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MULTIDOMAIN MULTIPHASE FLUID MECHANICS

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Abstract—A set of multiphase field equations—conservation of mass, momentum and energy—based on multiphase mechanics is developed. Multiphase mechanics applies to mixtures of phases which are separated by interfaces and are mutually exclusive. This is in contrast to the field equations of mixtures based on continuum mechanics which directly applies to molecular mixtures where the phases coexist at the same points in space. Based on the multiphase mechanics formulation, additional terms appear in the field equations when the physical size of the dispersed phase (bubble or droplet) is many times larger than the inter-molecular spacing. These terms are the inertial coupling due to virtual mass and the additional viscous coupling due to unsteadiness of the flow field. These physical effects as well as the continuum inertial coupling terms were neglected in many other two-phase calculations. By including this inertial coupling term, the one-dimensional multiphase equations are found to give real characteristics. Furthermore, the sum of momentum equations of all phases reduces to the momentum equations of the mixture as should be expected.

NOMENCLATURE

a,	bubble or droplet radius;
$a^{\alpha\beta}$,	metric tensor of interface;
B,	displacement factor;
c_p,	specific heat at constant pressure;
c_v,	specific heat at constant volume;
d,	domain;
D,	diffusivity;
D^*,	characteristic size of an element of a phase;
E,	total energy;
f,	field force;
F,	inverse relaxation time constant for momentum transfer;
G,	inverse relaxation time constant for energy transfer;
h,	enthalpy;
H,	total enthalpy or general relaxation time;
I,	inertial coupling in the momentum equation of momentum flux;
I',	force due to apparent mass;
$\mathbf{I}$,	unit tensor;
J,	general flux;
$\mathbf{J}_q$,	heat flux;
J_E,	heat source;
K,	effectiveness of particle-fluid momentum transfer;
L,	inertial coupling of energy in energy equation of energy flux;
L^*,	inertial coupling of energy in energy equation of energy per unit volume or characteristic length of a control volume;
L',	work done due to apparent mass and unsteadiness of flow field;
m,	mass per particle of dispersed phase;
$\dot{m}$,	mass transport per unit area per unit time;
$\mathbf{n}$,	unit outward normal vector;
N,	number;
n,	number density;
P,	pressure;
Q,	heat transfer coupling;
$\mathbf{r}, \mathbf{x}$,	space coordinate;
R,	radius of a pipe or gas constant;
S,	surface area;
S^*,	characteristic spacing of elements of a phase;
$\mathbf{S}$,	surface of interface;
t,	time;
t_α,	hybrid tensor;
T,	temperature;
T^*,	characteristic time for averaging in a control volume;
u,	internal energy;
$\mathbf{U}$,	velocity;
V,	viscous coupling or volume;
V',	force due to unsteadiness of flow field;
$\mathbf{x}$,	space coordinate;
X_0,	characteristic length of a flow passage.

Greek symbols

α,	volume fraction;
Γ,	mass generation rate per unit volume;
Δ,	shear tensor;
ν,	kinematic viscosity;
ρ,	density;

σ,	surface tension;
τ,	viscous stress or time;
Φ,	irreversible multiphase interaction;
ϕ,	general source term;
Ψ,	reversible multiphase interaction;
ψ,	general conservation quantity.

Superscript

(r),	domain (r);
$(^{-})$,	material property.

Subscript

c,	continuous phase;
d,	domain;
e,	evaporation;
E,	total energy;
k, l,	dispersed phase;
h,	enthalpy;
H,	total enthalpy;
i,j,	components;
ji,	tensorial components;
m,	mixture;
mc,	of continuous phase c in the mixture (such as stress of continuous phase in the mixture);
mk,	of phase k in the mixture;
s,	interface or interdomain;
u,	internal energy.

Operator

∇,	gradient;
$\nabla \cdot$,	divergence;

$d/dt_k = \partial/\partial + \mathbf{U}_k \cdot \frac{\partial}{\partial \mathbf{x}}$;

$:$,	scalar product of tensors;
$(\ )_{,\beta}$,	surface covariant derivative.

1. INTRODUCTION

REACTOR accident analysis, which stimulates interest in the rigorous multiphase formulation of the field equations, may be classified into the following two categories: (1) transient overpower, and (2) loss-of-coolant. Phase change, such as coolant boiling, fuel melting, vaporization of structure material—etc., normally takes place during the occurrence of each of these accidents. In order to predict a reactor accident sequence, as well as its consequence, the study of multiphase flow systems must be carried out in great detail.

There are two basic models of multiphase flow in the study of mass, energy and momentum transfers in a system. One is the particulate model by analogy to kinetic theory, and the other is the mixture model of continuum mechanics. In the kinetic model, the particulate phase is treated as discrete particles which are transported by the continuum phase where independent variables include both position coordinates and momentum coordinates. The resultant formulation is thus given in the coordinates of the phase space. In theory at least, proper statistical averaging will yield dynamic equations of average properties in the space coordinates with the independent momentum coordinates replaced by transport parameters. However, this has not been successful in the case of particulate (or bubble) suspensions. The approach, presented in this paper, is therefore to formulate the multiphase system outright by deriving from the continuum mechanics, with proper modifications to account for the multiphase behavior: mutual exclusion of phases, disparate mass motions and temperatures, and non-uniform inertia effects [1].

The continuum approach in a single-phase thermal-hydraulic problem is widely accepted and its validity is well proven. In some studies of two-phase flows, the conventional approach of continuum mechanics has also been applied [2]. In theory, a two-phase flow field can be subdivided into single-phase regions with moving boundaries between phases, and the two-phase flow problem can be formulated in terms of the local instantaneous variables. However, such a formulation would result in a multiboundary problem with the positions of the interfaces between two phases being unknown. Formulation based on a control volume smaller than an element of the phases, such as a bubble, remains to be completed [2].

The multiphase mechanics [3–5] is based on a control volume larger than an element of a phase, such as a bubble or a droplet, but much smaller than the characteristic volume of a flow system. It modifies the continuum mechanics to account for the discreteness of elements of phases:

(1) The partial pressure in a continuum molecular mixture is not meaningful when applied to bubbles in a liquid or droplets in a vapor.

(2) The mutual exclusion of phases gives rise to the effects of virtual mass and Basset force [6]. At the same time, multiphase mechanics introduces proper averaging over the phases to give a distributed representation of field variables such as density, velocity, and temperature. This duality yields a complete set of field equations for computing multiphase systems. In this set of basic equations, the significance of conservation based on the mixture and the gradient of concentration ($P\,d\alpha$) will be clarified in the section on Discussions of this paper.

When a bubble or droplet in a dispersion grows to a size approaching that of the characteristic dimension of the flow system, a provision is made for its transition to a new domain which interacts with other parts (domains) of the fluid via interfacial relations. This multidomain approach enables us to model the various flow regimes in a multiphase flow system: The phenomena of the flow of a boiling liquid in identifiable regimes [7] can be treated under this general scheme.

Within a domain, there is a continuous phase in which dispersed phases are suspended. The dispersed phases may consist of bubbles when the continuous phase is a liquid (or droplets in vapor). By invoking the multiphase principle [3], bubbles (droplets) of each size and density range constitute a phase. That is, the identifiable sizes of bubbles (droplets of liquid) are subdivided into k different ranges, and each range has the same density. Thus, k different ranges constitute correspondingly k dispersed phases.

Domains are separated by interfaces. Two adjacent domains are coupled to each other by mass, momentum, and energy transfer through the interface.

For the cases illustrated by boiling flow in a pipe [7], in the range of nucleate boiling, the system might start with one domain with bubbles of various size ranges identified as phases. Coalescence of bubbles lead to large bubbles or slugs, which are large in comparison to the characteristic dimension of the flow system. Each slug may then be identified as a new domain. The shape of each slug is describable in terms of the geometry of the interface. Inside these slugs, bubble burst may occur, producing droplets within each slug. These droplets may now be identified as a phase or phases when there is sufficient size range. Coalescence of slugs of vapor bubbles leads to flow of a liquid layer along the wall in the form of an annulus with a core of vapor. The interface divides a domain of boiling liquid with bubbles and a domain of vapor with suspended droplets. The number of domains becomes one when the fluid becomes a mist of droplets in vapor only, but droplets of different sizes can be identified as phases. Extension of these considerations to film boiling because of high heat flux can be made in an analogous manner.

The basic concept of multidomain multiphase fluid mechanics is that multiphase mechanics governs behavior of large numbers of small growing bubbles, whereas when a few large bubbles emerge, multidomain dynamic relations will be used. Given all the necessary transport parameters, interface properties, initial and boundary conditions, this general case will account for all of the ranges and regimes of flow of a boiling liquid, including various basic interactions.

Several different models [2, 8–10] have been proposed for two-phase flow in discussions at several conferences The objectives of this paper are: (1) to delineate a set of rigorous field equations of multiphase flow, and (2) to identify the source of differences among various proposed models.

2. GENERAL FORMULATION

The averaging procedure must be directly related to the experimental observation, thus, cross checks between the theoretical formulation and experimental data assure consistent procedures and meaningful predictions. Multiphase mechanics employs the space–time average over a control volume in a domain [5]. The relative magnitudes of three quantities which affect the method and means of averaging are the characteristic length of the elements of the dispersed phase D^*, the spacing between the elements S^*, and the volume V observed having characteristic length L^*. Specification of multiphase control volume calls for $L^* > S^*$, $L^* > D^*$, using a one-dimensional example. It is to be noted that variations in the number of bubbles N in a control volume V over a time interval $\Delta t \sim S^*/U$, U being the characteristic velocity, are considered as high frequency perturbations. However, the inertia of the system is such that dynamic response time is of the order of a characteristic time T^* which is, in general, many times the interval $\Delta t \sim (N/V)^{-1/3}/U$. The volume fraction α_k of phase k at a position in space where the mixture passes is given by:

$$\alpha_k = (\bar{U}_{k1}\Delta t_1 + \bar{U}_{k2}\Delta t_2 + \text{----}) \bigg/ \int_0^{T^*} U_k \,\mathrm{d}t = \frac{T_k^*}{T^*} \quad (1)$$

where $\bar{U}_{k1}$ is the mean velocity of phase k over duration Δt_1 within which it passes the observation station in space, $\bar{U}_{k2} \ldots$ etc., Δt_1, $\Delta t_2 \ldots$ are subtime intervals within T^* interval, and T_k^* is an equivalent time interval within T^* for the passage of phase k in which the correction on non-uniform velocity is included. As long as $L^* > S^*$, the instantaneous volume average of number density is N_k/V over the range L^*. α_k is the time average of $(N_k/V)v_k$, v_k being the bubble volume, over $T^* > \Delta t_k$. This space–time average over the same control volume is applicable for $L^*/U > T^* > S^*/U$. Note that this is not the case of averaging based on the jump condition [2], where α_k is as in equation (1), but given for $L^* < S^*$, $L^* < D^*$, and $\Delta t > L^*/U$. For this one-dimensional example, the corresponding volume average has to be taken over a length $X \sim UT^* > L^*$, not the space average within L^*, which now corresponds to a slit.

Thus, for a basic conservation quantity $\rho_m\psi_m$, where ρ_m is the density of the mixture, the time average is given by, for $T^* > \Delta t$,

$$\begin{aligned}\rho_m\psi_m &= \frac{1}{T^*}\int_{T^*} \rho'_m\psi'_m \,\mathrm{d}t = \frac{1}{T^*}\int_{T^*}\left(\sum_k \rho'_k\psi'_k\right)\mathrm{d}t \\ &= \frac{1}{T^*}\int_{T^*}\left(\sum_k \alpha'_k\bar{\rho}_k\psi'_k\right)\mathrm{d}t = \frac{1}{T^*}\sum_k\int_{T_k^*}\bar{\rho}_k\psi'_k\,\mathrm{d} \quad (2)\end{aligned}$$

where subscript k denotes a phase k of the mixture and $\bar{\rho}_k$ denotes the density of material constituting the phase.

When considering the general conservation of any quantity ψ_m of a mixture of phases, the general integral balance can be expressed in terms of instantaneous volume averages. For control volume $V(\mathbf{r}, t)$ of surface area $A(\mathbf{r}, t)$,

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_V \rho_m\psi_m \,\mathrm{d}V = -\int_A \mathbf{n}\cdot\mathbf{J}_m \,\mathrm{d}A + \int_V \rho_m\phi_m \,\mathrm{d}V \quad (3)$$

where ρ_m is the density, $\mathbf{J}_m$ is a general surface flux and ϕ_m is a general body source, $\mathbf{n}$ is a unit vector normal to surface $\mathrm{d}A$ and "a bold character" denotes a vector.

In equation (3), the basic conservation quantities: $\rho_m\psi_m$, $\mathbf{J}_m$, and $\rho_m\phi_m$ are time averages over time T^* such that, for the mixture m of components k, besides equation (2),

$$\mathbf{J}_m = \frac{1}{T^*}\int_{T^*} \mathbf{J}'_m \,\mathrm{d}t \quad (4)$$

$$\rho_m\phi_m = \frac{1}{T^*}\int_{T^*} \rho'_m\phi'_m \,\mathrm{d}t. \quad (5)$$

These time averages of basic quantities are in agreement with Delhaye and Achard [2] with generalization of volume fraction based on time adjusted for non-uniform velocity in the present study.

The Leibniz rule gives

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_V \rho_m\psi_m \mathrm{d}V = \int_V \frac{\partial}{\partial t}\rho_m\psi_m \mathrm{d}V + \int_A \rho_m\psi_m \mathbf{U}_m\cdot\mathbf{n}\,\mathrm{d}A \tag{6}$$

and the Gauss theorem gives

$$\left.\begin{aligned}\int_A \mathbf{n}\cdot\mathbf{J}_m \mathrm{d}A &= \int_V \nabla\cdot\mathbf{J}_m \mathrm{d}V\\ \int_A \rho_m\psi_m\mathbf{U}_m\cdot\mathbf{n}\,\mathrm{d}A &= \int_V \nabla\cdot(\rho_m\mathbf{U}_m\psi_m)\mathrm{d}V.\end{aligned}\right\} \tag{7}$$

Substitution of these relations into equation (3) for an arbitrary control volume gives a general differential balance equation as:

$$\frac{\partial}{\partial t}\rho_m\psi_m + \nabla\cdot(\mathbf{U}_m\rho_m\psi_m) = -\nabla\cdot\mathbf{J}_m + \rho_m\phi_m. \tag{8}$$

This relation has been derived for a single phase fluid [2, 10].

The basis of conservation of mass, momentum, and energy is applied to a given control volume encompassing the mixture, thus taking into account all internal actions and reactions. Components of phases k relate to the mixture according to:

$$\rho_m = \sum_k \rho_k \tag{9}$$

$$\rho_m\mathbf{U}_m = \sum_k \rho_k\mathbf{U}_k \tag{10}$$

$$\rho_m\psi_m = \sum_k \rho_k\psi_k \tag{11}$$

$$\mathbf{J}_m = \sum_k \mathbf{J}_{mk} \tag{12}$$

where $\mathbf{J}_{mk}$ is the general flux of k in the mixture m [3, 5], and for generation rate Γ_k, over the mixture:

$$\sum_k \Gamma_k = 0. \tag{13}$$

The relations given by equations (9) and (10) further defines the barycentric [11] frame of reference, that is, motion of the center of mass (c.g.) of the mixture in relation to those about the c.g.'s of the phases or components. In simple terms, for phases in disparate motion, the position coordinate and its conjugate velocity components are defined by the mixture. Therefore, when treating the motion of each phase k, a coordinate transformation which relates the c.g. of the mixture and the c.g.'s of phases can be expressed as:

$$\rho_m\mathbf{U}_m\psi_m = \sum_k \rho_k\mathbf{U}_k\psi_k - \sum_k \rho_k(\mathbf{U}_k-\mathbf{U}_m)(\psi_k-\psi_m) \tag{14}$$

$$\rho_m\phi_m = \sum_k \rho_k\phi_{mk} + \sum_k \Gamma_k\psi_m. \tag{15}$$

The last term on the RHS of equation (15) is equal to zero; the significance of its inclusion will be explained below. The crux of the coordinate transformation is represented by the last term of equation (14). This coordinate transformation enables expressing the general balance equation for ψ_m in terms of a phase k as:

$$\frac{\partial}{\partial t}\rho_k\psi_k + \nabla\cdot(\rho_k\mathbf{U}_k\psi_k) - \nabla\cdot\rho_k(\mathbf{U}_k-\mathbf{U}_m)(\psi_k-\psi_m) = -\nabla\cdot\mathbf{J}_{mk} + \rho_k\phi_{mk} + \Gamma_k\psi_m. \tag{16}$$

The third term on the LHS accounts for the coordinate transformation from the motion of c.g. of the mixture to that of phase k. The general body source term ϕ_{mk} in the mixture while satisfying equation (15), also includes mutual actions and reactions among the phases inside the mixture, or

$$\phi_{mk} = \phi_k + \sum_l H_{kl}(\psi_l-\psi_k) + (\Psi'_k/\rho_k) + (\Phi'_k/\rho_k) \tag{17}$$

where H_{kl}, is the inverse relaxation time of general transfer of ψ from phases l to k, Ψ'_k and Φ'_k are the other reversible and irreversible (dissipative) multiphase interactions due to mutual exclusions of phases, and the second term on the RHS of equation (17) is due to $\mathbf{J}_{mk}$ acting on the phase boundary to be given in the next section. Further

$$\sum_k \rho_k \sum_l H_{kl}(\psi_l-\psi_k) = 0 \tag{18}$$

and

$$\sum_k \Psi'_k = 0. \tag{19}$$

In the multiphase representation the detailed density, velocity, temperature fields in the immediate vicinity of the boundary layer around each particle [12] of a dispersed phase are of no concern. In this sense, each particle becomes a part of a distributed density of its own species which constitutes a particular phase. This cloud of particles is characterized by transport properties such as inverse relaxation times for mass, momentum and energy transfer and geometrical properties such as volume fractions of phases. Therefore, as long as a phase is defined as dispersed, the size of particles and the grid sizes for numerical computation are unrelated.

Transition occurs from a phase to a new domain when a bubble or slug is large in comparison to a characteristic physical dimension of the flow system. The boundary of the new domain becomes accurately defined with certainty according to classical mechanics. Consequently, for numerical computations, the computational grid will have to be smaller than the characteristic dimension of a domain.

3. RELATION OF MIXTURE TO PHASES

For the general description of a multiphase system, superscripts (r), (s), etc. denote the domains. Within each domain subscripts k, c and m denote dispersed phases (for example, bubbles of various size ranges), the continuous phase, and the mixture constituting a domain respectively. Different roles of the dispersed phase and the continuous phase in the conservative sients were relatively modest, indicating that some relations are as noted earlier [3]. The phase interactions within each domain and the interfacial relations between domains must be accounted for. Thus, for bubbles of species k in domain (r), the density of this bubble cloud is denoted as $\rho_k^{(r)}$ while its material density is denoted as $\bar{\rho}_k^{(r)}$, volume fraction $\alpha_k^{(r)}$, and its velocity $\mathbf{U}_k^{(r)}$. For domain (r), the mixture properties are governed by [3]:

$$\rho_m^{(r)} = \rho_c^{(r)} + \sum_k \rho_k^{(r)} \tag{20}$$

and the momentum by

$$\rho_m^{(r)}\mathbf{U}_m^{(r)} = \rho_c^{(r)}\mathbf{U}_c^{(r)} + \sum_k \rho_k^{(r)}\mathbf{U}_k^{(r)}. \tag{21}$$

The total energy E is defined according to:

$$E = u + \frac{\mathbf{U}\cdot\mathbf{U}}{2} \tag{22}$$

where u is the internal energy and $\mathbf{U}\cdot\mathbf{U}/2$ is the kinetic energy. The potential energy is accounted for in terms of a field force $\mathbf{f}$ per unit mass. The energy of a domain (r) is thus:

$$\rho_m^{(r)}E_m^{(r)} = \rho_c^{(r)}E_c^{(r)} + \sum_k \rho_k^{(r)}E_k^{(r)}. \tag{23}$$

Conformity with the kinetic theory of gases requires that the specific heats at constant volume c_v be related according to [13]:

$$\rho_m^{(r)}c_{vm}^{(r)} = \rho_c^{(r)}c_{vc}^{(r)} + \sum_k \rho_k^{(r)}c_{vk}^{(r)} \tag{24}$$

which leads to the relationship for static temperatures based on individual centers of mass (c.g.):

$$\begin{aligned}\rho_m^{(r)}c_{vm}^{(r)}T_m^{(r)} &= \rho_c^{(r)}c_{vc}^{(r)}T_c^{(r)} \\ &+ \sum_k \rho_k^{(r)}c_{vk}^{(r)}T_k^{(r)} + \frac{1}{2}\Big[\rho_c^{(r)}\mathbf{U}_c^{(r)}\cdot(\mathbf{U}_c^{(r)}-\mathbf{U}_m^{(r)}) \\ &+ \sum_k \rho_k^{(r)}\mathbf{U}_k^{(r)}\cdot(\mathbf{U}_k^{(r)}-\mathbf{U}_m^{(r)})\Big].\end{aligned} \tag{25}$$

The last term in equation (25) accounts for the relative motion between the respective centers of mass.

The definition in terms of total energy and internal energy does not prevent us from using the properties enthalpy and total enthalpy. Use of total enthalpy has the advantage of direct application of thermophysical property data and reduces the work term in the energy equation to $\partial P/\partial t$. Specifically, the enthalpy is defined in terms of

$$h_k^{(r)} = u_k^{(r)} + (P^{(r)}/\bar{\rho}_k^{(r)}) \tag{26}$$

in multiphase mechanics, which corresponds to:

$$h_k = u_k + (P_k/\rho_k) \tag{27}$$

in continuum mechanics. Modification of $P^{(r)}$ by surface tension can be readily accounted for. Further, the total enthalpy is given by:

$$H_k^{(r)} = h_k^{(r)} + \frac{\mathbf{U}_k^{(r)}\cdot\mathbf{U}_k^{(r)}}{2} \tag{28}$$

for both the multiphase and continuum mechanics formulations. Furthermore,

$$\alpha_c^{(r)} + \sum_k \alpha_k^{(r)} = 1. \tag{29}$$

The transport properties of a phase in a mixture were defined strictly [3], and in general, are different from those of each phase in pure form. In order to account for a variety of flow regimes based on viscous or turbulent flow conditions of the continuous phase, the viscous stresses within each domain are represented as that of the mixture $\tau_m^{(r)}$

$$\tau_m^{(r)} = \tau_{mc}^{(r)} + \sum_k \tau_{mk}^{(r)} \tag{30}$$

where $\tau_{mk}^{(r)}$ is the viscous stress of phase k in the mixture in domain (r), and $\tau_{mc}^{(r)}$ is the viscous stress of phase c in the mixture in the domain (r). It should be noted that $\tau_{mc}^{(r)}$ is in general not equal to $\tau_c^{(r)}$ based on the transport of momentum of the continuous phase alone, and $\tau_k^{(r)}$ might not be meaningful when there are insufficient collisions of species k. In general

$$\tau_{mc}^{(r)} \neq \tau_c^{(r)}, \quad \tau_{mk}^{(r)} \neq \tau_k^{(r)} \tag{31}$$

$\tau_{mk}^{(r)}$ may arise due to interaction of k with c alone when the k–k interaction is negligible compared to the k–c interaction. The latter gives rise to a "viscous" coefficient $\rho_k^{(r)}D_{kc}^{(r)}$. Momentum transfer is effected by bodily transfer of the particle cloud via diffusion through the continuous phase [14], with diffusivity $D_{kc}^{(r)}$

$$\tau_{mk}^{(r)} \sim \rho_k^{(r)}D_{kc}^{(r)}\Delta_k^{(r)} \tag{32}$$

where Δ_k is the shear strain tensor of species k in (r). Hence, even when phase c is in turbulent motion, the motion of species k, while in random motion, may actually be in the viscous or slip flow regime [3, 14].

Similarly, the conduction heat flux $J_m^{(r)}$ in the mixture is equal to:

$$\mathbf{J}_m^{(r)} = \mathbf{J}_{mc}^{(r)} + \sum_k \mathbf{J}_{mk}^{(r)} \tag{33}$$

where $\mathbf{J}_{mk}^{(r)}$ is the conduction heat flux of species k in the mixture in the domain (r), and $\mathbf{J}_{mc}^{(r)}$ is the conduction heat flux of the continuous phase c in the mixture in domain (r). Again, when there are negligible collisions among the species k themselves, the thermal conductivity of species k in the mixture is given by $c_{vk}^{(r)}\rho_k^{(r)}D_{kc}^{(r)}$ where $c_{vk}^{(r)}$ is the specific heat at constant volume of phase k; $c_{vk}^{(r)}$ is used instead of $c_{pk}^{(r)}$ (subscript p denotes constant pressure) because internal energy of the species k is transported by diffusion through the continuous phase c. The detailed derivation of the gradients of viscous stresses and heat fluxes of phases in the mixture were presented earlier [3–5]. Note that the inertial coupling terms are now identified separately [4, 5, 15].

4. CONTINUITY EQUATION

The continuity equations or the mass balance equations take the following form and the physical meaning of each of the terms in the balance equations is, with $\psi_k = 1$, $\mathbf{J}_{mk} = 0$, $\phi_{mk} = 0$ substituted into equations (11) and (16). For dispersed phase k:

$$\frac{\partial \rho_k^{(r)}}{\partial t} + \nabla \cdot (\rho_k^{(r)} \mathbf{U}_k^{(r)}) = \Gamma_k^{(r)}. \tag{34}$$

That is,

$$\begin{bmatrix}\text{Rate of change}\\ \text{of density of}\\ \text{dispersed phase}\end{bmatrix} + \begin{bmatrix}\text{Net rate of mass}\\ \text{flux of dispersed}\\ \text{phase (efflux–influx)}\end{bmatrix} = \begin{bmatrix}\text{Rate of}\\ \text{generation of}\\ \text{dispersed phase}\end{bmatrix}.$$

For continuous phase c:

$$\frac{\partial \rho_c^{(r)}}{\partial t} + \nabla \cdot (\rho_c^{(r)} \mathbf{U}_c^{(r)}) = \Gamma_c^{(r)} \tag{35}$$

with similar interpretations of terms as in equation (34). In equations (34) and (35), $\Gamma_k^{(r)}$ and $\Gamma_c^{(r)}$ are the rate of generation of phase k and c respectively in domain (r) per unit volume per unit time (t). The generation rates are given by breaking-up, agglomeration, evaporation and condensation [3]. For domain (r)

$$\sum_k \Gamma_k^{(r)} + \Gamma_c^{(r)} = 0. \tag{36}$$

It is only feasible to identify finite steps of sizes if k denotes different sizes in the distribution, while the change of particle size tends to be continuous. The approach chosen here is to approximate gradual change in size of all particles by a stepwise change in size, but gradual change in population or number of particles in each size is explicitly accounted for.

5. MOMENTUM EQUATION

The momentum equations are given by taking $\psi_k = \mathbf{U}_k$, $\mathbf{J}_{mk} = \alpha_k P\mathbf{I} - \tau_{mk}$, and

$$\phi_{mk} = \mathbf{f}_k + F_{kc}(\mathbf{U}_c - \mathbf{U}_k) + \sum_l F_{kl}(\mathbf{U}_l - \mathbf{U}_k) + (I_k'/\rho_k) + (V_k'/\rho_k),$$

and substituting into equation (16).

For the dispersed phase k:

$$(\partial/\partial t)\rho_k^{(r)}\mathbf{U}_k^{(r)} + \nabla \cdot \rho_k^{(r)}\mathbf{U}_k^{(r)}\mathbf{U}_k^{(r)} = -\alpha_k^{(r)}\nabla P^{(r)} - (1 - B_k^{(r)})P^{(r)}\nabla\alpha_k^{(r)} + \nabla \cdot \tau_{mk}^{(r)} + \rho_k^{(r)}\mathbf{f}_k^{(r)} + \mathbf{I}_k^{(r)} + \mathbf{V}_k^{(r)} + \mathbf{I}_k^{(r)\prime} + \mathbf{V}_k^{(r)\prime}. \tag{37}$$

The physical meaning of each term in equation (37) is:

$$\begin{bmatrix}\text{Rate of change of momentum}\\ \text{of dispersed phase}\end{bmatrix} + \begin{bmatrix}\text{Net rate of momentum flux of}\\ \text{dispersed phase (efflux–influx)}\end{bmatrix} = -\begin{bmatrix}\text{Force acting on dispersed}\\ \text{phase due to pressure gradient}\end{bmatrix} -$$

$$\begin{bmatrix}\text{Resistance force due to change}\\ \text{of volume of dispersed phase}\end{bmatrix} + \begin{bmatrix}\text{Force due to shear stress acting}\\ \text{on dispersed phase}\end{bmatrix} + \begin{bmatrix}\text{External field force acting on}\\ \text{dispersed phase}\end{bmatrix} +$$

$$\begin{bmatrix}\text{Rate of change of momentum}\\ \text{due to generation of dispersed}\\ \text{phase}\end{bmatrix} + \begin{bmatrix}\text{Inertial coupling force acting}\\ \text{on dispersed phase due to c.g.}\\ \text{of dispersed phase in relation}\\ \text{to c.g. mixture}\end{bmatrix} + \begin{bmatrix}\text{Viscous coupling force acting}\\ \text{on dispersed phase due to drag}\end{bmatrix} +$$

$$\begin{bmatrix}\text{Apparent mass effect on inertial}\\ \text{force of dispersed phase}\end{bmatrix} + \begin{bmatrix}\text{Resistance force acting on}\\ \text{dispersed phase due to}\\ \text{unsteadiness of flow field}\end{bmatrix}$$

where P is the pressure, $\mathbf{f}_k^{(r)}$ is the external force per unit mass of k in (r) and $\tau_{mk}^{(r)}$ is the shear stress of phase k in the mixture. The inertial coupling is given from equations (14) and (15)

$$\mathbf{I}_k^{(r)} = \nabla \cdot \rho_k^{(r)}(\mathbf{U}_k^{(r)} - \mathbf{U}_m^{(r)})(\mathbf{U}_k^{(r)} - \mathbf{U}_m^{(r)}) + \mathbf{U}_m\Gamma_k^{(r)}. \tag{38}$$

$\mathbf{I}_k$ is the inertial coupling which relates the center-of-mass frames of the mixture and the phases [5, 15]. $\mathbf{I}_k$ can be dropped only for very small relative motion between the phases. The uniqueness of the split was shown by Chao, *et al.* [16].

The viscous coupling is given by [3, 5]:

$$\begin{aligned}\mathbf{V}_k^{(r)} &= \rho_k^{(r)} F_{kc}^{(r)}(\mathbf{U}_c^{(r)} - \mathbf{U}_k^{(r)}) + \rho_k^{(r)} \sum_l F_{kl}^{(r)}(\mathbf{U}_l^{(r)} - \mathbf{U}_k^{(r)}) \\ &= \mathbf{V}_{kc}^{(r)} + \sum_l \mathbf{V}_{kl}^{(r)}\end{aligned} \tag{39}$$

where $F_{kc}^{(r)}$ is the inverse relaxation time of momentum transfer from the continuous phase c to k in (r) and $F_{kl}^{(r)}$, for $k \neq l$, is the inverse relaxation time of momentum transfer from other dispersed phases (other sizes and density) l to k. $\mathbf{V}_k^{(r)}$ accounts for the distribution of velocity in the immediate vicinity of the surface of a particle of a dispersed phase. The sum of all V's within a domain is zero because they are internal actions and reactions. In this way the effect of the presence of a physical interface of discrete particles is properly accounted for. For the multiphase system, the inertial effect due to virtual mass is given by [6]:

$$\mathbf{I}_k^{(r)\prime} = \tfrac{1}{2}\rho_k^{(r)} \frac{\bar{\rho}_c^{(r)}}{\bar{\rho}_k^{(r)}} \frac{\mathrm{d}}{\mathrm{d}t_k^{(r)}} (\mathbf{U}_c^{(r)} - \mathbf{U}_k^{(r)}) \tag{40}$$

which is known only for a dilute suspension and the influence of other dispersed phase l is not readily inferred. The multiphase viscous coupling due to unsteadiness of the flow field is [3, 5]:

$$\mathbf{V}_k^{(r)\prime} = \frac{9}{2(\pi)^{1/2}} \rho_k^{(r)} \frac{\nu_c^{1/2}}{a_k} \frac{\bar{\rho}_c^{(r)}}{\bar{\rho}_k^{(r)}} \int_{t_0}^{t} \frac{(\mathrm{d}/\mathrm{d}\tau)(\mathbf{U}_c^{(r)} - \mathbf{U}_k^{(r)})}{(t-\tau)^{1/2}} \, \mathrm{d}\tau \tag{41}$$

and

$$\frac{\mathrm{d}}{\mathrm{d}t_k^{(r)}} = \frac{\partial}{\partial t} + \mathbf{U}_k^{(r)} \cdot \nabla . \tag{42}$$

Two multiphase parameters stand out in equation (37): K_k and B_k. The effectiveness of momentum transfer, K_k, from the particle to the fluid arises from the dissipation by the wake of a particle in the fluid [3]. $K_k = 1$ for accelerating flow with F (see Table 1) defined by the force acting on the particle, while the drag forces contributed by the fluid include that by the friction at the particle surface and in the wake. The irreversibility of the wake is such that in decelerating flow, the force acting on the fluid by the particle is only fraction K_k of the resistance force while $(1-K_k)$ fraction of the force produces only random motion in the wake. This is diagrammatically

Table 1. Force and work relations between the continuous phase and the dispersed phase—irreversibility of wake flow

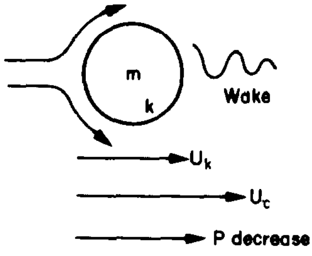
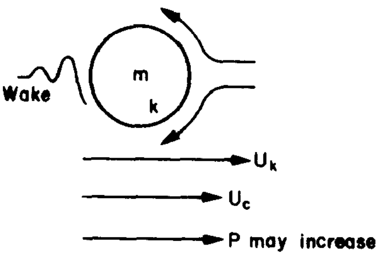
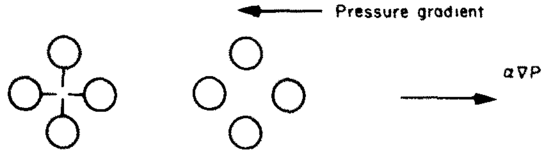
	Accelerating particle	Decelerating particle
		
Forces	Force acting on particles (→) $= Fm(U_c - U_k)$ Force acting on fluid and wake (←) $= Fm(U_c - U_k)$ (F defined by drag force acting on a stationary particle)	Force acting on particle (←) $= Fm(U_c - U_k)$ Force acting on fluid (→) $= KFm(U_c - U_k)$ Force to produce wake $= (1-K)Fm(U_c - U_k)$
Work	Work done by fluid $= U_c Fm(U_c - U_k)$ Work done by particle $= U_k Fm(U_c - U_k)$ Work dissipated in fluid $= Fm(U_c - U_k)^2$	Work done by fluid $= U_c KFm(U_c - U_k)$ Work done by particle $= U_k Fm(U_c - U_k)$ Work dissipated in fluid wake $= U_c(1-K)Fm(U_c - U_k)$ Work dissipated in fluid $= Fm(U_c - U_k)^2$

Table 2. Effects of pressure in multiphase system



Force	$-P\nabla\alpha+BP\nabla\alpha$ Diffusive or compressive force minus force at phase boundary	$-\alpha\nabla P$ Displacement
Work (in energy equation)	$P\delta\alpha$ Change of thermal state of particle	$\alpha\delta P$ Change of thermal state of fluid (displacement work)

illustrated in Table 1. Also shown in Table 1 is the distribution of work dissipated by this relative motion. This consideration is also applicable to the dissipation of unsteady motion. Only fraction K_k of V', as well as I and I' is transmitted to the fluid, excluding the random motion set in the wakes of particles. The parameter $B_k^{(r)}$ is called a displacement factor depending on the size of a dispersed phase (particle size), flow structure and fluid properties. As shown in Table 2, the term $(1-B_k^{(r)})\,P^{(r)}\nabla\alpha_k^{(r)}$ accounts for the force due to volumetric displacement or diffusion of phase k, and $0 \leqslant B_k^{(r)} \leqslant 1$. For the limiting cases, $B_k^{(r)} \geqslant 0$ for gas mixture or highly dispersed multiphase fluid, and $B_k^{(r)} \leqslant 1$ for a structured multiphase fluid such as a fluid with relatively large size of bubbles or droplets.

Note also the terms $\alpha_k\nabla P+(1-B_k)\,P\nabla\alpha_k$ in equation (37). It is seen that although the sum is equal to $\nabla\alpha_k P$ for $B_k = 0$, the concept of a partial pressure has no meaning when applied to a multiphase system where the phases are mutually exclusive. Here $\alpha_k\nabla P$ is a force acting on a phase due to a pressure gradient and $P\nabla\alpha_k$ is the force due to volumetric displacement. The term $P\nabla\alpha_k$ has further significance in that in the energy equation (in terms of enthalpy), it leads to the term $P\partial\alpha_k/\partial t$ which is the work of compression of the dispersed phase (Table 2). For spherical particles of radius a_k and number density n_k, it is given by:

$$P\frac{\partial}{\partial t}\left(\frac{4\pi}{3}a_k^3 n_k\right) = P\frac{\partial\alpha_k}{\partial t} \tag{43}$$

giving $\alpha_k\partial P/\partial t$ when displacement work is included.

For the continuous phase c, after subtracting the action–reaction terms from the momentum of the mixture, the following equation is obtained

$$\begin{aligned}(\partial/\partial t)\rho_c^{(r)}\mathbf{U}_c^{(r)}+\nabla\cdot\rho_c^{(r)}\mathbf{U}_c^{(r)}\mathbf{U}_c^{(r)} = {} & -\left(1-\sum_k K_k^{(r)}\alpha_k^{(r)}\right)\nabla P^{(r)} \\ & +P^{(r)}\sum_k K_k^{(r)}(1-B_k^{(r)})\nabla\alpha_k^{(r)}+\nabla\cdot\boldsymbol{\tau}_{mc}^{(r)}+\rho_c^{(r)}\mathbf{f}_c^{(r)} \\ & +\sum_k K_k^{(r)}\mathbf{I}_c^{(r)}+\sum_k K_k^{(r)}\mathbf{V}_c^{(r)}-\sum_k K_k^{(r)}\mathbf{I}_k^{(r)\prime}-\sum_k K_k^{(r)}\mathbf{V}_k^{(r)\prime}.\end{aligned} \tag{44}$$

The physical meaning of each term in equation (44) can be correspondingly interpreted as for equation (37).

6. ENERGY EQUATIONS

In formulating the energy equations, direct application of equation (16) would suggest substitutions of:

$$\psi_k = E_k, \quad \mathbf{J}_{mk} = \mathbf{U}_m\cdot(\alpha_k P\mathbf{I}-\boldsymbol{\tau}_{mk})+\mathbf{J}_{qmk},$$

and

$$\phi_{mk} = \mathbf{f}_k\cdot\mathbf{U}_k+(J_{Ek}/\rho)+\sum_i F_{kl}(\mathbf{U}_l-\mathbf{U}_k)\cdot\mathbf{U}_k+\sum_l G_{kl}(\mathbf{u}_l-\mathbf{u}_k)+(I_k'+V_k')\cdot\mathbf{U}_k/\rho_k$$

with subscripts k denoting both dispersed phase k and continuous phase c. However, this would lead to an incorrect relation for the dispersed phase where only thermal terms and work done on the phase k contribute to the change of its temperature while its motion is produced by the drag force exerted by the continuous phase c [3]. That is, the kinetic energy of the dispersed phase is, in effect, part of the energy of the continuous fluid phase. Conversion of kinetic energy of the dispersed phase into its thermal energy takes place via conversions in the fluid phase and subsequent heat transfer.

Application of the first law of thermodynamics leads to the following energy equation for the dispersed phase expressed in terms of enthalpy. It is noted that kinetic energy of particles and work for moving these particles are part of the energy of fluid phase c [3].

For the dispersed phase k:

$$(\partial/\partial t)(\rho_k^{(r)}h_k^{(r)})+\nabla\cdot(\rho_k^{(r)}\mathbf{U}_k^{(r)}h_k^{(r)}) = -\nabla\cdot\mathbf{J}_{qmk}^{(r)}+\mathbf{J}_{Ek}^{(r)}+\alpha_k^{(r)}\frac{\partial P}{\partial t}+L_{kh}^{(r)}+Q_k^{(r)}. \tag{45}$$

The physical meaning of each term in equation (45) is

$$\left[\begin{array}{l}\text{Rate of change of}\\ \text{enthalpy of}\\ \text{dispersed phase}\end{array}\right]+\left[\begin{array}{l}\text{Net rate of enthalpy}\\ \text{flux of dispersed}\\ \text{phase (efflux-influx)}\end{array}\right]=-\left[\begin{array}{l}\text{Heat transfer due to}\\ \text{conduction}\end{array}\right]+\left[\begin{array}{l}\text{Heat source in}\\ \text{dispersed phase}\end{array}\right]+$$

$$\left[\begin{array}{l}\text{Work due to}\\ \text{compression or}\\ \text{expansion by}\\ \text{pressure of dispersed}\\ \text{phase}\end{array}\right]+\left[\begin{array}{l}\text{Inertial coupling of}\\ \text{energy of dispersed}\\ \text{phase } k \text{ due to c.g. of}\\ \text{dispersed phase in}\\ \text{relation to c.g. of}\\ \text{mixture}\end{array}\right]+\left[\begin{array}{l}\text{Heat transfer}\\ \text{coupling of}\\ \text{dispersed phase to}\\ \text{continuous phase}\end{array}\right]$$

where $\mathbf{J}_{qmk}^{(r)}$ is the heat flux to species k in the mixture, J_{Ek} is the heat source in k, and $\alpha_k^{(r)}\,\partial P/\partial t$ is the work (including symmetric displacement work) due to compression or expansion of the k species. $L_{kh}^{(r)}$ gives the effect of inertial coupling on energy of the phases, since transfer based on enthalpy difference is accounted for via $Q_k^{(r)}$

$$L_{kh}^{(r)} = \Gamma_k^{(r)}h_m^{(r)} \tag{46}$$

$Q_k^{(r)}$ is the heat transfer coupling of species k to the continuous phase and the other dispersed phases:

$$Q_k^{(r)} = \rho_k^{(r)}c_{vk}^{(r)}G_{kc}^{(r)}(T_c^{(r)}-T_k^{(r)})+\rho_k^{(r)}c_{vk}^{(r)}\sum_l G_{kl}^{(r)}(T_l^{(r)}-T_k^{(r)}). \tag{47}$$

The inverse relaxation time of energy transfer (G) is seen to be consistent for both kinetic theory and multiphase calculations [13]. Details of the modification in equation (46) from [5] will be dealt with in a later paper.

The energy equation of the continuous phase is therefore obtained from subtracting the sum of equation (45) for all dispersed phases from the overall energy equation. The latter is obtained from

$$\psi_m = E_m,\quad \mathbf{J}_m = \mathbf{U}_m\cdot(P\mathbf{I}-\tau_m)+\mathbf{J}_{qm},$$

and

$$\rho_m\phi_m = (\sum\rho_k f_k)\mathbf{U}_m+J_{Em}+\sum_{k,c}\rho_k F_{kl}(\mathbf{U}_l-\mathbf{U}_k)(U_l-U_k)+\sum_k(I_k'+\mathbf{V}_k')(\mathbf{U}_l-U_k)$$

in equation (16), together with conversion from E to H. The energy equation of the continuous phase c thus obtained takes the form:

$$\begin{aligned}(\partial/\partial t)&\left(\rho_c^{(r)}H_c^{(r)}+\frac{1}{2}\sum_k\rho_k^{(r)}\mathbf{U}_k^{(r)}\cdot\mathbf{U}_k^{(r)}\right)+\nabla\cdot\left[\rho_c^{(r)}\mathbf{U}_c^{(r)}H_c^{(r)}+\frac{1}{2}\sum_k\rho_k^{(r)}\mathbf{U}_k^{(r)}(\mathbf{U}_k^{(r)}\cdot\mathbf{U}_k^{(r)})\right]\\ &= -\nabla\cdot\mathbf{J}_{qmc}^{(r)}+J_{Ec}^{(r)}+\alpha_c^{(r)}\frac{\partial P}{\partial t}+\nabla\mathbf{U}_m^{(r)}:\tau_m^{(r)}+\sum_k\rho_k^{(r)}F_{kc}^{(r)}(\mathbf{U}_c^{(r)}-\mathbf{U}_k^{(r)})\cdot(\mathbf{U}_c^{(r)}-\mathbf{U}_k^{(r)})\\ &\quad+\sum_k\rho_k^{(r)}\sum_l F_{kl}^{(r)}(\mathbf{U}_l^{(r)}-\mathbf{U}_k^{(r)})\cdot(U_l^{(r)}-\mathbf{U}_k^{(r)})+\rho_c^{(r)}\mathbf{f}_c^{(r)}\cdot\mathbf{U}_c^{(r)}+\sum_k\rho_k^{(r)}\mathbf{f}_k^{(r)}\cdot\mathbf{U}_k^{(r)}\\ &\quad+L_{cH}^{(r)}+L_c^{(r)'}+Q_c^{(r)}\end{aligned} \tag{48}$$

since $\sum_k P\dfrac{\partial\phi_k}{\partial t}+P\dfrac{\partial\phi_c}{\partial t}=0.$

The physical meaning of each term in equation (48) is

$$\left[\begin{array}{l}\text{Rate of change of total}\\ \text{enthalpy of continuous phase}\\ \text{including } KE \text{ of dispersed}\\ \text{phase}\end{array}\right]+\left[\begin{array}{l}\text{Net rate of total enthalpy flux}\\ \text{of continuous phase}\\ \text{(efflux-influx) including } KE \text{ of}\\ \text{dispersed phase}\end{array}\right]=-\left[\begin{array}{l}\text{Heat transfer due to}\\ \text{conduction}\end{array}\right]+$$

$$\left[\begin{array}{l}\text{Heat source in continuous}\\ \text{phase}\end{array}\right]+\left[\begin{array}{l}\text{Work due to displacement of}\\ \text{fluid excluding work due to}\\ \text{compression or expansion by}\\ \text{pressure of dispersed phase}\end{array}\right]+$$

$$\begin{bmatrix}\text{Energy dissipation due to shear}\\ \text{stress}\end{bmatrix} + \begin{bmatrix}\text{Viscous dissipation due to}\\ \text{relative motion of continuous}\\ \text{phase to dispersed phase}\end{bmatrix} + \begin{bmatrix}\text{Viscous dissipation due to}\\ \text{relative motion among}\\ \text{dispersed phases}\end{bmatrix} +$$

$$\begin{bmatrix}\text{Work done by field force on}\\ \text{continuous phase}\end{bmatrix} + \begin{bmatrix}\text{Work done by field force on}\\ \text{dispersed phases}\end{bmatrix} + \begin{bmatrix}\text{Total enthalpy and } KE\\ \text{adjustment for c.g. reference}\end{bmatrix} +$$

$$\begin{bmatrix}\text{Work done due to apparent}\\ \text{mass and flow field}\end{bmatrix} + \begin{bmatrix}\text{Heat transfer coupling}\end{bmatrix}$$

where

$$L_{kH}^{(r)} = \nabla \cdot \left[\rho_c^{(r)}(\mathbf{U}_c^{(r)} - \mathbf{U}_m^{(r)})(\tfrac{1}{2}\mathbf{U}_c^{(r)} \cdot \mathbf{U}_c^{(r)} - \tfrac{1}{2}\mathbf{U}_m^{(r)} \cdot \mathbf{U}_m^{(r)}) + \sum_k \rho_k^{(r)}(\mathbf{U}_k^{(r)} - \mathbf{U}_m^{(r)}) \right.$$
$$\left. \times (\tfrac{1}{2}\mathbf{U}_k^{(r)} \cdot \mathbf{U}_k^{(r)} - \tfrac{1}{2}\mathbf{U}_m^{(r)} \cdot \mathbf{U}_m^{(r)}) \right] - \sum_k \Gamma_k^{(r)} h_m^{(r)} \tag{49}$$

$$L_c^{(r)'} = \sum_k \left\{ \tfrac{1}{4}\rho_k^{(r)} \frac{\bar{\rho}_c^{(r)}}{\bar{\rho}_k^{(r)}} \frac{\mathrm{d}}{\mathrm{d}t_k^{(r)}} [(\mathbf{U}_c^{(r)} - \mathbf{U}_k^{(r)}) \cdot (\mathbf{U}_c^{(r)} - \mathbf{U}_k^{(r)})] + (\mathbf{U}_c^{(r)} - \mathbf{U}_k^{(r)}) \cdot \mathbf{V}_k^{(r)'} \right\} \tag{50}$$

$$Q_c^{(r)} = \sum_k \rho_k^{(r)} c_{vk}^{(r)} G_{kc}^{(r)} (T_k^{(r)} - T_c^{(r)}) \tag{51}$$

where G_{kc} is the inverse relaxation time for energy transfer from continuous phase in dispersed phase. The G's account for the distribution in temperature in the vicinity of the surface of a particle of a dispersed phase and

$$Q_c^{(r)} + \sum_k \rho_k^{(r)} c_{vk}^{(r)} \sum_l G_{kl}^{(r)} (T_l^{(r)} - T_k^{(r)}) = 0. \tag{52}$$

7. INTERFACIAL RELATIONS BETWEEN TWO ADJACENT DOMAINS

A simplified treatment of interfacial relations is given here. The layer which divides the domains is assumed to be a geometric surface of negligible thickness for a stepwise change to occur across the interface.

The challenging nature of the formulation of the interface is that the relations have to refer to the coordinate system constituting the interface $\mathbf{S}(\mathbf{r}, t)$, $\mathbf{r}$ being the space coordinate, while $\mathbf{S}$ remains to be determined from the overall calculations. For the present formulation, the approach of Ishii [10] and Aris [17] will be followed.

Interfacial mass conservation

The interfacial mass conservation equation is given in the form:

$$\sum_{(r)=1}^{2} \left[\rho_c^{(r)} \mathbf{n}^{(r)} \cdot (\mathbf{U}_c^{(r)} - \mathbf{U}_s) + \sum_k \rho_k^{(r)} \mathbf{n}^{(r)} \cdot (\mathbf{U}_k^{(r)} - \mathbf{U}_s) \right] \equiv \sum_{(r)=1}^{2} \left[\dot{m}_c^{(r)} + \sum_k \dot{m}_k^{(r)} \right] = 0 \tag{53}$$

and has the meaning of zero net flux from both sides of the interface; where $\mathbf{n}^{(r)}$ is the outward unit normal vector for domain (r) from the interface, and $\mathbf{U}_s = \mathrm{d}\mathbf{S}/\mathrm{d}t$ is the velocity of the interface.

Interfacial momentum conservation

The interfacial momentum equation is given by a balance between the momentum fluxes from the bulk fluids and the interfacial tension. This expression is given in terms of the transfer between mixtures in the domain on the two sides of the interface [10]:

$$\sum_{(r)=1}^{2} \{ \rho_c^{(r)} \mathbf{n}^{(r)} \cdot (\mathbf{U}_c^{(r)} - \mathbf{U}_s)\mathbf{U}_c^{(r)} + \sum \rho_k^{(r)} \mathbf{n}^{(r)} \cdot (\mathbf{U}_k^{(r)} - \mathbf{U}_s)\mathbf{U}_k^{(r)} - \mathbf{n}^{(r)} \cdot (-P^{(r)}\mathbf{I} + \boldsymbol{\tau}_m^{(r)}) \} + (t_\alpha a^{\alpha\beta}\sigma)_{,\beta} = 0 \tag{54}$$

and has the meaning:

$$\left\{ \begin{bmatrix}\text{Rate of change of momentum}\\ \text{fluxes of continuous phases}\end{bmatrix} + \begin{bmatrix}\text{Rate of change of momentum}\\ \text{fluxes of all dispersed phases}\end{bmatrix} - \begin{bmatrix}\text{Forces due}\\ \text{to stresses}\end{bmatrix} \right\} \begin{matrix}\text{Sum over both sides}\\ \text{of the interface}\end{matrix}$$

$$+ \begin{bmatrix}\text{Forces due to}\\ \text{surface tensions}\end{bmatrix} = 0$$

where $\sigma = \sigma(T_s)$ is a surface tension, T_s is the temperature at the interface, $\mathbf{t}_\alpha$ is the hybrid tensor between the space and the surface coordinates [17], $a^{\alpha\beta}$ is the metric tensor of the interface, and $(\ )_{,\beta}$ is the surface covariant derivative. The no slip condition is applicable to the continuous phases on both sides of the interface, but not to the dispersed phases as

$$\mathbf{U}_s = \mathbf{U}_c^{(r)} = \mathbf{U}_c^{(s)}. \tag{55}$$

Note that $\mathbf{U}_k^{(r)}$ is not limited by this condition, as a bubble may rise through a liquid interface and subsequently merge into the vapor phase.

Interfacial energy conservation

Based on the assumption of a geometrical surface of zero thickness, the interfacial energy equation is:

$$(\mathbf{t}_\alpha a^{\alpha\beta}\sigma\cdot\mathbf{U}_s)_{,\beta} + \sum_{(r)=1}^{2}\left\{\dot{m}_c^{(r)}\left(u_c^{(r)} + \frac{\mathbf{U}_c^{(r)}\cdot\mathbf{U}_c^{(r)}}{2}\right)\right. \\ \left. + \sum_k \dot{m}_k^{(r)}\left(u_k^{(r)} + \frac{\mathbf{U}_k^{(r)}\cdot\mathbf{U}_k^{(r)}}{2}\right) + \mathbf{n}^{(r)}\cdot[(-P^{(r)}\mathbf{I} + \tau_m^{(r)})\cdot\mathbf{U}_m] + \mathbf{n}^{(r)}\cdot\mathbf{J}_m^{(r)}\right\} = 0 \tag{56}$$

$$\begin{bmatrix}\text{Work done by}\\ \text{surface tension}\end{bmatrix} + \left\{\begin{bmatrix}\text{Flux of energy of}\\ \text{continuous fluid}\end{bmatrix} + \begin{bmatrix}\text{Fluxes of energy}\\ \text{of dispersed phases}\end{bmatrix} + \right. \\ \left. \begin{bmatrix}\text{Work done by}\\ \text{stress}\end{bmatrix}\begin{bmatrix}\text{Heat flux}\end{bmatrix}\right\}_{\substack{\text{Sum over both sides}\\ \text{of the interface}}} = 0$$

with $T_s = T_c^{(r)} = T_c^{(s)}$ in the limit.

Data on mass flux, momentum transfer, heat flux, bubble burst to droplets, droplet capture and coalescence are needed for the detailed specification of the interdomain boundary conditions.

8. INITIAL AND BOUNDARY CONDITIONS

The field equations for multidomain-multiphase fluid mechanics have been developed in the previous sections. In order to solve these simultaneous equations, both initial and boundary conditions need to be specified. Initial conditions are usually taken as the steady-state solution of the system equations or any known initial conditions. The typical boundary conditions encountered in the reactor problems of interest are listed below.

Heated wall—Variable heat flux or prescribed temperature distribution; nucleation sites, bubble size, detachment velocity and number density per surface area, normal and tangential velocity components, slip or non-slip.

Non-heated wall—Temperature or temperature gradient; normal and tangential velocity components, slip or non-slip.

In-flow boundary—Inlet temperature; normal component of velocity (inlet velocity) and tangential velocity components or inlet pressure.

Out-flow boundary—Temperature gradient; normal component of velocity gradient and tangential velocity components or outlet pressure.

9. TRANSITION FROM A PHASE TO A DOMAIN

When applied to the density of phase k, equation (1) becomes:

$$\rho_k = \frac{1}{T^*}\int_{T^*}\left[\frac{1}{V}\int_V N_k^0 m_k \,\mathrm{d}V\,\mathrm{d}t\right] \\ = \frac{1}{T^*}\int_{T^*}\rho_k'\,\mathrm{d}t \tag{57}$$

where N_k^0 is the total number of particles of mass m_k at the instant t and ρ_k' is the volume averaged density distributed in volume V.

While the mutually exclusive nature of the phases is accounted for by I' and V', the density ρ_k within the framework of multiphase mixtures is actually a distributed quantity. The discreteness of particles in a dispersed phase is removed by the basic averaging procedure in equation (57). Transition from the phases in a multiphase mixture to a new domain occurs when the net density of the largest of the phases k gives, in a volume constituted by the smallest characteristic physical dimension of the flow system x_0, a single particle, say, $(N_k^0/V)x_0^3 \gtrsim 1$, or

$$a_k^3 \gtrsim (3/4\pi)\alpha_k x_0^3. \tag{58}$$

In this way, a_k becomes radius R of a new spherical domain as an approximation, with

$$(4\pi/3)R^3\bar{\rho}_k = \int_0^R \sum_k \rho_k 4\pi r^2\,\mathrm{d}r \tag{59}$$

while the position and velocity of the center of the new domain are now at the c.g. of ρ_k. Additional domains may be generated and agglomeration of domains gives rise to new domains.

10. DISCUSSIONS

Deterministic nature of the problem

To summarize, the unknowns to be determined can be identified for d separate domains, each with k dispersed phases in Table 3.

Table 3 gives for $k \geqslant 1$ and $d \geqslant 1$ a total of $6d(k+2)-5$ dependent variables with $6d(k+2)-5$ equations; the system is deterministic. Computations for given initial and boundary conditions can cover, at least in theory, all flow regimes and their transitions.

Table 3. Variables and equations

Dependent variables	No. of unknowns*	No. of equations*	
ρ_c, ρ_k	$(k+1)d$	Continuity	$(k+1)d$
$\mathbf{U}_c, \mathbf{U}_k$	$3(k+1)d$	Momentum	$3(k+1)d$
h_c, h_k (or T_c, T_k)	$(k+1)d$	Energy	$(k+1)d$
P	d	Equation of state	$(k+1)d$
ϕ_c, ϕ_k	$(k+1)d$	Volume fractions	d
Total mass of each domain	$d-1$		
$\mathbf{S}(r, t)$	$3(d-1)$	Interface	$5(d-1)$
T_s	$d-1$		

*$k \geqslant 1$ and $d \geqslant 1$.

Inertial coupling term

A general discussion of the basic concepts in the formulation of conservation equations for multiphase systems seems appropriate. Most of the formulation of the conservation equations for multiphase systems begins with a consideration of the individual phases [7–10]. The conservation equations for the mixture are deduced by combining those for the individual phases. This might be considered a natural approach which appears feasible in principle. In practice, however, it often leads to errors [18] due to the inability of these investigators to include all relevant physical effects into the formulation. An example is their conspicuous omission of the inertial coupling forces [15, 19] in the momentum equation for the individual phases. This pitfall is recognized and the view [3] has been adopted that the formulation of the field equations should be based on conservation principles as applied to the mixture. Moreover, there is resistance to motion of a body through a non-viscous fluid. Consequently, it is believed that the global momentum and energy equation for the mixture of the multiphase system assumes the same form as those for a homogeneous medium, when viewed within the context of continuum mechanics. The foregoing statement has been adopted as a fundamental postulate. Most importantly, the formulation presented in this paper employs consistent coordinate transformation, independent of the procedures of averaging [2], size of control volume or jump condition [10], or flow regime [9]. It was shown rigorously that without the inertial coupling effect properly accounted for, the one-dimensional momentum equations of components give imaginary characteristics [20, 21]. Furthermore, the stability of computation of transient flow is significantly improved when the inertial coupling terms are properly accounted for [5]. The reason is that similar stability to that of the mixture momentum equation is retained via the inertial coupling terms. It is further noted that both the terms representing the effects of virtual mass and unsteady motion do not always stabilize the computation.

The $\mathrm{P}\nabla\alpha_k$ *terms*

Besides identifying the possible range of B_k in Section 5, distinction between homogeneous and structured multiphase fluid in terms of application of $P\nabla\alpha_k$ terms needs clarification.

An overview of the term $\nabla P\alpha_k = \alpha_k\nabla P + P\nabla\alpha_k$ includes those who favor (1) dropping $P\nabla\alpha_k$ for reasons of making computation easier [22, 23] or from consideration of an interfacial source force [10], (2) retaining part of it as a stabilizing force [22], and (3) retaining $P\nabla\alpha_k$ for the reason of an extension of the continuum mechanism, as a compressive (or expansive) force and validity of the laws of thermodynamics. While details of these views have been given [20, 24], it suffices to say that an all encompassing formulation for multiphase mechanics will be to replace, in the momentum equation, the term $\nabla P\alpha_k$ by

$$\nabla P\alpha_k - B_k P\nabla\alpha_k = \alpha_k\nabla P + (1-B_k)P\nabla\alpha_k \qquad (60)$$

with B_k as a displacement factor; B_k is a function of particle size, flow structure and fluid properties. The range of B_k covers: $B_k = 0$ for very small particles and $B_k \to 1$ for large particles because of low diffusivity. This factor includes all views and physical eventualities and its use is believed to facilitate the progress of the computer modeling of multiphase thermohydraulics.

It is interesting to note that the term $P\nabla\alpha_k$ has been attributed to as the source of imaginary characteristics in one-dimensional transient flow calculations, but realizing that dropping $P\nabla\alpha_k$ alone is not sufficient to give a system of real characteristics [22]. However, it is physically inconceivable that one-dimensional transient motion of air has real characteristics, yet when written separately in terms of oxygen and nitrogen, the equations would give imaginary characteristics. Significance is seen in the inertial coupling terms in equation (16) in general, and equations (37), (44), (45), and (46) in specifics actually account for consistent coordinate transformation, leading to real characteristics for one-dimensional transient flow of a suspension [21]. It was also shown that $P\nabla\alpha_k$ term contributes to the wave velocity in this case.

A thermodynamic and therefore a basic evidence for the existence of the $P\nabla\alpha_k$ term is seen in the physical case of adiabatic compression of a bubble, when the $P\nabla\alpha_k$ term is carried into the energy equation in the form of equation (45). When this is reduced to a single particle in a liquid at zero velocity of both phases and with negligible heat transfer or heat source, equation (45) reduces to the equation of adiabatic compression.

In exploring the continuation from continuum mechanics to multiphase mechanics, such as the case of continuum gas mixture of species 2 with a trace of species 1, the one-dimensional momentum equation of species 1 reduces to the diffusion equation when combined with the continuity equation. $P\nabla\alpha_k$ term gives the diffusion term via $(P/\bar{\rho}F)$ as diffusivity [24]. A complete discussion is given by Sha and Soo [5].

The range of $0 \lesssim B_k \lesssim 1$ will cover the whole range of reasoning and choices. Thus, the effects of $B_k P\nabla\alpha_k$ term on system behavior under various conditions can be investigated.

Comparison to other studies

To further the current knowledge on multiphase mechanics, it is desirable to compare the present formulation to other existing pertinent studies. The work of Harlow and Amsden [9], Solbrig and Hughes [8], and Ishii [10] were chosen for this comparison.

The field equations presented in this paper will reduce to: (1) Harlow and Amsden's formulation when both effectiveness of momentum transfer (K) and displacement parameter (B) are set equal to zero and unity respectively, inertial coupling term was dropped except that part due to mass generation and some simplifications of friction force between phases, (2) Solbrig and Hughes' equations when the control volume includes solid structures by introducing porosity, values of K and B are set equal to zero and unity respectively and the inertial coupling term is deleted except that part due to mass generation, (3) Ishii's set of governing equations, when the space–time average is replaced by the time average, the values of K and B are set equal to zero and unity respectively, and the inertial coupling term is substituted by interaction force.

Comparisons with other existing formulations [23, 26] and derivations are given in detail by Sha and Soo [5].

Consistent approximation

It is readily seen that, when applied to a one-dimensional transient flow, the problem is always well-posed (real characteristics) when $\mathbf{I}_k$, $\alpha_k\nabla P$, and $P\nabla\alpha_k$ are all retained. The relations for the characteristics are reducible to those of the case of a single-phase fluid. The possibility of ill-posedness raised by some authors [20] appears to be due to the inconsistent approximation via neglecting $\mathbf{I}_k$ but retaining $\alpha_k\nabla P$. Neglecting the latter always renders the problem well-posed. Such an approximation is also supported by the compensation of $\alpha_k\nabla P$ with $\mathbf{V}_k$ in an accelerated flow field in the case of a dilute suspension [27, 28]. However, without the term $(1-B_k)P\nabla\alpha_k$ the wave velocity of the two phase system is not reducible to the case of a single phase fluid and is not physically meaningful. Hence, for a dilute suspension (small α) of small particles ($\mathbf{U}_k \sim \mathbf{U}_c$), both $\alpha_k\nabla P$ and $\mathbf{I}_k$ can be dropped to maintain consistent approximations.

Worth noting is that $\mathbf{I}$ and $\mathbf{I}'$ are not directly related and can be treated as cumulative because $\mathbf{I}'$ is a field force due to the continuum phase. A valid question is that since $\mathbf{I}'$ and $\mathbf{V}'$ are known only for a dilute suspension [6], what should one do for a dense suspension? While it is obvious that $\mathbf{I}'$ and $\mathbf{V}'$ remain to be determined for a dense suspension, a conservative view is that a dense suspension is more readily treated as a continuum than a dilute suspension. $\mathbf{I}$ and $\mathbf{V}$ are expected to be much greater than $\mathbf{I}'$ and $\mathbf{V}'$ in a dense suspension while the reverse is likely for a dilute suspension. The error arising from ignoring $\mathbf{I}'$ and $\mathbf{V}'$ when calculating a dense suspension is expected to be small; the same is true when neglecting $\alpha_k\nabla P$ and $\mathbf{I}_k$ when calculating a dilute suspension.

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MECANIQUE DES FLUIDES MULTIPHASIQUES

Résumé—Un système d'équations est développé à partir de la mécanique des fluides multiphasiques· conservation de la masse, de la quantité de mouvement et de l'énergie La mécanique multiphasique s'applique aux mélanges de phases qui sont séparées par des interfaces et sont mutuellement exclusives. Ceci est en contraste avec les équations pour les mélanges, basées sur la mécanique des milieux contunus et qui s'appliquent directement aux mélanges moléculaires pour lesquels les phases coexistent aux même points dans l'espace. Dans la formulation de la mécanique multiphasique des termes suplémentaires apparaissent dans les équations quand la taille physique de la phase dispersée (bulle ou goutte) est plusieurs fois plus grande que la distance intermoléculaire. Ces termes représentent le couplage inertiel dû à la masse virtuelle et le couplage visqueux dû à la fluctuation du champ d'écoulement. Ces. effets physiques ainsi que les termes de couplage inertiel du continuum sont négligés dans beaucoup d'autres calculs en biphasique. En incluant ce couplage inertiel, les équations de l'écoulement unidirectionel et multiphasique donnent les caractéristiques réelles. La somme des équations de quantité de mouvement de toutes les phases se réduit aux équations de quantité de mouvement du mélange comme on peut l'espérer.

MEHRBEREICHSFLUIDMECHANIK FÜR MEHRPHASIGE SYSTEME

Zusammenfassung—Es wird ein Satz von Mehrphasenfeldgleichungen—Erhaltung der Masse des Impulses und der Energie—auf der Grundlage der Mehrphasenmechanik entwickelt. Mehrphasenmechanik wird angewendet bei Gemischen von Phasen, welche durch die Grenzflächen getrennt sind und sich gegenseitig ausschließen. Hierin unterscheiden sie sich von den Feldgleichungen für Gemische, die auf der Kontinuumsmechanik basieren und direkt für Molekulargemische gültig sind, bei denen sich die Phasen gleichzeitig an den gleichen Punkten im Raum befinden. Durch den Ansatz der Mehrphasenmechanik erscheinen zusätzliche Terme in den Feldgleichungen, wenn die kennzeichnende Größe der dispersen Phase (Blase oder Tropfen) mehrmals größer ist als der intermolekulare Abstand. Diese Terme sind die Inertialkopplung, entsprechend der virtuellen Masse und die zusätzliche Viskositätskopplung entsprechend der Veränderlichkeit des Strömungsfeldes. Diese physikalischen Effekte sowie die Kontinuums-Inertialkopplungsterme blieben in vielen anderen Zweiphasenberechnungen unberücksichtigt. Beim Einbeziehen dieses Inertialkopplungsterms ergeben die eindimensionalen Mehrphasengleichungen zutreffende Aussagen. Darüber hinaus führt die Summe der Impulsgleichungen für alle Phasen erwartungsgemäß auf die Impulsgleichungen des Gemisches.

МНОГОФАЗНАЯ ГИДРОМЕХАНИКА ДЛЯ НЕСМЕШИВАЮЩИХСЯ ФАЗ

Аннотация — На основе многофазной механики выведена система уравнений, представляющих полевые законы сохранения массы, импульса и энергии. Многофазная механика применяется к смеси взаимно нерастворимых фаз, разделенных поверхностями, что отличается от подхода, основанного на уравнениях сплошной среды для многокомпонентных молекулярных растворов. В тех случаях, когда физический размер дисперсной фазы (пузырька или капли) во много раз превышает межмолекулярное расстояние, в уравнениях многофазной механики появляются дополнительные члены, один из которых инерционный и обусловлен эффективной массой, а второй представляет собой вязкое взаимодействие, вызванное нестационарностью течения. Этими физическими эффектами, а также инерционными членами сплошной среды в других расчётах двухфазных смесей пренебрегали. Найдено, что учёт инерционного члена в одномерных многофазных уравнениях позволяет получить реальные характеристики смесей. Кроме того, как и следовало ожидать, найдено, что сумма уравнений импульсов для всех фаз сводится к уравнению импульса для смеси.