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Multidomain Multiphase Fluid Mechanics

By

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Prepared by

Components Technology Division

Argonne National Laboratory

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Washington, D.C. 20555

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MASTER

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Nomenclature

a	Bubble or droplet radius
$\dot{a}$	Rate of bubble or droplet growth
$a^{\alpha\beta}$	Metric tensor of interface
B	Displacement factor
c_p	Specific heat at constant pressure
c_v	Specific heat at constant volume
C_{B3}	Coefficient of bubble burst to droplet
C_{B4}	Coefficient of bubble burst to vapor
C_D	Drag coefficient
d	Domain
D	Diffusivity
$\hat{D}$	Self diffusivity
D_b	Bubble diameter at detachment
E	Total energy
E_o	Eotvos number
f	Field force
$\hat{f}$	Bubble frequency
F	Inverse relaxation time constant for momentum transfer
g	Gravitational constant
G	Inverse relaxation time constant for energy transfer
h	Enthalpy
$\hat{h}$	Heat transfer coefficient
h_{fg}	Latent heat
H	Total enthalpy
H_{42}	Mean curvature of the surface separating continuous phases 2 and 4
I	Inertial coupling

Nomenclature (contd.)

I'	Force due to apparent mass
I	Unit tensor
J	Heat flux
J_a	Jacob number
J_3	Droplet flux across the interface between two domains
J_4	Bubble flux across the interface between two domains
k	Boltzmann constant
$\hat{k}$	Agglomeration constant
k^*	Coefficient for diffusivity of pipe flow
$\bar{K}$	Effectiveness of particle-fluid momentum transfer
K	Particle-fluid interacting parameter
$\hat{L}$	Interacting length
L	Inertial coupling of energy
L'	Work done due to apparent mass and unsteadiness of flow field
m	Mass per particle of dispersed phase
M	Inverse relaxation time constant for mass transfer
n	Normal to characteristics
$\underline{n}$	Unit outward normal vector
N	Number density
$\dot{N}, \dot{S}$	Rate of generation of bubbles or droplets
N_o	Avogadro number
N_A	Nucleation sites per unit area
N_L	Probability of a spherical critical nucleus of radius a_k
Nu	Nusselt number
P	Pressure
Pr	Prandtl number
Q	Heat transfer coupling

Nomenclature (contd.)

$\underline{r}, \underline{x}$	Space coordinate
R	Radius of a pipe
Re	Reynolds number
$\dot{S}$	Rate of generation of bubbles or droplets
$\underline{S}$	Surface of interface
Sh	Sherwood number
t	Time
t_{α}	Hybrid tensor
T	Temperature
u	Internal energy
U	Velocity
U^*	Characteristic flow velocity
V	Viscous coupling
V'	Force due to unsteadiness of flow field
$\underline{x}$	Space coordinate
X_0	Characteristic length of a flow passage
Γ	Mass generation rate per unit volume
Δ	Shear strain
ΔF_g	Free nucleation energy
ζ	Bulk viscosity
θ	Dilatation
κ	Thermal conductivity
λ	Lagrangian integral
μ	Viscosity
μ^*	$\zeta - (2/3)\bar{\mu}$

Nomenclature (contd.)

ν	Kinematic viscosity
ρ	Density
σ	Surface tension
τ	Viscous stress
ϕ	Volume fraction

Superscript

(r)	Domain (r)
($\bar{}$)	Material property

Subscript

b	Bubble
c	Continuous phase
e	Evaporation
E	Total energy
k	Dispersed phase
h	Enthalpy
H	Total enthalpy
i,j	Components
ji	Tensorial components
l	Liquid
m	Mixture
mc	- of continuous phase c in the mixture (such as stress of continuous phase in the mixture)

Nomenclature (contd.)

m_k	- of phase k in the mixture
s	Interface or interdomain
t	Tangential direction
u	Internal energy
v	Vapor
$\underline{\quad}$	Vector

Operator

∇	Gradient
$\nabla \cdot$	Divergence
$d/dt_k = \partial/\partial t + \underline{u}_k \cdot \frac{\partial}{\partial \underline{x}}$	
$:$	Scalar product of tensors
$(\quad)_{,\beta}$	Surface covariant derivative
$\langle \quad \rangle$	Average

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 are usually ignored in continuum mechanics formulations. The continuum inertial coupling term has been neglected in all previous multiphase calculations. It can be shown that by including this inertial coupling term the multiphase field 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.

The multiphase formulation given here takes into account the discreteness of particles of dispersed phases and, at the same time, the necessity of the distributive representation of field variables via space-time averaging when handling a large number of particles. The provision for multidomain transition further permits us to treat dispersed phases which are large compared to the characteristic dimension of the flow system via inter-domain relations.

The multidomain multiphase approach provides a framework for us to model the various flow regimes. Because some of the transport parameters associated with the system equations are not well known at the present time, an idealized two-domain two-phase solution approach is proposed as a first step.

Finally, comparisons are made between the field equations formulated based on the multidomain-multiphase fluid mechanics and the pertinent existing models, and their relative significances are discussed. The desirability of consistent approximation and simplifications possible for dilute suspensions are discussed.

1.0 Introduction

The significance of two-phase flow in relation to nuclear reactor safety has led to several kinds of studies on multiphase flow. These include extensions of one-dimensional flow [1] to treat flow transients [2,3,4], extension of continuum mechanics to deal with three-dimensional systems [5,6], problems involving flow instabilities [7], and the suggestion of multiphase mechanics as a discipline of its own [8]. Extensive computer programs for two-phase flow have also been formulated [9,10]. The consistency of mathematical models used or proposed in these studies as well as those available in the open literature to describe two-phase flows has been questioned [6]. Open discussions [11] at several meetings have not led to a resolution or clarification of the differences. Hence, because of the importance of the problem a detailed re-examination of the models and a rigorous formulation is needed.

1.1 Theoretical Background

In many published studies on multiphase flow, there are two models used in the study of mass, energy and momentum transfer in a medium. One is the particulate model used in statistical mechanics and the other is the continuum model of continuum mechanics. In the particulate model, matter is made of discrete particles and mass is a discontinuous function of position. In the continuum model, matter is continuously distributed throughout space, except for surfaces of discontinuity which represent phase interfaces, physical boundaries and shock waves; mass is a continuous function of position within a single phase. Since matters are indeed made of discrete particles -- proton, neutron, electron, etc., -- the particulate model represents a much more realistic picture of the details of real materials. Furthermore, averages defined by the laws of statistical mechanics satisfy the laws of balance introduced in continuum mechanics. However, the continuum model has the distinct advantage of simplicity when one wishes to describe gross phenomena. Using the continuum formulation, the physical problem is represented by idealized boundary geometries, boundary conditions, initial conditions, field and constitutive equations. In summary, the continuum model has the advantage of simplicity; however, for multiphase systems the particulate nature needs to be accounted for in the mathematical formulation.

An item that deserves special attention even in the realm of continuum mechanics is the inertial coupling of the flow in a multicomponent mixture. When considering the motion of an individual component of a mixture, inertial

coupling gives rise to a resistant force acting on a component due to the presence of the other components. The actions and reactions of these forces cancel out when we consider an overall mixture. Physically it can be shown for the transient flow of a gaseous mixture the real characteristics obtained from the momentum equation based on Newton's Law can be correlated experimentally. It should come as no surprise that the momentum equation of individual components also give real characteristics when inertial coupling is properly included [8]; leaving out the inertial coupling force gives imaginary characteristics [11]. The concept of inertial coupling is especially clarified in this report.

The continuum approach in a single-phase thermal-hydraulic problem is widely accepted and its validity is well proven. In analyzing two-phase flows the conventional approach of continuum mechanics has also been applied. A two-phase flow is considered as a field which is subdivided into single-phase regions with moving boundaries between phases. In theory, it is possible to formulate a two-phase flow problem in terms of the local instantaneous variables. In practice, such a formulation would result in a multi-boundary problem with the positions of the interfaces between two phases being unknown. Mathematical difficulties encountered in solving the two-phase problems with instant local formulation are in general found to be unmanageable. In order to bypass some of these difficulties, an average of each phase over the time, or space, or time-space or space-time is employed with the assumption that each phase coexists over the same space. The purpose of the averaging process is to transform two phases with discontinuities at the interfaces to two simultaneous continua.

It is to be noted that there is the inherent limitation of continuum mechanics when applied to problems involving discrete particles whose sizes are many times larger than the inter-molecular spacing. For example, the existence of mutual exclusiveness of the phases in a multiphases system can not be accommodated. Consequently, such effects as virtual mass and Basset force cannot be accounted for, and the partial pressures in a mixture identified in continuum mechanics become meaningless when applied to bubbles in a liquid or droplets in a vapor at a given system pressure. However it is impractical to treat all discrete phases as interacting continua. The multiphase formulation proposed in this report taken into account the discreteness of

particles of dispersed phases, and at the same time the necessity of introducing a proper averaging when handling a large number of particles. The averaging yields a distributed representation of field variables such as density, velocity and temperature. This duality of approach results a set of field equations which give real characteristics.

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.

This transition from multiphase to a new domain corresponds to the "jump" considered by Ishii [6]. In choosing this approach, differences from the text of Ishii were introduced. In the two-fluid model of Ishii, the interfacial boundary condition or jump condition is included in the field equations. The aim of a multiphase-multidomain treatment is to facilitate computations; any difference with Ishii's formulation are attributable to a choice of control volume. Differences with other formalations are also discussed in this report.

An item which has been controversial among specialists of multiphase mechanics is the term (or terms) which correspond to the partial pressure in continuum mechanics. Various views on this subject matter are clarified, and a unified approach is presented in this report.

1.2 Physical Regime of Interest

Where physical examples are presented, the phenomena of multiphase flow are best illustrated in most cases via a steam-water system. The latter has a wealth of background data as seen in the proceedings of a recent International Symposium of Heat and Mass Transfer [12]. Even though a high degree of accuracy is needed in estimating a contingency situation such as loss of coolant in light water reactor systems, a realistic estimate of the consequence can be obtained from the available experimental data on boiling water flow under loss of flow conditions and other high velocity two-phase flow experiments [13].

When compared to a steam-water system, the sodium system needs a great deal more attention. Data on high velocity flow of boiling liquid metal are meager. Extrapolation of boiling water data [14] to sodium involves a three order of magnitude smaller Prandtl number, one order of magnitude larger surface tension, and two orders of magnitude higher thermal conductivity [15]. Hence, where experimental results are not yet available, a high degree of rigor in analysis and calculation is needed. High cost of experimentation can be reduced by a detailed theoretical study to identify the physical and transport properties to be determined, and the scaling relations for model studies and their experimental range.

The accident situations of a liquid metal fast breeder reactor (LMFBR) may be classified into the following two categories: (1) transient overpower (TOP) and (2) loss-of-coolant (LOC). Sodium boiling normally takes place during the occurrence of each of these accidents. The importance of studying sodium boiling in a fast breeder reactor system is threefold: (1) reactivity feedback associated with sodium voiding -- for the current design of FBR the sodium voiding most likely will result in positive reactivity feedback; (2) overheating due to sodium vapor blanket over structure surface -- one of the characteristics of LMFBR is its high specific power ($\sim .5$ MW/Liter for the oxide fuel), thus loss-of-coolant can readily cause severe damage of structure integrity; (3) mechanical work produced due to rapid voiding -- because of the rapid voiding characteristic of sodium and the very high ratio of specific volume of vapor to liquid ($V_g/V_l \sim 3000$ at atmospheric pressure for sodium, $V_g/V_l \sim 6$ for water), it is conceivable that tremendous amounts of mechanical work can be generated under certain accident conditions [16,17]. In order to predict a reactor accident sequence as well as its consequences, the study of two-phase flow of sodium systems must be carried out in great detail.

The dynamic equations of a boiling sodium system should account for both bubble generation at a surface and subsequent bubble growth after it leaves the surface because of high thermal conductivity, followed by bubble coalescence. The tendency of forming large bubbles because of large surface tension is also expected. The details of bubble dynamics are important, especially in relation to heat flux and flow conditions.

The basic concept of multidomain 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.

The boundary conditions of the multiphase mechanics approach include bubble generation, diffusion, and drift from a boundary. The interdomain relation will include symmetric bubble dynamics [18,19] at the beginning and later generalization to include wave motion of the interface of large bubbles due to varying surface tension [20].

In this study we shall first outline the basic relations of the general case of a multidomain-multiphase flow system (Fig. 1). 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. This will be followed by a detailed examination of available parameters and properties. Based on the accuracy of the available details, an idealized and simplified two-domain, two-phase flow will be formulated, with the degree of approximation consistent with the accuracy of the parameters and properties available at this time. The results of the computation will then be an idealized prediction of flow regimes and rates.

In summary, sodium boiling flow and heat transfer in a reactor core are complicated phenomena. At present, the mechanisms of mass, heat and momentum transfer between phases are not known in detail. The problem of two-phase flow of sodium systems is recognized as one of the most important problems in reactor safety analysis. Some concern about the consistency of mathematical models used or proposed in the literature to describe two-phase flows has been expressed. Therefore, the objectives of this report are: (1) to present a set of rigorous field equations to be used in multiphase flows and to point out the inconsistencies of existing models; (2) to propose a simplified two-domain, two-phase model as the basis of our computer program; and (3) to compare the proposed model with the pertinent existing work.

1.3 Terminology

For the sake of clarity and the readers' convenience, the definitions pertaining to multidomain-multiphase fluid mechanics are given below:

Multiphase Mechanics - Multiphase mechanics applies to mixtures of phases which are separated by interfaces and are mutually exclusive. This is in contrast to the continuum mechanics approach which is directly applicable to molecular mixtures where component coexist at the same point in space [8].

Phases (Thermodynamic) - In its conventional meaning they consist of liquid, vapor and solid phases.

Phases (Dynamic) - In multiphase mechanics each domain consists of a continuous phase and one or more dispersed phases. In the dispersed phase, such as bubbles in a liquid (continuous phase) or droplets in vapor (continuous phase), different size ranges (also density, electron charge, etc.) constitute different "phases". This is because of the different dynamic response behavior of these "phases". Hence, the term "multiphase" system [21].

Two-Phase - A dispersed phase in a continuous phase.

Domain - A portion of a multiphase mixture in a continuous phase bounded by a different continuous phase or a solid wall.

Flow Regimes - In the flow of a boiling liquid, bubble flow, slug flow, annular flow, droplet or mist flow are examples of flow regimes. Each regime may consist of one or many domains, each composed of a single phase or more phases (at least two for a mixture of phases [1])(Fig. 1).

Interphase Relations - Within a domain, dynamic conservation relations accounting for interactions between phases.

Intraphase Relations - Dynamic relations inside a pure material within a boundary inside a mixture.

Interface - A boundary separating two pure phases of liquid and vapor in its strict sense. It may be extended to include a boundary between two domains.

Interdomain Boundary - Boundary or interface separating two domains with different continuum phase, each consisting of a pure material, two-phase or multiphase mixtures.

Fig. 1 Flow and heat transfer regimes in rod array with vertical upflow [5].

2.0 Fundamentals of Multidomain-Multiphase Fluid Mechanics

The phenomena of flow of a boiling liquid in the identifiable regimes (Fig. 1) can be treated under the general scheme of multidomain-multiphase fluid mechanics.

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 [21], bubbles (droplets) of each size and density range constitute a phase. That is, if we subdivide the identifiable sizes into k different ranges, we have k dispersed phases when each range has the same density of vapor (droplets of liquid).

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 in Fig. 1, in the case of nucleate boiling (low heat flux), 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 passage. 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. In 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 leads to annular flow. 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 of high heat flux flow can be made in an analogous manner.

2.1 General Formulation

A general rigorous formulation of multiphase-multidomain flow is desirable as a reference for subsequent simplifications needed in developing a viable computer program. This development is visualized to be in stages with improving rigor and accuracy.

In formulating multiphase field equations within the Eulerian frame of reference, conceptually we are treating space average of a volume element to define field variables such as density and velocity of each phase which characterize the system behavior. The volume element must be small relative to the perturbations of interest in the medium but large enough to contain sufficient number of dispersed phases so that the averaging is meaningful. In the multiphase representation we are not concerned with velocity fields in the immediate

vicinity of the boundary layer around each particle [22] of a dispersed phase. In this sense, each particle becomes 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 relaxation time for momentum 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 numerical computational grid sizes are unrelated.

Measurements by sampling at a given location, however, involve time averages. This concern was noted by Ishii [6] in that the time mean values are consistently expressed by the spatial description. In a sense the microscopic formulation involves "time averaged" mean values in space. The time duration over which the average is taken should be greater than the mean interparticle spacing divided by the mean particle velocity. Except at defined interfaces between domains and at a solid wall, a dispersed phase such as a bubble within a domain is represented by the idealization of not having a velocity or temperature distribution, nor mass inside or outside of it. At a given point in space, however, that phase is identified by a mass density ρ_k , velocity $\underline{U}_k$ and enthalpy h_k (temperature T_k); the detailed distributions around each particle of the dispersed phase are represented by the corresponding relaxation times for mass, momentum and energy transfer. Phase change is represented by local averaged mass generation of the phase (including bubble coalescence).

Multiphase fluid mechanics employs the space-time average (see Appendix A) within a domain. 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 then will have to be smaller than the characteristic dimension of a domain.

The basic considerations of the field equations employed in the multiphase fluid mechanics within a domain are presented in Appendix B.

2.1.1 Relation of Mixture to Phases

For the general description of such a system we denote the domains with superscripts (r), (s), etc. Within each domain we denote dispersed phases (for example, bubbles of various size ranges) with subscript k, the continuous phase with subscript c, and the mixture constituting a domain with subscript m. Within each domain we have to account for phase interactions, and the

interfacial relations between domains. Thus, we have, 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 $\rho_k^{(r)}$, and volume fraction $\phi_k^{(r)}$; its velocity $\underline{U}_k^{(r)}$. For domain (r) we have the mixture properties governed by [21]:

$$\rho_m^{(r)} = \rho_c^{(r)} + \sum_k \rho_k^{(r)} \quad (2-1)$$

and the momentum by

$$\rho_m^{(r)} \underline{U}_m^{(r)} = \rho_c^{(r)} \underline{U}_c^{(r)} + \sum_k \rho_k^{(r)} \underline{U}_k^{(r)} \quad (2-2)$$

where " $\underline{\quad}$ " denotes a vector unless otherwise noted.

The energy is $E = u + \underline{U} \cdot \underline{U} / 2$

$$\rho_m^{(r)} E_m^{(r)} = \rho_c^{(r)} E_c^{(r)} + \sum_k \rho_k^{(r)} E_k^{(r)} \quad (2-3)$$

where u is the internal energy. The enthalpy of each phase is

$$h_k^{(r)} = u_k^{(r)} + \frac{p_k^{(r)}}{\rho_k^{(r)}} = u_k^{(r)} + \frac{\phi_k^{(r)} p^{(r)}}{\rho_k^{(r)}} \quad (2-4)$$

where

$$\phi_k^{(r)} p^{(r)} = \frac{\rho_k^{(r)}}{\rho_k^{(r)}} p^{(r)} \quad (2-5)$$

accounts for the effect of a general compressibility but not in the sense of partial pressure. Moreover, we have

$$\phi_c^{(r)} + \sum_k \phi_k^{(r)} = 1 \quad (2-6)$$

2.1.2 Continuity Equation

The continuity equations or the mass balance equations take the following forms and the physical meaning of each of the terms in the balance equations is (Appendix B.1):

For dispersed phase k ,

$$\frac{\partial \rho_k^{(r)}}{\partial t} + \nabla \cdot (\rho_k^{(r)} \underline{U}_k^{(r)}) = \Gamma_k^{(r)} \quad (2-7)$$

$\left[\begin{array}{c} \text{Rate of Change} \\ \text{of Density of} \\ \text{Dispersed Phase} \end{array} \right]$	+	$\left[\begin{array}{c} \text{Net rate of Mass} \\ \text{Flux of Dispersed} \\ \text{Phase (Efflux-} \\ \text{Influx)} \end{array} \right]$	-	$\left[\begin{array}{c} \text{Rate of Gen-} \\ \text{eration of} \\ \text{Dispersed} \\ \text{Phase} \end{array} \right]$
---	---	--	---	--

For continuous phase c,

$$\frac{\partial \rho_c^{(r)}}{\partial t} + \nabla \cdot (\rho_c^{(r)} \mathbf{u}_c^{(r)}) = \Gamma_c^{(r)} \quad (2-8)$$

$$\left[\begin{array}{l} \text{Rate of Change of} \\ \text{Density of Contin-} \\ \text{uous Phase} \end{array} \right] + \left[\begin{array}{l} \text{Net Rate of Mass} \\ \text{Flux of Continu-} \\ \text{ous Phase} \\ \text{(Efflux-Influx)} \end{array} \right] = \left[\begin{array}{l} \text{Rate of Gen-} \\ \text{eration of Con-} \\ \text{tinuous Phase} \end{array} \right]$$

In these relations, $\Gamma_k^{(r)}$ is the rate of generation of phase k with mass $m_k^{(r)}$ in domain (r) per unit volume per unit time (t). For each size range of similar material density, and thus of similar mass $m_k^{(r)}$ we have

$$\Gamma_k^{(r)} / m_k^{(r)} = \frac{1}{2} \sum_{m+n=k} \dot{N}_{mn} + \sum_{m=k}^{\infty} \dot{S}_{mk} - \sum_{m=0}^{\infty} \dot{N}_{mk} - \frac{1}{2} \sum_{m+n=k} \dot{S}_{mn} + (\Gamma_{ke}^{(r)} / m_k^{(r)}) \quad (2-9)$$

where $\dot{N}_{mn}$ is the number of effective collisions per unit volume per unit time between the m and n species to form a k bubble, $\dot{S}_{mk}$ is the number of m species which split to give k species, $\dot{N}_{mk}$ is the k species removed by collision with m species, $\dot{S}_{mn}$ is the number of k species removed by splitting of k into m and n, and Γ_{ke} is the rate of generation in k by phase change (evaporation in the case of bubbles and by growth or collapse of those of sizes larger or less than k; $\Gamma_{ke}^{(r)} < 0$ for condensation). For the continuous phase, we have:*

$$\sum_k \Gamma_k^{(r)} + \Gamma_c^{(r)} = \Gamma_e^{(r)} = 0 \quad (2-10)$$

where $\Gamma_e^{(r)}$ is the net phase change in domain (r) including interdomain mass transfer. The smallest radius (a_k) identified will also include bubbles or droplets produced by nucleation [23,24].

2.1.3 Generation Due to Phase Change

In the macroscopic form, phase change can be expressed in terms of a mass transfer coupling between the continuous phase and the dispersed phase:

$$\Gamma_{ke}^{(r)} = M_{kc}^{(r)} (\bar{\rho}_c^{(r)})' - \bar{\rho}_k^{(r)} \quad (2-11)$$

where $M_{kc}^{(r)}$ is an inverse relaxation time for the mass transfer and $\bar{\rho}_c^{(r)}$ denotes the density of the vapor of the continuous phase based on the temperature of the liquid phase whether it is superheated or compressed and $\bar{\rho}_k^{(r)}$ denotes the density

*Finite $\Gamma_e^{(r)}$ may arise from dissolved gases (having negligible effect on liquid properties) or species generated via nuclear excitation.

of the dispersed phase based on the temperature and pressure of the vapor phase whether it is superheated or supersaturated.

2.1.4 Momentum Equation

In treating the momentum balance of the system, there exists a need to clarify the concept of stress and flux of a phase in the mixture.

The transport properties of a phase in a mixture were defined strictly in [21], 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, we represent the viscous stresses within each domain as that of the mixture $\underline{I}_m^{(r)}$

$$\underline{I}_m^{(r)} = \underline{I}_{mc}^{(r)} + \sum_k \underline{I}_{mk}^{(r)} \quad (2-12)$$

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

$$\underline{I}_{mc}^{(r)} \neq \underline{I}_c^{(r)}, \quad \underline{I}_{mk}^{(r)} \neq \underline{I}_k^{(r)} \quad (2-13)$$

$\underline{I}_{mk}^{(r)}$ 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 transferring of the particle cloud via diffusion through the continuous phase [25,26].

$$\underline{I}_{mk}^{(r)} \sim \rho_k^{(r)} D_{kc}^{(r)} \underline{\Delta}_k^{(r)} \quad (2-14)$$

where $\underline{\Delta}_k$ 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 [21,26].

Similarly the conduction heat flux $\underline{J}_m^{(r)}$ in the mixture is equal to:

$$\underline{J}_m^{(r)} = \underline{J}_{mc}^{(r)} + \sum_k \underline{J}_{mk}^{(r)} \quad (2-15)$$

where $\underline{J}_{mk}^{(r)}$ is the conduction heat flux of species k in the mixture in the domain (r) , and $\underline{J}_{mc}^{(r)}$ 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 respectively are presented in Appendix C.

The momentum equations take the following forms [Appendix B.2]:

For the dispersed phase k :

$$\begin{aligned} (\partial/\partial t) \rho_k^{(r)} \underline{U}_k^{(r)} + \nabla \cdot \rho_k^{(r)} \underline{U}_k^{(r)} \underline{U}_k^{(r)} = & - \phi_k^{(r)} \nabla P^{(r)} - (1 - B_k^{(r)}) P^{(r)} \nabla \phi_k^{(r)} \\ & + \nabla \cdot \underline{T}_{mk}^{(r)} + \rho_k^{(r)} \underline{f}_k^{(r)} \\ & + \underline{I}_k^{(r)} + \underline{V}_k^{(r)} + \underline{I}_k^{(r)'} + \underline{V}_k^{(r)'} \end{aligned} \quad (2-16)$$

The physical meaning of each term in equation (2-16) is:

$\left[\begin{array}{l} \text{Rate of Change of} \\ \text{Momentum of Dis-} \\ \text{persed Phase} \end{array} \right]$	+	$\left[\begin{array}{l} \text{Net Rate of Momen-} \\ \text{tum Flux of Disper-} \\ \text{sed Phase (Efflux-} \\ \text{Influx)} \end{array} \right]$	= -	$\left[\begin{array}{l} \text{Force Acting on} \\ \text{Dispersed Phase} \\ \text{Due to Pressure} \\ \text{Gradient} \end{array} \right]$	-
$\left[\begin{array}{l} \text{Resistance Force} \\ \text{Due to Change of} \\ \text{Volume of Disper-} \\ \text{sed Phase} \end{array} \right]$	+	$\left[\begin{array}{l} \text{Force Due to Shear} \\ \text{Stress Acting on} \\ \text{Dispersed Phase} \end{array} \right]$	+	$\left[\begin{array}{l} \text{External Field} \\ \text{Force Acting On} \\ \text{Dispersed Phase} \end{array} \right]$	+
$\left[\begin{array}{l} \text{Rate of Change of} \\ \text{Momentum Due to} \\ \text{Generation of Dis-} \\ \text{persed Phase} \end{array} \right]$	+	$\left[\begin{array}{l} \text{Inertial Coupling} \\ \text{Force Acting On Dis-} \\ \text{persed Phase Due to} \\ \text{c.g. of Dispersed} \\ \text{Phase in Relation to} \\ \text{c.g. Mixture} \end{array} \right]$	+	$\left[\begin{array}{l} \text{Viscous Coupling} \\ \text{Force Acting On} \\ \text{Dispersed Phase} \\ \text{Due to Drag} \end{array} \right]$	+
$\left[\begin{array}{l} \text{Apparent Mass} \\ \text{Effect on Inertial} \\ \text{Force of Dispersed} \\ \text{Phase} \end{array} \right]$	+	$\left[\begin{array}{l} \text{Resistance Force} \\ \text{Acting On Disper-} \\ \text{sed Phase Due to} \\ \text{Unsteadiness of Flow} \\ \text{Field} \end{array} \right]$			

$B_k^{(r)}$ is a displacement factor depending on the size of a dispersed phase (particle size) flow structure and fluid properties, and $0 < B_k^{(r)} < 1$. For the limiting cases; $B_k^{(r)} \geq 0$ for gas mixture or homogeneous multiphase fluid (very fine size of disperse phase), $B_k^{(r)} \leq 1$ for a structured multiphase fluid such as a fluid with relatively large size of bubbles or droplets.

For the continuous phase c:

$$\begin{aligned} (\partial/\partial t) \rho_c^{(r)} \underline{u}_c^{(r)} + \nabla \cdot \rho_c^{(r)} \underline{u}_c^{(r)} \underline{u}_c^{(r)} = & - (1 - \sum_k K_k^{(r)} \phi_k^{(r)}) \nabla p^{(r)} \\ & + P^{(r)} \sum_k K_k^{(r)} (1 - B_k^{(r)}) \nabla \phi_k^{(r)} + \nabla \cdot \underline{\tau}_{mc}^{(r)} + \rho_c^{(r)} \underline{f}_c^{(r)} \\ & + \sum_k K_k^{(r)} \underline{I}_a^{(r)} + \sum_k K_k^{(r)} \underline{v}_c^{(r)} - \sum_k K_k^{(r)} \underline{I}_k^{(r)'} - \sum_k K_k^{(r)} \underline{v}_k^{(r)'} \quad (2-17) \end{aligned}$$

The physical meaning of each term in equation (2-17) is

$\left[\begin{array}{l} \text{Rate of Change of} \\ \text{Momentum of Con-} \\ \text{tinuous Phase} \end{array} \right]$	+	$\left[\begin{array}{l} \text{Net Rate of Momen-} \\ \text{tum Flux of Con-} \\ \text{tinuous Phase} \\ \text{(Efflux-Influx)} \end{array} \right]$	= -	$\left[\begin{array}{l} \text{Force Acting On} \\ \text{Continuous Phase} \\ \text{Due to Pressure} \\ \text{Gradient} \end{array} \right]$	+
$\left[\begin{array}{l} \text{Reactive Force On} \\ \text{Continuous Phase} \\ \text{Due to Volumetric} \\ \text{Displacement of} \\ \text{Dispersed Phases} \end{array} \right]$	+	$\left[\begin{array}{l} \text{Force Due to Shear} \\ \text{Stress Acting On} \\ \text{Continuous Phase} \end{array} \right]$	+	$\left[\begin{array}{l} \text{External Field} \\ \text{Force Acting On} \\ \text{Continuous Phase} \end{array} \right]$	+
$\left[\begin{array}{l} \text{Rate of Change of} \\ \text{Momentum Due to} \\ \text{Generation of Con-} \\ \text{tinuous Phase} \end{array} \right]$	+	$\left[\begin{array}{l} \text{Inertial Coupling} \\ \text{Force Acting On} \\ \text{Continuous Phase} \\ \text{Due to c.g. of Con-} \\ \text{tinuous Phase in} \\ \text{Relation to c.g. of} \\ \text{Mixture} \end{array} \right]$	+	$\left[\begin{array}{l} \text{Viscous Coupling} \\ \text{Force From Dis-} \\ \text{persed Phase to} \\ \text{Continuous Phase} \end{array} \right]$	-
$\left[\begin{array}{l} \text{Apparent Mass} \\ \text{Effect on Iner-} \\ \text{tial Force of} \\ \text{Continuous} \\ \text{Phase} \end{array} \right]$	-	$\left[\begin{array}{l} \text{Resistance Force} \\ \text{Acting On Contin-} \\ \text{uous Phase Due to} \\ \text{Unsteadiness of} \\ \text{Flow Field} \end{array} \right]$			

where P is the pressure and $\phi_k^{(r)} \nabla p^{(r)}$ is the force acting on the dispersed phase k by the pressure gradient; the $(1 - B_k^{(r)}) P^{(r)} \nabla \phi_k^{(r)}$ term accounts for the

force due to volumetric displacement of phase k: $\underline{f}_k^{(r)}$ is the external force per unit mass of k in (r) and $\underline{\tau}_{mk}^{(r)}$ is the shear stress of species k in the mixture. When the inertia force is written in terms of momentum flux in Eq. (2-16) the inertial coupling is given by:

$$\underline{I}_k^{(r)} = \nabla \cdot \rho_k^{(r)} (\underline{U}_k^{(r)} - \underline{U}_m^{(r)}) (\underline{U}_k^{(r)} - \underline{U}_m^{(r)}) + \underline{U}_m^{(r)} \Gamma_k^{(r)} \quad (2-18)$$

The detailed derivation of Eq. (2-18) and the "uniqueness" of the split are presented in Appendix D. Philosophical differences in formulation between the present study and that of others is discussed in Appendix E. The values of B_k associated with $PV\phi$ term is also discussed in Appendix E.

The viscous coupling is given by [21]:

$$\begin{aligned} \underline{V}_k^{(r)} &= \rho_k^{(r)} F_{kc}^{(r)} (\underline{U}_c^{(r)} - \underline{U}_k^{(r)}) + \rho_k^{(r)} \sum_{\ell} F_{k\ell}^{(r)} (\underline{U}_{\ell}^{(r)} - \underline{U}_k^{(r)}) \\ &= \underline{V}_{kc}^{(r)} + \sum_{\ell} \underline{V}_{k\ell}^{(r)} \end{aligned} \quad (2-19)$$

where $F_{kc}^{(r)}$ is the inverse relaxation time of momentum transfer from the continuous phase to k in (r) and $F_{k\ell}^{(r)}$, for $k \neq \ell$, is the inverse relaxation time of momentum transfer from other dispersed species (other sizes and density) ℓ on species k. $\underline{V}_k^{(r)}$ accounts for the distribution of velocity in the immediate vicinity of the surface of a particle of a dispersed phase. 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 [27].

$$\underline{I}_k^{(r)'} = \frac{1}{2} \bar{\rho}_k^{(r)} \frac{\bar{\rho}_c^{(r)}}{\bar{\rho}_k^{(r)}} \frac{d}{dt_k} (\underline{U}_c^{(r)} - \underline{U}_k^{(r)}) \quad (2-20)$$

which is known only for a dilute suspension and the influence of other dispersed species ℓ is not readily inferred. The multiphase viscous coupling due to [21]. unsteadiness of the flow field is:

$$\underline{V}_k^{(r)'} = \frac{9}{2\sqrt{\pi}} \rho_k^{(r)} \frac{\sqrt{\underline{v}_c}}{a_k} \frac{\bar{\rho}_c^{(r)}}{\bar{\rho}_k^{(r)}} \int_{t_0}^t \frac{(d/d\tau) (\underline{U}_c^{(r)} - \underline{U}_k^{(r)})}{\sqrt{t - \tau}} d\tau \quad (2-21)$$

and

$$\frac{d}{dt_k} = \frac{\partial}{\partial t} + \underline{U}_k^{(r)} \cdot \nabla \quad (2-22)$$

In the formulation of the continuous phase, K_k is the effectiveness of momentum transfer from the dispersed phase to the continuous phase depending on the momentum of phases; $1 > K_k \geq 0$ for decelerating flow; $K_k = 1$ for accelerating flow [21].

Worth noting is the term $\underline{I}_k$ in Equation (2-16). $\underline{I}_k$ is the inertial coupling which relates the center-of-mass frames of the mixture and the phases [28]. $\underline{I}_k$ can be dropped for very small relative motion between the phases. All of the previous general formulations neglect $\underline{I}_k$, thus, the approximation

$$\rho_m \underline{U}_m \cdot \nabla \underline{U}_m \sim \rho_c \underline{U}_c \cdot \nabla \underline{U}_c + \sum_k \rho_k \underline{U}_k \cdot \nabla \underline{U}_k \quad (2-23)$$

cannot account for the difference between co-current and counter-current flow.

Note also the terms $\phi_k \nabla P + (1-B_k) PV\phi_k$ in Equation (2-16). It is seen that although the sum is equal to $\nabla \phi_k P$ 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 $\phi_k \nabla P$ is a force acting on a phase due to a pressure gradient and $PV\phi_k$ is the force due to volumetric displacement. The term $PV\phi_k$ has further significance in that in the energy equation (in terms of enthalpy) it leads to the term $P \partial \phi_k / \partial t$ which is the work of compression in microscopic form. For spherical particles of radius a_k and number density N_k it is given by

$$P \frac{\partial}{\partial t} \left(\frac{4\pi}{3} a_k^3 N_k \right) = P \frac{\partial \phi_k}{\partial t}$$

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

2.1.5 Energy Equation

In formulating the energy equation, the center of mass relation and the relations among internal energy, kinetic energy, static temperature, and enthalpy need to be clarified (Appendix B.3).

The basic conservation relation is based on the total energy E of an entity defined according to:

$$E = u + \frac{\underline{U} \cdot \underline{U}}{2} \quad (2-24)$$

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

$$\rho_m^{(r)} E_m^{(r)} = \rho_c^{(r)} E_c^{(r)} + \sum_k \rho_k^{(r)} E_k^{(r)} \quad (2-25)$$

Conformity with the kinetic theory of gases requires that [29]

$$\rho_m^{(r)} c_{vm}^{(r)} = \rho_c^{(r)} c_{vc}^{(r)} + \sum_k \rho_k^{(r)} c_{vk}^{(r)} \quad (2-26)$$

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

$$\rho_m^{(r)} c_{vm}^{(r)} T_m^{(r)} = \rho_c^{(r)} c_{vc}^{(r)} T_c^{(r)} + \sum_k \rho_k^{(r)} c_{vk}^{(r)} T_k^{(r)} + \frac{1}{2} [\rho_c^{(r)} \underline{U}_c^{(r)} \cdot (\underline{U}_c^{(r)} - \underline{U}_m^{(r)}) + \sum_k \rho_k^{(r)} \underline{U}_k^{(r)} \cdot (\underline{U}_k^{(r)} - \underline{U}_m^{(r)})] \quad (2-27)$$

The last term in Equation (2-27) accounts for the relative motion between the respective centers of mass. Moreover, the relaxation times are calculated also in terms of c_v . The inverse relaxation time of energy transfer (G) is consistent for both kinetic theory and multiphase calculations [29,30].

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, we can define enthalpy in terms of

$$h_k^{(r)} = u_k^{(r)} + (P^{(r)} / \rho_k^{(r)}) \quad (2-28)$$

in multiphase mechanics, which corresponds to:

$$h_k = u_k + (P / \rho_k) \quad (2-29)$$

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

$$H_k^{(r)} = h_k^{(r)} + \frac{u_k^{(r)} \cdot u_k^{(r)}}{2} \quad (2-30)$$

for both the multiphase and continuum mechanics formulations.

Direct application of the first law of thermodynamics leads to the following energy equation for the dispersed phase expressed in terms of enthalpy.*

$$(\partial / \partial t) (\rho_k^{(r)} h_k^{(r)}) + \nabla \cdot (\rho_k^{(r)} \underline{U}_k^{(r)} h_k^{(r)}) = - \nabla \cdot \underline{J}_{mk}^{(r)} + J_{Ek}^{(r)} + \phi_k^{(r)} \frac{\partial P}{\partial t} + L_{kh}^{(r)} + Q_k^{(r)} \quad (2-31)$$

The physical meaning of each term in Equation (2-31) is

* Kinetic energy of particles and work for moving these particles are part of the energy of fluid phase c.

$$\begin{aligned}
 & \left[\begin{array}{l} \text{Rate of Change of} \\ \text{Enthalpy of Dis-} \\ \text{persed Phase} \end{array} \right] + \left[\begin{array}{l} \text{Net Rate of Enthal-} \\ \text{py Flux of Dispers-} \\ \text{ed Phase (Efflux-} \\ \text{Influx)} \end{array} \right] = \left[\begin{array}{l} \text{Heat Transfer} \\ \text{Due to Conduc-} \\ \text{tion} \end{array} \right] + \left[\begin{array}{l} \text{Heat Source} \\ \text{in Dispersed} \\ \text{Phase} \end{array} \right] + \\
 & \left[\begin{array}{l} \text{Work Due to Com-} \\ \text{pression or Ex-} \\ \text{pansion by Pres-} \\ \text{sure of Disper-} \\ \text{sed Phase} \end{array} \right] + \left[\begin{array}{l} \text{Inertial Coupling} \\ \text{of Energy of Dis-} \\ \text{persed Phase k Due} \\ \text{to c.g. of Disper-} \\ \text{sed Phase in Rela-} \\ \text{tion to c.g. of} \\ \text{Mixture} \end{array} \right] + \left[\begin{array}{l} \text{Heat Transfer} \\ \text{Coupling of Dis-} \\ \text{persed Phase} \\ \text{to Continuous} \\ \text{Phase} \end{array} \right]
 \end{aligned}$$

For the dispersed phase k, only thermal terms and work done on phase k are retained because its motion is due to drag of the continuous phase c [21].

For the continuous phase c we have

$$\begin{aligned}
 & (\partial/\partial t)(\rho_c^{(r)} H_c^{(r)}) + \frac{1}{2} \sum_k \rho_k^{(r)} \underline{U}_k^{(r)} \cdot \underline{U}_k^{(r)} + \nabla \cdot [\rho_c^{(r)} \underline{U}_c^{(r)} H_c^{(r)} + \frac{1}{2} \sum_k \rho_k^{(r)} \underline{U}_k^{(r)} (\underline{U}_k^{(r)} \cdot \underline{U}_k^{(r)})] \\
 & = - \nabla \cdot \underline{J}_{mc}^{(r)} + \underline{J}_{Ec}^{(r)} + \phi_c^{(r)} \frac{\partial P}{\partial t} + \nabla \cdot \underline{U}_m^{(r)} : \underline{T}_m^{(r)} \\
 & + \sum_k \rho_k^{(r)} \underline{F}_{kc}^{(r)} (\underline{U}_c^{(r)} - \underline{U}_k^{(r)}) \cdot (\underline{U}_c^{(r)} - \underline{U}_k^{(r)}) \\
 & + \sum_k \rho_k \sum_l \underline{F}_{kl}^{(r)} (\underline{U}_l^{(r)} - \underline{U}_k^{(r)}) \cdot (\underline{U}_l^{(r)} - \underline{U}_k^{(r)}) + \rho_c^{(r)} \underline{f}_c^{(r)} \cdot \underline{U}_c^{(r)} \\
 & + \sum_k \rho_k^{(r)} \underline{f}_k^{(r)} \cdot \underline{U}_k^{(r)} + L_{cH}^{(r)} + L_c^{(r)'} + Q_c^{(r)} \\
 & \text{since } \sum_k P \frac{\partial \phi_k}{\partial t} + P \frac{\partial \phi_c}{\partial t} = 0.
 \end{aligned} \tag{2-32}*$$

The physical meaning of each term in Equation (2-23) is

$$\begin{aligned}
 & \left[\begin{array}{l} \text{Rate of Change of} \\ \text{Total Enthalpy of} \\ \text{Continuous Phase} \\ \text{Including KE of} \\ \text{Dispersed Phase} \end{array} \right] + \left[\begin{array}{l} \text{Net Rate of Total} \\ \text{Enthalpy Flux of} \\ \text{Continuous Phase} \\ \text{(Efflux-Influx)} \\ \text{Including KE of} \\ \text{Dispersed Phase} \end{array} \right] = - \left[\begin{array}{l} \text{Heat Transfer Due} \\ \text{to Conduction} \end{array} \right] + \\
 & \left[\begin{array}{l} \text{Heat Source in} \\ \text{Continuous Phase} \end{array} \right] + \left[\begin{array}{l} \text{Work Due to Dis-} \\ \text{placement of Fluid} \\ \text{Excluding Work Due} \\ \text{to Compression or} \\ \text{Expansion by Pres-} \\ \text{sure of Dispersed} \\ \text{Phase} \end{array} \right]
 \end{aligned}$$

*: Denotes scalar product of tensors
See p. 76 for the term $\partial P/\partial t$

$$\begin{aligned}
 & \left[\begin{array}{l} \text{Energy Dissipation} \\ \text{Due to Shear} \\ \text{Stress} \end{array} \right] + \left[\begin{array}{l} \text{Viscous Dissipa-} \\ \text{tion Due to Rela-} \\ \text{tive Motion of} \\ \text{Continuous Phase} \\ \text{to Dispersed Phase} \end{array} \right] + \left[\begin{array}{l} \text{Viscous Dissipa-} \\ \text{tion Due to Rela-} \\ \text{tive Motion Among} \\ \text{Dispersed Phases} \end{array} \right] + \\
 & \left[\begin{array}{l} \text{Work Done by Field} \\ \text{Force on Continu-} \\ \text{ous Phase} \end{array} \right] + \left[\begin{array}{l} \text{Work Done by Field} \\ \text{Force on Dispersed} \\ \text{Phases} \end{array} \right] + \left[\begin{array}{l} \text{Total Enthalpy} \\ \text{and K.E. Adjust-} \\ \text{ment for c.g.} \\ \text{Reference} \end{array} \right] + \\
 & \left[\begin{array}{l} \text{Work Done Due to} \\ \text{Apparent Mass and} \\ \text{Flow Field} \end{array} \right] + \left[\begin{array}{l} \text{Heat Transfer} \\ \text{Coupling} \end{array} \right]
 \end{aligned}$$

where $J_{mk}^{(r)}$ is the heat flux to species k in the mixture, J_{Ek} is the heat source in k , and $\phi_k^{(r)} \partial P / \partial t$ 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 the energy of the phases, based on enthalpy as dependent variables:

$$L_{kh}^{(r)} = \nabla \cdot [\rho_k^{(r)} (\underline{u}_k^{(r)} - \underline{u}_m^{(r)}) (h_k^{(r)} - h_m^{(r)})] + \Gamma_k^{(r)} h_m^{(r)} \quad (2-33)$$

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

$$Q_k^{(r)} = \rho_k^{(r)} c_{vk}^{(r)} G_{kc}^{(r)} (T_c^{(r)} - T_k^{(r)}) + \rho_k^{(r)} c_{vk}^{(r)} \sum_l G_{kl}^{(r)} (T_l^{(r)} - T_k^{(r)}) \quad (2-34)$$

where c_v is the specific heat at constant volume.

For the continuous phase we further have:

$$L_{ch}^{(r)} = \nabla \cdot \{ [\rho_c^{(r)} (\underline{u}_c^{(r)} - \underline{u}_m^{(r)}) (h_c^{(r)} - h_m^{(r)}) + \sum_k \rho_k^{(r)} (\underline{u}_k^{(r)} - \underline{u}_m^{(r)}) (\frac{1}{2} \underline{u}_k^{(r)} \cdot \underline{u}_k^{(r)} - \frac{1}{2} \underline{u}_m^{(r)} \cdot \underline{u}_m^{(r)})] \} - \sum_k \Gamma_k^{(r)} h_m^{(r)} \quad (2-35)$$

$$\begin{aligned}
 L_c^{(r)'} &= \sum_k \{ \frac{1}{4} \rho_k^{(r)} \frac{\rho_c}{\rho_k} \frac{d}{dt_k} [(\underline{u}_c^{(r)} - \underline{u}_k^{(r)}) \cdot (\underline{u}_c^{(r)} - \underline{u}_k^{(r)})] + (\underline{u}_c^{(r)} - \underline{u}_k^{(r)}) \\
 &\cdot \underline{v}_k^{(r)'} \} \quad (2-36)
 \end{aligned}$$

$$Q_c^{(r)} = \sum_k \rho_k^{(r)} c_{vk}^{(r)} G_{kc}^{(r)} (T_k^{(r)} - T_c^{(r)}) \quad (2-37)$$

where G_{kc} is the inverse relaxation time for energy transfer from continuous phase to 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

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

2.2 Consistent Approximation

It is readily seen (Appendix F) that, when applied to a one-dimensional transient flow, the problem is always well-posed (real characteristics) when I_k , $\phi_k \nabla P$, and $P \nabla \phi_k$ 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 [1] appears to be due to the inconsistent approximation of neglecting I_k but retaining $\phi_k \nabla P$. Neglecting the latter always renders the problem well-posed. Such an approximation is also supported by the interaction of $\phi_k \nabla P$ with $\underline{V}_k$ in the case of a dilute suspension [31,32]. However, without the term $(1 - B_k) P \nabla \phi_k$ 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 ϕ) of small particles ($\underline{U}_k \sim \underline{U}_c$), both $\phi \nabla P$ and I can be dropped to maintain consistent approximations.

Table 1 is a summary of multiphase mechanics as compared to continuum mechanics.

Table 1
Comparison of Multiphase Mechanics
and Continuum Mechanics

	<u>MULTIPHASE</u>	<u>CONTINUUM</u>
Momentum Equation		
Coupling Terms (Coordinate Transformation)	I, V	I, V
Coupling Terms (Phase Exclusion)	I', V'	None
Force Due to Pressure Gradient	$\phi \nabla P$	$\nabla(\phi P)$
Net force due to volumetric displacement	$(1 - B) P \nabla \phi$	None
Energy Equation (in Enthalpy)*		
Work Due to Displacement of bulk	$P \frac{\partial \phi}{\partial t} **$	$\frac{\partial(\phi P)}{\partial t}$
Work Due to Volumetric Displacement of Phases (including Symmetric Displacement)	$\phi \frac{\partial P}{\partial t} *$	None
Flow Energy	In Continuous Phase Only	Distributed

*Refer to Table B-2 for equation in terms of energy.

**The term $\phi \partial P / \partial t$ in Eq. (2-32) is the work contributed to the continuous phase. This includes the flow work because the expression is in terms of enthalpy.

2.3 Interfacial Relations Between Two Adjacent Domains

We shall follow the simplified treatment of interfacial relations as outlined by Ishii [6]. The layer which divides the domains is assumed to be a geometric surface of negligible thickness for the interfacial jump to take place. The mass density of the interface is neglected so that its momentum and mechanical energy can also be neglected. All of the molecular diffusion fluxes within the surface are neglected, i.e., no surface viscous stress or surface heat flux exists. The surface sources are neglected, i.e., no particular body force other than that of gravity, and no radiation effect is accounted for.

The challenging nature of the formulation of the interface is in that the relations have to refer to the coordinate system constituting the interface $S(\underline{r}, t)$, $\underline{r}$ being the space coordinate, while S remains to be determined from the overall calculations. For our formulation, the symbolism and derivation of Ishii [6] and Aris [33] will be followed up to the point where we shall apply the theory to specific examples for computation.

2.3.1 Interfacial Mass Conservation

The interfacial mass conservation equation is given in the form:

$$\sum_{(r)=1}^2 [\rho_c^{(r)} \underline{n}^{(r)} (\underline{U}_c^{(r)} - \underline{U}_s) + \sum_k \rho_k^{(r)} \underline{n}^{(r)} (\underline{U}_k^{(r)} - \underline{U}_s)] = \sum_{(r)=1}^2 [\dot{m}_c^{(r)} + \sum_k \dot{m}_k^{(r)}] = 0 \quad (2-38)$$

and has the meaning:

$$\left\{ \left[\begin{array}{l} \text{Sum of Mass Fluxes of} \\ \text{Continuous Phase En-} \\ \text{tering from Both Sides} \\ \text{of the Interface} \end{array} \right] + \left[\begin{array}{l} \text{Sum of Mass Fluxes of} \\ \text{Dispersed Phases En-} \\ \text{tering from Both Sides} \\ \text{of the Interface} \end{array} \right] \right\} \text{Sum Over Both Sides} \\ \text{of the Interface} = 0$$

where $\underline{n}^{(r)}$ is the outward unit normal vector for domain (r) from the interface, and $\underline{U}_s = dS/dt$ is the velocity of the interface.

It is to be noted that Equation (2-38) assumes explicitly no net mass generation at the interface.

2.3.2 Interfacial Momentum Conservation

The interfacial momentum equation is given by a balance between the momentum fluxes from the bulk fluids and the interfacial tension. The expression of Ishii [6] is given in terms of the transfer between mixtures in the domain on the two sides of the interface:

$$\sum_{(r)=1}^2 \{ \rho_c^{(r)} \underline{n}^{(r)} \cdot (\underline{U}_c^{(r)} - \underline{U}_s) \underline{U}_c^{(r)} + \sum_k \rho_k^{(r)} \underline{n}^{(r)} \cdot (\underline{U}_k^{(r)} - \underline{U}_s) \underline{U}_k^{(r)} - \underline{n}^{(r)} \cdot (-P^{(r)} \underline{I} + \underline{\tau}_m^{(r)}) \} + (\underline{t}_\alpha a^{\alpha\beta} \sigma)_{,\beta} = 0 \quad (2-39)$$

and has the meaning:

$$\left\{ \begin{array}{l} \text{Rate of Change of} \\ \text{Momentum Fluxes} \\ \text{of Continuous} \\ \text{Phases} \end{array} \right\} + \left\{ \begin{array}{l} \text{Rate of Change of} \\ \text{Momentum Fluxes} \\ \text{of All Dispersed} \\ \text{Phases} \end{array} \right\} - \left\{ \begin{array}{l} \text{Forces Due to} \\ \text{Stresses} \end{array} \right\} \quad \text{Sum Over Both Sides} \\ \text{of the Interface} \\ + \left\{ \begin{array}{l} \text{Forces Due to Sur-} \\ \text{face Tensions} \end{array} \right\} = 0$$

where $P^{(r)}$ is the fluid pressure, $\underline{I}$ is the unit tensor, $\underline{\tau}_m^{(r)}$ is the viscous stress tensor, $\sigma = \sigma(T_s)$ is a surface tension, $\underline{t}_\alpha$ is the hybrid tensor between the space and the surface coordinates [33], $a^{\alpha\beta}$ is the metric tensor of the interface, and $(\)_{,\beta}$ is the surface covariant derivative. The no slip condition [6] is applicable to the continuous phases on both sides of the interface, but not to the dispersed phases as

$$\underline{U}_s = \underline{U}_c^{(r)} = \underline{U}_c^{(s)} \quad (2-40)$$

Note that $\underline{U}_k^{(r)}$ is limited by this condition, as a bubble may rise through a liquid interface and subsequently merges into the vapor phase.

2.3.3 Interfacial Energy Conservation

The interfacial energy equation presented below follows the derivation given by Ishii:

$$\begin{aligned} \frac{du_s}{dt_s} + u_s \nabla_s \cdot \underline{U}_s &= (\underline{t}_\alpha a^{\alpha\beta} \sigma \cdot \underline{U}_s)_{,\beta} \\ + \sum_{(r)=1}^2 \{ \dot{m}_c^{(r)} (u_c^{(r)} + \frac{u_c^{(r)} \underline{U}_c^{(r)}}{2}) + \sum_k \dot{m}_k^{(r)} (u_k^{(r)} + \frac{u_k^{(r)} \underline{U}_k^{(r)}}{2}) \} \\ + \underline{n}^{(r)} \cdot [(-P^{(r)} \underline{I} + \underline{\tau}_m^{(r)}) \cdot \underline{U}_m] + \underline{n}^{(r)} \cdot \underline{J}_m \} \end{aligned} \quad (2-41)$$

and has the meaning:

$$\left[\begin{array}{c} \text{Rate of Change of} \\ \text{Surface Energy} \end{array} \right] + \left[\begin{array}{c} \text{Rate of Change of} \\ \text{Energy Due to Sur-} \\ \text{face Dilatation} \end{array} \right] = \left[\begin{array}{c} \text{Work Done by} \\ \text{Surface Tension} \end{array} \right] +$$

$$\left\{ \begin{array}{c} \left[\begin{array}{c} \text{Flux of Energy} \\ \text{of Continuous} \\ \text{Fluid} \end{array} \right] \\ \left[\begin{array}{c} \text{Heat Flux} \end{array} \right] \end{array} \right\} + \left[\begin{array}{c} \text{Fluxes of Energy} \\ \text{of Dispersed} \\ \text{Phases} \end{array} \right] + \left[\begin{array}{c} \text{Work Done by} \\ \text{Stress} \end{array} \right] +$$

Sum Over Both Sides of the Interface

where the interface or surface energy per unit volume is given by:

$$u_s = T_s \left(\frac{d\sigma}{dT_s} \right) + \sigma \quad (2-42)$$

and d/dt_s is the surface convective derivative, and ∇_s is the surface divergence operator.

2.3.4 Interfacial Boundary

Thermal equilibrium, no slip condition and balance between the chemical potential and the sum of the relative kinetic energy difference and the normal stresses due to phase change are employed as interdomain boundary conditions. The data on mass flux, momentum transfer, heat flux, bubble burst to droplets, droplet capture and coalescence at the interdomain boundary are needed.

2.4 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. The typical boundary conditions encountered in the reactor problems of interest are listed below.

2.4.1 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.

2.4.2 Non-heated Wall

Temperature or temperature gradient; normal and tangential velocity components, slip or non-slip.

2.4.3 In-flow Boundary

Inlet temperature; normal component of velocity (inlet velocity) and tangential velocity components or inlet pressure.

2.4.4 Out-flow Boundary

Temperature gradient; normal component of velocity gradient and tangential velocity components or outlet pressure.

2.5 Deterministic Nature of the Problem

To summarize, we can identify the following unknowns to be determined for d separate domains each with k dispersed phases characterized by the following equations:

<u>Dependent Variables</u>	<u>No. of Unknowns</u> *	<u>No. of Equations</u> *	
ρ_c, ρ_k	$(k + 1)d$	Continuity	$(k + 1)d$
$\underline{U}_c, \underline{U}_k$	$3(k + 1)d$	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	$d-1$		
$\underline{S}(r,t)$	$3(d - 1)$	Interface	$5(d-1)$
T_s	$d-1$		

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.

2.6 Deficiency of Data

In theory, one might even think of this as a matter of computer power. We, however, should note our lack of detailed information on the following items (references indicate limited source):

- Virtual mass effect of a dense suspension
- Unsteadiness of flow field in a dense suspension,
- Agglomeration rates or probability of bubbles or droplets [34],
- Shattering rates or probability of bubbles or droplets [21,35],
- Surface tension of a liquid-vapor interface with vapor bubbles [36],
- Bubble burst, and formation rates of bubbles and droplets [37],

* $k \geq 1$ and $d \geq 1$

Coefficients of surface dilational viscosity and surface shear viscosity [20],

Effect of bursting of bubbles and merging of droplets at interface [18,37],

Transport properties of phases in a dense suspension [21],

Diffusivity of dispersed phase in a continuous phase [38],

Nucleation at the boundary in bulk fluid, bubble number, size, and detachment velocity [23,24].

It appears that, until detailed information in the above items become available, it would be more productive to formulate a realistic approximation consistent with the accuracy of the available data.

2.7 Transition From a Phase To a Domain

It is important to reiterate the nature of a phase in a multiphase mixture and its transition to become a new domain.

The field equations of a multiphase mixture are applicable to a volume element of the fluid which, on the time averaging, includes a number ($\gg 1$) of particles of the dispersed phase k , that is, the volume element V under consideration is much larger than the volume of a single particle in the dispersed phase. The time average is taken over a duration τ much greater than the interparticle spacing ($N^{-1/3}$) divided by the characteristic flow velocity U_k^* , or $\tau \gg N^{-1/3}/U_k^*$. The density of phase k is therefore

$$\begin{aligned}\rho_k &= \frac{1}{\tau} \int \left[\frac{1}{V} \int_V N_k^0 m_k dV \right] dt \\ &= \frac{1}{\tau} \int \rho_k' dV\end{aligned}\tag{2.43}$$

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 Eq. (2.43). Transition from the species 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,

$$(N_k^0/V) x_o^3 \gtrsim 1$$

or

$$a_k^3 \gtrsim (3/4\pi)\phi_k x_o^3$$

In this way, a_k becomes radius R of a new spherical domain which evolves, with

$$(4\pi/3)R^3 \bar{\rho}_k = \int_0^R \sum_k \rho_k 4\pi r^2 dr$$

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

3.0 Two-Domain, Two-Phase Flow System

In order to treat the two-phase flow system relevant to the problem under consideration we introduce the idealization of two-phase flow system as shown in Fig. 2, with an approximation of one species of dispersed phase at a given location and time. The reason to limit ourselves in this manner is that we can get started without waiting for the complete knowledge on transport properties and interacting parameters for a full-fledged multiphase flow treatment. It is believed that such an approach can already account for a range of two-phase flow regimes as shown in Figs. 3 and 4 comparable to those identified in [5] and [1], for instance, including the flow regime maps of Bennet, Baker and Govier [1].

In Fig. 2, we denote the continuous phases ll (2), vv (4) for liquid and vapor respectively, vl (1) thus denotes bubbles in liquid, while lv (3) denotes droplets in vapor. Any dissolved inert gas may be denoted as il and iv , which we shall leave out at this stage although its inclusion is straightforward. We shall also limit ourselves to vertical passages. The aim of this formulation will be toward the prediction of flow regimes and their transition with the idealizations rendered realistic via the introduction of proper transport parameters. The possible routes of computations are outlined in Table 2.

Because of the difference in the formulations of a bubble (phase 1) suspension in liquid (phase 2) and those of a droplet (phase 3) suspension in vapor (phase 4), the equations of each phase in the two domains will be given. Moreover, to facilitate computer programming, equations will be written in tensor components in this chapter.

3.1 General Description of a Two-Phase Domain with Non-Equilibrium Velocities and Temperatures

The dynamics of a two-phase single component mixture are defined according to the following (we use the bubble-liquid domain for our illustration):

- (1) A mean density ρ_m given by $\rho_m = \rho_1 + \rho_2$ where ρ_1 and ρ_2 are the densities of phases 1 and 2, each of which relates to the densities of materials constituting each phase $\bar{\rho}$ according to volume fraction ϕ , or $\rho_1 = \phi_1 \bar{\rho}_1$, $\rho_2 = \phi_2 \bar{\rho}_2$, $\phi_1 + \phi_2 = 1$.
- (2) A mean velocity U_{mj} given by $\rho_m U_{mj} = \rho_1 U_{1j} + \rho_2 U_{2j}$ where U_{1j} and U_{2j} are mass velocities of each phase of space component j .

ll = LIQUID IN LIQUID lv = DROPLET IN VAPOR
 vl = VAPOR IN LIQUID vv = VAPOR IN VAPOR

Fig. 2 General Two-Phase Flow System

Fig. 3 Idealized Flow Regimes

Fig. 4 Simplified Two-Domain Two-Phase Flow System

Table 2
Transition of Flow Regimes

- (3) A mean energy E_m per unit mass such that $\rho_m E_m = \rho_1 E_1 + \rho_2 E_2$, with $E = u + (U_j^2/2)$, u being the internal energy. Enthalpy is defined as $h_1 = u_1 + P/\rho_1$, P being the pressure of the domain. Modification for surface tension can be readily accounted for.
- (4) A mean specific heat at constant volume c_{vm} given by $\rho_m c_{vm} = \rho_1 c_{v1} + \rho_2 c_{v2}$.
- (5) The mean static temperature T_m is not independent after items (3) and (4) are defined, or $\rho_m c_{vm} T_m = \rho_1 c_{v1} T_1 + \rho_2 c_{v2} T_2 + \frac{1}{2} \frac{\rho_1 \rho_2}{(\rho_1 + \rho_2)} (U_{1j} - U_{2j})^2$. The last term accounts for the relative motion and amounts to a kinetic energy per unit volume of a reduced mass due to relative motion. T_1 and T_2 so defined are the actual static temperatures of the phases.

When the above definitions are applied to the continuity, momentum, and energy equations of multiphase mechanics based on the center of mass of the mixture [21], these equations can be expressed in terms of the center of mass of each phase.

3.1.1 Mass Balance Equations

Following the definition in Fig. 2, the continuity equations within the boundary of each domain are;

For the domain of liquid continuum (2) with dispersed bubbles (1),

$$\frac{\partial \rho_1}{\partial t} + \frac{\partial \rho_1 U_{1j}}{\partial x_j} = \Gamma \quad (3.1)$$

$$\frac{\partial \rho_2}{\partial t} + \frac{\partial \rho_2 U_{2j}}{\partial x_j} = -\Gamma \quad (3.2)$$

For the domain of vapor continuum (4) with dispersed droplets (3),

$$\frac{\partial \rho_3}{\partial t} + \frac{\partial \rho_3 U_{3j}}{\partial x_j} = -\Gamma' \quad (3.3)$$

$$\frac{\partial \rho_4}{\partial t} + \frac{\partial \rho_4 U_{4j}}{\partial x_j} = \Gamma' \quad (3.4)$$

where ρ 's denote the density of a phase in a mixture, x_j is the space coordinate, U_j is the conjugate velocity component, Γ is the evaporation rate in the liquid continuum, and Γ' is the evaporation rate in the vapor continuum.

The number density N , size (radius a), and material densities $\bar{\rho}$'s of dispersed phase are related according to:

$$\rho_1 = N_1 \frac{4\pi}{3} a_1^3 \bar{\rho}_1 \quad (3.5)$$

and

$$\rho_3 = N_3 \frac{4\pi}{3} a_3^3 \bar{\rho}_3 \quad (3.6)$$

while the continuum phases are

$$\rho_2 = (1 - N_1 \frac{4\pi}{3} a_1^3) \bar{\rho}_2 \quad (3.7)$$

and

$$\rho_4 = (1 - N_3 \frac{4\pi}{3} a_3^3) \bar{\rho}_4 \quad (3.8)$$

Hence all variations of number densities N_1 , N_3 , and sizes at given (x_j, t) are readily accounted for. Transition between domains ll (2) and vv (4) are accounted for by proper boundary conditions.

The usefulness of Eq. (3.5) can be seen from the change of ρ_1 as follows:

$$d\rho_1 = \frac{4\pi}{3} a_1^3 \bar{\rho}_1 dN_1 + 4\pi N_1 \bar{\rho}_1 a_1^2 da_1 + \frac{4\pi}{3} N_1 a_1^3 d\bar{\rho}_1 \quad (3.9)$$

The first term on the right hand side of Eq. (3.9) can account for addition (or subtraction) of number of bubbles; the first and second terms combined can account for breakup or coalescence; the second and the third terms combined can account for bubble growth or collapse. Starting from a reference state for a liquid with increasing number of bubbles, growth and coalescence will lead to a condition of a slug. The slug to be identified as a new domain leading to annular and droplet spray flow of vapor (Fig. 3). The limitation for handling these transitions will be the knowledge of transport properties, coalescence models, phase interactions, and bubble nucleation on heated wall boundary or in the liquid.

3.1.2 Momentum Balance Equations

For the present discussion, the mixture is taken to be Newtonian with viscosity μ_m , bulk viscosity ζ_m , and $\mu_m^* = \zeta_m - (2/3) \mu_m$. We further identify static pressure P , i -th component of field force f_{mi} per unit mass. Additional relations obtained by expressing these basic equations in terms of the center of mass motion of each phase are outlined in the following items with space coordinate x_j and time t . Again, we use the domain consisting of phases 1, 2 for illustration.

- (a) The stress due to viscosity of phase 1 fluid in the mixture μ_{m1} is given by

$$\mu_{m1} \Delta_{1ji} = \mu_m \frac{\rho_1}{\rho_1 + \rho_2} \Delta_{1ji} + \mu_m \frac{\rho_2}{(\rho_1 + \rho_2)^2} \left[(U_{1i} - U_{2i}) \frac{\partial \rho_1}{\partial x_j} + (U_{1j} - U_{2j}) \frac{\partial \rho_1}{\partial x_i} \right] \quad (3.10)$$

where $\Delta_{ji} = (\partial U_i / \partial x_j) + (\partial U_j / \partial x_i)$ is the deformation tensor and the dilatation is given by $\Theta = (1/2) \Delta_{jj}$. Note that the last term of Eq. (3.10) arises from the motion about the center of mass of phase 1 for shear stress defined according to the motion about the center of mass of the mixture. μ_{m1} so defined includes the adjustment to the motion referring to the center of mass of phase 1 in the mixture. In addition, we have

$$\mu_{m1}^* \Theta_1 = \mu_m^* \frac{\rho_1}{\rho_1 + \rho_2} \Theta_1 + \mu_m^* \frac{\rho_2}{(\rho_1 + \rho_2)^2} (U_{1j} - U_{2j}) \frac{\partial \rho_1}{\partial x_j} \quad (3.11)$$

In the case of a dilute suspension, $\mu_{m1} \sim \rho_1 D_1$ and $\mu_{m2} \sim \bar{\mu}_2$ are applicable where $\rho_1 D_1$ is defined as viscous coefficient and $\bar{\mu}_2$ is the viscosity of pure phase 2. (See Appendix G).

- (b) The viscous coupling (V) is as before [21]:

$$V_{12i} = \rho_1 F_{12} (U_{2i} - U_{1i}) = -V_{21i} \quad (3.12)$$

with

$$\rho_1 F_{12} = \rho_2 F_{21} \quad (3.13)$$

where F_{12} is the inverse relaxation time for momentum transfer to phase 1 from phase 2. The existence of these terms is also assured by consideration of molecular systems [30].

- (c) The inertial coupling I of the momenta of the phases is given by

$$I_{12i} = \frac{\partial}{\partial x_j} \left[\frac{\rho_2^2 \rho_1}{(\rho_1 + \rho_2)^2} (U_{2i} - U_{1i})(U_{2j} - U_{1j}) \right] + \Gamma U_{m1} \quad (3.14)$$

where the first term accounts for the inertial effect due to relative motion and the second term accounts for the fact that when phase 1 is generated, it was at the velocity of phase 2 from which it is converted. Γ is the rate of generation of phase 1 in mass per unit volume per unit time. The derivation for I_{12i} is given in Appendix D.

- (d) The feature of multiphase mechanics most distinctly different from continuum mechanics is that the phases in the heterogeneous configuration occupying the same space are mutually exclusive. Moreover, the velocity of mass motion of the continuous phase does not include velocity distributions around the dispersed phases or bubbles, and the velocity of mass motion of the dispersed phase does not include velocity distribution within each dispersed phase or bubble. The same applies to the temperature distributions. These distinctions are accounted for by the introduction of pertinent transport properties.

The virtual mass term of Basset I'_{12i} [27] is based on potential flow around the sphere in addition to the adjustment of inertial frame of reference by I_{12i} , and V'_{12i} is an additional viscous coupling due to an unsteady flow field [21]:

$$I'_{12i} = \frac{1}{2} \rho_1 \frac{\bar{\rho}_2}{\rho_1} \frac{d}{dt_1} (U_{2i} - U_{1i}) = - I'_{21i} \quad (3.15)$$

$$V'_{12i} = \frac{9}{2\sqrt{\pi}} \rho_1 \frac{\sqrt{\bar{v}_2} \bar{\rho}_2}{a_k \bar{\rho}_1} \int_{t_0}^t \frac{(d/d\tau_1)(U_{2i} - U_{1i})}{\sqrt{t - \tau}} d\tau = - V'_{21i} \quad (3.16)$$

The latter accounts for only relative motion in the viscous range and $\bar{v}_2$ is the kinematic viscosity of phase 2. The last equalities in Eqs. (3.15) and (3.16) account for the action and reaction. Actual transmission to phase 2 is affected by the dissipation of momentum in the wake of the dispersed phase. Note that the total time derivatives in Eqs. (3.15) and (3.16) are based on the motion of phase 1 because these forces exist only where the dispersed phases are present.

We now have for phase 1 of this mixture, momentum equation in the form:

$$\frac{\partial}{\partial t} (\rho_1 U_{1i}) + \frac{\partial}{\partial x_j} (\rho_1 U_{1j} U_{1i}) = - \phi_1 \frac{\partial P}{\partial x_i} - P(1 - B) \frac{\partial \phi_1}{\partial x_i} + \frac{\partial}{\partial x_j} [\mu_{ml} \Delta_{1ji} + \mu_{ml}^* \Theta_1 \delta_{ji}] + \rho_1 f_{1i} + I_{12i} + V_{12i} + I'_{12i} + V'_{12i} \quad (3.17)$$

where f_{1i} is the field force per unit mass of phase 1, $\delta_{ji} = 0$ for $j \neq i$, and $\delta_{ji} = 1$ for $i = j$. The loss of momentum due to dissipation in the wakes of the dispersed phase is accounted for via the effectiveness of dispersed phase to continuous phase momentum transfer K ; $K = 1$ for accelerating flow and $0 < K \leq 1$ for a decelerating flow [21]; $0 \lesssim B \lesssim 1$ depending on the flow range. (Appendix E).

The momentum equation of phase 2 is now given by

$$\begin{aligned} \frac{\partial}{\partial t} (\rho_2 U_{2i}) + \frac{\partial}{\partial x_j} (\rho_2 U_{2j} U_{2i}) = & - (1 - K\phi_1) \frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j} [\mu_{m2} \Delta_{2ji} + \mu_{m2}^* \theta_2 \delta_{ji}] \\ & + K [I_{21i} + V_{21i} + I'_{21i} + V'_{21i} + P(1 - B) \frac{\partial \phi_1}{\partial x_i}] + \rho_2 f_{2i} \end{aligned} \quad (3.18)$$

Note that for $K = 1$, the sum of Eq. (3.17) and Eq. (3.18) reverts the momentum equation of a continuum mixture.

The sum of Eqs. (3.17) and (3.18) is the overall momentum equation for domain 1-2:

$$\begin{aligned} \frac{\partial}{\partial t} (K \rho_1 U_{1i} + \rho_2 U_{2i}) + \frac{\partial}{\partial x_j} (K \rho_1 U_{1j} U_{1i} + \rho_2 U_{2j} U_{2i}) = & - \frac{\partial P}{\partial x_i} + \\ \frac{\partial}{\partial x_j} [(\mu_{m2} \Delta_{2ji} + \mu_{m2}^* \theta_2 \delta_{ji}) + K (\mu_{m1} \Delta_{1ji} + \mu_{m1}^* \theta_1 \delta_{ji})] + & K (I_{12i} + I_{21i}) + \\ K \rho_1 f_{1i} + \rho_2 f_{2i} \end{aligned} \quad (3.19)$$

where

$$I'_{12i} + I'_{21i} = 0$$

and

$$I_{12i} + I_{21i} = \frac{\partial}{\partial x_j} \left[\frac{\rho_1 \rho_2}{\rho_1 + \rho_2} (U_{2i} - U_{1i})(U_{2j} - U_{1j}) \right] \quad (3.20)$$

The sum as shown in Eq. (3.20) is negligible only if $U_{1j} \simeq U_{2j}$; it accounts for the effect of motion about the center of mass of the mixture. Note that the work done by I'_{12} and V'_{12} constitutes additional dissipation of energy.

For the phases in the domains and in terms of mass and momentum fluxes, the momentum equations for domain 1-2 are given above in Eqs. (3.17) and (3.18), and their sums given in Eq. (3.19). For domains 3-4 we have momentum equations as follows:

$$\frac{\partial \rho_3 U_{3i}}{\partial t} + \frac{\partial \rho_3 U_{3i} U_{3j}}{\partial x_j} = - P' (1 - B') \frac{\partial \phi_3}{\partial x_i} - \phi_3 \frac{\partial P'}{\partial x_i} + \frac{\partial}{\partial x_j} [\mu_{m3} \Delta_{3ji} + \mu_{m3}^* \theta_3 \delta_{ji}]$$

$$+ \frac{\partial}{\partial x_j} \left[\frac{\rho_4^2 \rho_3}{(\rho_4 + \rho_3)^2} (U_{4i} - U_{3i})(U_{4j} - U_{3j}) \right] - \frac{\rho_3 U_{3i} + \rho_4 U_{4i}}{\rho_3 + \rho_4} \Gamma' + \rho_3 F_{34} \\ (U_{4i} - U_{3i}) + \rho_3 f_{3i} \quad (3.21)$$

$$\frac{\partial \rho_4 U_{4i}}{\partial t} + \frac{\partial \rho_4 U_{4i} U_{4j}}{\partial x_j} = - (1 - K\phi_3) \frac{\partial P'}{\partial x_i} + K'P' (1 - B') \frac{\partial \phi_3}{\partial x_i} + \frac{\partial}{\partial x_j} [\mu_{m4} \Delta_{4ji} + \\ \mu_{m4}^* \Theta_4 \delta_{ji}] + K' \frac{\partial}{\partial x_j} \left[\frac{\rho_4 \rho_3^2}{(\rho_4 + \rho_3)^2} (U_{4i} - U_{3i})(U_{4j} - U_{3j}) \right] + K' \frac{\rho_3 U_{3i} + \rho_4 U_{4i}}{\rho_3 + \rho_4} \Gamma' \\ - K'\rho_3 F_{34} (U_{4i} - U_{3i}) + \rho_4 f_{4i} \quad (3.22)$$

The multiphase inertial and viscous coupling terms are negligible for most of the droplet suspensions because $\bar{\rho}_3 \gg \bar{\rho}_4$.

The sum of mass and momenta fluxes in domain 3-4 is now:

$$\frac{\partial (K'\rho_{3i} U_{3i} + \rho_{4i} U_{4i})}{\partial t} + \frac{\partial}{\partial x_j} (K'\rho_3 U_{3i} U_{3j} + \rho_4 U_{4i} U_{4j}) = - \frac{\partial P'}{\partial x_i} + \frac{\partial}{\partial x_j} \\ [K' (\mu_{m3} \Delta_{3ki} + \mu_{m3}^* \Theta_3 \delta_{ji}) + (\mu_{m4} \Delta_{4ji} + \mu_{m4}^* \Theta_4 \delta_{ji})] + K' \frac{\partial}{\partial x_j} \left[\frac{\rho_3 \rho_4}{\rho_3 + \rho_4} (U_{4i} - U_{3i}) \right. \\ \left. (U_{4j} - U_{3j}) \right] + K'\rho_3 f_{3i} + \rho_4 f_{4i} \quad (3.23)$$

Simplifications to treat dilute phases are readily made with $\rho_4 \gg \rho_3$ and $\phi_3 \frac{\partial P'}{\partial x_i} \sim 0$.

It is seen that while the viscous coupling can readily be handled for comparable values of ρ_1 and ρ_2 [9,21], the inertial coupling is not known for a dense suspension since Eq. (3.15) was derived for a single bubble or particle. A strict definition for a dilute suspension is the range where interaction between the dispersed phases is negligible compared to dispersed phase - continuous phase interaction [32].

3.1.3 Energy Balance Equations

Again, the mixture is taken to be Newtonian with thermal conductivity κ_m . J_{Em} is defined as energy source per unit volume. Additional relations obtained from expressing these basic equations in terms of the center of

mass motion of each phase are outlined in the following items with space coordinate x_j and time t . The same domain consisting of phases 1 and 2 is used here for illustration.

(a) The conduction heat flux is given for phase 1 as

$$\kappa_{m1} \frac{\partial T_1}{\partial x_j} = \kappa_m \frac{\partial}{\partial x_j} \left[\frac{c_{v1} \rho_1}{c_{vm} \rho_m} T_1 \right] + \kappa_m \frac{\partial}{\partial x_j} \left[\frac{\rho_1 \rho_2 U_{1j} (U_{1j} - U_{2j})}{c_{vm} (\rho_1 + \rho_2)^2} \right] \quad (3.24)$$

where κ_{m1} is the thermal conductivity of phase 1 in the mixture. The last term again adjusts for reference to the center of mass of phase 1.

(b) The thermal coupling (Q) is [21]:

$$Q_{12} = c_{v1} \rho_1 G_{12} (T_2 - T_1) = -Q_{21} \quad (3.25)$$

$$c_{v1} \rho_1 G_{12} = c_{v2} \rho_2 G_{21} \quad (3.26)$$

Where G_{12} is the inverse relaxation time for energy transfer to Phase 1 from Phase 2.

(c) The inertial coupling effect on the coupling of energy of phases is given by:

$$L_{12E} = \frac{\partial}{\partial x_j} \left[\frac{\rho_1 \rho_2^2}{(\rho_1 + \rho_2)^2} (U_{2j} - U_{1j}) (E_2 - E_1) \right] + \frac{\rho_1 E_1 + \rho_2 E_2}{\rho_1 + \rho_2} \Gamma \quad (3.27)$$

which includes work done by the inertial force, the energy transported by the relative motion, and the energy of the species generated.

$$L_{12E} + L_{21E} = \frac{\partial}{\partial x_j} \left[\frac{\rho_1 \rho_2}{\rho_1 + \rho_2} (U_{2j} - U_{1j}) (E_2 - E_1) \right] \quad (3.28)$$

These sums are negligible only if $U_1 \simeq U_2$ and $E_1 \simeq E_2$.

(d) The work done by I'_{12} and V'_{12} constitutes additional conversion of energy. Corresponding effects on the change of energy per unit volume via work performed by these forces is given by:

$$L'_{E1} = \frac{1}{4} \rho_1 \frac{\bar{\rho}_2}{\rho_1} \frac{d}{dt_1} [(U_{2j} - U_{1j})^2] + (U_{2j} - U_{1j}) v'_{12j} \quad (3.29)$$

giving the change in kinetic energy of relative motion induced by the void produced by the motion of dispersed phase and the rate of doing work by the unsteady flow field.

In terms of energy, the thermal state of each moving droplet or bubble is identified by its body temperature and the velocity of the dispersed phase is sustained by the drag force of the fluid phase 1. The energy equation of the dispersed phase is given by terms pertaining only to the body temperature (internal energy) or

$$\frac{\partial}{\partial t} \rho_1 u_1 + \frac{\partial}{\partial x_j} \rho_1 U_{1j} u_1 = \frac{\partial}{\partial x_j} [\kappa_{m1} \frac{\partial T_1}{\partial x_j}] + Q_{12} + L_{12u} + J_{E1} - U_{mj} P \frac{\partial \phi_1}{\partial x_j} \quad (3.30)$$

where J_{E1} is the heat source per unit volume of the suspension such as radiation input; L_{12u} consists of terms in Eq. (3.30) containing internal energy u_1 or

$$L_{12u} = \frac{\partial}{\partial x_j} \left\{ \frac{\rho_1 \rho_2^2}{(\rho_1 + \rho_2)^2} (U_{2j} - U_{1j})(u_2 - u_1) \right\} + \frac{\rho_1 u_1 + \rho_2 u_2}{\rho_1 + \rho_2} \Gamma \quad (3.31)$$

and

$$U_{mj} P \frac{\partial \phi_1}{\partial x_j} \equiv W_{12} \quad (3.32)$$

is the work done by phase 2 on phase 1 at the phase boundary such as bubble expansion or compression. The energy equation of phase 2 of the suspension is given by subtracting Eq. (3.30) from the overall energy equation to give:

$$\begin{aligned} \frac{\partial}{\partial t} (\rho_2 E_2 + \rho_1 \frac{U_{1j}^2}{2}) + \frac{\partial}{\partial x_j} (\rho_2 U_{2j} E_2 + \rho_1 U_{1j} \frac{U_{1j}^2}{2}) = - \frac{\partial}{\partial x_j} (U_{mj} P) + \\ U_{1j} P \frac{\partial \phi_1}{\partial x_j} + \frac{\partial}{\partial x_j} [U_{mj} (\mu_{m2} \Delta_{2ji} + \mu_{m2}^* \Theta_2 \delta_{ji} + \mu_{m1} \Delta_{1ji} + \mu_{m1}^* \Theta_1 \delta_{ji})] + \frac{\partial}{\partial x_j} [\kappa_{m2} \\ \frac{\partial T_2}{\partial x_j}] + L_{21E} + L'_E + \rho_1 F_{12} (U_{2j} - U_{1j})^2 + \rho_1 U_{1j} f_{1j} + \rho_2 U_{2j} f_{2j} + J_{E2} \end{aligned} \quad (3.33)$$

where

$$\begin{aligned} L_{21E} = \frac{\partial}{\partial x_j} \left[\frac{\rho_1^2 \rho_2}{(\rho_1 + \rho_2)^2} (U_{1j} - U_{2j})(E_1 - E_2) + \frac{\rho_1 \rho_2^2}{(\rho_1 + \rho_2)^2} (U_{2j} - U_{1j}) \left(\frac{U_{2j}^2}{2} - \frac{U_{1j}^2}{2} \right) \right] - \Gamma \\ \frac{\rho_1 u_1 + \rho_2 u_2}{\rho_2 + \rho_2} \end{aligned} \quad (3.34)$$

The energy equation of two-domain two-phase systems can be expressed in terms of total enthalpy content and total enthalpy flux as:

$$\frac{\partial}{\partial t} \rho_1 h_1 + \frac{\partial}{\partial x_j} \rho_1 U_{1j} h_1 = \phi_1 \frac{\partial P}{\partial t} + \frac{\partial}{\partial x_j} [\kappa_{m1} \frac{\partial T_1}{\partial x_j}] + Q_{12} + L_{12h} + J_{E1} \quad (3.35)$$

where

$$L_{12h} = \frac{\partial}{\partial x_j} \left[\frac{\rho_1 \rho_2^2}{(\rho_1 + \rho_2)^2} (U_{2j} - U_{1j})(h_2 - h_1) \right] + \Gamma \frac{\rho_1 h_1 + \rho_2 h_2}{\rho_1 + \rho_2} \quad (3.36)$$

Since the kinetic energy of the bubbles is really part of the kinetic energy of the continuous phase. Since $P \frac{\partial \phi_1}{\partial t} + P \frac{\partial \phi_2}{\partial t} = 0$

$$\begin{aligned} \frac{\partial}{\partial t} (\rho_2 H_2 + \rho_1 \frac{U_{1j}^2}{2}) + \frac{\partial}{\partial x_j} (\rho_2 U_{2j} H_2 + \rho_1 U_{1j} \frac{U_{1j}^2}{2}) &= \phi_2 \frac{\partial P}{\partial t} + \frac{\partial}{\partial x_j} (\kappa_{m2} \frac{\partial T_2}{\partial x_j}) - Q_{12} + \\ &+ L_{21h} + L_E + \rho_1 F_{12} (U_{2j} - U_{1j})^2 + \rho_1 U_{1j} f_{1j} + \rho_2 U_{2j} f_{2j} + J_{E2} + \frac{\partial}{\partial x_j} [U_{mj} (\mu_{m2} \Delta_{2ji} + \mu_{m2}^* \theta_2 \delta_{ji} + \mu_{m1} \Delta_{1ji} + \mu_{m1}^* \theta_1 \delta_{ji})] \end{aligned} \quad (3.37)$$

where

$$\begin{aligned} L_{21h} &= \frac{\partial}{\partial x_j} \left[\frac{\rho_1^2 \rho_2}{(\rho_1 + \rho_2)^2} (U_{1j} - U_{2j})(H_1 - H_2) + \frac{\rho_1 \rho_2^2}{(\rho_1 + \rho_2)^2} (U_{2j} - U_{1j}) (\frac{U_{2j}^2}{2} - \frac{U_{1j}^2}{2}) \right] \\ &- \frac{\rho_1 h_1 + \rho_2 h_2}{\rho_1 + \rho_2} \Gamma \end{aligned} \quad (3.38)$$

In domain 3-4, we have

$$\frac{\partial}{\partial t} \rho_3 h_3 + \frac{\partial}{\partial x_j} \rho_3 U_{3j} h_3 = \phi_3 \frac{\partial P'}{\partial t} + \frac{\partial}{\partial x_j} [\kappa_{m3} \frac{\partial T_3}{\partial x_j}] + Q_{34} + L_{34h} + J_{E3} \quad (3.39)$$

where

$$L_{34h} = \frac{\partial}{\partial x_j} \left[\frac{\rho_3 \rho_4^2}{(\rho_3 + \rho_4)^2} (U_{4j} - U_{3j})(h_4 - h_3) \right] - \Gamma \frac{\rho_3 h_3 + \rho_4 h_4}{\rho_3 + \rho_4} \quad (3.40)$$

and since $P' \frac{\partial \phi_3}{\partial t} + P' \frac{\partial \phi_4}{\partial t} = 0$,

$$\begin{aligned} \frac{\partial}{\partial t} (\rho_4 H_4 + \rho_3 \frac{U_{3j}^2}{2}) + \frac{\partial}{\partial x_j} (\rho_4 U_{4j} H_4 + \rho_3 U_{3j} \frac{U_{3j}^2}{2}) &= \phi_4 \frac{\partial P'}{\partial t} + \frac{\partial}{\partial x_j} (\kappa_{m4} \frac{\partial T_4}{\partial x_j}) - Q_{34} \\ &+ L_{43h} + \rho_3 F_{34} (U_{4j} - U_{3j})^2 + \rho_3 U_{3j} f_{3j} + \rho_4 U_{4j} f_{4j} + J_{E4} + \frac{\partial}{\partial x_j} \\ &[U_{mj} (\mu_{m4} \Delta_{4ji} + \mu_{m4}^* \theta_4 \delta_{ji} + \mu_{m3} \Delta_{3ji} + \mu_{m3}^* \theta_3 \delta_{ji})] \end{aligned} \quad (3.41)$$

Since $L_E \approx 0$ because $V', I' \approx 0$ for liquid droplets in vapor, in Eq. (3.41) P' is the pressure in domain 3-4, and

$$L_{43H} = \frac{\partial}{\partial x_j} \left[\frac{\rho_3^2 \rho_4}{(\rho_3 + \rho_4)^2} (U_{3j} - U_{4j})(H_3 - H_4) + \frac{\rho_3 \rho_4^2}{(\rho_3 + \rho_4)^2} \left(\frac{U_{4j}^2}{2} - \frac{U_{3j}^2}{2} \right) \right] + \Gamma \frac{\rho_3 h_3 + \rho_4 h_4}{\rho_3 + \rho_4} \quad (3.42)$$

3.1.4 Constitutive Equations

Constitutive equations are formulated based on experimental data characterizing specific behavior of materials together with postulated principles governing them. Thus, constitutive equations can be considered as mathematical models of a particular group of materials. We restrict our attention to particular type of constitutive equations which are relevant to the problems under consideration.

3.1.4.1 Equation of State

The standard form of the thermal equation of state for fluid is given by a functional relationship between temperature, pressure and density; or enthalpy, pressure, and density. Thus we have:

$$h = h(P, \rho), \quad T = T(P, \rho) \quad (3.43)$$

The most complete reference of sodium properties appears to be that of Golden and Tokar [15]. An approximation of temperature dependence on surface tension was given by Griffith [39].

3.1.4.2 Phase Changes

The rate of generation, evaporation, or condensation for a heterogeneous system is given by:

$$\Gamma = \frac{\rho_1}{\bar{\rho}_1} \left[\frac{3 N_{Sh} \hat{D}}{2 a_1^2} \right] (\bar{\rho}_2' - \bar{\rho}_1') \equiv M_{12} (\bar{\rho}_2' - \bar{\rho}_1') \quad (3.44)$$

where N_{Sh} is the Sherwood number for mass transfer, $\hat{D}$ is the self-diffusion coefficient of molecules in the vapor phase, $\bar{\rho}_1'$ is the density of the vapor at its temperature T_1 and pressure P_1 including the curvature effect and M_{12} is the inverse relaxation time for the mass transfer.

According to [40]

$$P_1 - P_2 = \frac{2\sigma}{a_1} + 4 \bar{\mu}_2 \frac{\dot{a}_1}{a_1} \quad (3.45)$$

where a_1 is the bubble radius and $\dot{a}_1$ is the rate of bubble growth.

$$\bar{\rho}_2' = \bar{\rho}_2' (T_2 \text{ saturation or superheated liquid})$$

$$\bar{\rho}_1' = \bar{\rho}_1' (T_1, P_1)$$

and for droplets

$$P_3 = P_{\text{sat}} (T_3) + \frac{2\sigma'}{a_3}$$

$$P_4 \sim P_3$$

$$\bar{\rho}_4' = \bar{\rho}_4' (P_3, T_4)$$

$$\bar{\rho}_3' = \bar{\rho}_3' (T_3 \text{ saturation or superheated liquid})$$

and

$$r' = M_{34} (\bar{\rho}_3' - \bar{\rho}_4') \quad (3.46)$$

3.1.4.3 Bubble Generation

Initial bubble generation at a heated wall is given in various studies of boiling. In this single domain two-phase flow, average growth of a spherical bubble is by agglomeration and evaporation via heat transfer. Quantities of interest are bubble diameter, bubble frequency, number per unit area in relation to nucleation sites, and their emerging velocity. Cases of interest are nucleate boiling, film boiling under the condition of forced convection and pool boiling. A survey in this section leads to an assemblage of the basic parameters to be used in the computations.

A survey in Rohsenow and Choi [14] gave bubble diameter D_b at detachment as

$$D_b = C_b \beta \sqrt{\frac{2\sigma}{g(\rho_l - \rho_v)}} \quad (3.47)$$

where $C_b \sim 0.0148$ for water and hydrogen, β is the bubble contact angle in degrees, g is the gravitational constant, ρ_v is the density of the vapor and ρ_l is that of the liquid. Eq. (.47) explains trend of parametric relationship, although no detailed data available for sodium system.

Bubble frequency, f , was given by Zuber [41] relating attached time and delay time. Cole [42] suggested a bubble frequency relation in the form

$$D_b f^2 = \frac{4}{3} \frac{g(\rho_l - \rho_v)}{C_D \rho_l} \quad (3.48)$$

where C_D is a drag coefficient ($C_D \sim 1$). Hence, we have approximately:

$$D_b f^2 \sim 1.32 g \quad (3.49)$$

In forced convection D_b decreases linearly with an increase in velocity [43]. In the case of LOCA transition to forced convection boiling is important. The bubble velocity U_b is given by [14]:

$$U_b \sim f D_b \quad (3.50)$$

A recent correlation by Cole and Rohsenow [44] gave a relation in the form:

$$(E_o)^{1/2} = (4.56 \times 10^{-4}) (J_a^*)^{5/4} \quad (3.51)$$

where $E_o = g (\rho_l - \rho_v) D_b^2 / \sigma$, $J_a^* = \rho_l c_l T_{sat} / \rho_v h_{fg}$, where c_p is the specific heat of the liquid, T_{sat} is the saturation temperature and h_{fg} is the latent heat. The nucleation sites N_A per unit area and bubble diameter D_b is related to the heat flux J_Q as given in [44]:

$$J_Q = N_A \left(\frac{\pi}{6} D_b^3 \rho_v \right) h_{fg} \hat{f} \quad (3.52)$$

In SI units note that $N_A \sim 3 \times 10^4$ to 10^5 per m^2 for polished metal surfaces. Further, special mention of the surface condition was also made by Griffith and Wallis [45]. A relation for nucleate boiling given by Scriven [46] is:

$$\frac{D_b}{2} = \frac{2 \Delta T}{h_{fg} \rho_v} \left[\frac{3 \kappa_l \rho_l c_p t}{\pi} \right]^{1/2} \quad (3.53)$$

where ΔT is the temperature difference between the wall and coolant, κ_l is the thermal conductivity of the liquid phase, and t is the time.

Film boiling is in general not correlated to nucleation sites [47,48].

Still another important relation is homogeneous nucleation which is likely to occur at high heat flux conditions [40]. Defay, et al., gave [49]

$$N_L = N_0 \exp (- \Delta F_g / kT) \quad (3.54)$$

where N_L is the probability of a spherical critical nucleus of radius a_k , $\Delta F_g = (4 \pi / 3) \sigma a_k^2$ is the free nucleation energy, N_0 is the Avogadro number and k is Boltzmann constant.

Bubble growth during boiling via heat transfer is significant in the case of liquid metal because of its high thermal conductivity. This was given by Singh, et al., [50] according to:

$$a_1 \dot{a}_1 = \frac{\pi}{2} \left[\sqrt{\frac{\kappa_l}{c_p \rho_l}} J_a \right]^2 \quad (3.55)$$

where $J_a = c_p \rho_l (T_l - T_v) / \rho_v h_{fg}$.

Other data on boiling sodium were given by Noyes and Lurie [51]. A comprehensive survey has been given by Rohsenow [52]. In general, there is an absence of specific details on bubble size, number, and velocity for a sodium system.

In summary, most of the previous efforts in correlating boiling processes have been toward generating results in terms of lumped parameters [14,53]. Bubble details were discussed for the purpose of explanation and interpretation only. Efforts

toward computer modeling such as ours calls for data in terms of bubble diameter (D_b), bubble velocity (U_b) and bubble number density (N_b) at the wall or in the liquid phase. We have sufficient base to proceed at present however, further experimental studies toward refining these data will be desirable.

3.1.4.4 Bubble Agglomeration

Bubble agglomeration has been studied and reported only in the idealized cases [34,54]. General relations for the agglomeration of a cloud of bubbles such as in a boiling liquid are not available. The mechanism of bubble agglomeration and break-up can be represented by the following rate relation:

$$\frac{dN_1}{dt_1} = -\frac{1}{2} \hat{k}_1 N_1^2 + \frac{1}{2} \hat{k}_2 N_{1+} \quad (3.56)$$

where $\hat{k}_1$ is an agglomeration constant of dimension m^3/sec and is a function of material composition of the liquid and the vapor, surface tension, relative velocities of the motion in the cloud, diffusivity and probability of coalescence; $\hat{k}_2$ is the rate constant for break-up, and N_{1+} is the density of those larger than N_1 . Experimental data have not been correlated in terms of the agglomeration constant consequently additional measurements are needed.

There appears to be a greater abundance of data on droplet coalescence [35, p. 604], expressed in terms of coalescence frequency.

The change in N_1 (and N_3) are applicable to the density of the phase in Eqs. (3.5) and (3.6). For these two domains, we have

$$\frac{\partial N_1}{\partial t} + U_{1j} \frac{\partial N_1}{\partial x_j} = -\frac{1}{2} \hat{k}_1 N_1^2 \quad (3.57)$$

$$\frac{\partial N_3}{\partial t} + U_{3j} \frac{\partial N_3}{\partial x_j} = -\frac{1}{2} \hat{k}_3 N_3^2 \quad (3.58)$$

3.1.4.5 Droplet Generation by Bubble Burst

Generation of droplets (phase 3) into domain 3-4 by bursting of bubbles (phase 1) from domain 1-2 occurs at the interface of 2-4. Past studies were made to study droplet carryover in boilers [55,56] and oceanography [37], basically for water or water-air systems. The data are not yet in the form that is readily applicable to the present study. It appears that this aspect of the study has not been made for liquid metals. Further experimental work is desirable to refine the estimation of quantities which we now can use.

Available data indicate that the number of droplets generated decrease with bubble size. These droplets were noted to be ejected to various heights against gravity rather than initial velocity, although conversion can be made by approximation [37].

3.1.4.6 Transport Properties

(a) Relaxation Time Constants [21]

In each domain we are concerned with the inverse relaxation time constants M , F and G , for mass, momentum, and energy transfer between the continuous and the dispersed phases, and between the dispersed phases, respectively.

In the case of a dilute suspension in a uniform flow field, M_{kc} , F_{kc} and G_{kc} are given by [21]:

$$M_{kc} = \frac{\rho_k}{\rho_c} \left(\frac{3 D_{kc}}{2 a_k} \right) \quad (3.59)$$

$$F_{kc} = \frac{9 \bar{u}_c}{2 a_k \bar{\rho}_k} \quad (3.60)$$

$$G_{kc} = \frac{3 \bar{\kappa}_c}{c_{vk} a_k \bar{\rho}_k} \quad (3.61)$$

for small relative motion, and for the Reynolds number of the relative motions less than 1 where

$$Re_{kc} = 2 a_k \bar{\rho}_c | \underline{U}_k - \underline{U}_c | / \bar{\mu}_c. \quad (3.62)$$

For large Reynolds number flow, the inverse relaxation time constant for mass transfer may be written:

$$M_{kc} = \frac{\rho_k}{\rho_c} \frac{3 Sh D_{kc}}{2 a_k} \quad (3.63)$$

where the Sherwood Number $Sh = \hat{h}_D 2 a_k / D_{kc}$ and D_{kc} in the mass transfer diffusion coefficient.

The drag coefficient C_{Dk} is given by:

$$C_{Dk} = C_D (Re_{kc}) \quad (3.64)$$

$$F_{kc} = \frac{3}{8} C_{Dk} \frac{\bar{\rho}_c}{\bar{\rho}_k} \frac{1}{a_k} | \underline{U}_c - \underline{U}_k | \quad (3.65)$$

G_{kc} is given in terms of the Nusselt number (Nu) as:

$$Nu_k = \frac{\hat{h}_{kc} (2a_k)}{\bar{\kappa}_c} = Nu (Re_{kc}, Pr_c) \quad (3.66)$$

$$G_{kc} = \frac{3 Nu_k \bar{\kappa}_c}{2 c_{vk} a_k^2 \bar{\rho}_k} \quad (3.67)$$

where Pr_c is Prandtl number of continuous phase and $\hat{h}$ is the heat transfer coefficient. With respect to a dense suspension some information is available for dense particle clouds, however, almost none for dense bubble clouds. A reasonable estimate at this time is:

$$F_{kc} = \frac{75}{2} \frac{\phi_k}{(1 - \phi_k)^2} \frac{\mu_c}{\bar{\rho}_k a_k^2} + \frac{1.75}{2(1 - \phi_k)} \frac{\bar{\rho}_c}{\bar{\rho}_k} \frac{|\bar{u}_{cj} - u_{kj}|}{a_k} \quad (3.68)$$

which has been proven for droplets [9,21] but not for bubbles. G_{kc} is given in terms of $\hat{h}_{kc} (Pr)^{2/3} / c_{vc} \bar{\rho}_c \bar{\mu}_c$ vs. Re_{kc} for a dense bed of particles as

$$G_{kc} = \frac{3 \hat{h}_{kc}}{c_{vk} \bar{\rho}_k a_k} \quad (3.69)$$

which might be applicable to droplets in vapor but not bubbles in liquid.

Interactions between dispersed phases call for a knowledge of F_{kl} and G_{kl} for the dispersed phases k and l . Some information exists for heated solid particles [21], but its usefulness in heated bubbles and droplets has to be studied further.

Continuing studies will determine the minimum amount of experimental effort needed on the transport properties.

(b) Viscosity and Thermal Conductivities

The viscosity and thermal conductivity of a mixture of phases, μ_m and κ_m , (Appendix C) have not been measured in detail. Some discussion concerning these properties is presented in Ref. [21]. In general, computation of the transport properties of a phase component in a mixture requires some approximation. This is an area of future experimental investigation.

In the case of a dilute suspension of a dispersed phase we know these transport properties with certainty. In this case, for domain 1-2

$$\begin{array}{ll} \mu_m \sim \bar{\mu}_2 & \kappa_m \sim \bar{\kappa}_2 \\ \mu_{m2} \sim \bar{\mu}_2 & \kappa_{m2} \sim \bar{\kappa}_2 \\ \mu_{m1} \sim \rho_1 D_{12} & \kappa_{m1} \sim \rho_1 D_{12} c_{v1} \end{array}$$

and similarly for domain 3-4. The diffusivity of phase 1 in phase 2 is known for limited cases (Appendix G).

These data are useful when we treat laminar flow. In the case of a turbulent flow we can express the stress in terms of a power law velocity distribution, however, data on turbulent diffusivities will still be required. Extensive data are available in single phase steady flow but not in a boiling liquid. Some data on turbulent diffusivity of liquid metals have been reported recently [57].

3.1.5 Initial and Boundary Conditions

Both initial and boundary conditions are the same as specified in Section 2.4.

3.2 Interdomain Boundary Conditions

Identification of a new domain is made via:

(a) When bubble growth and agglomeration leads to the emergence of a large bubble, large in comparison to the characteristic physical dimension, such as the minimum spacing X_0 between the pins in a reactor fuel assembly, the logical choice is to identify the beginning of slug flow when there is one bubble in X_0^3 with the radius of the order of $a_1 \sim (3 \phi_1 / 4\pi)^{1/3} X_0$, i.e., the radius of the spherical domain.

(b) When the bubble population at the wall is such that the inter-bubble spacing is equal to the order of the bubble diameter at one bubble diameter away from the wall, transition to film boiling is identified, giving a liquid ligament in an annular flow of vapor containing droplets.

These defined transitions are needed at this time because the procedure for a continuous transition from multiphase flow based on the time-averaged phase description according to multiphase mechanics, to the specific description of a domain with indefinite accuracy, remains to be discovered.

Once a domain is identified, case (a) will have "slugs" or "large" bubbles [58,59,60] containing droplets produced by bursting bubbles from the liquid domain. In theory at least, what follows is accountable via the basic relations in Section 2.3, the interdomain (interfacial) relations. Computation thereafter includes agglomeration and coalescence of growing slugs [61] and transition to annular flow [62] of a vapor core with droplets in a bubbly liquid annulus, and so on to a vapor flow with droplets and flow of pure vapor. In case (b) we have the case of annular flow of a bubbling liquid core in the annulus with droplets and the transition to droplet flow in the vapor alone as the ligament breaks up by oscillation and by thinning. As these processes occur over a number of pins in

a fuel assembly, and subsequent condensation by the reversal [63] of some of the above processes in regions of lower temperature the case of a large bubble in the reactor fuel assembly over a number of the pins is produced.

In carrying out such a calculation, one should note that the interdomain (interfacial) relations account for the interactions of transfer of mass, momentum and energy occurring over a surface whose shape is determined by these interactions. The relations describing these interactions have to be expressed in terms of a surface coordinate system which is itself to be determined from these relations. Hence, an iterative procedure is required and can be formulated. However, insufficient knowledge of the transport parameters such as surface dilatational and surface shear viscosities (Scriven's κ and ϵ) [20] at present suggests that an elaborate model may not be feasible. This limitation is also consistent with the present necessity of defining the emergence of a new domain.

The interdomain relations outlined below represent practical and meaningful boundary conditions in terms of an actual computational and physical situation. More detailed interdomain boundary conditions are given by Ishii [6].

3.2.1 Thermal Interdomain Boundary Conditions

$$a) \quad T_2 = T_4 = T_s \quad (3.70)$$

$$b) \quad \underline{n} \cdot \underline{J}_{2m} = \underline{n} \cdot \underline{J}_{4m} = \underline{n} \cdot \underline{J}_s \quad (3.71)$$

It is to be noted that the thermal equilibrium condition is assumed in both Eqs. (3.70) and (3.71).

3.2.2 No Slip Interdomain Boundary Conditions

$$U_{2t} = U_{4t} \quad (3.72)$$

where subscript t denotes the tangential direction. Under the assumption of a no slip boundary condition, the momentum jump conditions in the normal and tangential directions respectively become:

$$a) \quad \underline{n} \cdot \underline{P}_2 + \underline{n} \cdot \underline{P}_4 = -2 H_{42} \underline{n} \sigma \quad (3.73)$$

where H_{42} is the mean curvature of the surface separating continuous phases 4 and 2.

$$b) \quad \underline{\tau}_{2mt} + \underline{\tau}_{4mt} = (\underline{\tau}_\alpha a^{\alpha\beta}_\sigma)_\beta \quad (3.74)$$

3.2.3 Phase Change Interdomain Boundary Conditions

a) No mass transfer across the interface between two adjacent domains

$$\dot{m}_k = 0 \quad (3.75)$$

b) Mass transfer across the interface between two adjacent domains

$$\underline{n} \cdot \underline{J}_3 = C_{B3} N_1 \quad (3.76)$$

$$\underline{n} \cdot \underline{J}_4 = - \underline{n} \cdot D_4 \nabla_s \rho_4 + C_{B4} N_1 \quad (3.77)$$

where J_3 and J_4 are droplet and bubble flux across the interface between two adjacent domains, C_{B3} is the coefficient of bubble burst to droplets and C_{B4} is the coefficient of bubble burst to vapor.

3.3 Solution of Equations

For a single component, two-phase flow system, the minimum number of unknowns to be determined are: density of phases, ρ_1, ρ_2 ; velocities of phases, U_1, U_2 ; enthalpy of phases, h_1, h_2 ; pressure of the system P ; and ϕ_1, ϕ_2 . The number of independent equations are: two continuity equations from mass balance, six momentum equations (3-dimensional) from the coupled motion, and two energy equations, plus two equations of state, and volume fraction equation. Hence, with pertinent initial and boundary conditions, a problem of single component, two-phase dynamic system is deterministic. It appears that, while this fact has been identified in several references [9,10], the mass transfer equation, hence the determination of the phase generation Γ , has been outlined only in [6]. Therefore, for a single component two-phase domain and treating the average properties of the dispersed phase, we have altogether thirteen equations and thirteen unknowns to be determined.

Extending these considerations to the two-domain two-phase flow systems as outlined in Figs. 2-4, we have the following equations for a minimal description:

- 4 equations of continuity (2 per domain)
- 12 momentum equations (6 per domain)
- 4 energy equations (2 per domain)
- 4 equation of state or tabulated P-V-T relations or data
- 5 interfacial equations
- 2 equations of volume fractions

or a total of thirty one equations for thirty one dependent variables: P (2 each), S (boundary), ρ (4 each), U (12 each), h (4 each), Γ (1 each), ϕ (4 each), and T_S (interface). This checks with the general relation $6d(k + 2) - 5$ for $d = 2$, $k = 1$. This is under the simplification of treating the mean size of the spherical dispersed phase at a given position and time, or $a(x_j, t)$. Each additional domain (slug, for instance) increases the number of equations by eighteen.

Solution of these simultaneous equations will be determined by the boundary conditions of heat flux, bubble size, number density, and velocity at the boundary; overall flow quantity, inlet or initial temperature and pressure; and transport parameters to be identified for this study. Once an interdomain boundary becomes identifiable, additional boundary conditions are imposed on heat flux, mass flux (phase change, bubble burst to droplets, and droplet capture), and momentum transfer (effects of inertia and surface tension). The aim of this entire formulation will be toward the prediction of flow regimes and their transition with the idealizations rendered realistic by the introduction of the proper transport parameters.

Computations on single domain, two-phase flow system have been illustrated in several cases [9,21]. New computational techniques and strategies are needed in dealing with a multidomain situation and the criteria to identify a new domain in a multiphase flow field must also be developed. The latter has to be accomplished by identifying a bubble in a multiphase mixture as large enough (after growth via agglomeration and evaporation) compared to the characteristic physical dimensions of the flow system such that its presence is identified by distributions of velocities and temperatures around it.

The study of the mechanisms for such a transition is currently in progress, and will be reported at a later date.

4.0 Comparison to Other Studies

To further the current knowledge on multiphase mechanics, it is desirable to compare the present formulation (ANL) to those presented in other recent studies. This is in the spirit that "honest men differ".

Among many worthy studies in recent times, we chose to compare this ANL study to those of Harlow and Amsden (H.-A.) [9], Solbrig and Hughes (S.-H.) [5], Ishii [6] and various one dimensional studies [6,64]. In the (H.-A.) study the control volume is chosen to be smaller than the characteristic physical dimensions as in ANL, but (S.-H.) formulation chose a control volume larger than the smallest dimension of the flow passage. Hence, H.-A. and S.-H. differ from each other for at least this reason. Ishii included the possibility of volume elements smaller than the particle size and hence accounts for phase and domain on a common basis. Still another study of Hayday [65] gave formulation of components but referred to the center-of-mass of the mixture.

4.1 Comparison to Harlow and Amsden (H. - A.)

Table III shows a term-by-term comparison of ANL to H.-A. The major difference appears to be in the inertial coupling terms I, V', L', in ANL. Other differences appear to be that H.-A. uses (following their notation)

$$\theta U_{vj} + (1 - \theta) U_{dj} \equiv \bar{U}_j \quad (4.1)$$

for the mean velocity instead of U_m which is defined by, for c.g. frame of reference.

$$\rho'_m U_{mj} = \rho'_v U_{vj} + \rho'_d U_{dj} = \rho_v \theta U_{vj} + \rho_d (1 - \theta) U_{dj} \quad (4.2)$$

and

$$\rho'_m = \rho_v \theta + \rho_d (1 - \theta) \quad (4.3)$$

in their notation. The use of $\bar{U}_j$ has the advantage of $\bar{U}_j = \text{constant}$ in two-phase flow when material densities ρ_v and ρ_d are constants. In general, the continuity equation gives

$$\frac{\partial}{\partial x_j} \bar{U}_j + \theta \frac{d}{dt} \ln \rho_v + (1 - \theta) \frac{d}{dt} \ln \rho_d = 0$$

and the use of $\bar{U}_j$ has no particular advantage when dealing with compressible bubbles. Arbitrary use of $\bar{U}_j$ in place of mass mean velocity U_{mj} will lead to errors.

They also chose thermal conductivity of the vapor phase in the mixture as given by $k_v \theta$, k_v being the thermal conductivity of the pure vapor.

A recent study by Travis, Harlow and Amsden [66], used the kinetic equation based on continuum theory only. They appear to emphasize adjusting equations to forms which facilitate computation but missed the inertial coupling terms completely.

4.2 Comparison to Solbrig and Hughes (S. - H.)

Table IV shows a term-by-term comparison of the ANL formulation to that of S.-H. Besides the basic differences in the choice of the sizes of control volume in relation to the characteristic physical dimension of the flow system, S.-H. does not include the inertia coupling terms I and L in the momentum and the energy equations. The reason for not having direct correspondence of the terms in their momentum and energy equations in their formulation is not clear. While not included in their report, one of these investigators (Lyczkowski) [67] indicated that including the inertial coupling terms in their calculations significantly improved the stability of computations.

Table III

Comparison to Harlow and Amsden (H. - A.)

(Illustration with Droplets in Vapor)

<u>Equation</u>	<u>H. - A.</u>	<u>ANL</u>
Continuity Eq.	(3), (4)	(3.3), (3.4)
Density	ρ_v (vapor) ρ_d (droplet)	ρ_4 ρ_3
Velocity	U_v U_d	U_4 U_3
Mass Generation	$S_{me} - S_{mc}$	Γ'
Volume fraction	$\theta, 1 - \theta$	ϕ_3, ϕ_4
Momentum Eq.	(8) ⁺	(3.22)
Force due to mass generation	$U_d S_{me} - U_v S_{mc}$	$\frac{\rho_3 U_{31} + \rho_4 U_{41}}{\rho_3 + \rho_4} \Gamma' *$
Pressure gradient	$-\nabla P$	$(1 - \phi_3) \nabla P'$
Compression	--	$-(1 - B) P \nabla \phi_3$
Shear force	$V_v \frac{\partial}{\partial x_j} [\mu_{m4} \Delta_{4ji} + \mu_{m4}^* \theta_4 \delta_{ji} + \mu_{m3} \Delta_{3ji} + \mu_{m3}^* \theta_3 \delta_{ji}]$	
Field force	$\rho_v' g$	$\rho_4 f_{4i}$
Inertial coupling	--	I_{4i}
Viscous coupling	$K(U_v - U_d)$	$V_{4i} = \rho_3 F_{34} (U_{4i} - U_{3i})$
Multiphase inertial force	--	I_{4i}'
Multiphase viscous force	--	V_{4i}'
Energy Eq.	(10) ⁺	(3-33) ^{**}
Total energy	I_v	E_4
Generation	$S_{iev} - S_{icv}$	$-\Gamma' E_4$
Heat Source	E_v	J_{E4}
Heat transfer coupling	$R(T_d - T_v)$	$Q_{43} = c_{v4} \rho_4 G_{43} (T_3 - T_4)$
Drag force dissipation	$K(U_d - U_v)^2$	$+ \rho_4 F_{43} (U_3 - U_4)^2$
Heat conduction	$\nabla \cdot (k_v \nabla T_v)$	$\frac{\partial}{\partial x_j} \kappa_{m4} \frac{\partial T_4}{\partial x_j}$

* This term is included in I_{4i} .

** In the form of rate of energy change per unit volume. [68]

⁺ Similar comparisons can be made of eqs. (9) and (11) for the droplet phase.

Table III (Cont.d)

<u>Equation</u>	<u>H. - A.</u>	<u>ANL</u>
Viscous dissipation	$V_{iv} \frac{\partial}{\partial x_j} [U'_m (\mu_{m4} \Delta_{4ji} + \mu_{m4}^* \Theta_4 \delta_{ji} + \mu_{m3} \Delta_{3ji} + \mu_{m3}^* \Theta_3 \delta_{ji})]$	
Work due to displacement - $P \nabla_b \cdot [\Theta U_v + (1 - \Theta) U_d]$		$-\phi_4 \nabla U_m P$
Work due to compression	--	$-U_m P \nabla \phi_4$
Coupling term from c.g. reference	--	L_{43}
Coupling term from multiphase interaction	--	L'_{43}
Effect of kinetic energy of dispersed phase	--	All terms due to velocity effects of dispersed phase are added to the continuum phase
Other Details: Thermal Conductivity	$k_v \Theta$	κ_{m4}
	$k_d (1 - \Theta)$	κ_{m3}
Viscous dissipation	Implicit	Explicit for viscous motion
Use of multidomain concept	For different droplet sizes	For transition between flow regimes

Table IV

Comparison to Solbrig and Hughes (S. - H.)

Equation	S. - H.	ANL
Continuity Eq.	(19)	(3.1)
Phases	a, l, g	2,1
Density in mixture	$\rho^a \phi$	ρ_1
Velocity	v_i^a	U_{1i}
Mass Generation	$\dot{m}^a \phi$	Γ_1
Momentum Eq.	(59)	(3.17)
Control volume	Include details of geometry <u>larger than characteristic</u> physical dimension	<u>Smaller</u> than characteris- tic physical dimension
Force due to mass genera- tion	$\phi \dot{m}^a \hat{v}_i^a$	$\frac{\rho_1 U_{1i} + \rho_2 U_{2i}}{\rho_1 + \rho_2} \Gamma_1^*$
Shear force	$-\phi \sum_s \bar{A}_s^a B_s^a (\theta_s, \theta_a) v_i^a$ (solid wall) $-\phi A_{ab} B_{ab} (v_i^a - v_i^b)$ (phases) $(\phi \alpha_{ji}^a), j$ (viscous)	-- -- $\frac{\partial}{\partial x_j} (\mu_{m2} \Delta_{2ji} + \mu_{m2}^* \theta_2$ $\delta_{ji} + \mu_{m1} \Delta_{1ji} + \mu_{m1}^* \theta_1$ $\delta_{ji})$
Drag force	$-\phi \sum_s C_s^a \bar{A}_s^a v_i^c$ (solid wall) $-\phi C_{ab} \bar{A}_{ab} (v_i^a - v_i^b)$ (phases)	-- $V_{21i} = \rho_1 F_{12} (U_{2i} - U_{1i})$
Multiphase in- ertial force	$-\phi \bar{A}_{ab} C_{AM}^{ab} (\frac{\partial v_i^a}{\partial t} - \frac{\partial v_i^b}{\partial t})$ (phases) $-\phi \sum_s \bar{A}_s^a C_{AM}^a (\frac{\partial v_i^a}{\partial t})$ (solid wall)	V_{21i}' I_{21i}' --
Field force	$\phi \rho^a g_i$	$\rho_1 f_{1i}$
Inertial coupling	--	I_{21i}
Energy Eq.	(72)	(3.30)(3.33)
	(overall energy only)	(for each phase)
	(Does not include direct term-by-term correspond- ence with momentum eq. [59])	(Direct correspondence and derivation from our momentum eq.)
Heat conduction	$(\phi \sum_{l,g} \alpha_{k,i}^a T_i), i$	$-\frac{\partial}{\partial x_j} J_{m2j} = \frac{\partial}{\partial x_j} \kappa_{m2} \frac{\partial T_2}{\partial x_j}$
Heat source	ϕq	J_{E2}

* This term is included in I_{21i} .

Table IV (Cont.d)

<u>Equation</u>	<u>S. - H.</u>	<u>ANL</u>
Viscous dissipation	$(\phi_{\ell, g} \Sigma \alpha_{ji}^a \sigma_{vi}^a v_i^a),_i$	$\frac{\partial}{\partial x_j} [U_{mj} (\mu_{m2} \Delta_{2ji} + \mu_{m2}^* \Theta_2 \delta_{ji} + \mu_{m1} \Delta_{1ji} + \mu_{m1}^* \Theta_1 \delta_{ji})]$
Work due to displacement	$-(\phi P \Sigma \alpha_{vi}^g v_i^g),_i$	$-\frac{\partial}{\partial x_j} (U_m P \delta_{ji})$
Work due to compression	--	$-U_m P \delta_{ji} \frac{\partial \phi_1}{\partial x_j}$
Work by field force	$\phi_{\ell, g} \Sigma \rho_{gi}^a v_i^a$	$\rho_1 U_{1j} f_{1j}, \rho_2 U_{2j} f_{2j}$
Other energy terms:		
Coupling term from c.g. ref.	--	$L_{12u}, L_{21E}, L_{12(KE)}$ (See note below)
Viscous drag dissipation	--	$V_{12j} (U_{2j} - U_{1j})$
Multiphase dissipation	--	L'_{12}

Note:
$$L_{12(KE)} = \frac{\partial}{\partial x_j} \left[\frac{\rho_1 \rho_2^2}{(\rho_1 + \rho_2)^2} (U_{1j} - U_{2j}) \left(\frac{U_{1j}^2}{2} - \frac{U_{2j}^2}{2} \right) \right]$$

4.3 Comparison to Ishii's Two-fluid Model [6]

The formulation in terms of the two-fluid model of Ishii [6] accounts for averages over time durations shorter than the duration of passage of successive particles of the dispersed phase and volume elements larger or smaller than each of these particles. His formulation has the advantage of treating large and small particles alike, with averaging carried out across the interface. Complication if any, is in the averaging procedure including the jump condition. The present formulation simplifies the treatment of the dispersed phase by introducing a duality of discrete nature and distributive representation. The discreteness is accounted for via treating the virtual mass and unsteadiness of flow field of each finite size particle. The distributive nature of the particle cloud is accounted for by taking an elementary volume consisting of a sufficiently large number of particles. This latter condition calls for defining an elementary volume smaller than the volume based on the characteristic dimension of the flow system. The provision for the jump condition (but otherwise direct transition from small to large bubbles, for instance) as defined by Ishii [6] is replaced here by recognizing the transition from a phase to a domain, when the size of the dispersed phase becomes large compared to the characteristic volume, as the emergence of a new domain. The criteria of the proposed transition are to be determined by comparison to experimental data. This approach also provides for successive generation of domains and agglomeration of domains, and hence accounting for the transition of flow regimes. One feature of the present formulation is its provision for any number of phases in each domain: droplets in a domain of vapor (a large bubble for instance), or bubbles in a domain of liquid. Furthermore, it avoids the complication of handling an elemental volume containing the jump condition of an interface in the two-fluid model where "it is only possible to discuss the model in general terms rather than to give firmly established constitutive equations" (quoted from p.144 of Ref. [6]).

A detailed comparison of Ishii's two-fluid model [6] and the present study is presented in Table V. The relative merit of these different approaches is best left to the users of the equations.

Table V
Comparison to Ishii's Two-fluid Model

ISHII

ANL

Averaging over

$$V < \frac{4\pi}{3} a_k^3$$

$$\tau < N^{-1/3} U_k^*$$

$$V \gg \frac{4\pi}{3} a_k^3$$

$$\tau > N^{-1/3} U_k^*$$

Transition

Continuous

Stepwise to new domain

Equations

Continuity Eq. (IX 3.1)

$$\alpha_k \bar{\rho}_k$$

$$\rho_k = \phi_k \bar{\rho}_k$$

$$\bar{v}_k$$

$$\bar{U}_k$$

$$\bar{\Gamma}_k = \frac{D_k \bar{v}_k}{Dt}$$

$$\rho_k \frac{d\bar{U}_k}{dt_k} \text{ (in inertia force form)}$$

Momentum Eq. (IX 3.2)

$$- \alpha_k \nabla \bar{P}_k$$

$$- \phi_k \nabla P$$

$$- (1 - B_k) P \nabla \phi_k$$

$$\bar{\tau}_k$$

$$\bar{\tau}_{mk}$$

$$\tau_k^T$$

(turbulence not treated yet)

$$\alpha_k \bar{\rho}_k g$$

$$\rho_k \bar{f}_k$$

$$M_k^d$$

$$\rho_k F_{kc} (\bar{U}_c - \bar{U}_k)$$

$$\bar{\Gamma}_k (\bar{v}_i - \bar{v}_k)$$

$$\bar{\Gamma}_k (\bar{U}_m - \bar{U}_k) + \frac{\partial}{\partial x_j} \rho_k (\bar{U}_m - \bar{U}_k) (\bar{U}_m - \bar{U}_k)$$

Energy Eq.

(IX 3.3) Kinetic energy neglected

Thermal energy only in dispersed phase

$$\alpha_k \bar{\rho}_k \frac{D_k \bar{i}_k}{Dt}$$

$$\rho_k \frac{dh_k}{dt_k} \text{ (In enthalpy change per unit volume)}$$

Table V (Contd.)

Comparison to Ishii's Two-fluid Model

	<u>ISHII</u>	<u>ANL</u>
	$-\nabla \cdot \alpha_k (\bar{q}_k + \bar{q}_k)$	$-\nabla \cdot (-\kappa_{mk} \nabla T_k)^*$
	$\alpha_k \frac{D_k \bar{p}_k}{Dt}$	$\phi_k \frac{\partial P}{\partial t}$
	$\alpha_k \bar{\tau}_k : \nabla \bar{v}_k$	Viscous dissipation in continuous phase
	$\Gamma_k (\bar{i}_{ki} - \bar{i}_k)$	$\nabla \cdot [\rho_k (\bar{u}_k - \bar{u}_m) (h_k - h_m)]$
	$\frac{\bar{q}_k''}{L_s}$	$-\Gamma_k (h_k - h_m)$
		$c_k \rho_k G_k (T_c - T_k)$
		(Including transfer of dissipated energy from continuous phase)
<u>Details</u>		
Mass transfer term (IX 3.22)	Γ_1	$M_{kc} (\bar{\rho}_c^* - \bar{\rho}_k^*)$
Interface drag force (IX 3.24)	M_1^d	$\rho_k F_{kc} (\bar{u}_c - \bar{u}_k)$
Conduction heat flux	$\bar{q}_k = -\bar{\kappa}_k [\nabla \bar{T}_k - \frac{\nabla \alpha_k}{\alpha_k} (\bar{T}_1 - \bar{T}_k)]$	$-\kappa_{mk} \nabla T_k$
Convective coupling		$c_k \rho_k G_{kc} (\bar{T}_c - \bar{T}_k)$

*(Turbulence not treated)

4.4 Comparison to Various One-Dimensional Formulations

A correct one-dimensional formulation of a two-phase flow system in terms of the mixture velocities was given by Shapiro following Newton's Law [64]. Wallis [69] gave another version ([69] p. 44) in terms of mean velocity but ignored inertial coupling when converted to a two-phase formulation ([69] p. 65). Boure [4] proposed a unified presentation of non-equilibrium two-phase flow, but left the interphase relations in general form without spelling out the details.

Besides delineation in Appendix D, it is desirable to resolve the difference between the two-phase flow and mixture formulations by first identifying their correspondence. It is possible to visualize the I's as an interaction in the following manner:

$$\int I_{12i} dx_j = \frac{1}{\rho_1} \left[\frac{\rho_1 \rho_2}{\rho_1 + \rho_2} \right]^2 (U_{2i} - U_{1i}) (U_{2j} - U_{1j}) + \int \Gamma U_{mi} dx_j \quad (4.4)$$

if we define a reduced relative momentum as

$$M_{12}^* = \frac{\rho_1 \rho_2}{\rho_1 + \rho_2} (U_2 - U_1) \quad (4.5)$$

the above expression becomes

$$\int I_{12i} dx_j = \frac{1}{\rho_1} M_{12i}^* M_{12j}^* + \int \Gamma U_{mi} dx_j = \rho_1 \left(\frac{M_{12i}^*}{\rho_1} \right) \left(\frac{M_{12j}^*}{\rho_1} \right) + \int \Gamma U_{mi} dx_j \quad (4.6)$$

where M_{12}^*/ρ_1 is the relative momentum distributed to species 1 and

$$\int I_{12i} dx_j = \begin{array}{l} \text{Change of momentum input over } x_j \\ \text{due to relative motion} \end{array} + \begin{array}{l} \text{Change of momentum input over } x_j \\ \text{due to mass conversion} \end{array} \quad (4.7)$$

Similarly

$$\int I_{21i} dx_j = \rho_2 \left(\frac{M_{12i}^*}{\rho_2} \right) \left(\frac{M_{12j}^*}{\rho_2} \right) + \int \Gamma U_{mi} dx_j \quad (4.8)$$

Namely the first term on the right hand side is the resistance due to relative motion because of relative displacement and the second term is due to conversion.

Take a simple case of an one-dimensional steady-flow and convert to the rate of change of momentum per unit volume, then we get for species 1

$$\frac{d}{dx} (\rho_1 U_1^2) - \frac{d}{dx} [\rho_1 (M_{12}^*/\rho_1)^2] = - \frac{d}{dx} (\phi_1 P) + \Gamma U_m + \rho_1 f_1 + \rho_1 F_{12} (U_2 - U_1) \quad (4.9)$$

and for species 2

$$\frac{d}{dx} (\rho_2 U_2^2) - \frac{d}{dx} [\rho_2 (M_{12}^*/\rho_2)^2] = - \frac{d}{dx} (\phi_2 P) - \Gamma U_m + \rho_2 f_2 - \rho_2 F_{21} (U_2 - U_1) \quad (4.10)$$

Their sum gives

$$\frac{d}{dx} [\rho_1 U_1^2 + \rho_2 U_2^2 + \rho^* (M_{12}^*/\rho^*)^2] = \frac{d}{dx} (\rho_m U_m^2) = - \frac{dP}{dx} + \rho_1 f_1 + \rho_2 f_2 \quad (4.11)$$

in the simplest form where $\rho^* = \rho_1 \rho_2 / (\rho_1 + \rho_2)$ is the reduced density. A comparison in Fig. 5 shows the difference between countercurrent flow and cocurrent flow of two phases.

Perhaps the strongest indication of the significance of the inertial coupling term is that the distinction between cocurrent and counter-current flow such as given by Eq. (4.11), or

$$\frac{d}{dx} \left[\rho_1 U_1^2 + \rho_2 U_2^2 - \frac{\rho_1 \rho_2}{\rho_1 + \rho_2} (U_2 - U_1)^2 \right] = - \frac{dP}{dx} \quad (4.12)$$

without it, the distinction would have been absent. Note that for idealized counter-current flow, with $U_2 = -U_1$, $\rho_2 = \rho_1$, we get $dP/dx = 0$, as it should be.

The condition such as in a fluidized bed with $U_1 = 0$ gives us:

$$\frac{d}{dx} \left[- \frac{\rho_1 \rho_2^2}{(\rho_1 + \rho_2)^2} U_2^2 \right] = (1 - \phi_2) \frac{dP}{dx} + (1 - B) P \frac{d\phi_2}{dx} + \rho_1 f_1 + \rho_1 f_1 + \rho_1 F_{12} U_2 \quad (4.13)$$

$$\frac{d}{dx} (\rho_2 U_2^2) \left[1 - \left(\frac{\rho_1}{\rho_1 + \rho_2} \right)^2 \right] = - \phi_2 \frac{dP}{dx} - (1 - B) P \frac{d\phi_2}{dx} + \rho_2 f_2 - \rho_2 F_{21} U_2 \quad (4.14)$$

where $\phi_2 \frac{dP}{dx}$ is the force acting on phase 1 by pressure gradient, $(1 - B) P \frac{d\phi_2}{dx}$ is the force due to volumetric displacement, $\phi_1 + \phi_2 = 1$ and $\rho_1 F_{12} = \rho_2 F_{21}$.

The signs of $P \frac{d\phi_2}{dx}$ in Eqs. (4.13) and (4.14) show action and reaction. Their sum gives

$$\frac{d}{dx} \left[\rho_2 U_2^2 \left(1 - \frac{\rho_1}{\rho_1 + \rho_2} \right) \right] = - \frac{dP}{dx} + \rho_1 f_1 + \rho_2 f_2 \quad (4.15)$$

comparing this to fixed particles in a passage, then we have

$$\frac{d}{dx} \rho_2 U_2^2 = - \frac{dP}{dx} + \rho_2 f_2 - \rho_2 F_{21} U_2 \quad (4.16)$$

Hence a drag force determined by free particles will be different from that determined by fixed particles. Taking the difference of Eqs. (4.15) and (4.16), the drag force ($F_{12} U_2$) acting on fixed particles corresponds to the force given by $(-f_1 - \frac{d}{dx} U_2^2)$ acting on free particles. It is to be noted that Eqs. (4.15) and (4.16) would be identical without inertial coupling effect.

Fig. 5. Counter Current Flow of Two Phases.

5.0 Discussion and Conclusion

It appears pertinent to note some accomplishments and interim conclusions at this stage. It also appears worthwhile to discuss some of the approach to numerical modeling and the needed experimental information to generate the physical parameters required in advanced numerical modeling.

5.1 Basic Equations

The basic equations of the flow field and the interface have been formulated with:

- a. Inclusion of inertial coupling terms which is significant especially to the study of transient flow in multiphase systems [28].
- b. Inclusion of concepts of multiphase mechanics dealing with mutual exclusion of phases, force and work due to displacement in space; force and work due to displacement of inter-phase boundary (compression); and energy exchange with dispersed phases [8].
- c. Introduction of the multidomain concept and the transition from a growing dispersed phase to a new domain with an interface. The numerical technique was illustrated in Harlow and Amsden [9]. Phases of diverse configurations [70,71] have to be treated as domains if a specific solution to a problem is to be obtained quantitatively.
- d. Consideration of the feasibility of transition of flow regimes via agglomeration of domains, and the pertinent boundary conditions.

5.2 Feasibility of Numerical Modeling

Numerical modeling of two-domain two-phase flow appears feasible with the formulation given in this report. Even the general multidomain-multiphase formulation is readily applicable provided there exists sufficient number of transport parameters identified in this study. Based on a two-domain two-phase formulation, it appears that we have adequate information on transport parameters for a dilute system and the numerical modeling of two-phase flow is feasible at the present time.

5.3 Transport Parameters and Experimental Efforts

We have adequate data on transport parameters of a dilute two-phase flow system to proceed with some preliminary computations. However, to conduct

general computations on reactor systems, more detailed information on transport parameters is desirable. Data in useful form can be generated via experimental studies on:

- a. Bubbles in liquid metals - Bubble cloud properties; inverse relaxation time constants M , F , G ; nucleation in terms of size, number, and velocity of bubbles; and agglomeration rate constants.
- b. Droplet generation in liquid metals - Number of Droplets generated by bursting of bubbles at an interface, their size and velocity.
- c. Interface properties - Agglomeration of domains.

5.4 Future Work Needed on Basic Formulation

For the general case of a dense dispersed phase, the terms I' and V' , i.e., the forces due to apparent mass effect and the effect of unsteadiness of flow field remain to be determined. Also, there is the need to obtain more details on the effectiveness of momentum transfer between the phases.

5.5 Concluding Remarks

Numerical modeling of a complicated two-phase flow system is a long term effort, and this modeling is visualized in stages of improved rigor and accuracy. The work presented here represents, at least in our opinion, a most rigorously derived formulation to date of the two-phase flow system.

While working toward a rational set of governing equations for general use of computer programs, the various formulations are accommodated by providing user options; user can input values of parameters K and B with the range $0 \leq K \leq 1$ and $0 \leq B \leq 1$, and either retain or discard the inertial coupling terms (I and I'). In this way, the effect of each term on system behavior can be delineated, thus, it advances basic knowledge and understanding with eventual resolution of differences via experiments.

Because of the application of multiphase mechanics formulation to the new concept of multidomain described in this report, we are most anxious to disseminate the information. The detailed mechanistic approach on transition of flow regimes will be reported at a later date. Finally, any comments and suggestions are welcomed wholeheartedly.

Appendix A

AVERAGING IN MULTIPHASE FLUID MECHANICS

The averaging procedure in the present study is simplified by averaging over a phase in a domain without crossing an interface separating it from another domain. When an interface is reached, a new domain is identified.

For a volume element V much larger than the volume of a particle in the dispersed phase, at a given time t , we have, from averaging over a volume at time t

$$\rho'_k \Big|_t = \frac{1}{V} \int_V \rho''_k(t) dV \Big|_t \quad (A-1)$$

and we have, for the momentum

$$\rho'_k U'_{kj} \Big|_t = \frac{1}{V} \int_V \rho''_k(t) U''_k(t) dV \Big|_t \quad (A-2)$$

The above integration over volume V does not cross the boundary of a domain.

Approximation via a distributed quantity ρ_k and $\rho_k U_k$ is carried out by further averaging over time τ , $\tau \gg N_k^{-1/3}/U_k^*$ where N_k is the number density of species k , $N_k^{-1/3}$ is the mean interparticle spacing and U_k^* is the characteristic velocity. We note that

$$\rho_k = \frac{1}{\tau} \int_{\tau} \rho'_k d\tau \quad (A-3)$$

while for the momentum

$$\rho_k U_{kj} = \frac{1}{\tau} \int_{\tau} \rho'_k U'_{kj} d\tau \quad (A-4)$$

Other averaging of u_k , etc. is readily seen.

Appendix B

BASIC CONSIDERATIONS OF THE FIELD EQUATIONS

B.1 Continuity Equation

With a domain, conservation of mass over a volume V in the mixture (Fig. B-1) is given by (for simplicity in notation subscript m is dropped in this appendix unless otherwise noted):

Sum of mass in, out and generation = Rate of change of mass

- (1) Rate of gain or loss of mass through all surfaces of a volume

$$\int_S \rho U_j n_j ds = \int_V \frac{\partial}{\partial x_j} (\rho U_j) dV$$

- (2) Rate of net generation of mass in a volume

$$\int_V \Gamma_e dV = 0$$

when dissolved gas and species generated via nuclear excitation is neglected.

- (3) Rate of change of mass in a volume

$$\int_V \frac{\partial \rho}{\partial t} dV$$

Conservation of mass gives

$$\int_V \frac{\partial \rho}{\partial t} dV + \int_V \frac{\partial}{\partial x_j} (\rho U_j) dV = 0 \quad (B-1)$$

Since V is arbitrary, we have the continuity equation of the mixture:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho U_j}{\partial x_j} = 0 \quad (B-2)$$

which can be expressed in the alternate form:

$$\frac{d\rho}{dt} + \rho \frac{\partial U_j}{\partial x_j} = 0 \quad (B-3)$$

which gives, for later derivations:

$$\frac{\partial U_j}{\partial x_j} = - \frac{1}{\rho} \frac{d\rho}{dt} \quad (B-4)$$

and

$$P \frac{\partial U_j}{\partial x_j} = - \frac{P}{\rho} \frac{d\rho}{dt} = P \rho \frac{d}{dt} \left(\frac{1}{\rho} \right) \quad (B-5)$$

Further, we have the relation:

$$\rho \frac{d\bar{U}_i}{dt} = \frac{\partial}{\partial t} (\rho U_i) + \frac{\partial}{\partial x_j} (\rho U_j U_i) \quad (B-6)$$

B.2 Momentum equations

B.2.1 Momentum equation of the mixture

Conservation of momentum over a volume V in the mixture (Fig. B-1) is given by: (Sum of all forces) = Rate of change of momentum.

In the i-direction (use unsubscripted quantities for the mixture) we have:

(1) Stress:

$$\int_S p_i ds = \int_S P_{ji} n_j ds = \int_V \frac{\partial p_{ji}}{\partial x_j} dV$$

where the stress p_{ji} can be expressed as:

$$p_{ji} = -P\delta_{ji} + \partial\tau_{ji}/\partial x_j \quad (B-7)$$

and P is the static pressure. τ_{ji} is the viscous stress.

(2) Body force: for force f_i per unit mass in the direction given by (Fig. B-1):

$$\int_V f_i \rho dV$$

(3) Rate of change of momentum outside of the volume:

$$\int_S U_i \rho U_j n_j ds = \int_V \frac{\partial}{\partial x_j} (\rho U_j U_i) dV$$

(4) Rate of change of momentum inside of the volume:

$$\int_V \frac{\partial(\rho U_i)}{\partial t} dV$$

Conservation of momentum gives, by summing the above effects:

$$\int_V \left[\frac{\partial p_{ji}}{\partial x_j} + f_i \rho - \frac{\partial}{\partial x_j} (\rho U_j U_i) - \frac{\partial}{\partial t} (\rho U_i) \right] dV = 0 \quad (B-8)$$

Since V is arbitrary, we have the momentum equation of the mixture (with Eq. (B-7)):

$$\begin{aligned} \frac{\partial}{\partial t} (\rho U_i) + \frac{\partial}{\partial x_j} (\rho U_j U_i) &= - \frac{\partial}{\partial x_i} P + \frac{\partial \tau_{ji}}{\partial x_j} + f_i \rho \\ &= \rho \frac{dU_i}{dt} \end{aligned} \quad (B-9)$$

the last equality by substituting its continuity equation (B-6)

B.2.2 Momentum equation of phase k

When treating a dispersed phase k in the mixture, the conservation principle is applicable with the concerns of the discrete nature of the particles and the inertial and viscous coupling to the rest of the mixture (Fig.B.2).

When stress p is applied to an area ds on the control volume V only part of it is transmitted to phase k , in proportion to its volume fraction ϕ_k . Hence

$$\int_S p_{ki} ds = \int_S p_{kji} n_j ds = \int_V \frac{\partial p_{kji}}{\partial x_j} dV$$

and

$$p_{kji} = P \phi_k \delta_{ji} + \tau_{mkji} \quad (B-10)$$

$$\frac{\partial p_{kji}}{\partial x_j} = -\phi_k \frac{\partial}{\partial x_i} P - (1-\phi_k) P \frac{\partial \phi_k}{\partial x_i} + \frac{\partial \tau_{mkji}}{\partial x_j}$$

where the first term is the force acting on the particles by the pressure gradient in the fluid (or mixture) and the second term is the force due to the compressibility (yield in volume) of the particles. τ_{mk} is the viscous stress of component k in the mixture (Appendix C). Corresponding to the previous section B.2.1, the terms are:

(1) Stress:

$$\int_S p_{ki} ds = \int \left[-\phi_k \frac{\partial}{\partial x_i} p - (1 - B_k) p \frac{\partial}{\partial x_i} \phi_k + \frac{\partial \tau_{mkji}}{\partial x_j} \right] dV$$

(2) Body force:

$$\int_V n_i f_k \rho_k dV = \int_V f_{ki} \rho_k dV$$

(3) Rate of increase of the i-th component of momentum of k outside the volume consists of $\rho_k U_{ki}$ having the area ds with normal $\hat{n}$ at velocity U_{kj} and the resistance contribution by inertia of the rest of the mixture. This resistance may take the form of the momentum of the component k relative to the mean velocity of the mixture $\rho_k (U_{ki} - U_{mi})$ at relative velocity $(U_{kj} - U_{mj})$. Note that $\rho_k (U_{ki} - U_{mi})$ is also the flux of k in the mixture and the product $\rho_k (U_{ki} - U_{mi}) (U_{kj} - U_{mj})$ is a force due to rates of change of i-th component of momentum in the j-direction.

$$\begin{aligned} & \int_S \left[\rho_k U_{ki} U_{kj} - \rho_k (U_{ki} - U_{mi}) (U_{kj} - U_{mj}) \right] n_j ds \\ &= \int_V \frac{\partial}{\partial x_j} (\rho_k U_{ki} U_{kj}) dV - \int_V \frac{\partial}{\partial x_j} \left[\rho_k (U_{ki} - U_{mi}) (U_{kj} - U_{mj}) \right] dV \\ &= \int_V \frac{\partial}{\partial x_j} (\rho_k U_{ki} U_{kj}) dV - \int_V (I_{ki} - \Gamma_k U_{mj}) dV \end{aligned}$$

$$\text{where } I_{ki} = I_{kci} + \sum_l I_{kcli} = \frac{\partial}{\partial x_j} \rho_k (U_{ki} - U_{mi}) (U_{kj} - U_{mj}) + \Gamma_k U_{mj}$$

- (4) Rate of increase of momentum inside the volume

$$\int_V \frac{\partial}{\partial t} \rho_k U_{ki} dV$$

- (5) Viscous coupling forces: V_{ki} (Sum of V_{kci} and V_{kli}), V'_{ki} (Sum of V'_{kci} and V'_{kli} , where V'_{kli} is not known)

- (6) Virtual mass forces: I'_{ki} (Sum of I'_{kci} and I'_{kli} , where I'_{kli} is not known)

- (7) Rate of removal of phase k: $\int_V (-\Gamma_k) U_{ki} dV$

Conservation of momentum gives, by summing all the above effects: (also Appendix E)

$$\int_V \left[-\phi_k \frac{\partial P}{\partial x_i} - (1 - B_k) P \frac{\partial}{\partial x_i} \phi_k + \frac{\partial \tau_{mkji}}{\partial x_j} + f_{ki} \rho_k + \sum_l I_{kli} + I_{kci} + I'_{kci} + \sum_l V_{kli} + V_{kci} + V'_{kci} - \frac{\partial}{\partial x_j} (\rho_k U_{kj} U_{ki}) - \frac{\partial}{\partial t} (\rho_k U_{ki}) + \Gamma_k U_{ki} \right] dV = 0$$

or

$$\frac{\partial}{\partial t} (\rho_k U_{ki}) + \frac{\partial}{\partial x_j} (\rho_k U_{kj} U_{ki}) - U_k \Gamma_k = -\phi_k \frac{\partial P}{\partial x_i} - (1 - B_k) P \frac{\partial}{\partial x_i} \phi_k + \frac{\partial \tau_{mkji}}{\partial x_j} + f_{ki} \rho_k + \sum_l I_{kli} + I_{kci} + I'_{kci} + \sum_l V_{kli} + V_{kci} + V'_{kci} \quad (B-11)$$

where I_{kci} and I_{kli} are given in Appendix D.

B.2.3 Effectiveness of momentum transfer

The effectiveness of momentum transfer from the particle to the fluid arises from the dissipation by the wake of a particle in the fluid. This effectiveness K is given by the mixture momentum equation in the form (take one k species only):

$$\rho_c \frac{dU_{ci}}{dt_c} + K_k \rho_k \frac{dU_{ki}}{dt_k} = - \frac{\partial P}{\partial x_i} + \frac{\partial \tau_{ji}}{\partial x_j} + f_i^p + K_k (I_{kci} + I_{cki}) + - K_k (\Gamma_k U_{ki} + \Gamma_c U_{ci})$$

(B-12)

Where $K_k = 1$ for accelerating flow with F defined as the force acting on the particle, while the drag force 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 encountered by the particle while $(1-K_k)$ fraction of the force produces only random motion in the wake. This is diagrammatically illustrated in Table B-1. Also shown in Table B-1 is the distribution of work dissipated by this relative motion. This consideration is also applicable to the dissipation of unsteady motion. V' , as well as I and I' because only fraction K_k of the momentum of particles is transmitted to the fluid excluding the random motion set in the wakes of particles. [21]

Table B.1

Force and Work Relations between the continuous phase and the dispersed phase - irreversibility of wake flow.

	Accelerating Flow $K=1$	Decelerating Flow $K \leq 1$
Drag Force	Force acting on fluid and wake $F_m (U_c - U_k)$	Force acting on particle $F_m (U_c - U_k)$
Force acting on particle *
Work	<div>Work done by fluid $U_c F_m (U_c - U_k)$</div> <div>Work done by particle $U_k F_m (U_c - U_k)$</div>	<div>Work done by fluid $U_c K F_m (U_c - U_k)$</div> <div>Work done by particle $U_k F_m (U_c - U_k)$</div>
Work dissipated in fluid	$= F_m (U_c - U_k)^2$	$= F_m (U_c - U_k)^2$ Work dissipated in fluid wake $U_c (1-K) F_m (U_c - U_k)$

$$\frac{1}{N_k} V_{kc} = F_m (U_c - U_k)$$

$\frac{1}{N_k} V_{kc}$ can be replaced by $\frac{1}{N_k} V'_{kc}$ and $\frac{1}{N_k} I'_{kc}$ for drag and work relations of the latter.

* F is determined by the drag force acting on a stationary particle.

B.2.4 Case of a single solid particle

In the case of a single solid particle in a flowing incompressible fluid, Eq. (2.16) gives, with $\phi_k = \text{constant}$, $\Gamma_k = 0$, $\bar{\rho}_k = \text{constant}$:

$$m_k \frac{dU_k}{dt_k} = - \frac{m_k}{\rho_k} \nabla P + m_k f_k + \frac{m_k}{\rho_k} I_k + m_k \frac{V_k}{\rho_k} + m_k \frac{I'_k}{\rho_k} + m_k \frac{V'_k}{\rho_k} \quad (B.13)$$

We note that all the terms are as assembled by Tchen cited in [71] except the term:

$$\frac{m_k}{\rho_k} I_k = \frac{m_k}{\phi_k \rho_k} \nabla \cdot \bar{\rho}_k \phi_k (U_k - U_m) \cdot (U_k - U_m) = m_k \nabla (U_k - U_c) \cdot (U_k - U_c) \quad (B.14)$$

The last equality is because $U_m \sim U_c$. It is also readily shown that the motion of the fluid phase is unaffected by the presence of a single solid particle ($\phi_k \rightarrow 0$) as Eq. (2.17) reduces to:

$$\bar{\rho}_c \frac{dU_c}{dt_c} = - \nabla P + \nabla \cdot \tau_c + \bar{\rho}_c f_c \quad (B.15)$$

Note that the term in Eq. (B.14) did not appear in Tchen's formulation [72].

B.3 Energy equations

An outstanding feature of multiphase mechanics is that each particle of the dispersed phase may consist of many millions of molecules and the motion of the dispersed phase arises from the drag force of the continuous phase. Hence the kinetic energy of the dispersed phase is really part of the kinetic energy of the continuous phase; the state of each particle of the dispersed phase is affected directly by its displacement and shear motion through the continuous phase, its change of kinetic energy, and dissipation via relative motions affect its state via heat transfer coupling with the continuous phase. Conversely, the change of thermal state of a particle affects its motion via transferring heat to the continuous phase.

Hence it is important to identify separately the effects that produce changes in the kinetic energy of the system and those producing changes in the thermal state of the system.

B.3.1 Energy equation of the mixture

The kinetic energy of the mixture is given by:

$$\rho \frac{d}{dt} \left(\frac{U_j^2}{2} \right) = \rho f_j U_j - U_j \frac{\partial}{\partial x_j} P \delta_{ji} + U_j \frac{\partial \tau_{ji}}{\partial x_j}$$

$$\begin{aligned}
 &= \rho f_j U_j - \frac{\partial}{\partial x_j} U_j P + P \frac{\partial U_j}{\partial x_j} + \frac{\partial}{\partial x_j} U_j \tau_{ji} - \tau_{ji} \frac{\partial U_j}{\partial x_j} \\
 &= \left[\rho f_j U_j - \frac{\partial}{\partial x_j} U_j P + \frac{\partial}{\partial x_j} U_j \tau_{ji} \right] - \left[\tau_{ji} \frac{\partial U_j}{\partial x_j} \right] - \left[P \frac{1}{\rho} \frac{d\rho}{dt} \right] \quad (B.16)
 \end{aligned}$$

The last two terms of Eq. (B.16) resulted from using Eq. (B.5).

which reads:

$$\left[\begin{array}{c} \text{Rate of Change} \\ \text{in kinetic} \\ \text{energy} \end{array} \right] = \left[\begin{array}{c} \text{Work against} \\ \text{fluid re-} \\ \text{sistance} \end{array} \right] - \left[\begin{array}{c} \text{Dissipation} \\ \text{by friction} \end{array} \right] + \left[\begin{array}{c} \text{Work of} \\ \text{compression} \end{array} \right]$$

The thermal energy of the mixture is given by the first law of thermodynamics in the form:

$$\begin{aligned}
 \rho \frac{du}{dt} - \frac{P d\rho}{\rho dt} &= \left[\tau_{ji} \frac{\partial U_j}{\partial x_j} \right] + \left[\sum_k \rho_k F_{kc} (U_{cj} - U_{kj})^2 + \sum_k \sum_l \rho_l F_{lk} (U_{kj} - U_{lj})^2 + \sum_k L'_k \right] \\
 &+ \left[- \frac{\partial}{\partial x_j} J_{-m} \right] + \left[J_{Em} \right] \quad (B.17)
 \end{aligned}$$

which reads:

$$\left[\begin{array}{c} \text{Rate of Change} \\ \text{in Internal} \\ \text{energy} \end{array} \right] - \left[\begin{array}{c} \text{Work of} \\ \text{compression} \end{array} \right] = \left[\begin{array}{c} \text{Heat from} \\ \text{dissipation} \end{array} \right] + \left[\begin{array}{c} \text{Dissipation by} \\ \text{relative motion} \end{array} \right] \\
 + \left[\begin{array}{c} \text{Heat} \\ \text{conducted} \end{array} \right] + \left[\begin{array}{c} \text{Heat} \\ \text{generated} \end{array} \right]$$

The mechanism of dissipation by internal relative motion within the mixture is seen in that from the momentum equation (Table B-1):

$$\text{Work done by the particle on the fluid} = - U_k (V_{kc} + V'_{kc} + I'_{kc})$$

$$\text{Work done by the fluid} = U_c K_k (V_{kc} + V'_{kc} + I'_{kc})$$

$$\text{Energy dissipated in the wakes of particles} = U_c (1 - K_k) (V_{kc} + V'_{kc} + I'_{kc})$$

Their sum gives the dissipation due to relative internal motion:

$$(U_c - U_k) (V_{kc} + V'_{kc} + I'_{kc}) = (U_c - U_k) (V_{kc}) + L'_k$$

Similarly this dissipation for relative motion between the dispersed phases is given by

$$\rho_l F_{lk} (U_k - U_l) \text{ although } V'_k \text{ and } I'_k \text{ are not known.}$$

The sum of Eqs. (B.16) and (B.17) gives:

$$\begin{aligned}
 \rho \frac{d}{dt} \left(u + \frac{U_j^2}{2} \right) &= - \frac{\partial}{\partial x_j} U_j P + \frac{\partial}{\partial x_j} U_j \tau_{ji} + \rho f_j U_j - \frac{\partial}{\partial x_j} J_{mj} + J_{Em} \\
 &+ \sum_k \rho_k F_{kc} (U_{ij} - U_{kj})^2 + \sum_k \sum_l \rho_l F_{lk} (U_{kj} - U_{lj})^2 + \sum_k L'_k \quad (B.18)
 \end{aligned}$$

This is converted to an expression in terms of enthalpy via the following relation:

$$\begin{aligned}
 \rho \frac{du}{dt} &= \rho \frac{dh}{dt} - \rho \frac{d}{dt} \left(\frac{P}{\rho} \right) \\
 &= \rho \frac{dh}{dt} - \rho \left[\frac{1}{\rho} \frac{dP}{dt} - \frac{P}{\rho^2} \frac{d\rho}{dt} \right] \\
 &= \rho \frac{dh}{dt} - \frac{\partial P}{\partial t} - U_j \frac{\partial P}{\partial x_j} - \frac{P}{\rho} \rho \frac{\partial U_j}{\partial x_j} \\
 &= \rho \frac{dh}{dt} - \frac{\partial P}{\partial t} - \frac{\partial}{\partial x_j} P U_j
 \end{aligned} \tag{B-19}$$

Hence the overall energy equation can be given in terms of enthalpy, or^{*}

$$\begin{aligned}
 \rho \frac{d}{dt} \left(h + \frac{U_j^2}{2} \right) &= \frac{\partial P}{\partial t} + \frac{\partial}{\partial x_j} U_j \tau_{ji} + \rho f_j U_j + \frac{\partial}{\partial x_j} \kappa_m \frac{\partial T}{\partial x_j} + J_{Em} \\
 &\quad + \sum_k \rho_k F_{kc} (U_{cj} - U_{kj})^2 + \sum_k \sum_\ell \rho_\ell F_{\ell k} (U_{kj} - U_{\ell j})^2 + L'_c \\
 &= \rho \frac{dH}{dt} = \frac{\partial}{\partial t} \rho H + \frac{\partial}{\partial x_j} \rho U_j H
 \end{aligned} \tag{B-20}$$

where (Table B-2) (expressing components k and c separately)

$$\begin{aligned}
 \frac{\partial P}{\partial t} &= \frac{\partial}{\partial t} \left(\sum_k \phi_k + \phi_c \right) P = \sum_k \frac{\partial \phi_k P}{\partial t} + \frac{\partial \phi_c P}{\partial t} \\
 &= \sum_k \phi_k \frac{\partial P}{\partial t} + P \sum_k \frac{\partial \phi_k}{\partial t} + \phi_c \frac{\partial P}{\partial t} + P \frac{\partial \phi_c}{\partial t}, \phi_c + \sum_k \phi_k = 1
 \end{aligned} \tag{B-21}$$

$$P \frac{\partial \phi_c}{\partial t} = - P \sum_k \frac{\partial \phi_k}{\partial t} \tag{B-22}$$

which states that the fluid c is undergoing expansion if the phases are compressed. $\phi_k \frac{\partial P}{\partial t}$ includes the work due to displacement of k through c; its displacement includes that of a particle into and out of a control volume such as shown in Fig. (B-2).

* An alternate form, from substitution of momentum Eq. (B-9) is [83]

$$\rho \frac{dh}{dt} = \frac{dP}{dt} + \tau_{ji} \frac{\partial U_i}{\partial x_j} + \dots$$

Table B.2
Effects of Pressure in Multiphase System

Force

$$-P\Delta\phi + B P \Delta\phi$$

Compression or Expansion Minus
Force at Phase Boundary

Pressure
Gradient

$$-\phi \nabla P$$

Displacement

Work
(in E
Eq.)

$$P \delta \phi$$

Change of Thermal State
of Particle

$$\phi \delta P$$

Change of Thermal
State of Fluid
(Displacement work)

A corresponding consideration of energy balance of a control volume V in a similar manner of making this momentum balance gives (Fig. B-1):

(1) Rate of change of energy outside of the volume:

$$\int_s \rho E U_j n_j ds = \int_V \frac{\partial}{\partial x_j} \rho E U_j dV$$

(2) Rate of accumulation in the inside:

$$\int_V \frac{\partial}{\partial t} \rho E dV$$

(3) Heat transferred to the outside:

$$\int_s J_{mj} n_j ds = \int_V \frac{\partial}{\partial x_j} J_{mj} dV$$

(4) The work done:

$$-\int_s U_i p_i ds = -\int_V \frac{\partial}{\partial x_j} U_i p_{ji} dV$$

Overall balance gives:

$$\rho \frac{dE}{dt} + \frac{\partial J_{mj}}{\partial x_j} - \frac{\partial}{\partial x_j} (U_i p_{ji}) = 0$$

which is reducible to Eq. (B.18) by identifying the details.

When applied to species k (Fig. B-2), we get, in place of item (1)

$$\int_s \left[\rho_k E_k U_{kj} - \rho_k (U_{kj} - U_{mj})(E_k - E_m) \right] n_j ds$$

where the second term is the decrease in energy flux due to relative motion given by the difference in velocity $U_{kj} - U_{mj}$, corresponding to the inertial coupling. The energy flux phase k through the surface of a mixture domain B is reduced by the amount of a drift energy flux. The overall energy flux is then given by:

$$\sum_{k,c} \rho_k U_{mj} E_k = \rho_m U_{mj} E_m, \text{ because } \sum_{k,c} \rho_k E_k = \rho_m E_m.$$

B.3.2 Energy Equations of Phase k

The thermal state of the dispersed phase is affected by the fluid energy only through heat transfer coupling:

$$Q_{kc} = c_{vk} \rho_k G_{kc} (T_c - T_k) \quad (B-23)$$

and

$$Q_{k\ell} = c_{vk} \rho_k \sum_{\ell} G_{k\ell} (T_{\ell} - T_k) \quad (B-24)$$

The thermal state of the dispersed phase k is therefore (with Eqs. (B-13), B-23) and (B-24))

$$\frac{\partial}{\partial t} \rho_k h_k + \frac{\partial}{\partial x_j} \rho_k U_{kj} h_k = \frac{\partial}{\partial x_j} \kappa_{mk} \frac{\partial T_k}{\partial x_j} + J_{Ek} + \phi_k \frac{\partial P}{\partial t} + L_{kh} + Q_k \quad (B-25)$$

where

$$Q_k = Q_{kc} + \sum_{\ell} Q_{k\ell} \quad (B-26)$$

which is the same as Eq. (2.31). Subtracting the sum of all kth Eq. (B-25)

from the overall energy equation gives Eq. (2.32). Note that thermal coupling relations verify that

$$Q_c + \sum_k Q_{kc} = 0 \quad (B-27)$$

$$\sum_k \sum_{\ell} Q_{k\ell} = 0 \quad (B-28)$$

where Q_c is the energy transferred to the continuous phase.

Derivation of Eq. (2.32) can be made as follows:

$$\begin{aligned}
 & \sum_k \left[\frac{\partial}{\partial t} \rho_k H_k - \frac{\partial}{\partial t} \rho_k \frac{U_{kj}^2}{2} + \frac{\partial}{\partial x_j} \rho_k U_{kj} H_k - \frac{\partial}{\partial x_j} \rho_k U_{kj} \frac{U_{kj}^2}{2} \right] \\
 = & -\phi_c \frac{\partial P}{\partial t} + \frac{\partial}{\partial x_j} \kappa_m \frac{\partial T_m}{\partial x_j} - \frac{\partial}{\partial x_j} \kappa_{mc} \frac{\partial T_c}{\partial x_j} + \\
 & \sum_k \left[\frac{\partial}{\partial x_j} \rho_k (H_k - H_m) (U_{kj} - U_{mj}) - \frac{\partial}{\partial x_j} \rho_k \left(\frac{U_{kj}^2}{2} - \frac{U_{mj}^2}{2} \right) (U_{kj} - U_{mj}) \right] + \Gamma_k (H_m - \frac{U_{mj}^2}{2}) \\
 & + J_{Ek} - J_{Ec} + \sum_k Q_{kc} + \sum_k \sum_\ell Q_{k\ell} \tag{B-29}
 \end{aligned}$$

The last two terms are simplified according to Eqs. (B-27) (B-28).

Subtracting Eq. (B-29) in Eq. (B-20) in the form (with separate identification of phase c):

$$\begin{aligned}
 & \frac{\partial}{\partial t} \rho H + \frac{\partial}{\partial x_j} \rho U_j H \\
 = & \frac{\partial}{\partial t} \rho_c H_c + \frac{\partial}{\partial x_j} \rho_c U_{cj} H_c + \sum_k \frac{\partial}{\partial t} \rho_k H_k + \sum_k \frac{\partial}{\partial x_j} \rho_k U_{kj} H_k \\
 & - \frac{\partial}{\partial x_j} \rho_c (H_c - H_m) (U_{cj} - U_{mj}) - \sum_k \frac{\partial}{\partial x_j} \rho_k (H_k - H_m) (U_{kj} - U_{mj})
 \end{aligned}$$

gives

$$\begin{aligned}
 & \frac{\partial}{\partial t} \left[\rho_c H_c + \sum_k \rho_k \frac{U_{kj}^2}{2} \right] + \frac{\partial}{\partial x_j} \left[\rho_c U_{cj} H_c + \sum_k \rho_k U_{kj} \frac{U_{kj}^2}{2} \right] = \\
 & \phi_c \frac{\partial P}{\partial t} + \frac{\partial}{\partial x_j} \kappa_{mc} \frac{\partial T_c}{\partial x_j} + \frac{\partial}{\partial x_j} \left[\rho_c (H_c - H_m) (U_{cj} - U_{mj}) + \sum_k \rho_k \left(\frac{U_{kj}^2}{2} - \frac{U_{mj}^2}{2} \right) (U_{kj} - U_{mj}) \right] \\
 & + \Gamma_c h_m + J_{Ec} + \sum_k \rho_k F_{kc} (U_{ij} - U_{kj})^2 + \sum_k \sum_\ell \rho_\ell F_{\ell k} (U_{kj} - U_{\ell j})^2 + L'_c \\
 & + Q'_c + \rho_m f_{mj} U_{mj}
 \end{aligned}$$

which is Eq. (2.32) in terms of tensorial components.

Appendix C

DERIVATIVES IN TERMS OF CENTER OF MASS OF PHASES

(k's Denote Components in a Mixture)

Δ_{ji} denotes shear tensor and is given by ($i \neq j$)

$$\Delta_{ji} = \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \quad (C-1)$$

For the mixture, we have,

$$\Delta_{mji} = \frac{\partial U_{mi}}{\partial x_j} + \frac{\partial U_{mj}}{\partial x_i} \quad (C-2)$$

$$\begin{aligned} \frac{\partial U_{mi}}{\partial x_j} &= \sum_k \left\{ \frac{\rho_k}{\rho_m} \frac{\partial U_{ki}}{\partial x_j} + U_{ki} \frac{\partial}{\partial x_j} \left(\frac{\rho_k}{\rho_m} \right) \right\} \\ &= \sum_k \left\{ \frac{\rho_k}{\rho_m} \frac{\partial U_{ki}}{\partial x_j} + \frac{U_{ki}}{\rho_m} \frac{\partial \rho_k}{\partial x_j} - \frac{U_{ki} \rho_k}{\rho_m^2} \frac{\partial \rho_m}{\partial x_j} \right\} \\ &= \sum_k \left\{ \frac{\rho_k}{\rho_m} \frac{\partial U_{ki}}{\partial x_j} + \frac{U_{ki} - U_{mi}}{\rho_m} \frac{\partial \rho_k}{\partial x_j} + \frac{U_{mi}}{\rho_m} \frac{\partial \rho_k}{\partial x_j} - \frac{U_{ki} \rho_k}{\rho_m^2} \frac{\partial \rho_m}{\partial x_j} \right\} \\ &= \sum_k \left\{ \frac{\rho_k}{\rho_m} \frac{\partial U_{ki}}{\partial x_j} + \frac{U_{ki} - U_{mi}}{\rho_m} \frac{\partial \rho_k}{\partial x_j} \right\} + \frac{U_{mi}}{\rho_m} \frac{\partial \rho_m}{\partial x_j} - \frac{U_{mi} \rho_m}{\rho_m^2} \frac{\partial \rho_m}{\partial x_j} \end{aligned} \quad (C-3)$$

$$\Delta_{mji} = \frac{1}{\rho_m} \sum_k \rho_k \Delta_{kji} + \frac{1}{\rho_m} \sum_k \left\{ (U_{ki} - U_{mi}) \frac{\partial \rho_k}{\partial x_j} + (U_{kj} - U_{mj}) \frac{\partial \rho_k}{\partial x_i} \right\} \quad (C-4)$$

Alternately, let $J_{ki} = \rho_k (U_{ki} - U_{mi})$

$$\begin{aligned} \Delta_{mji} &= \sum_k \frac{\rho_k}{\rho_m} \Delta_{kji} + \frac{1}{\rho_m} \sum_k \left\{ \frac{\partial}{\partial x_j} \rho_k (U_{ki} - U_{mi}) - \rho_k \frac{\partial}{\partial x_j} (U_{ki} - U_{mi}) \right. \\ &\quad \left. + \frac{\partial}{\partial x_i} \rho_k (U_{kj} - U_{mj}) - \rho_k \frac{\partial}{\partial x_i} (U_{kj} - U_{mj}) \right\} \\ &= \sum_k \frac{\rho_k}{\rho_m} \Delta_{kji} + \frac{1}{\rho} \sum_k \left(\frac{\partial J_{ki}}{\partial x_j} + \frac{\partial J_{kj}}{\partial x_i} \right) - \frac{1}{\rho_m} \sum_k \rho_k \left(\frac{\partial U_{ki}}{\partial x_j} + \frac{\partial U_{kj}}{\partial x_i} \right) \\ &\quad + \frac{1}{\rho_m} \sum_k \rho_k \left(\frac{\partial U_{mi}}{\partial x_j} + \frac{\partial U_{mj}}{\partial x_i} \right) \end{aligned}$$

$$= \sum_k \left\{ \frac{\rho_k}{\rho_m} \Delta_{kji} + \frac{1}{\rho} \left(\frac{\partial J_{ki}}{\partial x_j} + \frac{\partial J_{kj}}{\partial x_i} \right) \right\} \quad (C-5)$$

Temperature Gradient: For notational simplicity c denotes c_v

$$\rho_m c_m T_m + \rho_m \frac{U_m^2}{2} = \sum_k \left[\rho_k c_k T_k + \rho_k \frac{U_k^2}{2} \right] \quad (C-6)$$

$$\begin{aligned} T &= \sum_k \frac{\rho_k c_k}{\rho_m c_m} T_k + \frac{1}{2\rho_m c_m} \left[\sum_k (\rho_k U_{ki}^2) - \rho_m U_{mi}^2 \right] \\ &= \frac{1}{\rho_m c_m} \left\{ \sum_k \rho_k c_k T_k + \frac{1}{2} \sum_k \rho_k (U_{ki}^2 - U_{mi}^2) U_{ki} \right\} \\ &= \frac{1}{\rho_m c_m} \left\{ \sum_k \rho_k c_k T_k + \frac{1}{2} \sum_k \rho_k (U_{ki} - U_{mi}) \cdot U_{ki} \right\} \\ &= \frac{1}{\rho_m c_m} \left\{ \sum_k \rho_k c_k T_k + \frac{1}{2} \sum_k U_{ki} \cdot J_{ki} \right\} \end{aligned} \quad (C-7)$$

$$\frac{\partial T}{\partial x_j} = \sum_k \left\{ \frac{\rho_k c_k}{\rho_m c_m} \frac{\partial T_k}{\partial x_j} + T_k \frac{\partial}{\partial x_j} \left(\frac{\rho_k c_k}{\rho_m c_m} \right) + \frac{\partial}{\partial x_j} (U_{ki} J_{ki} / 2\rho_m c_m) \right\} \quad (C-8)$$

Shear Stress:

For a mixture

$$\mu_m \Delta_{mji} = \sum_k \mu_m \frac{\rho_k}{\rho_m} \Delta_{kji} + \sum_k \mu_m \frac{\rho_k}{\rho_m} \left[(U_{ki} - U_{mi}) \frac{\partial \ln \rho_k}{\partial x_j} + (U_{kj} - U_{mj}) \frac{\partial \ln \rho_k}{\partial x_i} \right]$$

In general

$$\tau_{mji} = \sum_k \tau_{kji} \equiv \sum_k (\mu_{mk} \Delta_{kji} + \mu_{mk}^* \theta_k) \quad (C-9)$$

which defines the viscosity of phase k (phase c) in the mixture. μ_{mk} is not a mole-

Heat Flux: cular property in general.

For Mixture

$$\kappa_{mk} \frac{\partial T}{\partial x_j} = \sum_k \left\{ \kappa_m \frac{\partial}{\partial x_j} \left(\frac{\rho_k c_k}{\rho_m c_m} T_k \right) + \kappa_m \frac{\partial}{\partial x_j} \frac{\rho_k U_{kj} (U_{kj} - U_{mj})}{2 \rho_m c_m} \right\} \quad (C-10)$$

where

$$J_{mji} = \sum_k J_{kji} \quad (C-11)$$

$$J_{kji} = \kappa_m \frac{\partial}{\partial x_j} \left(\frac{\rho_k c_k}{\rho_m c_m} T_k \right) + \kappa_m \frac{\partial}{\partial x_j} \frac{\rho_k U_{kj} (U_{kj} - U_{mj})}{2 \rho_m c_m} \equiv \kappa_{mk} \frac{\partial}{\partial x_j} T_k \quad (C-13)$$

which defines the thermal conductivity of phase k in the mixture. κ_{mk} is, in general, not a molecular property.

Appendix D

DERIVATION OF DYNAMIC TERMS OF PHASES TO THOSE OF OVERALL MIXTURE

(k's Denote Components in a Mixture)

When treating the dynamics of a mixture, the barycentric frame of reference specifies

$$\rho_m = \sum_k \rho_k \quad (D-1)$$

$$\rho_m U_{mi} = \sum_k \rho_k U_{ki} \quad (D-2)$$

$$\rho_m E_m = \sum_k \rho_k E_k \quad (D-3)$$

where ρ , U and E denote densities, velocities, and energies, respectively; subscripts m and k denote mixture and phase k , respectively. The relations for the inertia force $\rho_m dU_m/dt_m$ and change of energy $\rho_m dE_m/dt_m$ of the mixture were given in Reference [21]. New derivations, although straight-forward, have not been published before. They are now given, together with their application to a two-phase system. Note that the main point of attention is that for a mixture

$$\frac{d}{dt_m} = \frac{\partial}{\partial t} + U_{mj} \frac{\partial}{\partial x_j} \quad (D-4)$$

which for each phase

$$\frac{d}{dt_k} = \frac{\partial}{\partial t} + U_{kj} \frac{\partial}{\partial x_j} \quad (D-5)$$

D.1 Inertial Force

We drop the subscript (m) when referring to the mixture.

$$\rho \frac{dU_i}{dt} = \rho \frac{\partial U_i}{\partial t} + \rho U_j \frac{\partial U_i}{\partial x_j} \quad (D-6)$$

$$\begin{aligned} \rho \frac{\partial U_i}{\partial t} &= \frac{\partial}{\partial t} (\rho U_i) - U_i \frac{\partial \rho}{\partial t} = \sum_k \frac{\partial}{\partial t} (\rho_k U_{ki}) - U_i \frac{\partial}{\partial t} \sum_k \rho_k \\ &= \sum_k \rho_k \frac{\partial U_{ki}}{\partial t} + \sum_k U_{ki} \frac{\partial \rho_k}{\partial t} - \sum_k U_i \frac{\partial \rho_k}{\partial t} \\ &= \sum_k \rho_k \frac{\partial U_{ki}}{\partial t} + \sum_k (U_{ki} - U_i) \frac{\partial \rho_k}{\partial t} \end{aligned} \quad (D-7)$$

$$\begin{aligned}
 \rho U_j \frac{\partial U_i}{\partial x_j} &= U_j \frac{\partial \rho U_i}{\partial x_j} - U_j U_i \frac{\partial \rho}{\partial x_j} = U_j \frac{\partial}{\partial x_j} \sum_k \rho_k U_{ki} - U_i U_j \frac{\partial}{\partial x_j} \sum_k \rho_k \\
 &= U_j \sum_k \rho_k \frac{\partial U_{ki}}{\partial x_j} + U_j \sum_k U_{ki} \frac{\partial \rho_k}{\partial x_j} - U_j \sum_k U_i \frac{\partial \rho_k}{\partial x_j} \\
 &= \sum_k (U_j - U_{kj}) \rho_k \frac{\partial U_{ki}}{\partial x_j} + \sum_k U_{kj} \rho_k \frac{\partial U_{ki}}{\partial x_j} + U_j \sum_k (U_{ki} - U_i) \frac{\partial \rho_k}{\partial x_j} \\
 &= \sum_k \rho_k U_{kj} \frac{\partial U_{ki}}{\partial x_j} - \sum_k (U_{kj} - U_j) \rho_k \frac{\partial (U_{kj} - U_i)}{\partial x_j} - \sum_k (U_{kj} - U_j) \rho_k \frac{\partial U_i}{\partial x_j} \\
 &\quad - \sum_k (U_{kj} - U_j) (U_{ki} - U_i) \frac{\partial \rho_k}{\partial x_j} + \sum_k U_{kj} (U_{ki} - U_i) \frac{\partial \rho_k}{\partial x_j} \\
 &= \sum_k \rho_k U_{kj} \frac{\partial U_{ki}}{\partial x_j} - \sum_k (U_{kj} - U_j) \frac{\partial}{\partial x_j} \rho_k (U_{ki} - U_i) + \sum_k U_{kj} (U_{ki} - U_i) \frac{\partial \rho_k}{\partial x_j} \\
 &= \sum_k \rho_k U_{kj} \frac{\partial U_{ki}}{\partial x_j} - \sum_k (U_{kj} - U_j) \frac{\partial}{\partial x_j} [\rho_k (U_{ki} - U_i)] + \sum_k (U_{ki} - U_i) \frac{\partial \rho_k U_{kj}}{\partial x_j} \\
 &\quad - \sum_k \rho_k (U_{ki} - U_i) \frac{\partial}{\partial x_j} (U_{kj} - U_j) - \sum_k \rho_k (U_{ki} - U_i) \frac{\partial U_i}{\partial x_j} \quad (D-8)
 \end{aligned}$$

with $\rho_k \frac{dU_{ki}}{dt_k} = \rho_k \frac{\partial U_{ki}}{\partial t} + \rho_k U_{kj} \frac{\partial U_{ki}}{\partial x_j}$, we get

$$\rho \frac{dU_i}{dt} = \sum_k \left\{ \rho_k \frac{dU_{ki}}{dt_k} + (U_{ki} - U_i) \Gamma_k - \frac{\partial}{\partial x_j} \rho_k (U_{ki} - U_i) (U_{kj} - U_j) \right\} \quad (D-9)$$

Hence $\Gamma_{ki} = \frac{\partial}{\partial x_j} \rho_k (U_{ki} - U_i) (U_{kj} - U_j) + (U_i - U_{ki}) \Gamma_k$ gives inertial coupling of species k in the mixture when inertia force per unit volume is used in the momentum equation.

D.2 Energy Relations

$$\begin{aligned}
 \rho \frac{d}{dt} \left(\frac{U_i^2}{2} \right) &= \rho U_i \frac{dU_i}{dt} = \sum_k U_i \left[\rho_k \frac{dU_{ki}}{dt_k} + (U_{ki} - U_i) \Gamma_k - \frac{\partial}{\partial x_j} \rho_k (U_{ki} - U_i) (U_{kj} - U_j) \right] \\
 &= \sum_k \left\{ U_{ki} \rho_k \frac{dU_{ki}}{dt_k} - (U_{ki} - U_i) \rho_k \frac{d(U_{ki} - U_i)}{dt_k} - (U_{ki} - U_i) \rho_k U_i \frac{dU_i}{dt_k} \right. \\
 &\quad \left. + U_i (U_{ki} - U_i) \Gamma_k - U_i \frac{\partial}{\partial x_j} \rho_k (U_{ki} - U_i) (U_{kj} - U_j) \right\}
 \end{aligned}$$

$$\begin{aligned}
 &= \sum_k \left\{ \rho_k \frac{d}{dt_k} \left(\frac{U_{ki}^2}{2} \right) - \rho_k \frac{d}{dt_k} \left(\frac{U_{ki} - U_i}{2} \right)^2 - (U_{ki} - U_i) \rho_k U_i \frac{dU_i}{dt_k} + U_i (U_{ki} - U_i) \Gamma_k \right. \\
 &\quad - (U_{ki} - U_i) \rho_k U_j (U_{kj} - U_j) \frac{\partial U_i}{\partial x_j} - (U_{ki} - U_i) \rho_k U_i U_j \frac{\partial U_i}{\partial x_j} - U_i \frac{\partial}{\partial x_j} \rho_k \\
 &\quad \left. (U_{ki} - U_i) (U_{kj} - U_j) \right\} \\
 &= \sum_k \left\{ \rho_k \frac{d}{dt_k} \left(\frac{U_{ki}^2}{2} \right) - \rho_k \frac{d}{dt_k} \left(\frac{U_{ki} - U_i}{2} \right)^2 + U_i (U_{ki} - U_i) \Gamma_k \right. \\
 &\quad \left. - \frac{\partial}{\partial x_j} U_i \rho_k (U_{ki} - U_i) (U_{kj} - U_j) \right\} \quad (D-10)
 \end{aligned}$$

Further $E = u + \frac{U_i^2}{2}$

$$\begin{aligned}
 \rho \frac{dE}{dt} &= \rho \frac{\partial E}{\partial t} + \rho U_j \frac{\partial E}{\partial x_j} = \frac{\partial \rho E}{\partial t} - E \frac{\partial \rho}{\partial t} + \frac{\partial \rho U_j E}{\partial x_j} - E \frac{\partial \rho U_j}{\partial x_j} \\
 &= \frac{\partial \rho E}{\partial t} + \frac{\partial}{\partial x_j} \rho U_j E \\
 &= \frac{\partial}{\partial t} \sum_k \rho_k E_k - \frac{\partial}{\partial x_j} \sum_k \rho_k E_k (U_{kj} - U_j) + \frac{\partial}{\partial x_j} \sum_k U_{kj} \rho_k E_k \\
 &= \sum_k \left\{ \rho_k \frac{\partial}{\partial t} E_k + E_k \frac{\partial \rho_k}{\partial t} + \rho_k U_{kj} \frac{\partial}{\partial x_j} E_k + E_k \frac{\partial \rho_k U_{kj}}{\partial x_j} - \frac{\partial}{\partial x_j} \rho_k (U_{kj} - U_j) E_k \right\} \\
 &= \sum_k \left\{ \rho_k \frac{dE_k}{dt_k} + (E_k - E) \Gamma_k - \frac{\partial}{\partial x_j} \rho_k (E_k - E) (U_{kj} - U_j) \right\} \quad (D-11)
 \end{aligned}$$

or substituting $H = E + \frac{P}{\rho}$ we get

$$\rho \frac{dH}{dt} = \rho \frac{\partial H}{\partial t} + \rho U_j \frac{\partial H}{\partial x_j} = \sum_k \left\{ \rho_k \frac{dH_k}{dt} + (H_k - H) \Gamma_k - \frac{\partial}{\partial x_j} \rho_k (H_k - H) (U_{kj} - U_j) \right\}$$

referring to the change of H_k from H . (D-12)

D.3 Two-Phase System

When applied to a two-phase system, $k = 1, 2$

$$\rho_m = \rho_1 + \rho_2 \quad (D-13)$$

$$\rho_m U_m = \rho_1 U_1 + \rho_2 U_2 = (\rho_1 + \rho_2) U_m \quad (D-14)$$

Hence we get for all terms in the form $U_k - U_m$

$$U_1 - U_m = \frac{\rho_1 U_1 + \rho_2 U_1 - \rho_1 U_1 - \rho_2 U_2}{(\rho_1 + \rho_2)} = \frac{\rho_2 (U_1 - U_2)}{(\rho_1 + \rho_2)} \quad (D-15)$$

and

$$U_2 - U_m = \frac{\rho_1 (U_2 - U_1)}{(\rho_1 + \rho_2)} \quad (D-16)$$

thus for $\Gamma_2 = -\Gamma_1$, we get

$$\begin{aligned} \rho_m \frac{dU_{mi}}{dt_m} &= \rho_1 \frac{dU_{1i}}{dt_1} + \frac{\rho_2}{\rho_1 + \rho_2} (U_{1i} - U_{2i}) \Gamma_1 - \frac{\partial}{\partial x_j} \frac{\rho_1 \rho_2^2}{(\rho_1 + \rho_2)^2} (U_{1i} - U_{2i}) (U_{1j} - U_{2j}) \\ &+ \rho_2 \frac{dU_{2i}}{dt_2} + \frac{\rho_1}{\rho_1 + \rho_2} (U_{2i} - U_{1i}) \Gamma_2 - \frac{\partial}{\partial x_j} \frac{\rho_2 \rho_1^2}{(\rho_1 + \rho_2)^2} (U_{2i} - U_{1i}) (U_{2j} - U_{1j}) \\ &= \rho_1 \frac{dU_{1i}}{dt_1} + \rho_2 \frac{dU_{2i}}{dt_2} + (U_{1i} - U_{2i}) \Gamma_1 - \frac{\partial}{\partial x_j} \left[\frac{\rho_1 \rho_2}{(\rho_1 + \rho_2)} (U_{1i} - U_{2i}) (U_{1j} - U_{2j}) \right] \end{aligned} \quad (D-17)$$

and

$$\begin{aligned} \rho_m \frac{dE_m}{dt_m} &= \rho_1 \frac{dE_1}{dt_1} + E_1 \Gamma_1 - \frac{\partial}{\partial x_j} \left[\rho_1 E_1 \frac{\rho_2}{\rho_1 + \rho_2} (U_{1j} - U_{2j}) \right] \\ &+ \rho_2 \frac{dE_2}{dt_2} + E_2 \Gamma_2 - \frac{\partial}{\partial x_j} \left[\rho_2 E_2 \frac{\rho_1}{\rho_1 + \rho_2} (U_{2j} - U_{1j}) \right] \\ &= \rho_1 \frac{dE_1}{dt_1} + \rho_2 \frac{dE_2}{dt_2} + \Gamma_1 (E_1 - E_2) - \frac{\partial}{\partial x_j} \left[\frac{\rho_1 \rho_2}{\rho_1 + \rho_2} (U_{1j} - U_{2j}) (E_1 - E_2) \right] \end{aligned} \quad (D-18)$$

The same is applicable to H_1 , ϕ , H_2 , and H_m .

D.4 Expression in Terms of Fluxes

Combining with the continuity equation gives:

$$\rho_k \frac{dU_{ki}}{dt_k} = \rho_k \frac{\partial U_{ki}}{\partial t} + \rho_k U_{kj} \frac{\partial U_{ki}}{\partial x_j} = \frac{\partial}{\partial t} (\rho_k U_{ki}) + \frac{\partial}{\partial x_j} (\rho_k U_{kj} U_{ki}) - U_{ki} \Gamma_k \quad (D-19)$$

$$\rho_k \frac{dE_k}{dt_k} = \frac{\partial \rho_k E_k}{\partial t} + \frac{\partial}{\partial x_j} (\rho_k U_{kj} E_k) - E_k \Gamma_k \quad (D-20)$$

$$\rho_k \frac{dH_k}{dt_k} = \frac{\partial \rho_k H_k}{\partial t} + \frac{\partial}{\partial x_j} (\rho_k U_{kj} H_k) - H_k \Gamma_k \quad (D-21)$$

when conversion between H_k and E_k is given by:

$$\rho_k \frac{dH_k}{dt_k} = \rho_k \frac{dE_k}{dt_k} - \frac{P}{\rho_k} \Gamma_k + \frac{\partial \phi_k P}{\partial t} + \frac{\partial}{\partial x_j} \phi_k U_{kj} P \quad (D-22)$$

When applied to Chapter 2, k in the above includes c for the continuous phase. c differs from k only when considering I' and V' and the fact that the kinetic energy of c includes that of the k'_s .

I_k is seen as an accelerating force due to the relative motion between the k - th phase and the mixture:

$$I_{ki} = \frac{\partial}{\partial x_j} \rho_k (U_{ki} - U_i) (U_{kj} - U_j) + (U_i - U_{ki}) \Gamma_k \quad (D-23)$$

when inertial force per unit volume is used in the momentum equation. When the inertia force is written in terms of momentum flux (Eq. D-19), I_{ki} becomes that given by Eq. (2-18).

D.5 Uniqueness of Split to Component Equation -- Continuum Mechanics

For a continuum non-reactor mixture with disparate mass motion and static temperatures the split into components is determined by: (1) the evidenced condition that the predominating component c is not significantly affected by the trace component. (2) The sum of equation of all components will revert the equation of the mixture.

The continuity equation defines the generation ratio Γ_k such that:

$$\frac{\partial \rho_k}{\partial t} + \frac{\partial}{\partial x_j} \rho_k U_{kj} = \Gamma_k \quad (D-24)$$

The momentum equation takes the form:

$$\begin{aligned} \rho_k \frac{\partial U_{ki}}{\partial t} + \rho_k U_{kj} \frac{\partial U_{ki}}{\partial x_j} = & - \frac{\partial P_k}{\partial x_j} + \frac{\partial}{\partial x_j} (\tau_{mkji}) + \rho_k F_{kc} (U_{ci} - U_{ki}) + \rho_k f_{kj} + \\ & + \frac{\partial}{\partial x_j} \rho_k (U_{kj} - U_{mj}) (U_{ki} - U_{mi}) - \Gamma_k (U_{ki} - U_{mi}) \end{aligned} \quad (D-25)$$

The energy equation takes the form in terms of total energy E_k :

$$\begin{aligned} \rho_k \frac{\partial E_k}{\partial t} + \rho_k U_{kj} \frac{\partial E_k}{\partial x_j} = & - \frac{\partial P_k}{\partial x_j} U_{kj} + \frac{\partial}{\partial x_j} (U_{mj} \tau_{mkji}) + \frac{\partial}{\partial x_j} \kappa_{mk} \frac{\partial T_k}{\partial x_j} + \rho_k F_{kc} \\ & (U_{cj} - U_{kj})^2 + \rho_k f_{kj} U_{kj} + \frac{\partial}{\partial x_j} \rho_k (U_{kj} - U_{mj}) (E_k + \frac{P_k}{\rho_k} - H_m) - \Gamma_k (E_k - E_m) + \Gamma_k \frac{P}{\rho_m} \end{aligned} \quad (D-26)$$

This is because

$$-\frac{\partial}{\partial x_j} P_k U_{kj} + \frac{\partial}{\partial x_j} \rho_k (U_{kj} - U_{mj}) \frac{P_k}{\rho_k} = -\frac{\partial}{\partial x_j} P_k U_{mj} \quad (D-27)$$

conforms to the derivation in Appendix D².

In terms of total enthalpy H_k , we have by direct substitution of $H_k = E_k + (P_k/\rho_k)$ and rearranging, we get

$$\begin{aligned} \rho_k \frac{\partial H_k}{\partial t} + \rho_k U_{kj} \frac{\partial H_k}{\partial x_j} &= \frac{\partial P_k}{\partial t} + \frac{\partial}{\partial x_j} (U_{mj} \tau_{mkji}) + \frac{\partial}{\partial x_j} \kappa_{mk} \frac{\partial T_k}{\partial x_j} + \rho_k F_{kc} (U_{cj} - U_{kj})^2 \\ &+ \rho_k f_{kj} U_{kj} + \frac{\partial}{\partial x_j} \rho_k (U_{kj} - U_{mj}) (H_k - H_m) - \Gamma_k (H_k - H_m) \end{aligned} \quad (D-28)$$

For a two component mixture, we have,

$$\begin{aligned} \frac{\partial}{\partial x_j} \rho_k (U_{kj} - U_{mj}) (U_{ki} - U_{mi}) &\rightarrow \frac{\partial}{\partial x_j} \frac{\rho_1 \rho_2^2}{(\rho_1 + \rho_2)^2} (U_{1i} - U_{2i}), \\ -\Gamma_k (U_{ki} - U_{mi}) &\rightarrow -\Gamma_1 \frac{\rho_2}{\rho_1 + \rho_2} (U_{1i} - U_{2i}), \\ \frac{\partial}{\partial x_j} \rho_k (U_{kj} - U_{mj}) (H_k - H_m) &\rightarrow \frac{\partial}{\partial x_j} \frac{\rho_1 \rho_2^2}{(\rho_1 + \rho_2)^2} (U_{1j} - U_{2j}) (H_1 - H_2), \end{aligned}$$

and

$$-\Gamma_k (H_k - H_m) \rightarrow -\Gamma_1 \frac{\rho_2}{\rho_1 + \rho_2} (H_1 - H_2) \quad (D-29)$$

for $\rho_2 \gg \rho_1$ the above 4 terms become, for component 1

$$\begin{aligned} \frac{\partial}{\partial x_j} \rho_1 (U_{1j} - U_{2j}) (U_{1i} - U_{2i}), \\ -\Gamma_1 (U_{1i} - U_{2i}), \\ \frac{\partial}{\partial x_j} \rho_1 (U_{1j} - U_{2j}) (H_1 - H_2), \end{aligned}$$

and

$$-\Gamma_1 (H_1 - H_2) \quad (D-30)$$

while all these four terms for component 2 include (ρ_1/ρ_2) and approach zero.

Appendix E

GENERAL DISCUSSION OF INERTIAL COUPLING AND $PV\phi$ ($P\nabla\alpha$) TERMS

Two major areas of prime concern in mutliphase formulation are discussed in this Appendix. One is the existence of the inertial coupling term and its "uniqueness" of splitting. The other is $PV\phi$, ($P\nabla\alpha$) term in momentum equation.

E.1 Inertial Coupling Term

A general discussion of the philosophical difference 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 [5,6,9,69]. 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 due to investigators' inability to include all relevant physical effects into the formulation. An example is the conspicuous absence of the inertial coupling forces [28] in the momentum equation for the individual phases. This pitfall is recognized in this report, we have adopted the view [21] that the formulation of the field equations should begin with the mixture. The basic reasoning for such a choice stems from the observation that all experimental evidence supports the use of Navier-Stokes equation for describing air motion despite the fact that air is a mixture of nitrogen and oxygen. Consequently, the present authors believe 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 by us as a fundamental postulate which we shall not abandon unless evidence to the contrary can be demonstrated. Based on this concept, the conservation equations given in this report are rigorously derived; they are not merely stated here.

To illustrate our viewpoint, and for simplicity, we present the following derivation of the momentum and energy equation for a one-dimensional, two-phase system. The results can be readily generalized for multiphase systems. Our line of reasoning leads to the inertial coupling force in the momentum equation for the individual phases. On the other hand, such a contribution, conspicuously, has not been correctly accounted for in all other published derivations. It is interesting to note that the use of the momentum equation without the inertial coupling term gives rise to imaginary characteristics in transient flow, when the equation of the mixture gives real characteristics. Experimental verifications of the latter is well known.

Neglecting field forces and capillarity, the one-dimensional momentum equations for individual phases are:

$$\rho_1 \frac{dU_1}{dt_1} = \rho_1 \frac{\partial U_1}{\partial t} + \rho_1 U_1 \frac{\partial U_1}{\partial x} = -\phi_1 \frac{\partial P}{\partial x} + I_{12} + V_{12} \quad (E-1a)^*$$

$$\rho_2 \frac{dU_2}{dt_2} = \rho_2 \frac{\partial U_2}{\partial t} + \rho_2 U_2 \frac{\partial U_2}{\partial x} = -\phi_2 \frac{\partial P}{\partial x} + I_{21} + V_{21}. \quad (E-1b)^*$$

The inertial interaction forces I_{12} and I_{21} are to include the contribution resulting from phase change. A consideration of the physical origin of the viscous interaction forces leads to the simple relation $V_{12} = V_{21}$. The evaluation of I_{12} and I_{21} is made possible via the mixture momentum equation for which we write

$$\rho_m \frac{dU_m}{dt_m} = \rho_m \frac{\partial U_m}{\partial t} + \rho_m U_m \frac{\partial U_m}{\partial x} = -\frac{\partial P}{\partial x} \quad (E-2)$$

where $\rho_m = \rho_1 + \rho_2$ and $\rho_m U_m = \rho_1 U_1 + \rho_2 U_2$. Thus, U_m is seen to be the mass center velocity. In (E-2), the viscosity of the mixture is purposely dropped since we wish to focus our attention to the nature of I_{12} and I_{21} , which are independent of the viscosities of the media.

By making use of the continuity equations for the individual phases:

$$\frac{\partial \rho_1}{\partial t} + \frac{\partial \rho_1 U_1}{\partial x} = \Gamma_1 \quad (E-3a)$$

$$\frac{\partial \rho_2}{\partial t} + \frac{\partial \rho_2 U_2}{\partial x} = \Gamma_2 \quad (E-3b)$$

where $\Gamma_1 + \Gamma_2 = 0$, and the continuity equation for the mixture:

$$\frac{\partial \rho_m}{\partial t} + \frac{\partial \rho_m U_m}{\partial x} = 0, \quad (E-4)$$

we find after a straightforward calculation that (E-2) can be written as

$$\rho_1 \frac{dU_1}{dt_1} + \Gamma_1 (U_1 - U_m) + \rho_2 \frac{dU_2}{dt_2} + \Gamma_2 (U_2 - U_m) - \frac{\partial}{\partial x} \left[\frac{\rho_1 \rho_2}{\rho_1 + \rho_2} (U_2 - U_1)^2 \right] = -\frac{\partial P}{\partial x}. \quad (E-5)$$

*Whether the pressure gradient term written as $-\phi_1 \frac{\partial P}{\partial x}$ or $-\frac{\partial(\phi_1 P)}{\partial x}$, is immaterial insofar as the resulting forms for I_{12} and V_{12} are concerned; $p \partial \phi / \partial x$ is left out here for later clarification.

Since

$$\frac{\rho_1 \rho_2}{\rho_1 + \rho_2} (U_1 - U_2)^2 = \rho_1 (U_1 - U_m)^2 + \rho_2 (U_2 - U_m)^2, \quad (E-6)$$

it follows then from a comparison of (E-5) with (E-1a) and (E-1b) that

$$I_{12} = \frac{\partial}{\partial x} \left[\rho_1 (U_1 - U_m)^2 \right] - \Gamma_1 (U_1 - U_m) \quad (E-7)$$

$$I_{21} = \frac{\partial}{\partial x} \left[\rho_2 (U_2 - U_m)^2 \right] - \Gamma_2 (U_2 - U_m). \quad (E-8)$$

Note that the above I's are redefined when the momentum flux forms are used.

Equation (2-18) is a generalization of the foregoing results. From (E-7) and (E-8), one sees that the inertial coupling force originates from the difference in the velocity of individual phase and that of the mass center of the mixture. The existence of this force and its effect on the dynamics of the individual phase has not been recognized by all other investigators. It was hinted by some investigators [2], [6], [73], but not rigorously accounted for. As a matter of fact, it is unlikely that these inertial coupling terms could be overlooked, had one tried to derive the equation rigorously. If one denotes the viscous interaction force V_{12} by $\rho_1 F_{12} (U_2 - U_1)$, where F_{12} is the inverse relaxation time, then the momentum equation for phase 1 becomes,

$$\rho \frac{dU_1}{dt_1} - \frac{\partial}{\partial x} \left[\rho_1 (U_1 - U_m)^2 \right] + \Gamma_1 (U_1 - U_m) = - \phi_1 \frac{\partial P}{\partial x} + \rho_1 F_{12} (U_2 - U_1). \quad (E-9)$$

Equivalently, in flux form, it becomes

$$\frac{\partial \rho_1 U_1}{\partial t} + \frac{\partial \rho_1 U_1^2}{\partial x} - \frac{\partial}{\partial x} \left[\rho_1 (U_1 - U_m)^2 \right] - \Gamma_1 U_m = - \phi_1 \frac{\partial P}{\partial x} + \rho_1 F_{12} (U_2 - U_1). \quad (E-10)$$

We now turn our attention to the energy equation. Denoting the sum of the internal and kinetic energy per unit mass by E , the energy equations for adiabatic flow of the mixture, in the absence of heat source and disposition, are

($H = E + P/\rho$):

$$\rho_1 \frac{dH_1}{dt_1} = \frac{\partial \phi_1 P}{\partial t} + L_{12} + Q_{12} \quad (E-11a)$$

$$\rho_2 \frac{dH_2}{dt_2} = \frac{\partial \phi_2 P}{\partial t} + L_{21} + Q_{21} \quad (E-11b)$$

for the individual phases, and

$$\rho_m \frac{dH_m}{dt_m} = \frac{\partial P}{\partial t} \quad (E-12)$$

for the mixture. In (E-11), L_{12} and L_{21} denote the coupling of energy of phase associated with inertial effects, while Q_{12} and Q_{21} denote heat transfer coupling. The mixture enthalpy H_m is defined by $\rho_m H_m = \rho_1 H_1 + \rho_2 H_2$ and $Q_{12} = Q_{21}$.

Following a procedure completely analogous to that used for the momentum equations, we find that (E-12) can be rewritten as

$$\begin{aligned} \rho_1 \frac{dH_1}{dt_1} - \frac{\partial}{\partial x} \left[\frac{\rho_1 \rho_2}{\rho_1 + \rho_2} (U_1 - U_2) H_1 \right] + \Gamma_1 H_1 + \rho_2 \frac{dH_2}{dt_2} \\ - \frac{\partial}{\partial x} \left[\frac{\rho_1 \rho_2}{\rho_1 + \rho_2} (U_2 - U_1) H_2 \right] + \Gamma_2 H_2 = - \frac{\partial P}{\partial t} \end{aligned} \quad (E-13)$$

By comparing with (E-11a) and (E-11b), we readily identify

$$\begin{aligned} L_{12} &= \frac{\partial}{\partial x} \left[\frac{\rho_1 \rho_2^2}{(\rho_1 + \rho_2)^2} (U_1 - U_2) (H_1 - H_2) \right] - \Gamma_1 (H_1 - H_2) \frac{\rho_2}{\rho_1 + \rho_2} \\ &= \frac{\partial}{\partial x} \left[\rho_1 (U_1 - U_m) (H_1 - H_m) \right] - \Gamma_1 (H_1 - H_m), \end{aligned} \quad (E-14)$$

and

$$\begin{aligned} L_{21} &= \frac{\partial}{\partial x} \left[\frac{\rho_1 \rho_2^2}{(\rho_1 + \rho_2)^2} (U_2 - U_1) (H_2 - H_1) \right] - \Gamma_2 (H_2 - H_1) \frac{\rho_1}{\rho_1 + \rho_2} \\ &= \frac{\partial}{\partial x} \left[\rho_2 (U_2 - U_m) (H_2 - H_m) \right] - \Gamma_2 (H_2 - H_m), \end{aligned} \quad (E-15)$$

where H denotes the total enthalpy, $E + \frac{\phi P}{\rho}$, of the phases. As is the case of the inertial coupling force in the momentum equation for the individual phases, energy exchange associated with inertial effects, L_{12} and L_{21} , has not been recognized by other investigators.

In summary, the momentum and energy exchange between phases arising from their unequal velocities and associated with inertial effects can only be recognized through simultaneous consideration of the corresponding conservation equation for the mixture and for the individual phases. While experimental evidence

is always the ultimate means for validating a formulation or resolving a controversy, evidences favoring the inclusion of inertial coupling terms are cited as follows:

a) Uniqueness of inertial coupling terms

The desirability of such a split is evidenced by the fact that, for a dilute suspension of particle phase 1 in continuous phase 2, $\rho_2 \gg \rho_1$ the presence of 1 does not affect the motion of 2. The above equations and Eq. (2.16) then gives

$$\rho_1 \frac{dU_1}{dt_1} - \frac{\partial}{\partial x} \rho_1 (U_2 - U_1) = - \frac{\partial P \phi_1}{\partial x} + \rho_1 F (U_2 - U_1) \quad (E-16a)$$

$$\rho_2 \frac{dU_2}{dt_1} = - \frac{\partial P(1 - \phi_1)}{\partial x} - \rho_1 F (U_2 - U_1) \quad (E-16a)$$

as expected.

Similar consideration is applicable to the energy equation; the case $\rho_2 \gg \rho_1$ gives

$$\rho_1 \frac{dH_1}{dt_1} = \frac{\partial P \phi_1}{\partial t} + \frac{\partial}{\partial x} \rho_1 (U_2 - U_1) (H_2 - H_1) + \Gamma (H_2 - H_1) + Q_{12} \quad (E-17a)$$

$$\rho_2 \frac{dH_2}{dt_2} = \frac{\partial P(1 - \phi_1)}{\partial t} + Q_{12} \quad (E-17b)$$

that is the thermal state of 2 is not affected by the presence of 1.

b) Transient flow

The Newton's law is applicable to the mixture with disparate motion of phases and gives real characteristics. With the above split, the equations of the phases also give real characteristics as they should. Inas much as we could write the components of air and expect the unsteady motion to give real characteristics, the illustration in Appendix F demonstrates this point with an example. The example is, of course, not the limit of the scope of the present study. The wave phenomenon in this case arises from $\bar{\rho}_1 \phi_1 + \bar{\rho}_2 (1 - \phi_1)$ with ϕ_1 as a variable.

It was shown (Appendix F) rigorously that without the inertial coupling effect properly accounted for, momentum equations of components give imaginary characteristics when the momentum equation of this mixture gives real characteristics. Such a result is contradictory to the experimental evidence which have been observed in the case of air. When the flow phenomenon is such that the mixture (air) has real characteristics, no physical reasons are available for the equations for oxygen and nitrogen to have imaginary characteristics.

c) Stability of computation of transient flow

Worth mentioning is that the stability of computation of transient flow is significantly improved when the inertial coupling terms are properly accounted for. This was found independently by Krier [74] and Lyczkowski [75]. 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 effects of virtual mass and unsteady motion do not always stabilize the computation.

2.0 The $PV\phi$ ($PV\alpha$) terms

Extensive discussion of the $PV\phi$ term in multiphase formulation has been carried out in the past several years. However, distinction between homogeneous and structured multiphase fluid in terms of application of $PV\phi$ terms needs clarification.

An overview of the term $\nabla P\phi = \phi \nabla P + PV\phi$ includes those who favor (1) dropping $PV\phi$ for reasons of making computation easier or for consideration of an interfacial source force, (2) retaining part of it as a stabilizing force, and (3) retaining $PV\phi$ 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 are given below, it suffices to say that an all encompassing formulation for multiphase mechanics will be to replace, in the momentum equation, the term $\nabla P\phi_k$ by

$$\nabla P\phi_k - B_k PV\phi_k = \phi_k \nabla P + (1 - B_k) PV\phi_k \quad (E-18)$$

with B_k as a displacement factor; B_k is a function of particle size, fluid and flow properties, etc. The range of B_k covers: $B_k = 0$ for very small particles

and $B_k = 1$ for large particles.* This factor includes all views and physical eventualities and its use is believed to facilitate the progress of the computer modeling of multiphase thermohydraulics. The range of reasoning is outlined below.

a) Views favoring the choice of $B_k \sim 1$ are:

i) A derivation toward eliminating $PV\phi$ term from the momentum equation was given by Ishii [2]. He defines ϕ (α) as a time (void) fraction and suggested that the term $\bar{p}_k \nabla \alpha_k$ is cancelled out via the interfacial source term

$$M_k = (\bar{p}_{ki} - \bar{p}_k) \nabla \phi_k + (\bar{v}_{ki} - v_k) \Gamma_k + M_k^d \quad (E-19)$$

with $\bar{p}_{ki} \sim \bar{p}_k$.

It is seen that in M_k : $(\bar{v}_{ki} - v_k) \Gamma_k$ and M_k^d have corresponding terms in our derivations. In our derivation for the multiphase system $\bar{p}_{ki}$ and $\bar{p}_k$ exist in separate phases and $PV\phi_k$ cancels out in the mixture equation but not in the individual phase equations. Ph. Vernier [76] suggested that the coefficient to $\nabla \phi$ in Ishii's Eq. V2.9 should be zero and should not have an effect on the $PV\alpha$ term via $\nabla \phi P$.

Dr. Ishii introduced, via his Eqs. V1.17, V2.8, IX1.11, IX1.14, IX1.15, the term $\nabla P \phi_k$. He showed via IX3.2 that while $-\nabla P \phi_k = -\phi_k \nabla P - PV\phi_k$, $PV\phi_k$ drops out by the substitution of momentum sources M_k for phase k at interface, as a special case of $\bar{p}_{ki} \sim \bar{p}_k$ (or interfacial mean pressure is nearly equal to bulk mean pressure). The basis of his substitution is that in his formulation, the boundary of the control volume may cross an interface with the help of the interfacial transfer condition.

ii) The concern of Cidaspow and Solbrig [77] is how to get real characteristics. We have shown that the imaginary characteristics had arisen solely from omission of inertial coupling and there is no need to drop $PV\phi$ for the sake of stabilizing the solution. They suggested that "since unreasonably high pressure are obtained, the partial pressure model without compensating large relative forces must be regarded as unrealistic in general".

* A simple case is hydrostatic force due to hydrostatic pressure acting on a wedge, or a pile of particles in the shape of a wedge as suggested by Professor G. Birkoff. In that case, $PV\phi$ on the slanted surface of the wedge is balanced by the force exerted on its end at the boundary.

iii) Harlow, et. al., [66] dropped $PV\phi$ via a derivation for "if an individual particle is small compared with the scale of pressure variation in the continuum phases" and made provision that "this may not be valid for turbulent flow". It appears that all those "for" dropping $PV\phi$ came from one source -- to make the computer program manageable when inertial coupling was omitted.

b) Views favoring the choice of $0 < B_k < 1$ are:

i) A review was given by Gidaspow and Solbrig [77]. They attributed $PV\phi$ as an "extra type diffusive force". They cited Roberts and Donnelly [78] as having "such a force in their equations". They also cited Wallis and others and pointed out that "although there exist forces that depend upon gradients of volume fraction, the coefficient should not be simply the thermodynamic pressure P ".

ii) Jackson, et. al., [79] uses a force in his momentum equation $P_s \nabla\phi$, calling $P_s \nabla\phi$ an "effective force without giving an exact value". Gidaspow and Solbrig had expected that $PV\phi$ contributes to "reduce the region of imaginary characteristics, but alone is not sufficient to give a system of partial differential equations that can be solved by stable finite difference techniques". They also called

$$(P - P_{\text{interface}}) \nabla\phi \quad (E-20)$$

Ishii's stabilizing force, but it was insufficient to give real characteristics.

iii) G. B. Wallis [11] confirmed the above and suggested that $PV\phi$ might be dropped for the case of stratified flow but not in suspensions. He suggested "careful experiments".

c) Evidence that favors $B_k \gtrsim 0$ are:

i) The characteristic analysis in Appendix F shows that the term $PV\phi$ gives rise to a wave velocity in transient flow as in the case of transient one dimensional single phase flow.

ii) A thermodynamic and therefore a basic evidence for the existence of the $PV\phi$ term is seen in the physical case of adiabatic compression of a bubble, when the $PV\phi$ term is carried into the energy equation in the form of Eq. (3.30). 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, and $dx_j/U_j \rightarrow dt$, Eq. (3.30) reduces, with the continuity equation, to

$$\phi \bar{\rho}_1 \frac{dU_1}{dt} = - P \frac{d\phi}{dt} \quad (E-21)$$

For a bubble which can be approximated as that of a perfect gas, $P/\bar{\rho}_1 = RT$, $du_1 = c_{v1} dT$, $d\phi/\phi = dV/V$, V being the volume of the bubble and u is the internal energy

$$\frac{c_v}{R} \frac{dT}{T} + \frac{dV}{V} = 0 \quad (E-22)$$

or for ratios of specific heats γ , we get

$$TV^\gamma - 1 = \text{constant} \quad (E-23)$$

the well known adiabatic relation when dissipation is absent. It is believed that resolution of a dilemma of this kind should be made in favor of the validity of the Laws of Thermodynamics. For the same adiabatic relation per unit volume,

$$\phi_1 \bar{\rho}_1 du_1 + P d\phi_1 = 0 \quad (E-24)$$

becomes, in terms of enthalpy h ($h_1 = u_1 + P\phi_1/\rho_1$)

$$\phi_1 \bar{\rho}_1 dh_1 - d(P\phi_1) + P d\phi_1 = 0 \quad (E-25)$$

or

$$\phi_1 \bar{\rho}_1 dh_1 - \phi_1 dP = 0 \quad (E-26)$$

For $dh_1 = c_{p1} dT$ for specific heat at constant pressure c_p . For perfect gas, we get next

$$\frac{c_p}{R} \frac{dT}{T} - \frac{dP}{P} = 0 \quad (E-27)$$

or

$$T \frac{(c_p/R)}{P} = \text{constant} \quad (E-28)$$

for the adiabatic compression of a bubble. The term $\phi_1 d\bar{p}$ became $\phi_k \frac{\partial P}{\partial t}$ in Eq. (2.31) and in Eq. (2.32) $\phi_c \frac{\partial P}{\partial t}$ remains while $\sum_k P \frac{\partial \phi_k}{\partial t} + P \frac{\partial \phi_c}{\partial t} = 0$ since h includes flow work.

Alternate forms derivable from each other are:

$$h_1 = u_1 + \frac{P\phi_1}{\rho_1} \quad (E-29)$$

$$\rho_1 \frac{du_1}{dt_1} + \Gamma_1 u_1 - \frac{\partial}{\partial x_j} \rho_1 (U_{1j} - U_{mj}) u_1 = - \frac{\partial}{\partial x_j} U_{mj} P\phi_1 + \text{heat input} \quad (E-30)$$

and

$$\rho_1 \frac{dh_1}{dt_1} + \Gamma_1 h_1 - \frac{\partial}{\partial x_j} \rho_1 (U_{1j} - U_{mj}) h_1 = \frac{\partial}{\partial t} P\phi_1 + \text{heat input} \quad (E-31)$$

when no term is omitted.

iii) Continuation from continuum mechanics to multiphase mechanics.

In the case of a continuum gas mixture of species 2 with a trace of species 1, the one dimensional momentum equation of species 1 can be written as:

$$\frac{\partial \rho_1 U_1}{\partial t} + \frac{\partial \rho_1 U_1^2}{\partial x} - \frac{\partial}{\partial x} \rho_1 (U_1 - U_2)^2 = - \frac{\partial P_1}{\partial x} + \rho_1 F_1 (U_2 - U_1) \quad (E-32)$$

where

ρ_1 = density of species 1

U_1 = velocity of species 1

P_1 = partial pressure of species 1 = $P\phi_1 = P \frac{\rho_1}{\bar{\rho}_1}$

$\bar{\rho}_1$ = material density of species 1 at

pressure P and temperature T

F = inverse relaxation time of momentum transfer

For the case of $U_2 = 0$, $P = \text{constant}$ and with concentration gradient $\partial\phi_1/\partial x$ initially, Eq. (E-32) becomes

$$\frac{\partial \rho_1 U_1}{\partial t} = - P \frac{\partial \phi_1}{\partial x} - F \rho_1 U_1 \quad (E-33)$$

For a constant P and T (a stipulation which simplifies the problem but not a necessary condition), Eq. (E-33) can be written as:

$$\frac{\partial \rho_1 U_1}{\partial t} + F \rho_1 U_1 = - \frac{P}{\bar{\rho}_1} \frac{\partial \rho_1}{\partial x} \quad (E-34)$$

The continuity equation with no generation of species 1 can be written:

$$\frac{\partial \rho_1}{\partial t} = - \frac{\partial \rho_1 U_1}{\partial x} \quad (E-35)$$

We take derivative of Eq. (3) with respect to x to give:

$$\frac{\partial}{\partial t} \frac{\partial \rho_1 U_1}{\partial x} + F \frac{\partial \rho_1 U_1}{\partial x} = - \frac{P}{\rho_1} \frac{\partial^2 \rho_1}{\partial x^2} \quad (E-36)$$

U_1 can be eliminated by combining Eqs. (E-35) and (E-36)

$$\frac{\partial^2 \rho_1}{\partial t^2} + F \frac{\partial \rho_1}{\partial t} = - \frac{P}{\rho_1} \frac{\partial^2 \rho_1}{\partial x^2} \quad (E-37)$$

Eq. (E-37) is a diffusion equation with the inertial term $\frac{\partial^2 \rho_1}{\partial t^2}$, which by itself gives a wave equation with RHS. $\partial^2 \rho_1 / \partial t^2$ is negligible for large viscous resistance, and the resulting diffusion equation has a diffusivity of $P/(\rho_1 F)$. For a perfect gas, the diffusivity becomes $RT/(\bar{U}/\Lambda)$, where $\bar{U}$ is the mean molecular speed of $\sqrt{8RT/\pi}$, and Λ is the mean free path of species 1 in 2, i.e., this diffusivity is nearly $\bar{U}\Lambda$.

Hence, $PV\phi_1$ term contributes to the spread of species 1 which has an initial concentration gradient. The velocity U_1 can be determined then from Eq. (E-35) or by expressing Eq. (E-37) in flux form

$$\frac{\partial^2 (\rho_1 U_1)}{\partial t^2} + F \frac{\partial (P_1 U_1)}{\partial t} = - \frac{P}{\rho_1} \frac{\partial^2 (\rho_1 U_1)}{\partial x^2} \quad (E-38)$$

Now we apply to a multiphase mixture of fine particles of neutral buoyancy in water in a tube. If we apply Eqs. (E-37) and (E-38) then $P/(\rho_1 F)$ corresponds to a Brownian diffusivity. If we have solid spheres of neutral buoyancy in water in a tube, in the absence of field forces and adhesion, and if we started out with a concentration gradient of these spheres, over a long time the mixture will become homogeneous in the concentration of these spheres. This is because of the diffusion mechanism inherent in the continuum approximation via the continuity and the momentum equations of the trace species. Velocity U_1 becomes zero, once $\partial \phi_1 / \partial x$ becomes zero. The $PV\phi_1$ exists in this case in view of the mechanism embodied in Eq. (E-37).

d) Concluding remarks:

The range of $0 \leq B \leq 1$ will cover the whole range of reasoning and choices. Thus, the effects of $\bar{B}P\nabla\phi$ term on system behavior can be investigated.

E.3 Some of the Features of This Formulation

Some of the features originated or amplified in this report which differ from other publications are outlined below:

1. Since the representation via a distributive quantity such as density ρ_k calls for a large number of particles (droplets or bubbles) in a control volume and particles much smaller than this volume, continuum representation of conservation of mass (ρ_k), momentum ($\rho_k U_k$), and energy ($\rho_k E_k$) is not applicable to a control volume containing one or two bubbles, for instance. Hence, the introduction of multidomain makes possible treating a bubble which is large when compared to the characteristic dimension of a physical system. The jump condition becomes a boundary condition. Details of the evolution from particles in a multiphase mixture into a new domain are being formulated.

2. The fact that for a two-phase system, when the mixture momentum is represented by (neglecting friction boundary and field force in this illustration): (Newton's Law)

$$\rho_m \frac{dU_{mi}}{dt_m} = - \frac{\partial P}{\partial x}$$

and definition of $\rho_m = \rho_1 + \rho_2$, $\rho_m U_{mj} = \rho_1 U_{1j} + \rho_2 U_{2j}$, we must have the following equality to be correct:

$$\begin{aligned} \rho_m \frac{dU_{mi}}{dt_m} &= \rho_1 \frac{dU_{1i}}{dt_1} + \rho_2 \frac{dU_{2i}}{dt_2} - \frac{\partial}{\partial x_j} \left(\frac{\rho_1 \rho_2}{\rho_1 + \rho_2} \right) (U_{2j} - U_{1j}) (U_{2i} - U_{1i}) = - \frac{\partial P}{\partial x} \\ &\equiv \rho_1 \frac{dU_{1i}}{dt_1} + \rho_2 \frac{dU_{2i}}{dt_2} - (I_{12i} + I_{21i}) \end{aligned}$$

This was rigorously derived by simple substitution. We do not expect alteration of Newton's Law in the above form; it gives real characteristics in transient flow problems.

3. The split of the last term of the above equation has to be made according to:

$$\begin{aligned} I_{12i} &= \frac{\partial}{\partial x_j} \rho_1 (U_{1j} - U_{mj}) (U_{1i} - U_{mi}) - \Gamma_1 (U_{1i} - U_{mi}) \\ I_{21i} &= \frac{\partial}{\partial x_j} \rho_2 (U_{2j} - U_{mj}) (U_{2i} - U_{mi}) - \Gamma_2 (U_{2i} - U_{mi}) \end{aligned}$$

for phases 1 and 2 for example. It is seen that if phase 1 (particles) is dilute the inertial coupling is only felt by phase 1, while the motion of phase 2 is

unaffected by the presence of phase 1. This is supported by extensive experimental evidence. Modifications of I's for momentum flux form of formulation are used in Chapters 2 and 3 of our report. Other published formulations without the I's (or inertial coupling) in the formulation of individual phases or without I's split in the above form give imaginary characteristics in transient flow (certainly one does not expect the situation of air flow formulated as a mixture to have real characteristics and to have imaginary characteristics when one considers oxygen and nitrogen separately). All formulations and computer programs without proper inertial coupling needs rectification.

4. Identification of the mutual exclusiveness of phases in a multiphase mixture (as compared to a continuum mixture) and accounting for this mutual exclusiveness via the force due to virtual mass and that due to unsteady flow field even though ρ_k identifies with a distributed density and finite ρ_k and ρ_c are to be found at a given location in space. Formulations aimed at a few bubbles in a control volume should not use distributed densities. The energy state of the particle phase is influenced by heat source, heat transfer, and compression or expansion; kinetic energy of particle phase is part of that of the continuous phase. The forces due to virtual mass and unsteady flow field were determined to exist only where particles are present, hence d/dt_k for the rates. The contents of relaxation times also account for mutual exclusiveness of phases.

5. Amplification of the concept of effectiveness of momentum transfer between phases, thus accounting for the irreversibility of dissipation in the wakes of particles.

6. Amplification of the transport properties of a component in a mixture and viscous stress and heat flux of a component in a mixture.

7. The concept of multidomain enables us to model the various flow regimes in a multiphase flow system. This concept is particularly important for three dimensional analysis, although additional work is needed in this area.

Appendix F

NATURE OF THE PROBLEM OF TRANSIENT FLOW

Conditions for the solution of the equations are examined via a one-dimensional characteristic analysis. For the sake of simplicity we shall illustrate with the case of one dimensional incompressible flow since the nature of the solution is unaffected by the compressibility of the phases. We further choose the case $\rho_2 \gg \rho_1$ for the example of such an initial value problem.

First, we consider the formulation based on continuum mechanics. For the case of incompressible fluids, $\rho_1 = \phi \bar{\rho}_1$, $\rho_2 = (1 - \phi) \bar{\rho}_2$ and $\rho_2 \gg \rho_1$; the continuity and momentum equations of the phases can be expressed as

$$\bar{\rho}_1 \frac{\partial \phi}{\partial t} + \bar{\rho}_1 U_1 \frac{\partial \phi}{\partial x} + \bar{\rho}_1 \phi \frac{\partial U_1}{\partial x} = \Gamma \quad (F-1)$$

$$-\bar{\rho}_2 \frac{\partial \phi}{\partial t} - \bar{\rho}_2 U_2 \frac{\partial \phi}{\partial x} + \bar{\rho}_2 (1 - \phi) \frac{\partial U_2}{\partial x} = -\Gamma \quad (F-2)$$

$$\bar{\rho}_1 \phi \frac{\partial U_1}{\partial t} - [\bar{\rho}_1 (U_1 - U_2)^2 - (1 - B) P] \frac{\partial \phi}{\partial x} + \phi \frac{\partial P}{\partial x} + \bar{\rho}_1 \phi [U_1 -$$

$$2 (U_1 - U_2)] \frac{\partial U_1}{\partial x} + 2 \bar{\rho}_1 \phi (U_1 - U_2) \frac{\partial U_2}{\partial x} = (\bar{\rho}_1 \phi F - \Gamma) (U_1 - U_2) \quad (F-3)$$

$$\bar{\rho}_2 (1 - \phi) \frac{\partial U_2}{\partial t} + (1 - \phi) \frac{\partial P}{\partial x} - (1 - B) P \frac{\partial \phi}{\partial x} + \bar{\rho}_2 (1 - \phi) U_2 \frac{\partial U_2}{\partial x} = -\bar{\rho}_1 \phi F (U_1 - U_2) \quad (F-4)$$

or in the terms of the operator,

$$A' \underline{U}_t + B' \underline{U}_x = f \quad (F-5)$$

where

$$\underline{U} = \begin{pmatrix} \phi \\ P \\ U_1 \\ U_2 \end{pmatrix}$$

and f includes all the inhomogeneous terms. The normals (n_1, n_2) to the characteristics are given by the determinant

$$\det (A' n_1 + B' n_2) = 0 \quad (F-6)$$

or

$$\begin{aligned}
 & -\bar{\rho}_1^2 \bar{\rho}_2 (1 - \phi)^2 \phi n_2^2 (n_1 + U_1 n_2)^2 + (n_1 + U_2 n_2)^2 \left(\frac{\phi}{1 - \phi} \frac{\bar{\rho}_2}{\bar{\rho}_1} \right) \\
 & - 2 n_2 (U_1 - U_2) \left[(n_1 + U_1 n_2) + (n_1 + U_2 n_2) \frac{\phi}{1 - \phi} \right] + n_2^2 (U_1 - U_2)^2 \\
 & \left[1 - \frac{(1 - B) P}{(1 - \phi) \bar{\rho}_1 (U_1 - U_2)^2} \right] \} = 0 \quad (F-7)
 \end{aligned}$$

Equation (F-7) gives four characteristic curves. Two have normals to $n_2 = 0$, or

$$\underline{n} = (1, 0) \text{ and } \underline{n} = (1, 0) \quad (F-8)$$

The nature of the other two normals for the present case, $\rho_2 > \rho_1$, or $\bar{\rho}_2/\bar{\rho}_1 > \phi/(1 - \phi)$ are seen in the following cases:

Case 1 (General): Writing Equation (F-7) in the form

$$a n_1^2 + b n_1 n_2 + c n_2^2 = 0 \quad (F-9)$$

we have

$$\begin{aligned}
 a &= 1 + \frac{\phi}{1 - \phi} \frac{\bar{\rho}_2}{\bar{\rho}_1} \\
 b &= 2 U_2 \left[\frac{\phi}{1 - \phi} \frac{\bar{\rho}_2}{\bar{\rho}_1} + \frac{\phi}{1 - \phi} - \frac{U_1}{U_2} \frac{\phi}{1 - \phi} \right] \\
 c &= U_2^2 \left[\frac{\phi}{1 - \phi} \frac{\bar{\rho}_2}{\bar{\rho}_1} + \frac{1 + \phi}{1 - \phi} - 2 \frac{U_1}{U_2} \frac{\phi}{1 - \phi} - \frac{(1 - B) P}{(1 - \phi) \bar{\rho}_1 U_2^2} \right]
 \end{aligned}$$

It is readily seen from Equation (F-7) that the characteristics are real since

$$b^2 - 4ac = 4 U_2^2 \left[\left(\frac{\phi}{1 - \phi} \right)^2 \left(\frac{U_1}{U_2} - 1 \right)^2 + \frac{(1 - B) P}{(1 - \phi) \bar{\rho}_1 U_2^2} \left(1 + \frac{\phi}{1 - \phi} \frac{\bar{\rho}_2}{\bar{\rho}_1} \right) \right] > 0 \quad (F-10)$$

Hence the characteristics are real and the problem is, in general well-posed.

This is because the formulations based on the mixtures give real characteristics.

Case 2 (Absence of Inertial Coupling): We get, for the bracketed terms in Equation (F-7)

$$(n_1 + U_1 n_2)^2 + (n_1 + U_2 n_2)^2 \left(\frac{\phi}{1 - \phi} \frac{\bar{\rho}_2}{\bar{\rho}_1} \right) \quad (F-11)$$

The characteristics are complex and the problem is ill-posed; i.e., the ill-posed nature results because of the absence of the inertial coupling terms.

Case 3 - When phase 1 is unaffected by the pressure gradient, the term in Eq. (F-7) gives

$$n_1 = n_2 \left[\frac{-(U_2 - \phi U_1)}{1 - \phi} \pm \frac{\phi(U_1 - U_2)}{1 - \phi} \sqrt{1 + \frac{P}{\rho_1 \phi^2 (U_1 - U_2)^2} \frac{(1-B)(1-\phi)^2}{\rho_1}} \right] \quad (F-12)$$

which is always real, and the problem is well-posed. Further, if the inertial coupling term is absent, besides $n_2^2 = 0$, we have for $B = 0$

$$n_1 = n_2 \left[-U_1 \pm \sqrt{\frac{P}{\rho_1}} \right] \quad (F-13)$$

which is also always real, and the problem is well-posed, $\sqrt{P/\rho_1}$ is the wave velocity for incompressible flow.

Case 4 - Next we consider the multiphase heterogeneous system, whence Eq. (F-3) is replaced by

$$\begin{aligned} \rho_1 \left(1 + \frac{1}{2} \frac{\bar{\rho}_2}{\rho_1} \right) \frac{\partial U_1}{\partial t} + \rho_1 \left(1 + \frac{1}{2} \frac{\bar{\rho}_2}{\rho_1} \right) U_1 \frac{\partial U_1}{\partial x} - \frac{1}{2} \rho_1 \frac{\bar{\rho}_2}{\rho_1} \frac{\partial U_2}{\partial t} \\ - \frac{1}{2} \rho_1 \frac{\bar{\rho}_2}{\rho_1} U_1 \frac{\partial U_2}{\partial x} + \phi_1 \frac{\partial P}{\partial x} + (1 - B) P \frac{\partial \phi_1}{\partial x} = - (U_1 - U_2) \Gamma + \rho_1 F(U_2 - U_1) \end{aligned} \quad (F-14)$$

together with Eqs. (F-1), (F-2), and (F-4) and still for $\rho_2 > \rho_1$. We further note that in the case of a dilute suspension of liquid droplets, $\bar{\rho}_1 \gg \bar{\rho}_2$, while in the case of a dilute suspension of bubbles, $\bar{\rho}_1 \ll \bar{\rho}_2$. I_{12} is neglected for the present to test the effect of I' .

The normals (n_1, n_2) to the characteristics as determined by a similar determinant as in Eq. (F-6) are:

$$\begin{aligned} - \rho_1^2 \rho_2 (1 - \phi) \phi n_2^2 [(n_1 + U_1 n_2)^2 (1 - \phi) \left(1 + \frac{\bar{\rho}_2}{2\rho_1} \right) + (n_1 + U_2 n_2)^2 \left(\frac{\bar{\rho}_2}{\rho_1} \right) \phi \\ + \frac{1}{2} (n_1 + U_1 n_2)(n_1 + U_2 n_2) \phi \left(\frac{\bar{\rho}_2}{\rho_1} \right) - \frac{(1 - B) P}{\rho_1} n_2^2] \end{aligned} \quad (F-15)$$

The problem is ill-posed or well-posed depending on the relative magnitude of ϕ_1 , $\bar{\rho}_2/\bar{\rho}_1$, U , and $P/\bar{\rho}_1$, but well-posed in general because of the inertial effect accounted for by the Basset Term. When the term $\phi \partial P/\partial x$ is dropped from Eq. (F-14), the bracketed term in Eq. (F-15) becomes

$$\begin{aligned} [] = & \left[\left(1 + \frac{\bar{\rho}_2}{2\bar{\rho}_1}\right)(1 - \phi)(n_1 + U_1 n_2)^2 + \frac{\bar{\rho}_2}{2\bar{\rho}_1} \frac{\phi}{(1 - \phi)} (n_1 + U_1 n_2)(n_1 + U_2 n_2) - \right. \\ & \left. - \frac{(1 - B)P n_2^2}{\bar{\rho}_1 (1 - \phi)} \right] \end{aligned} \quad (F-16)$$

and the problem is always well-posed.

The ill-posed nature of the problem therefore arises from the partial gradient of pressure when the inertial coupling term is neglected in treating a suspension of droplets or bubbles.

It is seen that the ill-posed nature of the transient flow problem arose basically because the inertial coupling terms were ignored in some multiphase formulations. This is understandable because the formulation based on the mixture is always well-posed and ignoring the inertial coupling term in multiphase formulation represents an inconsistency between the mixture and the phases. Note that, setting $\phi = 0$, $\bar{\rho}_1 = \bar{\rho}_2 = \bar{\rho}$, $U_1 = U_2 = U$, $B=0$, we get from Eqs. (F-7), (F-10) and (F-12)

$$n_1 = [-U \pm \sqrt{P/\bar{\rho}}] n_2 \quad (F-17)$$

which agrees with one-dimensional isothermal transient flow; $\sqrt{P/\bar{\rho}}$ is the speed of the wave.

Consistent approximation requires dropping the pressure gradient term when ignoring the inertial coupling term to keep the problem well-posed.

Appendix G

Transport Properties of a Species in a Mixture

This appendix summarizes previous considerations [21] for the present study. Using species 1 in a mixture m for our illustration, it was shown for a fluid which is Newtonian in nature, the shear stress of species 1 in the mixture is given by:

$$(\tau_{m1})_{ji} = \mu_{m1} \Delta_{1ji} + \mu_{m1}^* \theta_1 \quad (G-1)$$

and

$$\mu_{m1} \Delta_{1ji} = \mu_m \frac{\rho_1}{\rho_m} \Delta_{1ji} + \frac{\mu_m}{\rho_m} \left[(U_{1i} - U_{mi}) \frac{\partial \rho_1}{\partial x_j} + (U_{1j} - U_{mj}) \frac{\partial \rho_1}{\partial x_i} \right] \quad (G-2)$$

where μ_{m1} is the viscosity of species 1 in the mixture of viscosity μ_m . $\Delta_{1ji} = (\partial U_{1i} / \partial x_j) + (\partial U_{1j} / \partial x_i)$ is the shear tensor. For the shear due to dilatation, we have

$$\mu_{m1}^* \theta_1 = \mu_m^* \frac{\rho_1}{\rho_m} \theta_1 + \frac{\mu_m^*}{\rho_m} (U_{1k} - U_{mk}) \frac{\partial \rho_1}{\partial x_k} \quad (G-3)$$

where $\mu_m^* = \zeta_m - \frac{2}{3} \mu_m$, ζ_m is the bulk viscosity of the mixture, and μ_{m1}^* has analogous meaning of μ_{m1} . Then viscosity of species 1 in the mixture is therefore

$$\frac{\mu_{m1}}{\mu_m} = \frac{\rho_1}{\rho_m} + \frac{\rho_1}{\rho_m} \frac{(U_{1i} - U_{mi})(\partial \ln \rho_1 / \partial x_j) + (U_{1j} - U_{mj})(\partial \ln \rho_1 / \partial x_i)}{(\partial U_{1i} / \partial x_j) + (\partial U_{1j} / \partial x_i)} \quad (G-4)$$

$$\frac{\mu_{m1}^*}{\mu_m^*} = \frac{\rho_1}{\rho_m} + \frac{\rho_1}{\rho_m} (U_{1k} - U_{mk}) \frac{\partial \ln \rho_1}{\partial U_{1k}} \quad (G-5)$$

Note that these relations also gave at $i = j = k$

$$\mu_{m1}^* = \zeta_{m1} - \frac{2}{3} \mu_{m1} \quad (G-6)$$

The viscosities of the mixture μ_m , ζ_m are, in general, only known empirically, unless for cases of (a) $\rho_1 \sim \rho_m$,

$$\mu_{m1} \sim \mu_m \sim \bar{\mu}_1 \quad (G-7)$$

where $\bar{\mu}_1$ is the viscosity of the pure material constituting species 1; and for case (b) $\rho_1 \ll \rho_m$

$$\mu_{m1} \sim \rho_1 D_1 \quad (G-8)$$

where D_1 is the diffusivity of species 1 in the mixture.

The diffusivity of particles in a flowing suspension affects the distribution of density and velocity of particles and various transport processes between the phases [21]. For a dilute suspension in which the fluid motion is unaffected by the presence of particles, the particle (dispersed phase) diffusivity D_1 is that arising from particle-fluid interaction only for diffusivity D_2 of the fluid. There is not an abundance of experimental data of D_2 and estimation of the latter for a given physical system is not easily made. The previous relation of D_1 to the nature of particle fluid interactions is reconsidered in light of recent findings. [38]

Take the case of a spherical particle of radius a and of material density $\bar{\rho}_1$ in a turbulent fluid of intensity $\langle U_2^2 \rangle^{1/2}$ of random component of velocity U_2 and Lagrangian integral scale λ : Several studies [21, 72] treated the particle as a randomly excited oscillator to give, in the absence of other field forces, the particle intensity $\langle U_1^2 \rangle^{1/2}$ of its random velocity U_1 in the form:

$$\langle U_1^2 \rangle / \langle U_2^2 \rangle = (\pi)^{1/2} \hat{K}^{-1} \exp(\hat{K}^{-2}) \operatorname{erfc}(\hat{K}^{-1}) \quad (G-9)$$

where $\hat{K}$ is a particle-fluid interacting parameter given by the ratio of the response time of momentum of a particle to the time in which a fluid element remains in a region of correlated velocities, or $\hat{K} = \sqrt{\pi} \langle U_2^2 \rangle^{1/2} / \lambda F_{12}$; $F_{12} = 9 \bar{\mu}_2 / 2 a^2 \bar{\rho}_1 [1 + (\bar{\rho}_2 / 2 \bar{\rho}_1)]$ where F_{12} is the inverse of relaxation time of momentum transfer between particle and fluid; and $\bar{\mu}, \bar{\rho}$ are the viscosity and the density of the material constituting the fluid phase. The assumptions leading to Eq.(G-9) include small relative motion between the phases giving $D_1/D = 1$ as a result.

Eq. (G-9) also gives an intensity of relative motion $\langle (\Delta U)^2 \rangle^{1/2}$ between the phases, and $\langle (\Delta U)^2 \rangle = \langle U_2^2 \rangle - \langle U_1^2 \rangle$. This leads to a particle-fluid interaction length [80.] $L_1 = \langle (\Delta U)^2 \rangle^{1/2} / F_{12}$, by analogy to the kinetic mean free path, and for flow in a pipe of radius R , we get:

$$D_1 = \langle U_1^2 \rangle^{1/2} R \quad (G-10)$$

for $L_1 > R$. The relation in Eq. (G-10) has been verified from correlating experimental results of the density distribution in a suspension of large particles in small pipes or passages [25].

For a more general situation of a free particle in a fluid with negligible wall effect, it is readily seen that for a very small particle, or $K \rightarrow 0$, $D_1/D \rightarrow 1$. For $D =$

$\langle U_2^2 \rangle^{1/2} \lambda$ [21] and $D_1 = \langle (\Delta U)^2 \rangle^{1/2} L_1$, we have

$$D_1/D = 1 - (\hat{K}^3 / 2(\pi)^{1/2}) + [0 (\hat{K}^5)] \quad (G-11)$$

since Eq. (G-9) gives, as $\hat{K} \rightarrow 0$, $\langle U_1^2 \rangle / \langle U_2^2 \rangle = 1 - (\hat{K}^2/2) + [0 (\hat{K}^4)]$.

For a large particle or a large value of K , large relative motion of a particle to the fluid has to be recognized; however, we still have $\langle U_1^2 \rangle < \langle U_2^2 \rangle$ when there is the absence of gravity [21] or other field forces. The scale of particle motion is also smaller than λ . However, the diffusivities result from displacements over a long time t , are $\langle U_1^2 \rangle t$ and $\langle U_2^2 \rangle t$ with $\langle U_1^2 \rangle$ given by Eq.(G-9). We note that

$$D_1/D \leq \langle U_1^2 \rangle / \langle U_2^2 \rangle \quad (G-12)$$

and at large $\hat{K}$, Eq. (G-9) gives $\langle U_1^2 \rangle / \langle U_2^2 \rangle = (\pi)^{1/2} / \hat{K}$.

For the intermediate range of $\langle U_1^2 \rangle$ given by Eq. (G-9) and scale limited by λ or R , and $D_1/D \sim \langle U_1^2 \rangle^{1/2} / \langle U_2^2 \rangle^{1/2}$ for $R < \lambda$ and as an approximation

$$D_1/D = \pi^{1/4} / \hat{K}^{1/2} \quad (G-13)$$

Equations (G-11), (G-12), and (G-13) are shown in Fig. (G-1) together with the theoretical results of Peskin [81] and measurements made on glass particles [21] and coal dusts [82]. In a pipe flow system, Fig. (G-1) permits an estimation of D_1 from D given by [21]:

$$D = (k^*) 2RU \cdot 10^{-3} \quad (G-14)$$

where k^* is an empirical coefficient with value ranging from 0.8 to 5.6 for flow at mean velocity U giving Reynolds numbers $(2RU\bar{\rho}/\bar{\mu})$ ranging from $2 \cdot 10^4$ to $6 \cdot 10^5$.

Note that the above diffusivity relations at small relative motion are applicable to laminar flow where besides Brownian motion, D could be induced by wall interaction (that is, motion induced by the shear layer of the fluid) and perturbation of the flow field by the particle (such as via action and reaction of the wake of a particle [83]). In these situations, D and D_1 may become self-consistent, or D may become prominent only in the vicinity of a particle. This is because in laminar flow of a simple fluid, only molecular diffusivity is active. Presence of particles and their diffusivity may induce additional diffusivity in the fluid phase.

Fig. G-1 Diffusivity Ratio as a Function of Parameter $\hat{K}$

(λ_E is Eulerian Microscale; ○— from Peskin [81])

□ — from Cheng, et al [74] and

△ — from Soo, et al [21].

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