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GENERAL PARTICLE TRANSPORT EQUATION

FINAL REPORT

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Office of Energy Research
University Nuclear Engineering Research Program

By

Dr. A.Y. Lafi
Dr. José N. Reyes, Jr.

Department of Nuclear Engineering
Oregon State University
Radiation Center C116
Corvallis, Oregon 97331-5902
(503) 737-2343

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J.N. Reyes, Jr.

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EXECUTIVE SUMMARY

This report was developed as part of a research program performed for the U.S. Department of Energy's Office of Energy Research (DOE-OER) through Grant No. DE-FG07-90ER13034. The general objectives of this research are as follows:

1. To develop fundamental models for fluid particle coalescence and breakage rates for incorporation into statistically based (Population Balance Approach or Monte Carlo Approach) two-phase thermal hydraulics codes.

2. To develop fundamental models for flow structure transitions based on stability theory and fluid particle interaction rates.

This report details the derivation of the mass, momentum and energy conservation equations for a distribution of spherical, chemically non-reacting fluid particles of variable size and velocity. To study the effects of fluid particle interactions on interfacial transfer and flow structure requires detailed particulate flow conservation equations.. The equations are derived using a particle continuity equation analogous to Boltzmann's transport equation. When coupled with the appropriate closure equations, the conservation equations can be used to model nonequilibrium, two-phase, dispersed, fluid flow behavior. Unlike the Eulerian volume and time averaged conservation equations, the statistically averaged conservation equations contain additional terms that take into account the change due to fluid particle interfacial acceleration and fluid particle dynamics. Two types of particle dynamics are considered; coalescence and breakage. Therefore, the rate of change due to particle dynamics will consider the gain and loss involved in these processes and implement phenomenological models for fluid particle breakage and coalescence.

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NOMENCLATURE

a_i	average interfacial acceleration
C_d	mass concentration of dispersed phase
C_D	drag coefficient
D	diameter
f	friction factor
$\hat{F}$	force per unit mass
$\hat{g}$	body force per unit mass
G	particle size distribution function
$\hat{G}_d$	mass flux
h_d	virtual enthalpy of dispersed phase
$\underline{I}$	identity tensor
$\hat{J}_d$	volumetric flux
m	mass particle
P_d	dispersed phase pressure
$\hat{q}_d$	dispersed phase heat flux
R	fluid particle radius
Re	Reynolds number
t	time
u	internal energy
$\hat{v}$	fluid particle velocity
v_i	fluid particle interfacial velocity or growth rate
V_D	diffussion velocity
$\hat{v}_d$	dispersed phase velocity
V	fluid particle volume

Greek symbols

α	volume fraction
ρ	density
σ	surface tension
ε	energy dissipated per unit mass
ε_d	average dispersed phase fluid energy
ν	kinematic viscosity
λ	coalescence efficiency
η	Kolmogorov length parameter
μ	dynamical viscosity
ϕ	holdup fraction
$\underline{\tau}_d$	viscous stress tensor
$\beta(R',R)$	daughter droplet volume density
υ	daughter droplet production

Subscripts

c	continuous phase
d	dispersed phase
max.	maximum
p	pipe
r	relative

1. INTRODUCTION

The study of fluid particle dynamics is of continuous interest because of its importance to the many industrial applications involving multiphase fluid flow. The design of nuclear reactors, chemical reactors, and boiling and condensation equip-ment present some examples of the areas of application. Recently, a renewed interest in fluid particle dynamics has been generated because of advancements in computer technology which may permit the next-generation of thermal hydraulic analysis codes to implement highly detailed statistical approaches for the treatment of fluid particle distributions. This may significantly improve the codes' ability to predict interfacial transfer processes and flow pattern transitions.

Thermal hydraulic computer codes of the future, will require detailed conservation equations for a distribution of fluid particles (bubbles and droplets) transported by a continuous fluid medium. These conservation equations will demand detailed fluid particle breakage and coalescence rates and thus detailed phenomenological models that predict the nature of the interaction between the fluid particles and the surrounding continuous field and between the fluid particles themselves. They may also predict certain transitions in the flow structure.

The aim of this report is to support the development of the next generation of thermal hydraulic computer codes by introducing a set of complete conservation equations that describe the particle behavior in a continuous surrounding medium. /1/, /2/

The behavior of particle fields within continuous fluid media has long been the subject of investigation in the scientific and industrial communities. Continued interest in this subject arises because of the variety of applications which depend on an accurate knowledge of particle field behavior. For example, the behavior of water droplets in a heated nuclear fuel channel is of significant interest to nuclear reactor safety studies /3/. Prediction of liquid droplet behavior in this instance is particularly complicated because the size distribution of the droplets will vary as evaporation occurs. In order to simplify the task of predicting the effects of droplet fields on interfacial mass, momentum and energy transport, most nuclear reactor thermal hydraulics codes use very simple models to predict an average droplet size during vaporization. A Weber number criteria is often implemented. Another simplification is to neglect droplet breakup and coalescence.

This report presents the derivation of the mass, momentum and energy conservation equations for a distribution of fluid particles (bubbles or droplets) transported by a continuous fluid medium. When coupled with the appropriate closure equations, the conservation equations can be used to model nonequilibrium, two-phase, dispersed, fluid flow behavior.

The general form of particle transport equation is analogous to Boltzmann's transport equation. This form represents an eight dimensional phase continuity equation that treats a system of chemically non-reacting fluid particles of variable size and velocity. Unlike the Eulerian volume and time averaged fluid field conservation equations generally used to describe flows of this nature, the statistical averaging approach presented in this report results in additional terms in each of the conservation equations. These terms arise because of the fluid particle interfacial velocity (i.e., expansion or collapse rate) and the particle dynamics (breakage and coalescence).

This report is divided into eight chapters. Chapter 2 describes the derivation of the eight dimensional phase space particle continuity equation. Chapter 3 shows how the particle continuity equation is integrated to obtain a general transport equation. Chapter 4 presents basic definitions that will be implemented in the formulation of the particle field conservation equations. Chapters 5 through 7 show how the general transport equation is used to derive the fluid particle field mass, momentum and energy conservation equations respectively. Finally, the conclusion derived from this study is presented in Chapter 8.

2. PARTICLE CONTINUITY EQUATION IN EIGHT DIMENSIONS

Hulburt and Katz [4] and Williams [5] present excellent overviews of the derivation of multi-dimensional phase space continuity equations. For the problem of interest to this research we shall assume spherical particles establishing an eight dimensional phase space consisting of a set of external coordinates represented by three spatial coordinates (x_1,x_2,x_3) and a set of internal coordinates represented by three velocity coordinates (v_1,v_2,v_3), one interfacial velocity coordinate (v_i) and a particle size coordinate (R). In formulating a set of averaged fluid particle phase conservation equations, the internal coordinate system will be the basis for the development of the interfacial transfer terms. The internal coordinate system has been carefully selected to include the effects of particle size on particle interfacial velocity (expansion or collapse rates). These effects will become evident in the averaged conservation equations developed in a later chapter.

A point in the phase space characterizes the instantaneous state of the fluid particle. A trajectory through multiple points would show how the fluid particle state changes in time. For the case of many fluid particles, each simultaneously tracing a trajectory in the phase space, we may define a phase space particle number density distribution function, $f(\hat{x},\hat{v},v_i,R,t)$. This function is assumed to be continuous and specifies the probable number of fluid particles in the phase space at a given time t, in the spatial range $d\hat{x}$ about a position $\hat{x}$, with velocities in the range $d\hat{v}$ about $\hat{v}$, interfacial velocities in the range dv_i about v_i and particle sizes in the range dR about R. The terms $d\hat{v}$ and $d\hat{x}$ represent simplified expressions for the three dimensional velocities and physical spatial positions (i.e., dv_1, dv_2, dv_3 and dx_1, dx_2, dx_3).

In order to develop a governing differential equation for the conservation of particle number density, we may treat the range $d\hat{x},d\hat{v},dv_i,dR$ as an eight dimensional phase space control volume. Unfortunately, unlike a conventional three-dimensional control volume, an eight dimensional control volume does not lend itself to simple visual aids such as an infinitesimal cube with each face representing a physical two-dimensional surface. Nonetheless, the procedure is the same and simple accounting of the fluid particles entering and leaving the control volume via the different mechanisms yields the eight dimensional phase space particle continuity equation:

$$\frac{\partial f}{\partial t} + \nabla_x \cdot (f\hat{v}) = -\nabla_v \cdot (f\hat{F}) - \frac{\partial}{\partial R}(fv_i) - \frac{\partial}{\partial v_i}(fa_i) + I \qquad (1)$$

In this equation, $\partial f/\partial t$ term represents the time rate of change in the number density distribution because of all different mechanisms considered in the formulation. The $\nabla_x \cdot (f\hat{v})$ term represents the change in the number density distribution because of fluid particle convection into and out of the range $d\hat{x}$. The $\nabla_v \cdot (f\hat{F})$ term represents the change in the number density distribution because of acceleration of the fluid particle into or out of the range $d\hat{v}$. The subscripts x and v on the gradient operator indicate the derivatives with respect to spatial and velocity coordinates respectively. The vector $\hat{F}$, represents the acceleration or deceleration or the forces per unit mass of particles acting to accelerate or decelerate the fluid particle. These forces include body and drag forces per unit mass. The force is expressed as follows:

$$\hat{F} = \frac{d\hat{v}}{dt} \qquad (2)$$

The $\partial(fv_i)/\partial R$ term represents the change in the number density distribution because of fluid particle growth into and out of the range dR. The average interfacial velocity represents the time rate of change of the particle size. This velocity (or particle growth rate) depends on the particle's mechanical and thermal interactions with the surrounding continuous medium. It is expressed as follows:

$$v_i = \frac{dR}{dt} \qquad (3)$$

The $\partial(fa_i)/\partial v_i$ term represents the change in the number density distribution because of acceleration of the fluid particle interface into or out of the range dv_i. The value a_i is the average interfacial acceleration for a fluid particle. Unlike the force per unit mass term, acceleration of a fluid particle interface may arise due to mechanical effects such as pressure and surface tension, as well as thermal effects such as evaporation or condensation. The interfacial acceleration is expressed as:

$$a_i = \frac{dv_i}{dt} \qquad (4)$$

The I term represents the interaction rate in eight dimensional phase space $I(\hat{x},\hat{v},v_i,R,t)$ that is the rate of change in the density distribution due to particle dynamics (breakage and coalescence).

Typically, the interaction term primarily addresses the gain and loss within particle phase space due to breakage and coalescence processes. Therefore, the I term may be expressed in terms of the algebraic sum of four components as follows:

$$I = I_{BG} - I_{BL} + I_{CG} - I_{CL} \tag{5}$$

where the subscripts B, C, G and L define the breakage, coalescence, gain and loss, respectively.

In order to evaluate these terms, accurate interaction rate models for fluid particle breakage and coalescence must be incorporated. These models are typically functions of the physical and operating conditions of the system.

3. GENERAL TRANSPORT EQUATION

The particle continuity equation described in the previous section is much too detailed for most flow studies where the primary focus is on the average fluid particle field behavior. Therefore it would be advantageous to develop a general transport equation that has been averaged over all particle sizes, particle velocities and interfacial velocities. We begin by defining some mathematical operators that will simplify the derivation. An arbitrary function, $\varphi(\hat{x},\hat{v},v_i,R,t)$, is used for illustrative purposes. The substantial derivatives for the external coordinate system, the internal coordinate system and the total phase space are defined as follows:

$$\frac{D_e\varphi}{Dt} = \frac{\partial\varphi}{\partial t} + \hat{v}\cdot\nabla_x\varphi \tag{6}$$

$$\frac{D_i\varphi}{Dt} = \hat{F}\cdot\nabla_v\varphi + v_i\frac{\partial\varphi}{\partial R} + a_i\frac{\partial\varphi}{\partial v_i} \tag{7}$$

$$\frac{D_{ps}\varphi}{Dt} = \frac{D_e\varphi}{Dt} + \frac{D_i\varphi}{Dt} \tag{8}$$

The following operator will be used to denote integration over the internal coordinate system that serves for elimination of the internal coordinates dependence:

$$\langle\varphi\rangle = \int_0^\infty\int_0^\infty\int_0^\infty \varphi\, d\hat{v}\, dv_i\, dR \tag{9}$$

Substituting equation (5) into equation (1) and then muiltiplying by ψ (an arbitrary fluid property which is independent of the external coordinate system) yields the following equation:

$$\frac{\partial}{\partial t}(f\psi) + \nabla_x\cdot(f\hat{v}\psi) = -\psi\nabla_v\cdot(f\hat{F}) - \psi\frac{\partial}{\partial R}(fv_i) - \psi\frac{\partial}{\partial v_i}(fa_i) + \psi I_{BG} - \psi I_{BL} + \psi I_{CG} - \psi I_{CL} \tag{10}$$

Adding $f\, D_i\psi/Dt$ to both sides and integrating over all $\hat{v}$, v_i and R yields:

$$\begin{aligned}\langle\frac{\partial}{\partial t}(f\psi)\rangle + \langle\nabla_x\cdot(f\hat{v}\psi)\rangle = &-\langle\nabla_v\cdot(f\hat{F}\psi)\rangle - \langle\frac{\partial}{\partial R}(fv_i\psi)\rangle - \langle\frac{\partial}{\partial v_i}(fa_i\psi)\rangle \\ &+\langle f\frac{D_i\psi}{Dt}\rangle + \langle\psi I_{BG}\rangle - \langle\psi I_{BL}\rangle + \langle\psi I_{CG}\rangle - \langle\psi I_{CL}\rangle\end{aligned} \tag{11}$$

Noting that the distribution function goes to zero as $\hat{v}$, v_i, and R go to zero or infinity results in the following simplifications:

$$\langle \nabla_v \cdot (f\hat{F}\psi) \rangle = 0 \tag{12}$$

$$\langle \frac{\partial}{\partial R}(fv_i\psi) \rangle = 0 \tag{13}$$

$$\langle \frac{\partial}{\partial v_i}(fa_i\psi) \rangle = 0 \tag{14}$$

Applying these simplifications and Liebnitz rule to equation (11) yields the following equation:

$$\frac{\partial}{\partial t}\langle f\psi \rangle + \nabla_x \cdot \langle f\hat{v}\psi \rangle = \langle f\frac{D_i\psi}{Dt} \rangle + \langle \psi I_{BG} \rangle - \langle \psi I_{BL} \rangle + \langle \psi I_{CG} \rangle - \langle \psi I_{CL} \rangle \tag{15}$$

It is noted that this equation still implements a particle number density distribution that is dependent on particle velocity, interfacial velocity and particle size. Such a distribution would be extremely difficult to develop. Thus in order to increase the usefulness of this equation, the following definition of a particle property, averaged over all particle and interfacial velocities, will be implemented. Once again the value, φ, is used for illustrative purposes.

$$\overline{\varphi} = \frac{1}{G(R)} \int_0^\infty \int_0^\infty \varphi f \, d\hat{v} \, dv_i \tag{16}$$

In this equation, G(R) is a particle size distribution which may be readily obtained from the literature. It is developed from the phase space number density distribution as follows:

$$G(R) = \int_0^\infty \int_0^\infty f \, d\hat{v} \, dv_i \tag{17}$$

Applying equation (16) to equation (9) yields the following relation:

$$\langle f\varphi \rangle = \int_0^\infty G\,\overline{\varphi}\, dR \tag{18}$$

Applying this result to the first term on the RHS of equation (15) yields:

$$\frac{\partial}{\partial t}\langle f\psi \rangle + \nabla_x \cdot \langle f\hat{v}\psi \rangle = \int_0^\infty G\,\overline{\frac{D_i\psi}{Dt}}\, dR + \langle \psi I_{BG} \rangle - \langle \psi I_{BL} \rangle + \langle \psi I_{CG} \rangle - \langle \psi I_{CL} \rangle \tag{19}$$

In order to evaluate the last four terms on RHS of equation (19), it is necessary to rewrite the particle population in eight dimensional phase space. For example, the breakage rate density (R_B) can be expressed as: [6]

$$R_B(\hat{x},\hat{v},v_i,R,t) = g(\hat{v}',v_i',R')\, f(\hat{x},\hat{v}',v_i',R',t) \tag{20}$$

where g is the breakage frequency of a particle characterized by internal coordinates $\hat{v}'$, v_i', R'. Equation (20) represents the breakage rate density at any point in the system.

When dealing with the particle gain due to breakage, we are interested in the number of daughter particles produced upon breakage. Therefore, the breakage rate density is multiplied by the average number of particles produced upon breakage of a parent particle of internal coordinates $\hat{v}'$,v_i', R'; that is υ ($\hat{v}'$, v_i', R'). It is most likely that these daughter particles have different sizes and velocities and if we assume the distribution density of these particles is given by β, then

$$\beta\,(\hat{v}',\hat{v};v_i',v_i;R',R)\, d\hat{v}\, dv_i\, dR \tag{21}$$

represents the number fraction of daughter particles of velocities between $\hat{v}$ and $\hat{v}$+d$\hat{v}$, interfacial velocities between v_i and v_i+ dv_i and radii between R and R+dR produced upon breakage of a particle characterized by the internal coordinates $\hat{v}'$, v_i', R'. Therefore the number of particles having velocities between $\hat{v}$ and $\hat{v}$+d$\hat{v}$, interfacial velocities between v_i and v_i+dv_i, and radii between R and R+dR produced per unit time upon breakage is:

$$\begin{aligned}&\beta(\hat{v}',\hat{v};v_i',v_i;',R',R)\,\upsilon(\hat{v}',v_i',R')\\ &g(\hat{v}',v_i',R')\, f(\hat{x},\hat{v}',v_i',R',t)\, d\hat{v}\, dv_i\, dR\end{aligned} \tag{22}$$

To evaluate the total gain component of breakage (I_{BG}) we integrate equation (22) over all possible velocities, interfacial velocities, and from radius R to R_{max} (the maximum attainable radius that a particle may possess before breakage) thus:

$$\begin{aligned}I_{BG}(\hat{x},\hat{v},v_i,R,t) = &\int_0^{\infty} d\hat{v}' \int_0^{\infty} dv_i' \int_R^{R_{max}} dR'\\ &\beta(\hat{v}',\hat{v};v_i',v_j;R',R)\\ &\upsilon(\hat{v},v_i',R')\\ &g(\hat{v}',v_i',R')\\ &f(\hat{x},\hat{v}',v_i',R',t)\end{aligned} \tag{23}$$

The same conceptual procedure can be applied to evaluate other components. The loss due to breakage can be readily evaluated for the case of a breakage event that results in destroying the particle. Therefore

$$I_{BL}(\hat{x},\hat{v},v_i,R,t) = g(\hat{v},v_i,R)\, f(\hat{x},\hat{v},v_i,R,t) \tag{24}$$

The gain due to a binary coalescence occurring at $\hat{x}$, t between two particles of velocities $\hat{v}$' and $\hat{v}$-$\hat{v}$', interfacial velocities v_i' and v_i- v_i', and radii R' and R-R' is expressed by a collision frequency $h(\hat{v}-\hat{v}',\hat{v}'; v_i-v_i',v_i'; R-R',R')$ multiplied by the product of the number densities of the respective particles $f(\hat{x},\hat{v}',v_i', R', t)$ and $f(\hat{x},\hat{v}-\hat{v}',v_i-v_i',R-R',t)$. This multiplication represents the collision rate density in eight dimensional phase space.

Since not every collision leads to coalescence, the total gain through coalescence can be given by multiplying the collision rate density by the coalescence efficiency $\lambda(\hat{v}-\hat{v}', \hat{v}'; v_i-v_i',v_i'; R-R',R')$ and integrating over all possible velocities and radii as follows:

$$\begin{aligned} I_{CG}(\hat{x},\hat{v},v_i,R,t) = .5[R/(R-R')]^2 \int_0^{\infty} d\hat{v}' \int_0^{\infty} dv_i' \int_0^{R} dR' \\ \lambda(\hat{v}-\hat{v}',\hat{v}'; v_i-v_i',v_i'; R-R',R') \\ h(\hat{v}-\hat{v}',\hat{v}'; v_i-v_i',v_i'; R-R',R') \\ f(\hat{x},\hat{v}',v_i',R',t) \\ f(\hat{x},\hat{v}-\hat{v}', v_i-v_i', R-R',t) \end{aligned} \tag{25}$$

where the minimum radius was set to zero for simplicity.

This equation describes how the coalescence between the two particles results in a new particle characterized by $\hat{v}$, v_i, and R coordinates. The factor .5 is included to prevent "double-counting" of collisions between particles of $\hat{v}$' and $\hat{v}$-$\hat{v}$', v'_i and v_i-v'_i, and R' and R-R' for a given particle of $\hat{v}$', v_i', R'.

The last component of equation (19) is the loss term due to coalescence which can easily be written as:

$$\begin{aligned} I_{CL}(\hat{x},\hat{v},v_i,R,t) = f(\hat{x},\hat{v},v_i,R,t) \int_0^{\infty} d\hat{v}' \int_0^{\infty} dv_i' \int_0^{R_{max}-R} dR' \\ \lambda(\hat{v},\hat{v}'; v_i,v_i'; R,R') \\ h(\hat{v},\hat{v}'; v_i,v_i'; R,R') \\ f(\hat{x},v',v_i',R',t) \end{aligned} \tag{26}$$

The idea behind this component is that whenever a particle of $(\hat{v},v_i,R)$ has coalesced with another particle, this particle is lost from the system. Now applying equation (16) allows us to write:

$$\overline{\beta \upsilon g} = \frac{\int_0^\infty d\hat{v}' \int_0^\infty dv_i' \beta(\hat{v}',\hat{v};v_i',v_i;R',R)\upsilon(\hat{v}',v_i',R')g(\hat{v}',v_i',R')f(\hat{x}',\hat{v}',v_i',R',t)}{\int_0^\infty d\hat{v}' \int_0^\infty dv_i' \, f(\hat{x},\hat{v}',v_i',R',t)} \tag{27}$$

Thus equation (23) may be written as:

$$I_{BG} = \int_R^{R_{max}} dR' \overline{\beta \upsilon g} \, G(R') \tag{28}$$

where

$$G(R') = \int_0^\infty d\hat{v}' \int_0^\infty dv_i' f(\hat{x},\hat{v}',v_i',R',t)$$

$$\therefore \quad \langle \psi I_{BG} \rangle = \langle \psi \int_R^{R_{max}} dR' G(R') \overline{\beta \upsilon g} \rangle \tag{29}$$

Similarly:

$$\langle \psi I_{BL} \rangle = \langle \psi g f \rangle \tag{30}$$

$$\langle \psi I_{CG} \rangle = .5 \left(\frac{R}{R-R'} \right)^2 \int_0^R dR' \overline{\lambda h} \, G(R') \langle \psi f \rangle \tag{31}$$

$$\langle \psi I_{CL} \rangle = \int_0^{R_{max}-R} dR' \overline{\lambda h} \, G(R') \langle \psi f \rangle \tag{32}$$

Equations (29,30,31, and 32) can be substituted into equation (19) to get:

$$\begin{aligned} \frac{\partial}{\partial t}\langle f\psi \rangle + \nabla_x \cdot \langle f\hat{v}\psi \rangle = & \int_0^\infty G(R) \frac{\overline{Di\psi}}{Dt} dR \\ & + \langle \int_R^{R_{max}} dR' \, G(R') \, \overline{\beta \upsilon g} \, \psi \rangle - \langle \psi g f \rangle \\ & + .5 \left(\frac{R}{R-R'} \right)^2 \int_0^R dR' \overline{\lambda h} \, G(R') \langle \psi f \rangle \\ & - \int_0^{R_{max}-R} dR' \overline{\lambda h} \, G(R') \langle \psi f \rangle \end{aligned} \tag{33}$$

This integro-differential equation is the general particle transport equation that will serve as the basis for the development of the particle field conservation equations.

4. DISPERSED PHASE PROPERTIES AND PARAMETERS

4.1 Properties

In order to derive a set of particle field conservation equations, it would be useful to define the total particle field properties in terms of the integrated fluid particle distribution. Equations for the various properties that describe the dispersed phase (droplets or bubbles) will be presented.

The volumetric flux of the dispersed phase is the total volume of fluid particles per unit volume of physical space passing through a cross-sectional area per unit time. It is defined as follows:

Volumetric Flux:

$$\hat{J}_d = \langle f\hat{v}V \rangle \tag{34}$$

where V is the volume of each particle and related to the particle radius by the following:

Particle Volume:

$$V = \frac{4\pi}{3} R^3 \tag{35}$$

Similarly, the mass flux of the dispersed phase is the total mass of particles per unit volume of physical space passing through a cross-sectional area per unit time. It is defined as follows:

Mass Flux:

$$\hat{G}_d = \langle f\hat{v}m \rangle \tag{36}$$

where m is the mass of each particle of given size as expressed by the simple relation:

Particle Mass:

$$m = \rho V \tag{37}$$

The total volume of particles per unit volume of physical space is known as the volume fraction of the dispersed phase and is defined as follows:

Volume Fraction:

$$\alpha_d = \langle fV \rangle \tag{38}$$

Similarly, the dispersed phase mass concentration is the total mass of particles per unit volume of physical space. It is defined as follows:

Mass Concentration:

$$C_d = \langle fm \rangle \tag{39}$$

For purposes of this study, the mass flux and the mass concentration can be simplified by assuming that the density of the fluid inside the particle is independent of the particle size, velocity and interfacial velocity. Thus by applying this assumption, in conjunction with equations (37) and (38), the definition of the mass concentration becomes the following:

$$C_d = \rho_d \alpha_d \tag{40}$$

Applying these same conditions simplifies the definition of the mass flux to the following:

$$\hat{G}_d = \rho_d \hat{J}_d \tag{41}$$

For the case under consideration, the average velocity of the dispersed phase can be expressed as follows:

$$\hat{v}_d = \frac{\langle f\hat{v}V \rangle}{\langle fV \rangle} \tag{42}$$

This simplifies the volumetric flux to the following:

$$\hat{J}_d = \alpha_d \hat{v}_d \tag{43}$$

Applying this definition to equation (41) yields:

$$G_d = \rho_d \alpha_d \hat{v}_d \tag{44}$$

In deriving the momentum and energy conservation equations, a definition for the averaged fluid particle pressure and energy will be required. The combined stress acting on the fluid particles shall be defined as:

$$\alpha_d(P_d \underline{I} - \underline{\tau}_d) \equiv \langle fm \hat{V}_D \cdot \hat{V}_D \rangle \tag{45}$$

In this equation, P_d, is the component of the partial pressure that can be attributed to the relative translational motion of the particles. $\underline{I}$ is the identity tensor. The stress tensor, $\underline{\tau}_d$, represents the sum of the viscous and turbulent stresses. The diffusion velocity, $\hat{V}_D$, is the difference between the particle velocity, $\hat{v}$, and the averaged dispersed phase velocity, $\hat{v}_d$. Thus:

$$\hat{V}_D = \hat{v} - \hat{v}_d \tag{46}$$

The sum of all the diffusion velocities, at a given location, is equal to zero. Therefore, the following can be shown to be true:

$$\langle fm\hat{V}_D \rangle = 0 \tag{47}$$

The average energy and heat flux of the liquid phase can be defined as follows: [7]

$$\varepsilon_d \equiv \frac{\langle fm\,(\tfrac{1}{2}\hat{V}_D \cdot \hat{V}_D + u)\rangle}{\langle fm \rangle} \tag{48}$$

$$\hat{q}_d = \langle fm\,(\tfrac{1}{2}\hat{V}_D \cdot \hat{V}_D + u)\hat{V}_D \rangle \tag{49}$$

where u is the internal energy contained by the molecules in the fluid particles. Unlike molecular theory, it may include turbulent kinetic energy in addition to the standard internal energy. The heat flux, $\hat{q}_d$, has units of energy per unit area per unit time. It also includes mean conduction, turbulent, and diffusion heat fluxes.

The last concept to be presented in this section is that of virtual enthalpy, h_d, defined as: [7]

$$h_d \equiv \varepsilon_d + P_d/\rho_d \tag{50}$$

4.2 Breakage Parameters

The parameters involved in the breakage components are the maximum radius, the average number of daughter particles produced by breakage of a parent particle, the average daughter particle distribution function, and the average breakage frequency. The parameters involved in the coalescence component are the minimum radius of the particle, the average collision frequency, and the average coalescence efficiency.

4.2.1 Breakage Radius

Breakage radius depends on the type of flow and the physical properties of the system. For example, for a particle in a non-flow (stagnant) media, breakage is due to the Rayleigh-Taylor instability. When the particle exists in a shear flow, the velocity gradient overcomes the interfacial surface tension forces leading to particle breakage. Furthermore, in the case of turbulent flow, the breakage of a particle is the final stage of the deformation that the particle can experience. This deformation, which is a physical properties-related phenomenon, is caused by the shear stress or the pressure variation along the particle surface.

Many expressions for the maximum attainable radius that a particle can possess before breakage occurs have been proposed. /8/ Based on the particle diameter as compared to the Kolmogorov length parameter (the microscale of the turbulence defined by $\eta = (\nu^3/\varepsilon)^{.25}$) two simplified cases can be considered. The first is the case of turbulent flow where the particle diameter greatly exceeds the Kolmogorov parameter. The maximum radius using Levich's definition of critical Weber number can be written as:

$$R_{max} = .33 \frac{\sigma^{.6}}{\rho_d^{.2}} \frac{1}{(\varepsilon \rho_c)^{.4}} \tag{51}$$

This definition takes into account the fluid (continuous and dispersed) properties and the flow and physical geometry conditions included in the energy dissipated per unit mass parameter (ε). The second is the case where the particle diameter is much less than the Kolmogorov length parameter. This represents the case where the viscous and surface tension forces are competing (laminar flow) and therefore R_{max} will be a function of surface tension and the viscosity of both dispersed and continuous phases. /8/

4.2.2 Average Daughter Particle Production, $\upsilon(R')$

This parameter determines the average number of daughter particles produced by breakage of a parent particle of internal coordinates $\hat{v}'$, v_i', and R'. Various experimental data indicate that 2 to 7 particles are produced in each breakage /9/. This parameter is

needed in two places, one in the integral kernel of the breakage gain component and the other in the evaluation of the daughter particle distribution $\beta(R',R)$.

4.2.3 Velocity Averaged Daughter Particle Distribution Function $\beta(R',R)$

This parameter is introduced due to the possible random production of non-equal (velocities, interfacial velocities, and radii) daughter particles upon breakage. It is reasonable to assume that these particles are distributed normally [10] and therefore

$$\beta(v',v) = \frac{1}{\delta\sqrt{2\pi}} \exp\left\{\frac{-(v-\bar{v})^2}{2\delta^2}\right\} \tag{52}$$

This relation is based on the variance δ^2 which is chosen in such a manner that 99.6% of the particle density lies within the volume range $v\pm3\delta$. v' is the volume of the breaking particle (parent particle) and $\bar{v}$ is the mean volume of the daughter particles. Or in terms of particle radius and υ, the velocity averaged daughter particle distribution function $\beta(R',R)$ can be written as follows:

$$\beta(R',R) = \frac{3.6\upsilon R^2}{R'^3} \exp\left\{-\frac{4.5\,(\upsilon R^3 - R'^3)^2}{R'^6}\right\} \tag{53}$$

It is worth mentioning that $\beta(R',R)$ can be expressed in terms of any other suitable distribution function.

4.2.4 Average Breakage Frequency

Several phenomenological models have been developed for breakage frequency in liquid-liquid and gas-liquid dispersions.[8] These models depend on the molecular decomposition analogy, dispersion hydrodynamics, breakage critical velocity, and particle oscillation in addition to arbitrarily chosen models.

By examining these models it can be concluded that they are related to one single concept; two components are affecting the breakage frequency, one affects the time of breakage and the other affects the fraction of particles being breaking. It is obvious that

an attempt to develop a general analytical model for breakage frequency is not easy task. This is because breakage frequency should include all the parameters affecting the breakage process like the fluid (continuous and dispersed) properties, the flow conditions and the physical geometry. However, the following basic phenomonological model is recommended. This model may be used for both gas-liquid and liquid-liquid dispersions. It is based on what so called transitional probability (P_t). The breakage frequency is therefore proportional to this probability as follows:

$$g \sim P_t = \frac{P}{t_b} \tag{54}$$

where t_b is the breakage time and P is the probability that a collision will lead to a breakage event. The breakage time is proportional to the ratio of the particle diameter to the breakage velocity u_b (velocity at which breakage may occur). This ratio is derived from the celebrated imbalance relation:

$$\rho_c u_b^2 D^3 > \sigma D^2 \tag{55}$$

from which one can relate the breakage time to the physical properties and particle diameter as:

$$t_b \sim \sqrt{\frac{\rho_c D^3}{\sigma}} \tag{56}$$

The probability P is derived from the same (but general) imbalance relation and may be expressed in terms of the ratio of surface energy to the kinetic energy transferred by the eddies in the turbulent flow regime as follows:

$$P \sim \exp\left(-\frac{c\sigma}{\rho_c D^{5/3} \varepsilon^{2/3}}\right) \tag{57}$$

by expressing the turbulent mean square velocity in terms of energy dissipation per unit mass (ε) as follows

$$u^2 \sim (D\varepsilon)^{2/3}. \tag{58}$$

Therefore

$$g = c_1 \sqrt{\frac{\sigma}{\rho_c R^3}} \exp\left(-\frac{c_2 \sigma}{\rho_c \varepsilon^{2/3} R^{5/3}}\right) \tag{59}$$

where c_1 and c_2 are constants to be evaluated based on experimental data.

The parameter ε must be defined according to the flow condition and physical geometry. For example, the energy dissipated per unit mass in turbulent pipe line can be given as a function of geometry (pipe diameter), friction factor (which is a function of fluid properties, geometry, and flow) and continuous superficial velocity (J_c) as follows:

$$\varepsilon = \bar{\varepsilon} = \frac{2 f J_c^3}{D_p} \tag{60}$$

where

$$f = .079\, Re^{-.25} \tag{61}$$

$$\therefore \quad \varepsilon = .158 \left(\frac{J_c^{11} \mu_c}{D_p^5 \rho_c}\right)^{.25} \tag{62}$$

A different expression for ε can be used in case of agitated turbulent flow in vessels.[8] Substituting equation (62) into equation (59) results in:

$$g(R) = c_1 \sqrt{\frac{\sigma}{\rho_c R^3}} \exp\left[-c_3 \sigma \left(\frac{D_p^5}{R^{10}}\right)^{1/6} \left(\frac{1}{\rho_c^5 J_c^{11} \mu_c}\right)^{1/6}\right] \tag{63}$$

for gas-liquid dispersion. The same expression can be used for liquid-liquid dispersion except ρ_c in the exponential term is to be replaced by ρ_d.

It is worth mentioning that the volume fraction of the dispersed phase affects the breakage and coalescence frequencies in the following manner. As the dispersed volume

fraction increases, the energy dissipated per unit mass, and thus the energy required to destabilize the particle, will decrease. Therefore, the breakage rate will decrease. On the contrary, the probability of collision, and thus the coalescence rate, will increase. The energy dissipated per unit mass in the presence of highly dispersed medium can be related to that of diluted medium (ε_D) as follows,

$$\varepsilon = \varepsilon_D(1 + n\phi)^{-m} \tag{64}$$

where n and m are constants. Reference /10/ used the values 1 and 2 for n and m respectively in correlating liquid-liquid dispersions in agitated vessels, while reference /11/ used 2.5 and 3 respectively for these constants in correlating liquid-liquid stirred tank contractors data. Therefore it is recommended that the ε term in breakage and coalescence parameters be modified based on the relation above in the case of highly dispersed systems.

4.3 COALESCENCE PARAMETERS

Two elements are usually considered in coalescence analyses; particle collision frequency, because coalescence cannot occur without particle collision and particle coalescence efficiency, because not every collision leads to coalescence. When two particles collide, this collision leads to either the change in the original direction of the colliding particles, if the collision takes place in a very short time or, coalescence, if the contact time is sufficient to destroy (rupture) the interface between the two particles.

The coalescence process after a collision event can be briefly described as a film trapping-thinning-rupturing process. Many efforts have been devoted to study these film-related issues. /12/, /13/ Based on the physical aspects of the coalescence process, the collision frequency and coalescence efficiency are discussed below.

4.3.1 Collision Frequency

Many definitions for the collision frequency between two particles of radii R and R' were proposed based on the type of flow./8/ The suggested expression for the velocity averaged collision frequency for small particles in a turbulent flow may be written as:

$$h(R,R') = 1.336\,(R+R')^3\sqrt{\varepsilon/\nu} \tag{65}$$

where $\sqrt{\varepsilon/\nu}$ is the velocity gradient.

In addition to the collision frequency's dependence on particle size compared to the size of the eddies, the density of both dispersed and continuous phases play an important role in shaping the collision frequency. Other correlations can be found in the literature for small and large sizes with equal or non-equal phase distributions. For the more realistic situation of non-equal large particle sizes in liquid-liquid dispersions, Coulaloglou and Tavlarides/10/ proposed the following expression based on molecular collision analogy:

$$h(R,R') = c(R^2+R'^2)(R^{2/3}+R'^{2/3})^{1/2}\,\varepsilon^{1/3} \tag{66}$$

A similar expression for h in gas-liquid dispersions was proposed by Prince et al. [12] For turbulent flow in pipe lines, one can substitute equation (62) in equation (66) to get:

$$h(R,R') = c(R^2 + R'^2)(R^{2/3} + R'^{2/3})\left(\frac{J_c^{11}\mu_c}{D_p^5 \rho_c}\right)^{1/12} \tag{67}$$

where c is a constant.

4.3.2 Coalescence Efficiency

The coalescence efficiency $\lambda(R,R')$ may be defined as the fraction of collisions between particles of radii R and R′ that results in coalescence. In order to determine the coalescence efficiency it is important to define two terms; the average contact time and the average coalescence time. The average contact time is defined as the average time two colliding particles remain in contact before coalescence occurs. The average coalescence time is the average time required for the liquid film trapped between the two colliding particles to thin to a critical value so that rupture, and consequently coalescence, can occur. Mathematically the velocity averaged coalescence efficiency may be written as:

$$\lambda = \exp(-\gamma) \tag{68}$$

where γ is the ratio of the average coalescence time to the average contact time (i.e., $\gamma = t/\tau$).

Different models have been used to determine the coalescence efficiency in turbulent and laminar regimes for liquid-liquid dispersions. These models are based on the bimolecular gas reaction analogy, sufficiency of the time of contact, impact of colliding particles, as well as combined approaches for collision efficiency. [8] An expression for coalescence efficiency in gas-liquid dispersions was also proposed by Prince, et al. [12] Since the fluid particles are deformable, a model that combines the deformable particle approach, which considers the existence of an attracting force that holds two particles for a time sufficient for the film of the continuous phase trapped

between them to be drained out, and the impact of the colliding particle approach, which is based on the possibility of immediate coalescence after collision, is recommended. According to this approach the coalescence efficiency for turbulent flow in pipe lines, for example, may be written as:

$$\lambda(R,R') = \exp\left[-c_3\left(\frac{J_c^{11}\mu_c^5\rho_c^3}{D_p^5\sigma^8}\right)^{1/4}\left(\frac{RR'}{R+R'}\right)^4\right] + \exp\left[-\frac{c_4\sigma(R^2+R'^2)(R^3+R'^3)}{\rho_d R^3 R'^3(R^{2/3}+R'^{2/3})}\left(\frac{D_p^5\rho_c}{J_c^{11}\mu_c}\right)^{1/6}\right] - \exp\left[-c_3\left(\frac{J_c^{11}\mu_c^5\rho_c^3}{D_p^5\sigma^8}\right)^{1/4}\left(\frac{RR'}{R+R'}\right)^4\right] \cdot \exp\left[-\frac{c_4\sigma(R^2+R'^2)(R^3+R'^3)}{\rho_d R^3 R'^3(R^{2/3}+R'^{2/3})}\left(\frac{D_p^5\rho_c}{J_c^{11}\mu_c}\right)^{1/6}\right] \quad (69)$$

where c_3 (in $1/\ell^2$ units) and c_4 are empirical constants.

With respect to the particle size distribution G(R), the log normal distribution, or any other suitable distribution may be used (see the appendix).

5. MASS CONSERVATION EQUATION

The mass conservation equation for the dispersed phase will be derived by setting $\psi = m$ and substituting into equation (33), the general transport equation. This yields:

$$\frac{\partial}{\partial t}\langle fm\rangle + \nabla_x \cdot \langle fm\hat{v}\rangle = \int_0^\infty G\,\frac{\overline{D_i m}}{Dt}\,dR + \left\langle \int_R^{R_{max}} dR' G(R')\overline{\beta v_g}\, m\right\rangle - \langle mgf\rangle$$
$$+ .5\left(\frac{R}{R-R'}\right)^2 \int_0^R dR'\,\overline{\lambda h}\, G(R')\,\langle fm\rangle \qquad (70)$$
$$- \int_0^{R_{max}-R} dR'\,\overline{\lambda h}\, G(R')\,\langle fm\rangle$$

Using equation (18) and substituting equations (36) and (39) into equation (70) yields:

$$\frac{\partial C_d}{\partial t} + \nabla_x \cdot G_d = \int_0^\infty G\,\frac{\overline{D_i m}}{Dt}\,dR + \left\langle \int_R^{R_{max}} dR' G(R')\overline{\beta v_g}\, m\right\rangle$$
$$- \int_0^\infty G(R')\,\overline{gm}\,dR'$$
$$+ .5\,C_d\left(\frac{R}{R-R'}\right)^2 \int_0^R dR'\,\overline{\lambda h}\, G(R') \qquad (71)$$
$$- C_d \int_0^{R_{max}-R} dR'\,\overline{\lambda h}\, G(R')$$

For the case where the density of the fluid inside the particles is independent of particle velocity, particle size and interfacial velocity, we may substitute equations (40) and (44) into equation (71) to obtain:

$$\frac{\partial}{\partial t}\rho_d \alpha_d + \nabla_x \cdot (\rho_d \alpha_d \hat{v}_d) = \int_0^\infty G \frac{\overline{D_i m}}{Dt} dR + \langle \int_R^{R_{max}} dR'(R')\overline{\beta v g}\, m\rangle$$
$$- \int_0^\infty G(R')\,\overline{gm}\, dR'$$
$$+ .5\,\rho_d \alpha_d \left(\frac{R}{R-R'}\right)^2 \int_0^R dR'\,\overline{\lambda h}\, G(R') \qquad (72)$$
$$- \rho_d \alpha_d \int_0^{R_{max}-R} dR'\,\overline{\lambda h}\, G(R')$$

Expanding the first term on the RHS of this equation yields:

$$\int_0^\infty G \frac{\overline{D_i m}}{Dt} dR = \int_0^\infty G\,\overline{\hat{F}\cdot\nabla_v m}\, dR + \int_0^\infty G\,\overline{v_i \frac{\partial m}{\partial R}}\, dR + \int_0^\infty G\,\overline{a_i \frac{\partial m}{\partial v_i}}\, dR \qquad (73)$$

However since the mass is not a function of velocity, the first term on the RHS of equation (73) is zero. Applying equations (35) and (37), the definitions of particle volume and mass, to equation (73) enables us to write the dispersed phase mass conservation equation as:

$$\frac{\partial\, \rho_d \alpha_d}{\partial t} + \nabla_x \cdot (\rho_d \alpha_d \hat{v}_d) = 4\pi \rho_d \int_0^\infty G R^2 \overline{\left(v_i + a_i \frac{\partial R}{\partial v_i}\right)} dR$$
$$+ \langle \int_R^{R_{max}} dR'\, G(R')\,\overline{\beta v g}\, m\rangle - \int_0^\infty G(R')\,\overline{gm}\, dR' \qquad (74)$$
$$+ .5 \left(\frac{R}{R-R'}\right)^2 \rho_d \alpha_d \int_0^R dR'\,\overline{\lambda h}\, G(R')$$
$$- \rho_d \alpha_d \int_0^{R_{max}-R} dR'\,\overline{\lambda h}\, G(R')$$

This equation has additional terms that are usually not included in the standard dispersed phase mass conservation equations. (See Williams[5] for example.) The first additional term is the mass transfer term associated with interfacial acceleration. That is:

$$4\pi \rho_d \int_0^\infty G R^2 \overline{a_i \frac{\partial R}{\partial v_i}} dR \tag{75}$$

This term takes into account the fact that the fluid particle mass transfer (i.e., expansion or collapse rate) is a function of thermal and mechanical effects which are themselves dependent on the particle size. Thus, as the particle size changes due to interactions with the surrounding medium, the mass transfer rate will accelerate or decelerate (i.e., expansion or collapse rate increases or decreases). For example, as droplets travel a distance dx within a heated control volume, their sizes decrease. As their sizes decrease, their evaporation accelerates.

The dependence of the interfacial velocity on the particle size may be given as:

$$v_i = -\frac{k}{R^n} \tag{76}$$

where k is a function of the dispersed and continuous fluid properties and n is a constant dependent on the mechanism controlling the process that results in the size change. This type of growth rate has been used in droplet vaporization studies, fluid particle combustion studies[5] and bubble growth rate studies (the well known Rayleigh solution). Growth rates may be inertially or heat diffusion controlled. Therefore various expressions may be used to represent the growth rate depending on the flow conditions. [14]

The last four terms in equation (74) are not usually included in the standard dispersed phase mass conservation equation. They represent the mass exchanges associated with particle dynamics and play a very significant role in dispersion systems.

6. MOMENTUM CONSERVATION EQUATION

To derive the dispersed fluid momentum conservation equation, we first set ψ equal to $m\hat{v}$ in the general transport equation to obtain:

$$\frac{\partial}{\partial t}\langle fm\hat{v}\rangle + \nabla_x \cdot \langle fm\hat{v}\hat{v}\rangle = \int_0^\infty G\,\overline{\frac{D_i m\hat{v}}{Dt}}\,dR + \langle \int_R^{R_{max}} dR' G(R')\overline{\beta vg}\, mv\rangle - \langle mvgf\rangle$$
$$+ .5\left(\frac{R}{R-R'}\right)^2 \int_0^R dR'\,\overline{\lambda h}\, G(R')\langle fmv\rangle \qquad (77)$$
$$- \int_0^{R_{max}-R} dR'\,\overline{\lambda h}\, G(R')\langle fmv\rangle$$

Substituting the definition of the diffusion velocity given in equation (46) into the second term on the LHS of equation (77), and expanding yields:

$$\nabla_x \cdot \langle fm\hat{v}\hat{v}\rangle = \nabla_x \cdot \langle fm\hat{V}_D\hat{V}_D\rangle + \nabla_x \cdot (2\hat{v}_d \langle fm\hat{V}_D\rangle) + \nabla_x \cdot \langle fm\rangle \hat{v}_d\hat{v}_d \qquad (78)$$

Substituting equations (45) and (47) into equation (78) and rearranging yields:

$$\nabla_x \cdot \langle fm\hat{v}\hat{v}\rangle = \nabla_x \cdot (\alpha_d P_d) - \nabla_x \cdot (\alpha_d \underline{\tau}_d) + \nabla_x \cdot \langle fm\rangle \hat{v}_d\hat{v}_d \qquad (79)$$

Substituting equation (79), (36) and (39) into equation (77) yields:

$$\frac{\partial}{\partial t}\hat{G}_d + \nabla_x \cdot C_d \hat{v}_d \hat{v}_d = -\nabla_x \cdot (\alpha_d P_d) + \nabla_x \cdot (\alpha_d \underline{\tau}_d)$$
$$+ \int_0^\infty G\,\overline{\frac{D_i m\hat{v}}{Dt}}\,dR$$
$$+ \langle \int_R^{R_{max}} dR'\, G(R')\,\overline{\beta vg}\, mv\rangle - \langle mvgf\rangle \qquad (80)$$
$$+ .5\, G_D\left(\frac{R}{R-R'}\right)^2 \int_0^R dR'\,\overline{\lambda h}\, G(R')$$
$$- G_D \int_0^{R_{max}-R} \overline{\lambda h}\, G(R')$$

Substituting equations (40) and (44) into equation (80) and expanding the third term on the RHS yields:

$$\frac{\partial}{\partial t}(\rho_d \alpha_d \hat{v}_d) + \nabla_x \cdot \rho_d \alpha_d \hat{v}_d \hat{v}_d) = -\nabla_x (\alpha_d P_d) + \nabla_x \cdot (\alpha_d \underline{\tau}_d)$$

$$+ \langle \int_R^{R_{max}} dR' \, G(R') \, \overline{\beta v g} \, mv \rangle - \langle mvgf \rangle$$

$$+ .5 \, \rho_d \alpha_d v_d \left(\frac{R}{R - R'} \right)^2 \int_0^R dR' \, \overline{\lambda h} \, G(R')$$

$$- \rho_d \alpha_d v_d \int_0^{R_{max}-R} dR' \, \overline{\lambda h} \, G(R') \qquad (81)$$

$$+ \int_0^\infty G \, \overline{\hat{F} \cdot \nabla_v (m\hat{v})} \, dR$$

$$+ \int_0^\infty G \, \overline{v_i \frac{\partial m\hat{v}}{\partial R}} \, dR$$

$$+ \int_0^\infty G \, \overline{a_i \frac{\partial m\hat{v}}{\partial v_i}} \, dR$$

Since the particle mass is not a function of the particle velocity, the seventh term on the RHS of equation (81) can be evaluated to obtain:

$$\int_0^\infty G \, \overline{\hat{F} \cdot \nabla_v (m\hat{v})} \, dR = \rho_d \, \alpha_d \, \hat{F} \qquad (82)$$

where $\hat{F}$ is assumed to be independent of internal coordinates and typically broken into a drag force component, $\hat{F}_d$, and a gravitational or body force component, $\hat{g}$ as follows:

$$\hat{F} = \hat{g} + \hat{F}_d \qquad (83)$$

Other components of the system forces such as the lifting forces due to particle rotation and forces of the boundary layer developed around the particle were neglected due to their insignificance. Assuming that the particle velocity is not a function of particle size, and substituting the definitions of particle mass and volume, the eighth term on the RHS of equation (81) becomes:

$$\int_0^\infty G\,\overline{v_i \frac{\partial m\hat{v}}{\partial R}}\,dR = 4\pi\rho_d \int_0^\infty G\,\overline{v_i R^2 \hat{v}}\,dR \tag{84}$$

Assuming that the particle velocity is not a function of interfacial velocity, and substituting the definitions of particle mass and volume, the last term on the RHS of equation (81) becomes:

$$\int_0^\infty G\,\overline{a_i \frac{\partial m\hat{v}}{\partial v_i}}\,dR = 4\pi\rho_d \int_0^\infty G\,\overline{a_i R^2 \hat{v} \frac{\partial R}{\partial v_i}}\,dR \tag{85}$$

Substituting equations (82) through (85) into equation (81) yields the momentum conservation equation for the dispersed phase.

$$\begin{aligned}\frac{\partial}{\partial t}(\rho_d\alpha_d\hat{v}_d) + \nabla_x\cdot\rho_d\alpha_d\hat{v}_d\hat{v}_d) = &-\nabla_x\cdot(\alpha_d P_d) + \nabla_x\cdot(\alpha_d\underline{\tau}_d)\\ &+\langle\int_R^{R_{max}} dR'\,G(R')\,\overline{\beta v g}\,mv\rangle - \langle mvgf\rangle\\ &+.5\,\rho_d\alpha_d v_d\left(\frac{R}{R-R'}\right)^2\int_0^R dR'\,\overline{\lambda h}\,G(R')\\ &-\rho_d\alpha_d v_d\int_0^{R_{max}-R} dR'\,\overline{\lambda h}\,G(R')\\ &+\rho_d\alpha_d\hat{g} + \rho_d\alpha_d\hat{F}_d\\ &+4\pi\rho_d\int_0^\infty G\,\overline{\hat{v}R^2\left(v_i + a_i\frac{\partial R}{\partial v_i}\right)}\,dR\end{aligned} \tag{86}$$

The drag force per unit mass is in the eighth term of the RHS of equation (86) can be expressed in terms of local volumetric interfacial area, drag coefficient, and the relative velocity between the two phases. The interfacial area is a very important paramater that plays a significant role in interfacial transfer processes in liquid-liquid and gas-liquid dispersions systems if it is connected to the particle distribution, concentration, and interaction rates. The drag coefficient could be chosen for multi-particle system and not for single-particle system. Furthermore, the relative velocity may also be expressed in

terms of drift velocity to account for the relative motion between the particles system and the whole mixture containing these particles. As in the derivation of the mass conservation equation, equation (86) contains several terms not usually contained in the standard engineering dispersed phase conservation equation. The first is:

$$4\pi \rho_d \int_0^\infty G \overline{a_i R^2 \hat{v} \frac{\partial R}{\partial v_i}} dR \tag{87}$$

Studies conducted by Prosperetti and Jones /15/ and by Biesheuvel and van Wijngaarden /16/ have also resulted in an additional term in the momentum conservation equation. Equation (86) qualitatively agrees with the work of Biesheuvel. In that study, the contribution of the particles to the bulk pressure was found to consist of a component that stems from the relative translational motion of the particles and a component that stems from the volume changes of the particles. Also, the pressure due to the relative translational motion of the particles was included in the term P_d, and the pressure forces due to the volume changes of the particles is included in equation (88).

The third through the sixth terms on the RHS of equation (86) are also usually excluded from the standard engineering dispersed phase conservation equation. They represent the exchange of momentum due to particle interactions.

7. ENERGY CONSERVATION EQUATION

The derivation of the dispersed phase energy conservation equation requires that we set:

$$\psi = m\left(\frac{\hat{v}\cdot\hat{v}}{2} + u\right) \tag{88}$$

where u is the internal energy per particle mass. Substituting the definition of the diffusion velocity into equation (88) yields:

$$\psi = m\left(\frac{\hat{V}_D\cdot\hat{V}_D}{2} + \hat{V}_d\cdot\hat{v}_d + \frac{\hat{v}_d\cdot\hat{v}_d}{2} + u\right) \tag{89}$$

Substituting equation (89) into the general transport equation given by equation (33) yields:

$$\frac{\partial}{\partial t}\left[\left\langle fm\left(\frac{\hat{V}_D\cdot\hat{V}_D}{2}+u+\frac{\hat{v}_d\cdot\hat{v}_d}{2}\right)\right\rangle + \hat{v}_d\cdot\langle fm\hat{V}_D\rangle\right] +$$

$$\nabla_x\cdot\left[\left\langle fm\hat{v}_d\left(\frac{\hat{V}_D\cdot\hat{V}_D}{2}+u+\frac{\hat{v}_d\cdot\hat{v}_d}{2}\right)\right\rangle + \langle fm\hat{v}_d(\hat{V}_D\cdot\hat{V}_D)\rangle + \frac{\hat{v}_d\cdot\hat{v}_d}{2}\cdot\langle fm\hat{V}_D\rangle\right] +$$

$$\nabla_x\cdot\left[\left\langle fm\hat{V}_D\left(\frac{\hat{V}_D\cdot\hat{V}_D}{2}+u\right)\right\rangle + (\hat{v}_d\cdot\hat{v}_d)\langle fm\hat{V}_D\rangle\right] =$$

$$\int_0^\infty G\,\overline{\frac{D_i}{Dt}\left[m\left(\frac{\hat{v}\cdot\hat{v}}{2}+u\right)\right]}\,dR + \tag{90}$$

$$\left\langle\int_R^{R_{max}} dR'\,G(R')\,\overline{\beta\upsilon g}\,m\left(\frac{\hat{v}\cdot\hat{v}}{2}+u\right)\right\rangle - \left\langle m\left(\frac{\hat{v}\cdot\hat{v}}{2}+u\right)gf\right\rangle +$$

$$.5\left(\frac{R}{R-R'}\right)^2\int_0^R dR'\,\overline{\lambda h}\,G(R')\left\langle fm\left(\frac{\hat{v}\cdot\hat{v}}{2}+u\right)\right\rangle -$$

$$-\int_0^{R_{max}-R}\overline{\lambda h}\,G(R')\left\langle fm\left(\frac{\hat{v}\cdot\hat{v}}{2}+u\right)\right\rangle$$

Substituting equations (45), (47), (48) and (49) into equation (90) yields:

$$\frac{\partial}{\partial t}\left[\rho_d \alpha_d \left(\varepsilon_d + \frac{\hat{v}_d \cdot \hat{v}_d}{2}\right)\right] +$$

$$\nabla_x \cdot \left[\rho_d \alpha_d \hat{v}_d \left(\varepsilon_d + \frac{\hat{v}_d \cdot \hat{v}_d}{2}\right)\right] = -\nabla_x \cdot \hat{q}_d -$$

$$\nabla_x \cdot (\alpha_d \hat{v}_d)(P_d \underline{I} - \underline{\tau}_d) +$$

$$\int_0^\infty G \overline{\frac{D_i}{Dt}\left[m\left(\frac{\hat{v} \cdot \hat{v}}{2} + u\right)\right]} dR + \tag{91}$$

$$\left\langle \int_0^{R_{max}} dR' \, G(R') \overline{\beta \upsilon g} \; m\left(\frac{\hat{v} \cdot \hat{v}}{2} + u\right)\right\rangle - \left\langle m\left(\frac{\hat{v} \cdot \hat{v}}{2} + u\right) gf \right\rangle +$$

$$.5\left(\frac{R}{R-R'}\right)^2 \rho_d \alpha_d \left(\varepsilon_d + \frac{\hat{v}_d \cdot \hat{v}_d}{2}\right) \int_0^R dR' \overline{\lambda h} \, G(R') -$$

$$\rho_d \alpha_d \left(\varepsilon_d + \frac{\hat{v}_d \cdot \hat{v}_d}{2}\right) \int_0^{R_{max}-R} dR' \, \overline{\lambda h} \, G(R')$$

Expanding the third term on the RHS of equation (91) yields:

$$\int_0^\infty G \overline{\frac{D_i}{D_t}\left[m\left(\frac{\hat{v} \cdot \hat{v}}{2} + u\right)\right]} dR = \int_0^\infty G \overline{\left[\hat{F} \cdot \nabla_v m\left(\frac{\hat{v} \cdot \hat{v}}{2} + u\right)\right]} dR +$$

$$\int_0^\infty G \overline{v_i \frac{\partial}{\partial R}\left[m\left(\frac{\hat{v} \cdot \hat{v}}{2} + u\right)\right]} dR + \int_0^\infty G \overline{a_i \frac{\partial}{\partial v_i}\left[m\left(\frac{\hat{v} \cdot \hat{v}}{2} + u\right)\right]} dR \tag{92}$$

Since the particle mass and internal energy are not functions of the particle velocity, the first term on the RHS of equation (92) can be evaluated to obtain:

$$\rho_d \alpha_d (\hat{F}_d + \hat{g}) \cdot \hat{v}_d \,. \tag{93}$$

In this equation, the force $\hat{F}$ has been assumed independent of internal coordinates and divided into two components by using equation (84), and $\rho_d \alpha_d \hat{F}_d \cdot \hat{v}_d$ can be again expressed in terms of interfacial area, drag coefficient, and relative velocity, as discussed in chapter (6). Assuming that the particle velocity and internal energy are not functions of particle size, and substituting the definitions of particle mass and volume, the second term on the RHS of equation (92) becomes:

$$2\pi \rho_d \int_0^\infty G \overline{v_i R^2 (\hat{v} \cdot \hat{v})}\, dR . \tag{94}$$

Assuming that the particle velocity and internal energy are not functions of interfacial velocity, and substituting the definitions of particle mass and volume, the last term on the RHS of equation (92) becomes:

$$2\pi \rho_d \int_0^\infty G \overline{a_i R^2 (\hat{v} \cdot \hat{v}) \frac{\partial R}{\partial v_i}}\, dR . \tag{95}$$

Substituting equations (93) through (95) into equation (91) yields the total energy conservation equation for the dispersed phase:

$$\frac{\partial}{\partial t}\left[\rho_d \alpha_d \left(\varepsilon_d + \frac{\hat{v}_d \cdot \hat{v}_d}{2}\right)\right] +$$

$$\nabla_x \cdot \left[\rho_d \alpha_d \hat{v}_d \left(\varepsilon_d + \frac{\hat{v}_d \cdot \hat{v}_d}{2}\right)\right] = -\nabla_x \cdot \hat{q}_d -$$

$$\nabla_x \cdot (\alpha_d P_d \hat{v}_d) + \nabla_x \cdot (\alpha_d \hat{v}_d) \underline{\tau}_d + \rho_d \alpha_d (\hat{F}_d + \hat{g}) \cdot \hat{v}_d +$$

$$2\pi \rho_d \int_0^\infty G \overline{\left(v_i + a_i \frac{\partial R}{\partial v_i}\right)(\hat{v} \cdot \hat{v}) R^2}\, dR + \tag{96}$$

$$\left\langle \int_0^{R_{max}} dR' \, G(R') \overline{\beta \upsilon g}\, m \left(\frac{\hat{v} \cdot \hat{v}}{2} + u\right)\right\rangle - \left\langle m \left(\frac{\hat{v} \cdot \hat{v}}{2} + u\right) gf \right\rangle +$$

$$.5 \left(\frac{R}{R-R'}\right)^2 \rho_d \alpha_d \left(\varepsilon_d + \frac{\hat{v}_d \cdot \hat{v}_d}{2}\right) \int_0^R dR' \overline{\lambda h}\, G(R') -$$

$$\rho_d \alpha_d \left(\varepsilon_d + \frac{\hat{v}_d \cdot \hat{v}_d}{2}\right) \int_0^{R_{max}-R} dR' \, \overline{\lambda h}\, G(R')$$

Once again we find additional terms not usually included in the standard dispersed phase energy conservation equation. The first is:

$$2\pi \rho_d \int_0^\infty \overline{G\, a_i R^2 (\hat{v} \cdot \hat{v}) \frac{\partial R}{\partial v_i}}\, dR \tag{97}$$

This term represents a component of the expansion or contraction work associated with particle volume changes. The last four terms on the RHS of equation (96) represent the energy exchanges due to particle dynamics.

8. CONCLUSIONS

This report presents a statistical derivation of the mass, momentum and energy conservation equations for a distribution of chemically non-reacting fluid particles. The resulting equations contain additional terms not usually included in the standard engineering formulations of dispersed phase conservation equations. These terms take into account the effects of interfacial acceleration on the mass, momentum and energy transfer associated with particle volume changes and the effects of particle dynamics. It is expected that these terms may be useful to the development of models for interfacial mass, momentum and energy transfer for fluid particle fields transported by continuous media. The lack of experimental data hampered the effort to find numerical values for different parameters involved in the formulation.

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APPENDIX

PARTICLE SIZE DISTRIBUTION

The particle sizes system is considered a statistical system. Therefore this system can be described by a distribution function with some sort of mean size and some measure of deviation from that mean. Numerous particle size distributions have been proposed over the years and have been frequently used in the literature. We list some of them as an example.

1. Γ-distribution Function

A continuous random variable (R) will be said to have a Γ-distribution if the probability distribution function of R is:

$$G(R) = f(R,\alpha,\beta) = \frac{R^{\alpha-1} e^{-R/\beta}}{\beta^{\alpha}\Gamma(\alpha)} \quad \text{for } R \geq 0 \qquad (A.1)$$

$$= 0 \quad \text{otherwise}$$

where $\alpha>0$, $\beta>0$.

When $\beta=1$, the above distribution is called standard Γ-distribution given by:

$$f(R,\alpha) = \frac{R^{\alpha-1} e^{-R}}{\Gamma(\alpha)} \quad \text{for } R \geq 0 \qquad (A.2)$$

$$= 0 \quad \text{otherwise}$$

The standard deviation δ is defined in terms of β and α parameters as:

$$\delta = \beta\sqrt{\alpha}\,.$$

If we define $\alpha=1/\beta$ then:

$$G(R) = \frac{1}{\alpha^{-\alpha}\Gamma(\alpha)} R^{\alpha-1} e^{-R\alpha}$$

in terms of α, or

$$G(R) = \left(\frac{1}{\delta^2}\right)^{1/\delta^2} R^{1/\delta^2-1} \frac{e^{-R/\delta^2}}{\Gamma(1/\delta^2)} \tag{A.3}$$

in terms of δ^2 which can be found from the experimental data.

For this distribution the basic property:

$$\int_0^\infty f(R,\alpha)\,dR = 1 \tag{A.4}$$

can be easily verified using the definition:

$$F(\alpha) = \int_0^\infty e^{\alpha-1} e^{-R} dR \tag{A.5}$$

2. Normal Distribution

The normal distribution can be written as follows:

$$G(R) = \frac{1}{\sqrt{2\pi}} \frac{1}{\delta} e^{\frac{-(R-\bar{R})^2}{2\delta^2}} \tag{A.6}$$

This distribution is characterized by the symmetry at the mean $\bar{R}$ with respect to vertical line, also it reaches the maximum at this mean and the area of the half to the left of the mean equals the area of the half to the right.

Another form that can be derived from the normal distribution is called log normal distribution. This distribution has been widely used and is given by:

$$G(R) = \frac{\eta}{\sqrt{2\pi}} \frac{1}{R} e^{(-\frac{\eta^2}{2})(\ell n\, R + \gamma/\eta)^2} \tag{A.7}$$

where η and γ are related to the standard deviation δ and the mean μ of $\ell n(R)$ as follows:

$$\eta = 1/\delta$$

$$\gamma = -\mu/\delta$$

where:

$$\mu = \frac{1}{N} \sum_{i=1}^{N} \ell n R \tag{A.8}$$

$$\delta = \left[\frac{N \sum_{i=1}^{N} (\ell n\, R)^2 - (\sum_{i=1}^{N} \ell n\, R)^2}{N(N-1)} \right]^{1/2} \tag{A.9}$$

where N is the total number of fluid particles.

This distribution was used in FLECHT-SEASET analyses. Another form of this distribution which has also been used is called the upper limit log normal distribution. /A1/, /A2/

3. Rossin-Rammler Distribution

This distribution is strictly an empirical distribution given by:

$$G(R) = \frac{6bn}{\pi} R^{n-4} e^{-bR^n} \tag{A.10}$$

where b and n are constants.

4. Nukiyama-Tanasawa Distribution

The general form of the Nukiyama-Tanasawa distribution function may be written as:

$$G(R) = aR^{b} e^{-cR^{d}} \tag{A.11}$$

where:

a is the normalization constant,

b is a constant normally set equal to 2,

c is the size parameter, and

d is the distribution parameter.

The normalization constant, a, can be written as:

$$a = \frac{d\, c^{3/d}}{\Gamma(3/D)} \tag{A.12}$$

By using the normalization condition:

$$\int_0^{\infty} G(R)\, dR = 1\,, \tag{A.13}$$

one can write:

$$G(R) = \frac{d c^{3/d}}{\Gamma(3/d)} R^{2} e^{-cR^{d}}. \tag{A.14}$$

By setting d=1, c=1/β, and α=3 we get:

$$G(R) = \frac{R^{2} e^{-R/\beta}}{\beta^{3}\, \Gamma(3)} \tag{A.15}$$

This is similar to the Γ-distribution function given by (A.1) with α=3.

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