geq 34.65, \Delta p = \rho_2 - \rho_1 $				
Distorted Particle Regime C_D	$C_D = \frac{4}{3} \times \frac{\sqrt{g \Delta p}}{\alpha} \left\{ \frac{1 + 17.67[f(\alpha)]^{6/7}}{18.67 f(\alpha)} \right\}^2$			
$\frac{\mu_2}{(\rho_2 \alpha \sqrt{g \Delta p})^{1/2}} \geq 0.11(1+\psi)^{8/3}$	$f(\alpha) = (1-\alpha)^{1.5} \quad (1-\alpha)^3 \quad (1-\alpha)^{2.25}$			
$\psi = 0.55(1 + 0.08r^3)^{4/7} - 1)^{3/4}$	$f(\alpha) = \sqrt{1-\alpha} \left(\frac{\mu_2}{\mu_m} \right)$			

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