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Notes On Well-Posed, Ensemble Averaged Conservation Equations For Multiphase, Multi-Component, And Multi-Material Flows

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Preface

At the INL researchers and engineers routinely encounter multiphase, multi-component, and/or multi-material flows. Some examples include:

- Reactor coolant flows
- Molten corium flows
- Dynamic compaction of metal powders
- Spray forming and thermal plasma spraying
- Plasma quench reactor
- Subsurface flows, particularly in the vadose zone
- Internal flows within fuel cells
- Black liquor atomization and combustion
- Wheat-chaff classification in combine harvesters
- Generation IV pebble bed, high temperature gas reactor

The complexity of these flows dictates that they be examined in an averaged sense. Typically one would begin with known (or at least postulated) microscopic flow relations that hold on the "small" scale. These include continuum level conservation of mass, balance of species mass and momentum, conservation of energy, and a statement of the second law of thermodynamics often in the form of an entropy inequality (such as the Clausius-Duhem inequality). The averaged or macroscopic conservation equations and entropy inequalities are then obtained from the microscopic equations through suitable averaging procedures. At this stage a stronger form of the second law may also be postulated for the mixture of phases or materials. To render the evolutionary material flow balance system unique, constitutive equations and phase or material interaction relations are introduced from experimental observation, or by postulation, through strict enforcement of the constraints or restrictions resulting from the averaged entropy inequalities. These averaged equations form the governing equation system for the dynamic evolution of these mixture flows.

Most commonly, the averaging technique utilized is either *volume* or *time averaging* or a combination of the two. The flow restrictions required for volume and time averaging to be valid can be severe, and violations of these restrictions are often found. A more general, less restrictive (and far less commonly used) type of averaging known as *ensemble averaging* can also be used to produce the governing equation systems. In fact volume and time averaging can be viewed as special cases of ensemble averaging. Ensemble averaging is beginning to gain some notice, for example the general-purpose multi-material flow simulation code CFDLib under continuing developed at the Los Alamos National Laboratory [Kashiwa and Rauenzahn 1994] is based on an ensemble averaged formulation.

The purpose of this short note is to give an introduction to the ensemble averaging methodology and to show how ensemble averaged balance equations and entropy inequality can be obtained from the microscopic balances. It then details some seven-equation, two-pressure, two-velocity hyperbolic, well-posed models for two-phase flows. Lastly, a simple example is presented of a model in which the flow consists of two barotropic fluids with no phase change in which an *equilibrium pressure equation* is obtained in the spirit of pressure-based methods of computational fluid dynamics.

Chapter 1: Ensemble Averaged Conservation Equations

Introduction

Many important "fluid" flows involve a combination of two or more materials having different properties. The multiple phases or components often exhibit relative motion among the phases or material classes. The microscopic motions of the individual constituents are complex and the solution to the micro-level evolutionary equations is difficult. Characteristic of such flows of multi-component materials is an uncertainty in the exact locations of the particular constituents at any particular time. For most practical purposes, it is not possible to exactly predict or measure the evolution of the details of such systems, nor is it even necessary or desirable. Instead, we are usually interested in more gross features of the motion, or the "average" behavior of the system. Here we present descriptive equations that will predict the evolution of this averaged behavior. Due to the complexities of interfaces and resultant discontinuities in fluid properties, as well as from physical scaling issues, it is essential to work with averaged quantities and parameters. We begin by tightening up, or more rigorously defining, our concept of an average. There are several types of averaging. The published literature predominantly contains two types of averaging: *volume averaging* [Whitaker 1999, Dobran 1991] and *time averaging* [Ishii 1975]. Occasionally combinations of the two are used. However, we utilize a more general approach by adopting what is known as *ensemble averaging*.

When the physical system has a large amount of variability, a natural interpretation of the meaning of predictions is in terms of *expected values* and variances. If there are many different events, or *realizations*, possible, then the expected value is naturally an "average" over all of these events, or the *ensemble* of realizations. The *ensemble* then is the set of all experiments with the same boundary- and initial-conditions, with some properties that we would like to associate with the mean and distribution of the components and their velocities. A *realization* of the flow is a possible motion that could have happened. Implicit in this concept is the intuitive idea of a "more likely" and a "less likely" realization in the ensemble. Therefore, as we shall see shortly each ensemble of realizations, corresponding to a given physical situation, has a probability measure on subsets of realizations. The ensemble average is the generalization of the elementary idea of adding the values of the variable for each realization, and dividing by the number of observations. The ensemble average then allows the interpretation of phenomena in terms of repeatability of multi-component flows.

One of the nice features of ensemble averaging, as opposed to volume averaging, is that ensemble averaging does not require that a control volume contain a large quantity of a particular component in any given realization. Consider the following example, taken directly from Drew and Lahey (1993), where the average of a particle-fluid mixture is of interest. Gas turbines are eroded by particulate matter suspended in the gas stream passing through the inlet and impacting on the various parts of the machine, e.g. the turbine blades. The trajectories of individual particles moving through the gas turbine are very complicated, depending on where and when the particles enter the inlet of the device. Such predictions are, fortunately, seldom required. A prediction, however, that is of interest to the designer is the average, or *expected values*, of the particle flux (or the concentration and velocities of particles) near parts in the device that are susceptible to erosion. Since the local concentration of particles is proportional to the probability that particles will be at the various points in the device at various times, and the particle velocity field will be the mean velocity that the particles will have if they are at that position in the device, the design engineer will be able to use this information to assess the places where erosion due to particle impact may occur. Notice it may be that there are no times for which there will be many particles in some representative control volume (or representative elementary volume, REV). So, volume averaging, which depends on the concept of having many representative particles in the averaging volume at any instant, will fail. The appropriateness of ensemble averaging is obvious. Here the ensemble is the set of motions of a single particle through the device, given that it started at a random point at the inlet at a random time during the transient flow through the device. Clearly the solution for the average concentration and average velocity gives little information about the behavior of a single particle in the device; however, the information is very appropriate for assessing the probability of damage to the device. Similar examples could be given where time averaging will fail, but where ensemble averaging is again appropriate.

The ensemble average is the more fundamentally based than either time or volume averaging. In fact, both time and volume averaging can be viewed as approximations to the ensemble average, which can be justified, respectively, for steady or homogeneous flow [Drew and Passman 1999].

Ensemble Averaging

A general method is presented here, based on the ensemble averaging concept [Kashiwa & Rauenzahn 1994, Lhuillier 1996, Brackbill et.al. 1997, Drew & Passman 1999], for developing averaged conservation equations for multiple materials, any one of which may be at point $\vec{x}$, at a given instant *t*. With this procedure, the most likely state at a point (the *expected value*) will be determined simultaneously with which material is most likely to be found at that point. Imagine running an experiment many times and collecting data about the state of the flow at each point $\vec{x}$ and time *t*. This information could include which material or phase is present, material density, velocity, pressure, temperature, concentration, etc. From this information, one can compute the ensemble average. The ensemble average of a generic property Q_0 of a fluid or material in a process is an average over the realizations

$$\langle Q_0 \rangle (\vec{x},t) = \frac{1}{N_R} \sum_{r=1}^{N_R} Q_{0,r} (\vec{x},t) , \tag{1}$$

where N_R is the number of times the process or experiment is repeated, and is a large number. Now imagine that many of the realizations are near duplicates, i.e. they are essentially the same state, with N occurrences. We can then rewrite the sum over the realizations as a sum over the number of states N_Γ

$$\begin{aligned}\langle Q_0\rangle(\vec{x},t) &= \frac{1}{N_R}\sum_{\Gamma=1}^{N_\Gamma} N(\vec{x},t,\Gamma)\,Q_0(\Gamma)\\ &= \sum_{\Gamma=1}^{N_\Gamma} \frac{N(\vec{x},t,\Gamma)}{N_R} Q_0(\Gamma)\\ &= \int_{all\,\Gamma} Q_0(\Gamma) f(\vec{x},t,\Gamma)\,d\Gamma\,,\end{aligned} \tag{2}$$

where $f(\vec{x},t,\Gamma)=\dfrac{N(\vec{x},t,\Gamma)}{N_R}$ is the probability of the state Γ in the ensemble. Note that in the limit of an infinite number of repetitions of the experiment, with a sum over all of the states, we have replaced the summation with an integral form in the definition of the ensemble average. More correctly, because $\int_{all\,\Gamma} f(\vec{x},t,\Gamma)\,d\Gamma = 1.0$, we refer to $f(\vec{x},t,\Gamma)$ as the probability density.

The state is the full thermodynamic description of the matter at a point $\vec{x}$ and time t. For example,

$$\Gamma = \left\{\begin{array}{l}\rho_0, \vec{u}_0, h_0, p_0, \underset{\sim}{\tau}_0,\\ \rho_0^1, \vec{u}_0^1, h_0^1, \rho_0^2, \vec{u}_0^2, h_0^2, \cdots,\\ X_1, X_2, \cdots\end{array}\right\} \tag{3}$$

where:

$X_k(\vec{x},t)$	*phase or material indicator function* $:= 1$ *if material k is present* $= 0$ *otherwise*
ρ_0	*phase or material density*
$\vec{u}_0$	*phase or material velocity*
h_0	*phase or material specific enthalpy*
p_0	*pressure*
$\underset{\sim}{\tau}_0$	*deviatoric stress*
ρ_0^s	*species partial density*
$\vec{u}_0^s$	*species velocity*
h_0^s	*species partial enthalpy ,*

with

$$\rho_0 = \sum_{species} \rho_0^s$$

$$\rho_0 \vec{u}_0 = \sum_{species} \rho_0^s \vec{u}_0^s$$

$$\rho_0 h_0 = \sum_{species} \rho_0^s h_0^s \, .$$

Other properties may also appear in the above thermodynamic state such as the phase or material temperature θ_0, the phase or material specific internal energy e_0, and the phase or material specific entropy s_0.

In a typical multiphase flow, the ensemble averages of interest may include

Material k volume fraction : $\alpha_k \equiv \langle X_k \rangle$

Material k bulk average density : $\hat{\rho}_k \equiv \langle X_k \rho_0 \rangle$

Material k intrinsic average density : $\rho_k \equiv \dfrac{\langle X_k \rho_0 \rangle}{\alpha_k}$

Species s in material k bulk average density : $\hat{\rho}_k^s \equiv \langle X_k \rho_0^s \rangle$

Species s in material k intrinsic average density : $\rho_k^s \equiv \dfrac{\langle X_k \rho_0^s \rangle}{\alpha_k}$

Material k velocity : $\vec{u}_k \equiv \dfrac{\langle X_k \rho_0 \vec{u}_0 \rangle}{\hat{\rho}_k} = \dfrac{\langle X_k \rho_0 \vec{u}_0 \rangle}{\alpha_k \rho_k}$

Material k total energy : $E_k \equiv \dfrac{\langle X_k \rho_0 E_0 \rangle}{\hat{\rho}_k} = \dfrac{\langle X_k \rho_0 E_0 \rangle}{\alpha_k \rho_k}$

Material k entropy : $s_k \equiv \dfrac{\langle X_k \rho_0 s_0 \rangle}{\hat{\rho}_k} = \dfrac{\langle X_k \rho_0 s_0 \rangle}{\alpha_k \rho_k}$

Mean mixture stress : $\underset{\sim}{T} \equiv \langle \underset{\sim}{T}_0 \rangle$

Mean k – material stress : $\underset{\sim}{T}_k \equiv \dfrac{\langle X_k \underset{\sim}{T}_0 \rangle}{\alpha_k}$

Pressure (single pressure model) : $p \equiv \langle p_0 \rangle$

Pressure in k – material : $p_k \equiv \dfrac{\langle X_k p_0 \rangle}{\alpha_k}$.

From a physical viewpoint, the *bulk average density* of a phase represents a summation of all of the density values that occurred for that phase, divided by the total number of experiments run. The bulk average density corresponds intuitively to the idea of the mass of phase k per unit volume of mixture, or the observed material density. On the other hand, the *intrinsic average density* physically corresponds to a summation of all of the density values that occurred for that phase, dividing by the number of times in which that phase occurred in the experiments. The intrinsic average density corresponds intuitively to the idea of the mass of phase k per unit volume of phase k, or the true material density. Some researchers prefer to work with bulk average densities [e.g. Kashiwa and Rauenzahn 1994] while others prefer working with intrinsic densities [e.g. Drew and Passman 1999]. This is mostly an issue of convenience, since one can easily be converted to the other. Here we will use intrinsic averages. Henceforth, when we say average, we shall mean intrinsic average unless indicated otherwise.

For a reasonably broad range of conditions (with common substances), the exact balance equations, valid inside each material, are

$$\dot{\rho}_0 = -\rho_0 \nabla \cdot \vec{u}_0 \qquad \textit{Material mass conservation} \tag{4}$$

$$\dot{\rho}_0^s = -\rho_0^s \nabla \cdot \vec{u}_0 - \nabla \cdot \rho_0^s \left(\vec{u}_0^s - \vec{u}_0\right) + \dot{r}_0^s \qquad \textit{Species mass conservation} \tag{5}$$

$$\rho_0 \dot{\vec{u}}_0 = \nabla \cdot \underset{\sim}{T}_0 + \rho_0 \vec{g} \qquad \textit{Material momentum balance} \tag{6}$$

$$\rho_0 \dot{E}_0 = \nabla \cdot \left(\underset{\sim}{T}_0 \cdot \vec{u}_0\right) + \nabla \cdot \vec{q}_0 + \rho_0 \vec{g} \cdot \vec{u}_0 + \rho_0 \varepsilon_0 \qquad \textit{Material energy conservation} \tag{7}$$

$$\rho_0 \dot{s}_0 \geq \frac{\rho_0 \varepsilon_0}{\theta_0} - \nabla \cdot \left(\frac{\vec{q}_0}{\theta_0}\right) \qquad \textit{Material entropy inequality}, \tag{8}$$

For these microscopic balance laws the material derivative has been used, which is defined as

$$\dot{Q}_0 \equiv \frac{\partial Q_0}{\partial t} + \vec{u}_0 \cdot \nabla Q_0 \qquad \textit{Material derivative}\,. \tag{9}$$

Let us assume that the total variation of f in the phase space $\left(\vec{x}, t, \Gamma\right)$ is [Kashiwa and Rauenzahn 1994]

$$\frac{\partial f}{\partial t} + \vec{u}_0 \cdot \nabla f + \dot{\Gamma} \cdot \frac{\partial f}{\partial \Gamma} = \frac{df}{dt} = 0 \tag{10}$$

where we are assuming that as we follow a material point through phase space its probability of occurrence remains constant. Various *moments* of this equation can be formed, first by multiplying equation (10) by Q_0, and then averaging this result. It can be shown [Kashiwa and Rauenzahn 1994, *here corrected*] that the resulting equation is

$$\frac{\partial}{\partial t}\left\langle Q_0 \right\rangle + \nabla \cdot \left\langle Q_0 \vec{u}_0 \right\rangle = \left\langle \dot{Q}_0 + Q_0 \nabla \cdot \vec{u}_0 \right\rangle. \tag{11}$$

This result is called the ***moment evolution equation*** and the details of its derivation are given in the Appendix. The averaged conservation equations are obtained by letting our generic Q_0 be replaced by various "meaningful" functions and then by performing judicious manipulations on the equations to bring about physically useful forms of the equation.

Mass Conservation

By letting $Q_0 = X_k \rho_0$ in equation (11) we get

$$\frac{\partial \langle X_k \rho_0 \rangle}{\partial t} + \nabla \cdot \langle X_k \rho_0 \vec{u}_0 \rangle = \langle \dot{X}_k \rho_0 + X_k \dot{\rho}_0 + X_k \rho_0 \nabla \cdot \vec{u}_0 \rangle$$
$$= \langle \dot{X}_k \rho_0 + X_k \left(\dot{\rho}_0 + \rho_0 \nabla \cdot \vec{u}_0 \right) \rangle .$$

Introducing the pure material (microscopic) mass conservation equation and the definition of average results in

$$\frac{\partial \alpha_k \rho_k}{\partial t} + \nabla \cdot \alpha_k \rho_k \vec{u}_k = \langle \dot{X}_k \rho_0 \rangle . \tag{12}$$

Since we are taking time- and spatial-derivatives of functions that are not smooth, this averaged mass conservation equation is to be interpreted in the sense of distributions, or generalized functions [Gelfand and Shilov 1964]. Let us examine the right hand side of this equation in more detail. From the definition of a material derivative we know that

$$\dot{X}_k = \frac{\partial X_k}{\partial t} + \vec{u}_0 \cdot \nabla X_k$$

in a generalized function sense. On the other hand, letting $\vec{u}_{int}$ denote the velocity of an interface of phase or material k, the material derivative of X_k following the interface velocity vanishes

$$\frac{\partial X_k}{\partial t} + \vec{u}_{int} \cdot \nabla X_k = 0 .$$

This result can be easily seen by first considering points not on the interface where either $X_k = 0$ or $X_k = 1$ and the partial derivatives both vanish, and thus the left side of this equation vanishes identically. For points on the interface, which also move with the interface velocity, the function X_k is a jump that remains constant so their material derivatives following the interface vanish. Therefore we can write

$$\begin{aligned}\left\langle \dot{X}_k \rho_0 \right\rangle &= \left\langle \rho_0 \left[\left(\frac{\partial X_k}{\partial t} + \vec{u}_0 \cdot \nabla X_k \right) - \underbrace{\left(\frac{\partial X_k}{\partial t} + \vec{u}_{int} \cdot \nabla X_k \right)}_{=0} \right] \right\rangle \\ &= \left\langle \rho_0 \left(\vec{u}_0 - \vec{u}_{int} \right) \cdot \nabla X_k \right\rangle ,\end{aligned} \tag{13}$$

and the ***averaged mass conservation equation*** becomes

$$\begin{aligned}\frac{\partial \alpha_k \rho_k}{\partial t} + \nabla \cdot \alpha_k \rho_k \vec{u}_k &= \left\langle \rho_0 \left(\vec{u}_0 - \vec{u}_{int} \right) \cdot \nabla X_k \right\rangle \\ &\equiv \Omega_k^{mass} .\end{aligned} \tag{14}$$

We note that ∇X_k has the sifting property of the Dirac delta function(al). Thus the only contributors are the material interfaces. ∇X_k is aligned with the surface unit normal vector pointing to phase k [Drew 1983, Kataoka and Serizawa 1988]

$$\nabla X_k = \vec{n}_k \delta \left(\vec{x} - \vec{x}_{int}, t \right) .$$

Thus the Ω_k^{mass} represents the flux of mass to phase k from the other phases via the interface, usually just referred to as phase change. With no storage of mass at an interface the mass conservation further requires

$$\sum_{k=1}^{no.of\ phases} \Omega_k^{mass} = 0 . \tag{15}$$

At this point, it is convenient to introduce for later use, the concept of *interfacial area density* of component k. Defined as

$$A_k = -\left\langle \hat{n}_k \cdot \nabla X_k \right\rangle ,$$

where $\hat{n}_k$ is the unit external normal to component k, it is the expected value of the ratio of the interfacial area (in a small volume) to the (small) volume, in the limit as that volume approaches zero.

Generic Conservation Equation

To more expeditiously derive the other conservation equations, let us first derive the averaged balance equation resulting from a generic, microscopic balance equation. Consider the generic, microscopic balance equation

$$\frac{\partial \rho_0 \psi_0}{\partial t} + \nabla \cdot \rho_0 \psi_0 \vec{u}_0 = \nabla \cdot J_0 + \rho_0 g_0 , \tag{16}$$

or

$$\frac{d\left(\rho_0 \psi_0\right)}{dt} + \left(\rho_0 \psi_0\right) \nabla \cdot \vec{u}_0 = \rho_0 \dot{\psi}_0 = \nabla \cdot J_0 + \rho_0 g_0 . \tag{17}$$

Equation (16) and (17) hold at each point where sufficient smoothness occurs for the derivatives to be taken, as does its generic jump condition

$$[\![\rho_0 \psi_0 \left(\vec{u}_0 - \vec{u}_{int} \right) + J_0]\!] \cdot \hat{n} = m \tag{18}$$

where ψ_0 is the conserved quantity, J_0 is a molecular or diffusive flux, g_0 is a source density, and m is the interfacial source of ψ_0. The symbol $[\![\cdot]\!]$ here denotes the jump in the enclosed quantity across an interface. Obviously, these quantities must be added to our state space, e.g.

$$\Gamma = \begin{Bmatrix} \rho_0, \vec{u}_0, \psi_0, J_0, \cdots \\ X_1, X_2, \cdots \end{Bmatrix} . \tag{19}$$

Let us also define averages of these quantities as

$$\begin{aligned} \psi_k &\equiv \frac{\left\langle X_k \rho_0 \psi_0 \right\rangle}{\alpha_k \rho_k} \\ J_k &\equiv \frac{\left\langle X_k J_0 \right\rangle}{\alpha_k} \\ g_k &\equiv \frac{\left\langle X_k \rho_0 g_0 \right\rangle}{\alpha_k \rho_k} . \end{aligned}$$

By letting $Q_0 = X_k \rho_0 \psi_0$ in equation (11) we get

$$
\begin{aligned}
\frac{\partial\left\langle X_k\rho_0\psi_0\right\rangle}{\partial t}+\nabla\cdot\left\langle X_k\rho_0\psi_0\vec{u}_0\right\rangle &= \left\langle\frac{d\left(X_k\rho_0\psi_0\right)}{dt}+X_k\rho_0\psi_0\nabla\cdot\vec{u}_0\right\rangle \\
&= \left\langle\dot{X}_k\rho_0\psi_0+X_k\frac{d\left(\rho_0\psi_0\right)}{dt}+X_k\rho_0\psi_0\nabla\cdot\vec{u}_0\right\rangle \\
&= \left\langle\dot{X}_k\rho_0\psi_0\right\rangle+\left\langle X_k\left(\frac{d\left(\rho_0\psi_0\right)}{dt}+\rho_0\psi_0\nabla\cdot\vec{u}_0\right)\right\rangle \\
&= \left\langle\dot{X}_k\rho_0\psi_0+X_k\nabla\cdot J_0+X_k\rho_0 g_0\right\rangle \\
&= \left\langle\nabla\cdot X_k J_0\right\rangle-\left\langle J_0\cdot\nabla X_k\right\rangle+\left\langle\dot{X}_k\rho_0\psi_0\right\rangle+\left\langle X_k\rho_0 g_0\right\rangle \\
&= \left\langle\nabla\cdot X_k J_0\right\rangle-\left\langle J_0\cdot\nabla X_k\right\rangle+\left\langle\rho_0\psi_0\left(\vec{u}_0-\vec{u}_{int}\right)\cdot\nabla X_k\right\rangle+\left\langle X_k\rho_0 g_0\right\rangle \\
&= \nabla\cdot\left\langle X_k J_0\right\rangle+\left\langle X_k\rho_0 g_0\right\rangle+\left\langle\left[\rho_0\psi_0\left(\vec{u}_0-\vec{u}_{int}\right)-J_0\right]\cdot\nabla X_k\right\rangle .
\end{aligned}
$$

Introducing the fluctuating velocity

$$\vec{u}_k' = \vec{u}_0-\vec{u}_k$$

into this expression finally results in

$$
\begin{aligned}
\frac{\partial\alpha_k\rho_k\psi_k}{\partial t}+\nabla\cdot\alpha_k\rho_k\psi_k\vec{u}_k &= \nabla\cdot\alpha_k J_k-\nabla\cdot\left\langle X_k\rho_0\psi_0\,\vec{u}_k'\right\rangle+\alpha_k\rho_k g_k+\left\langle\left[\rho_0\psi_0\left(\vec{u}_0-\vec{u}_{int}\right)-J_0\right]\cdot\nabla X_k\right\rangle \\
&= \nabla\cdot\alpha_k J_k-\nabla\cdot\left\langle X_k\rho_0\psi_0\,\vec{u}_k'\right\rangle+\alpha_k\rho_k g_k+\left\langle\rho_0\psi_0\left(\vec{u}_0-\vec{u}_{int}\right)\cdot\nabla X_k\right\rangle-\left\langle J_0\cdot\nabla X_k\right\rangle \\
&= \nabla\cdot\alpha_k J_k+\nabla\cdot\alpha_k J_k^{Fluct}+\alpha_k\rho_k g_k+\Omega_k^{mass}\psi_k^{int}+\Omega_k^{\psi}\ ,
\end{aligned}
\tag{20}
$$

where $J_k^{Fluct}=-\dfrac{\left\langle X_k\rho_0\psi_0\,\vec{u}_k'\right\rangle}{\alpha_k}$ is the flux of ψ due to fluctuations in the phase k velocity, ψ_k^{int} is the effective value of ψ that is transferred to phase k from the other phases due to mass transfer, or phase change, and Ω_k^{ψ} is a flux of ψ to phase k not due to bulk mass transfer from the other phases. This is our ***generic, averaged balance equation***. To obtain balance at the interface, our generic jump balance equation requires the constraint

$$\sum_{k=1}^{no.\,of\ phases}\Omega_k^{mass}\psi_k^{int}+\Omega_k^{\psi}=M\ , \tag{21}$$

where $M=\left\langle m\right\rangle$ is the expected net effect of all the interfacial ψ-source terms.

Species Mass Conservation

The microscopic species mass balance equation can be written as

$$\frac{\partial \rho_0^s}{\partial t} + \nabla \cdot \rho_0^s \vec{u}_0^s = \dot{r}^s \ , \tag{22}$$

where ρ_0^s is the species partial density, $\vec{u}_0^s$ is the species bulk velocity, and $\dot{r}^s$ is the generation or source of the species due to chemical reactions. The species mass balance equation is not usually written this way because we usually don't know much about individual species velocities. Instead, it is usually cast as

$$\frac{\partial \rho_0^s}{\partial t} + \nabla \cdot \rho_0^s \vec{u}_0 = \nabla \cdot \rho_0^s \left(\vec{u}_0 - \vec{u}_0^s \right) + \dot{r}^s \tag{23}$$

because we have (to a certain extent) acquired empirical knowledge of the behavior of the first term on the right hand side of this equation, as we shall see shortly. Let us now recast this equation as

$$\frac{\partial}{\partial t}\left(\rho_0 \frac{\rho_0^s}{\rho_0} \right) + \nabla \cdot \left(\rho_0 \frac{\rho_0^s}{\rho_0} \vec{u}_0 \right) = \nabla \cdot \left[\rho_0 \frac{\rho_0^s}{\rho_0} \left(\vec{u}_0 - \vec{u}_0^s \right) \right] + \rho_0 \frac{\dot{r}^s}{\rho_0} \ , \tag{24}$$

which is in the form of our generic, averaged balance equation (20) with the assignments of

$$\psi_0 = \frac{\rho_0^s}{\rho_0} \qquad J_0 = \rho_0 \frac{\rho_0^s}{\rho_0} \left(\vec{u}_0 - \vec{u}_0^s \right) \qquad g_0 = \frac{\dot{r}^s}{\rho_0} \ .$$

Thus the averaged species mass balance equation is

$$\frac{\partial}{\partial t}\left\langle X_k \rho_0^s \right\rangle + \nabla \cdot \left\langle X_k \rho_0^s \vec{u}_0 \right\rangle = \nabla \cdot \left\langle X_k \rho_0^s \left(\vec{u}_0 - \vec{u}_0^s \right) \right\rangle + \left\langle X_k \dot{r}^s \right\rangle + \left\langle \left[\rho_0^s \left(\vec{u}_0 - \vec{u}_{int} \right) - \rho_0^s \left(\vec{u}_0 - \vec{u}_0^s \right) \right] \cdot \nabla X_k \right\rangle .$$

Again introducing the fluctuating velocity and the definitions of averaged quantities, our final form of the ***averaged species mass balance equation*** is

$$\begin{aligned}
\frac{\partial \alpha_k \rho_k^s}{\partial t} + \nabla \cdot \alpha_k \rho_k^s \vec{u}_k = {} & \nabla \cdot \left\langle X_k \rho_0^s \left(\vec{u}_0 - \vec{u}_0^s \right) \right\rangle && \textit{relative species flux} \\
& - \nabla \cdot \left\langle X_k \rho_0^s \vec{u}_k' \right\rangle && \textit{fluctuational diffusion} \\
& + \left\langle \rho_0^s \left(\vec{u}_0 - \vec{u}_{int} \right) \cdot \nabla X_k \right\rangle && \textit{phase change} \\
& - \left\langle \rho_0^s \left(\vec{u}_0 - \vec{u}_0^s \right) \cdot \nabla X_k \right\rangle && \textit{mass exchange} \\
& + \dot{R}_k^s && \textit{chemical reactions}
\end{aligned} \tag{25}$$

where we have defined the average generation rate in phase k due to chemical reactions as $\dot{R}_k^s \equiv \dfrac{\left\langle X_k \dot{r}^s \right\rangle}{\alpha_k}$.

Momentum Balance

The ***averaged momentum balance equation*** results from the generic, averaged balance equation (20) with the assignment of

$$\psi_0 = \vec{u}_0 \qquad J_0 = \underset{\sim}{T}_0 \qquad g_0 = \vec{g}_0$$

to give

$$\frac{\partial \alpha_k \rho_k \vec{u}_k}{\partial t} + \nabla \cdot \alpha_k \rho_k \vec{u}_k \vec{u}_k = \nabla \cdot \alpha_k \left(\underset{\sim}{T}_k + \underset{\sim}{T}_k^{Fluct} \right) + \alpha_k \rho_k \vec{g}_k + \Omega_k^{mom} + \vec{u}_k^{int} \Omega_k^{mass} \text{ ,} \tag{26}$$

where the *fluctuating stress* $\underset{\sim}{T}_k^{Fluct}$ and the *interfacial momentum source* Ω_k^{mom} are given by

$$\underset{\sim}{T}_k^{Fluct} \equiv -\frac{\left\langle X_k \rho_0 \vec{u}_k' \, \vec{u}_k' \right\rangle}{\alpha_k} \qquad \Omega_k^{mom} \equiv -\left\langle \underset{\sim}{T}_0 \cdot \nabla X_k \right\rangle .$$

The averaged interfacial momentum balance constraint (jump condition) is

$$\sum_{k=1}^{no.\,of\ phases} \Omega_k^{mom} + \vec{u}_k^{int} \Omega_k^{mass} = \vec{M}_{surface\ tension} \text{ ,} \tag{27}$$

where $\vec{M}_{surface\ tension}$ is the *interfacial momentum source*, i.e. surface tension source.

Energy Conservation

The assignment of

$$\psi_0 = E_0 = e_0 + \frac{1}{2} \vec{u}_0 \cdot \vec{u}_0 \qquad J_0 = \underset{\sim}{T}_0 \cdot \vec{u}_0 + \vec{q}_0 \qquad g_0 = \vec{g}_0 \cdot \vec{u}_0 + \varepsilon_0$$

to the variables of the generic, averaged balance equation (20) gives the ***averaged energy conservation equation***

$$\begin{aligned}\frac{\partial}{\partial t}\alpha_k\rho_k\left(e_k+\frac{1}{2}\vec{u}_k\cdot\vec{u}_k+e_k^{Fluct}\right)+\nabla\cdot\alpha_k\rho_k\vec{u}_k\left(e_k+\frac{1}{2}\vec{u}_k\cdot\vec{u}_k+e_k^{Fluct}\right)&=\nabla\cdot\left[\alpha_k\left(\underset{\sim}{T}_k+\underset{\sim}{T}_k^{Fluct}\right)\cdot\vec{u}_k\right]\\&\quad-\nabla\cdot\alpha_k\left(\vec{q}_k+\vec{q}_k^{Fluct}\right)+\alpha_k\rho_k\left(\varepsilon_k+\vec{g}_k\cdot\vec{u}_k\right)\\&\quad+\Omega_k^{energy}+\Omega_k^{mom}\cdot\vec{u}_k^{int}\\&\quad+\Omega_k^{mass}\left(e_k^{int}+\frac{1}{2}\vec{u}_k^{int}\cdot\vec{u}_k^{int}\right),\end{aligned}\tag{28}$$

where

$$e_k^{Fluct}\equiv\frac{1}{2}\frac{\left\langle X_k\rho_0\vec{u}_k'\cdot\vec{u}_k'\right\rangle}{\alpha_k\rho_k}\qquad\textit{fluctuation kinetic energy}$$

$$\vec{q}_k^{Fluct}\equiv\underbrace{\frac{\left\langle X_k\rho_0\vec{u}_k'e_k'\right\rangle}{\alpha_k}}_{\textit{fluctution internal energy flux}}+\underbrace{\frac{\left\langle X_k\underset{\sim}{T}_0\cdot\vec{u}_k'\right\rangle}{\alpha_k}}_{\textit{fluctuation shear working}}+\underbrace{\frac{1}{2}\frac{\left\langle X_k\rho_0\vec{u}_k'\left(\vec{u}_k'\cdot\vec{u}_k'\right)\right\rangle}{\alpha_k}}_{\textit{fluctuation kinetic energy flux}}\qquad\textit{fluctuation energy flux}$$

$$\varepsilon_k\equiv\frac{\left\langle X_k\rho_0\varepsilon_0\right\rangle}{\alpha_k\rho_k}\qquad\textit{energy source}$$

$$\Omega_k^{energy}\equiv\left\langle\vec{q}_0\cdot\nabla X_k\right\rangle\qquad\textit{interfacial heat source}$$

$$\Omega_k^{mom}\cdot\vec{u}_k^{int}\equiv-\left\langle\underset{\sim}{T}_0\cdot\vec{u}_0\cdot\nabla X_k\right\rangle\qquad\textit{interfacial work}\ .$$

The averaged interfacial energy balance constraint (jump condition) is

$$\sum_{k=1}^{no.\ of\ phases}\Omega_k^{energy}+\Omega_k^{mom}\cdot\vec{u}_k^{int}+\Omega_k^{mass}\left(e_k^{int}+\frac{1}{2}\vec{u}_k^{int}\cdot\vec{u}_k^{int}\right)=\xi\ ,\tag{29}$$

where ξ is the interfacial energy source.

The kinetic energy associated with the velocity fluctuations, e_k^{Fluct} , is a type of "turbulent" kinetic energy. Sometimes the sum $e_k+e_k^{Fluct}$ is interpreted as the effective internal energy per unit mass of phase k .

It is sometimes useful to have an expression for the balance of fluctuation kinetic energy, e_k^{Fluct} . Its evolutionary description is derived by introducing the partition $\vec{u}_k'=\vec{u}_0-\vec{u}_k$ into the microscopic pure phase momentum balance, taking the dot product of this equation with $X_k\vec{u}_k'$, then performing the statistical average over configurations (keeping in mind that $\left\langle X_k \rho_0 \vec{u}' \right\rangle$ vanishes) to obtain [details are left to the reader, see e.g. Nigmatulin 1990]

$$\begin{aligned} \alpha_k \rho_k \frac{\partial e_k^{Fluct}}{\partial t} + \alpha_k \rho_k \vec{u}_k \cdot \nabla e_k^{Fluct} &= \alpha_k \underset{\sim}{T}_k^{Fluct} : \nabla \vec{u}_k \\ &\quad - \nabla \cdot \left\langle \frac{X_k \rho_0 \left(\vec{u}'_k \cdot \vec{u}'_k \right) \vec{u}'_k}{2} \right\rangle + \left\langle X_k \vec{u}'_k \cdot \left(\nabla \cdot \underset{\sim}{T}_0 + \rho_0 \vec{g}_0 \right) \right\rangle \end{aligned} \tag{30}$$

This equation bares some similarity to the equation of evolution of the fluctuational kinetic energy in a single-phase turbulent fluid [Wilcox 1998]. The first term on the right side describes the influence of the gradient of $\vec{u}_k$ on the development of e_k^{Fluct}, the second term is expected to diffuse e_k^{Fluct}, and the last term represents the power developed by the stresses and external forces [Lhuillier 1996].

For most multiphase flows, including some very (conceptually) simple flows such as gas flow through a packed bed or through a pebble-bed nuclear reactor, the nature of e_k^{Fluct} is somewhat different than that of a turbulent single-phase flow. Contrary to a one-phase fluid in which the fluctuations disappear for slow flows, these fluctuations for a multiphase flow exist however slow the flow. For this reason, e_k^{Fluct} that is produced by hydrodynamic interactions between the phases is sometimes called pseudo-turbulence [Lhuillier 1996].

Entropy Inequality

The local form of the entropy inequality (8), sometimes called the "Second Law of Thermodynamics," is used to place restrictions on the constitutive relations used to give unique phase or material behaviors. With the assignment of

$$\psi_0 = s_0 \qquad J_0 = -\frac{\vec{q}_0}{\theta_0} \qquad g_0 = \frac{\varepsilon_0}{\theta_0}$$

to the variables of the generic, averaged balance relationship (20) the ***averaged entropy inequality*** results,

$$\frac{\partial \alpha_k \rho_k s_k}{\partial t} + \nabla \cdot \alpha_k \rho_k s_k \vec{u}_k \geq \nabla \cdot \alpha_k \left(\Phi_k + \Phi_k^{Fluct} \right) + \alpha_k \rho_k S_k + \Omega_k^{entropy} + \Omega_k^{mass} s_k^{int} \tag{30}$$

where

$$\vec{\Phi}_k \equiv - \frac{\left\langle X_k \dfrac{\vec{q}_0}{\theta_0} \right\rangle}{\alpha_k} \qquad \textit{entropy flux}$$

$$\vec{\Phi}_k^{Fluct} \equiv -\frac{\left\langle X_k \rho_0 s_k' \vec{u}_k' \right\rangle}{\alpha_k} \qquad \textit{fluctuation entropy flux}$$

$$S_k \equiv \frac{\left\langle X_k \dfrac{\rho_0 \varepsilon_0}{\theta_0} \right\rangle}{\alpha_k \rho_k} \qquad \textit{entropy source}$$

$$\Omega_k^{entropy} \equiv \left\langle \frac{\vec{q}_0}{\theta_0} \cdot \nabla X_k \right\rangle \qquad \textit{interfacial entropy source}\,.$$

This entropy inequality corresponds to what Drew and Passman (1999) call the microscopic entropy inequality. A macroscopic entropy inequality can be obtained by summing inequalities (30) over all of the phases or materials present in the mixture [Truesdell 1984 and the other authors contained therein]. The macroscopic entropy inequality is useful for placing restrictions on the phasic or material interaction constitutive relations. The averaged interfacial entropy inequality (jump condition) is

$$\sum_{k=1}^{no.\,of\ phases} \Omega_k^{entropy} + \Omega_k^{mass} s_k^{int} \geq 0\,. \tag{31}$$

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Appendix: Moment Evolution Equation

It is critical that special attention be given to functional dependencies in deriving the moment evolution equation. Let us begin first by defining the ***ensemble average*** of some property Q_0 as

$$\langle Q_0\rangle(\vec{x},t) \equiv \int Q_0(\Gamma_0)\, f(\vec{x},t,\Gamma_0)\, d\Gamma_0 \,, \tag{A.1}$$

where, for example, $\Gamma_0 = \{\rho_0, \vec{u}_0, e_0, X_1, X_2, \cdots\}$. Note that, while Q_0 depends explicitly upon the state Γ_0, its average value $\langle Q_0\rangle$ depends upon position $\vec{x}$ and time t, which it acquired from the probability function $f(\vec{x},t,\Gamma_0)$. In fact, $\langle Q_0\rangle$ loses its explicit dependence upon Γ_0 by its very definition as an integral over all possible states Γ_0.

The variation of the probability is

$$df = \frac{\partial f}{\partial t}dt + \frac{\partial f}{\partial \vec{x}}\cdot d\vec{x} + \frac{\partial f}{\partial \Gamma_0}\cdot d\Gamma_0 \,,$$

so the ***time variation of the probability*** can be written

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \vec{u}_0 \cdot \nabla f + \dot{\Gamma}_0 \cdot \frac{\partial f}{\partial \Gamma_0}. \tag{A.2}$$

If we now multiply this equation by $Q_0(\Gamma_0)$ and integrate over Γ_0-space we get

$$\int Q_0 \frac{df}{dt} d\Gamma_0 = \int Q_0 \frac{\partial f}{\partial t} d\Gamma_0 + \int Q_0 \vec{u}_0 \cdot \nabla f \, d\Gamma_0 + \int Q_0 \Gamma_0 \cdot \frac{\partial f}{\partial \Gamma_0} d\Gamma_0. \tag{A.3}$$

Let us now further examine each term of this expression. Since Q_0 does not depend explicitly on time, t,

$$\begin{aligned} \int Q_0(\Gamma_0) \frac{\partial f}{\partial t} d\Gamma_0 &= \int \frac{\partial (Q_0 f)}{\partial t} d\Gamma_0 \\ &= \frac{\partial}{\partial t} \int Q_0 f \, d\Gamma_0 \\ &= \frac{\partial}{\partial t} \langle Q_0 \rangle (\vec{x}, t). \end{aligned}$$

Similarly, since Q_0 is independent of $\vec{x}$, we have

$$\begin{aligned} \int Q_0 \vec{u}_0 \cdot \nabla f \, d\Gamma_0 &= \int \nabla (Q_0 f) \cdot \vec{u}_0 \, d\Gamma_0 \\ &= \int \nabla \cdot (Q_0 \vec{u}_0 f) d\Gamma_0 - \int Q_0 f (\nabla \cdot \vec{u}_0) d\Gamma_0 \\ &= \nabla \cdot \int Q_0 \vec{u}_0 f \, d\Gamma_0 - \int Q_0 (\nabla \cdot \vec{u}_0) f \, d\Gamma_0 \\ &= \nabla \cdot \langle Q_0 \vec{u}_0 \rangle (\vec{x}, t) - \langle Q_0 \nabla \cdot \vec{u}_0 \rangle (\vec{x}, t). \end{aligned}$$

We also know that the $\dot{\Gamma}_0$ are independent of Γ_0, so

$$
\begin{aligned}
\int Q_0 \dot{\Gamma}_0 \cdot \frac{\partial f}{\partial \Gamma_0} d\Gamma_0 &= \dot{\Gamma}_0 \cdot \int Q_0 \frac{\partial f}{\partial \Gamma_0} d\Gamma_0 \\
&= \dot{\Gamma}_0 \cdot \left[\int \frac{\partial (Q_0 f)}{\partial \Gamma_0} d\Gamma_0 - \int f \frac{\partial Q_0}{\partial \Gamma_0} d\Gamma_0 \right] \\
&= \dot{\Gamma}_0 \cdot Q_0 f \big|_{\text{limit of } \Gamma_0} - \int \dot{\Gamma}_0 \cdot \frac{\partial Q_0}{\partial \Gamma_0} f \, d\Gamma_0 \\
&= 0 - \left\langle \dot{\Gamma}_0 \cdot \frac{\partial Q_0}{\partial \Gamma_0} \right\rangle \\
&= -\left\langle \frac{\partial Q_0}{\partial \Gamma_0} \cdot \frac{d\Gamma_0}{dt} \right\rangle \\
&= -\left\langle \frac{dQ_0}{dt} \right\rangle = -\left\langle \dot{Q}_0 \right\rangle (\vec{x}, t) .
\end{aligned}
$$

As long as the Q_0 are physically conserved quantities we also have

$$\int Q_0 \frac{df}{dt} d\Gamma_0 = 0 .$$

Putting all these expressions back into the integral equation above gives the ***moment evolution equation*** (11)

$$\frac{\partial \langle Q_0 \rangle}{\partial t} + \nabla \cdot \langle Q_0 \vec{u}_0 \rangle = \left\langle \dot{Q}_0 + Q_0 \nabla \cdot \vec{u}_0 \right\rangle .$$

⟦ **Notice:** By comparison with Equation (1.1) of [Kashiwa and Rauenzahn 1994],

$$\frac{\partial \langle Q_0 \rangle}{\partial t} + \nabla \cdot \langle Q_0 \vec{u}_0 \rangle = \left\langle \dot{\Gamma}_0 \cdot \frac{\partial Q_0}{\partial \Gamma_0} \right\rangle + \int Q_0 \frac{Df}{Dt} d\Gamma_0 ,$$

theirs should read

$$
\begin{aligned}
\frac{\partial \langle Q_0 \rangle}{\partial t} + \nabla \cdot \langle Q_0 \vec{u}_0 \rangle &= \left\langle \dot{\Gamma}_0 \cdot \frac{\partial Q_0}{\partial \Gamma_0} \right\rangle + \langle Q_0 \nabla \cdot \vec{u}_0 \rangle + \int Q_0 \frac{Df}{Dt} d\Gamma_0 \\
&= \left\langle \dot{Q}_0 + Q_0 \nabla \cdot \vec{u}_0 \right\rangle + \int Q_0 \frac{Df}{Dt} d\Gamma_0
\end{aligned}
$$

to be correct. ⟧

Chapter 2: Seven Equation, Two-Pressure, Two-Velocity Hyperbolic, Well-Posed Models for Two-Phase Flows

Prior to 1981 there had been attempts to remove the ill-posed nature from the full, two-phase flow equations, e.g. [Ransom and Scofield, 1976], [Stuhmiller, 1977], [Rousseau and Ferch, 1979], [Banerjee and Chan, 1980], [Hancox et.al., 1980], as well as others. All of these researchers were trying to gain closure of this equation system (the classical 6-equations system) through algebraic means – and were meeting some limited success. But they all seemed to be missing some key ingredient.

In 1981 [Nguyen, 1981] presented a paper identifying the missing ingredient in compressible two-phase flow. {Note: the author's paper drew considerable "fire" at the time, and the paper received little attention subsequently (in fact I don't believe I've ever seen it referenced). However, upon closer examination, this paper contains a key point that was developed independently (later) by other researchers, who now seem to have received credit for its invention.} In this paper Nguyen utilized the entropy production for each phase to perform an Onsager-type analysis wherein a bilinear form in the thermodynamic fluxes and their conjugate forces was obtained. From this he arrived at the so-called *phenomenological laws*, one of which, in first approximation is:

$$p_k - p_i = L_{\alpha k}\left(\frac{\partial \alpha_k}{\partial t} + w_k \frac{\partial \alpha_k}{\partial z}\right) \tag{1}$$

where the notation is standard, with w_k denoting the z -component of phase k velocity and $L_{\alpha k}$ denoting a phenomenological coefficient, possibly to be "obtained from the flow structure." To complete the set of closure equations, Nguyen proposed to define the interface pressure p_i as

$$p_i = \frac{1}{2}\sum_{k=1}^{2}\left[p_k - \alpha_k \rho_k \xi_k\left(w_1, w_2\right)\right] \tag{2}$$

where ξ_k was to be defined consistently with the physical situation of interest. Nguyen furthermore deemed it reasonable to assume that the phenomenological coefficients were equal or

$$L_{\alpha 1} = L_{\alpha 2} = L_{\alpha} \ .$$

With these assumptions Nguyen then obtained a 7-equation model with real characteristics which was hyperbolic and which could be formulated as a well-posed initial-value problem.

However, what Nguyen did not do (at least in that paper) was the following useful manipulation. Adding his equations (49) and (50) to eliminate p_i gives

$$\frac{\partial \alpha}{\partial t}+\frac{w_1+w_2}{2}\frac{\partial \alpha}{\partial z}=\frac{p_1-p_2}{2L_\alpha} \ .$$

While we are enhancing the equations of Nguyen's paper, let us also do the following: Let us assume that the phenomenological coefficients are <u>not</u> equal. It is easily obtained that

$$\frac{\partial \alpha}{\partial t}+\left(\frac{L_1 w_1+L_2 w_2}{L_1+L_2}\right)\frac{\partial \alpha}{\partial z}=\frac{p_1-p_2}{L_1+L_2} \ . \tag{3}$$

Now, if $L_2 \gg L_1$ and w_1 is of the same order as w_2 then the above relationship is approximately

$$\frac{\partial \alpha}{\partial t}+w_2\frac{\partial \alpha}{\partial z}\approx\frac{p_1-p_2}{L_2} \ .$$

These relationships are appealing because now the volume fraction change is governed by a dynamical relationship in which the pressure difference between the two phases drove the phase change. If the phases had the same pressure there would be no change in volume fraction. The denominators on the right hand side, i.e. combinations of the phenomenological coefficients for the two phases would determine how "fast" pressure equilibrium was attained. The phasic advection equation, or *volume fraction propagation equation*, also exhibited an advection velocity that was a weighted combination of phasic velocities (weighted with the phenomenological coefficients).

In March 1983 Stephen Passman and Jace Nunziato at Sandia and E.K. Walsh at U. of Florida published a report, later to become Appendix 5C [Passman, Nunziato, and Walsh 1983] of Clifford Truesdell's classical work [Truesdell, 1984]. In their elegant work, in addition to the traditional axioms of balance, an additional balance axiom was postulated which describes changes in volume fraction. They utilized the idea of workless constraints to describe a method of accounting, in the entropy inequality for the mixture, for the constraint requiring that the mixture be saturated. This resulted in a volume fraction propagation equation, which they called *balance of equilibrated force*, which accounts for the fact that the constituent volume fractions can change without affecting the gross motion. As they point out, this equation, in a sense, models the microstructural force systems operative in multiphase mixtures.

{Note: This approach has not seen much acceptance in the two-phase fluid flow community, probably because the equation derivation was postulational [Truesdell, 1984] (as opposed to using some type of averaging) and because of the lack of physical familiarity with the terminology. However, some years later Flavio Dobran at New York University published a monograph [Dobran, 1991] in which rigorous volume averaging is utilized, along with a basic *material deformation postulate*, to derive additional transport equations for multiphase mixtures that are very similar.}

In December 1983 Mel Baer and Jace Nunziato of Sandia released a two-phase mixture theory describing the deflagration-to-detonation transition (DDT) in reactive granular materials [Baer and Nuziato, 1983]. In this work the entropy inequality for the two-phase mixture was utilized to directly establish a constitutive volume fraction propagation equation, which (in the context of their application) they called the *compaction equation* (with phase change)

$$\frac{\partial \alpha_s}{\partial t} + v_s \frac{\partial \alpha_s}{\partial z} = \frac{\alpha_s \alpha_g}{\mu_c} \left[p_s - \left(p_g + \beta_s \right) \right] + \frac{c_s^+}{\gamma_s} \tag{4}$$

where β_s is a configuration pressure which resists changes in the packing of the bed or compaction and the coefficient μ_c is a compaction viscosity (again in their application context) which controls the rate at which pressure equilibrium is reached. Though derived in a different manner, this equation can also be viewed as a simpler, special case of Passman et.al.'s balance of equilibrated force equation, mentioned above. This 7-equation compressible two-phase model of Baer and Nunziato was hyperbolic and well-posed. They also constructed apparently successful numerical solution algorithms for this equation set. While the motivating applications for this model are far different from those of the two-phase fluid dynamics community, the foundational principles are very similar. Notice the similarities between their volume fraction propagation equation and that of Nguyen over two years earlier.

{Note added later: This research was published later in the open literature [Baer and Nunziato, 1986]. However, perhaps this time because of the application context and because of its postulational derivation, this method received little attention from the two-phase fluid dynamics community.}

Baer and Nunziato's volume fraction evolutionary equation can be more generally stated as

$$\frac{\partial \alpha_a}{\partial t} + v_a \frac{\partial \alpha_a}{\partial z} = \sum_j \frac{\alpha_a \alpha_j}{\mu_{j,a}} \left[p_a - \beta_a - \left(p_j - \beta_j \right) \right] + \frac{c_a^+}{\gamma_a} \tag{5}$$

where β_a are configuration pressures and exchange coefficients $\mu_{j,a}$ reflect interactions between the phases. These rate equations, which provide closure of the mixture model, are force balances involving the configurational pressures, phase pressures, and a viscous-like stress associated with rate-dependent volume fraction changes. The relaxation coefficients, $\mu_{j,a}$, have the units of viscosity. Moreover, like Nguyen's (but unlike Passman et.al.'s), these equations are constitutive equations, not field equations. As pointed out in [Baer, 1997], *they reflect boundary conditions at the microscale*. [Saurel et.al.] recast the volume fraction evolution equation as a microscopic mass density evolution equation {see notes}. [Kashiwa and Gaffney 2003] derive a mass density evolution equation having a somewhat different character.

To more easily see the need for a dynamic volume fraction evolution equation let us consider a cell mixture-intuitive physics model for two-phase flow. Consider a fixed volume V with two immiscible constituents present (e.g. the two constituents may have been advected into a fixed cell volume). They have masses m_1 and m_2 occupying volumes V_1 and V_2, respectively, such that

$$V_1 + V_2 = V\ .$$

Each constituent phase has material density ρ_1 and ρ_2, so

$$\begin{aligned} V &= V_1 + V_2 \\ &= \frac{m_1}{\rho_1} + \frac{m_2}{\rho_2} \end{aligned}$$

or

$$\begin{aligned} 1 &= \frac{V_1}{V} + \frac{V_2}{V} \\ &= \alpha_1 + \alpha_2 \\ &= \frac{m_1}{V\rho_1} + \frac{m_2}{V\rho_2} \end{aligned}$$

where $\alpha_1 = \dfrac{V_1}{V}$ and $\alpha_2 = \dfrac{V_2}{V}$ are volume fractions of each phase. For each constituent

$$\rho_1 = \frac{m_1}{V_1} \quad and \quad \rho_2 = \frac{m_2}{V_2} \tag{6}$$

and

$$\begin{aligned} p_1 &= f_1(\rho_1, I_1) \\ &= f_1\left(\frac{m_1}{V_1}, I_1\right) \end{aligned} \tag{7}$$

$$\begin{aligned} p_2 &= f_2(\rho_2, I_2) \\ &= f_2\left(\frac{m_2}{V_2}, I_2\right) \end{aligned} . \tag{8}$$

Now if V_1 and V_2 are adjusted (subject to the $V_1 + V_2 = V$ constraint) until the phase pressures are equal to

$$p = f_1\left(\frac{m_1}{V_1}, I_1\right) = f_2\left(\frac{m_2}{V_2}, I_2\right) \tag{9}$$

with the equilibrium (or equilibration) pressure, p . At this equilibrium pressure the corresponding phase volumes yield the equilibrium volume fractions

$$\alpha_1^e = \frac{V_1}{V}$$
$$\alpha_2^e = \frac{V_2}{V} \ .$$

This can be accomplished more generally in a dynamical fashion as follows. First, note that

$$\begin{aligned} p_1 &= f_1\left(\rho_1, I_1\right) \\ &= f_1\left(\frac{m_1}{\alpha_1 V}, I_1\right) \end{aligned}$$

$$\begin{aligned} p_2 &= f_2\left(\rho_2, I_2\right) \\ &= f_2\left(\frac{m_2}{\alpha_2 V}, I_2\right) \end{aligned}$$

and also that

$$\frac{d\alpha_1}{dt} = -\frac{d\alpha_2}{dt}$$
$$\frac{d^2\alpha_1}{dt^2} = -\frac{d^2\alpha_2}{dt^2} \ .$$

Intuitively, we now consider the dynamical equation

$$\frac{d\alpha_1}{dt} = \frac{p_1 - p_2}{\tau} \ . \tag{10}$$

If α_1 is compressed too much $\left(p_1 > p_2\right)$ then α_1 will increase with time (relax) letting p_1 reduce while α_2 decreases letting p_2 increase. This process ends when $p_1 = p_2 = p$ and thus $\frac{d\alpha_1}{dt} = 0$. The relaxation rate, τ , controls the rate at which the phases (pressures) equilibrate.

More generally yet, we could even write

$$\begin{aligned} \left(microinertia\right)\cdot\frac{d^2\alpha_1}{dt^2} + \left(compaction\ viscosity\right)\cdot\frac{d\alpha_1}{dt} &= \left(microstructural\ \ forces\right) \\ &= F \end{aligned} \tag{11}$$

The microstructural force F is a relaxation term that is intended to model the driving force or "resistance" exhibited by the mixture to changes in its configuration. For example, if we were compacting a gas-solid particle bed,

$$F = \begin{cases} \alpha_s \alpha_g \left(p_s - p_g - \beta_s \right) & for \quad p_s - \beta_s > 0 \\ -\alpha_s \alpha_g p_g & for \quad p_s - \beta_s \leq 0 \end{cases} \tag{12}$$

in accordance with the view of compaction as an irreversible process. β_s is the "configuration pressure" of the bed.

If we set the "microinertial" and the "configuration pressure" to zero we are left with

$$\mu \frac{d\alpha_1}{dt} = \alpha_1 \alpha_2 \left(p_1 - p_2 \right)$$

or

$$\frac{d\alpha_1}{dt} = \frac{\alpha_1 \alpha_2 \left(p_1 - p_2 \right)}{\mu} \tag{13}$$

Note the multiplicative coefficient $\alpha_1 \alpha_2$ in the driving force F . This term is included for a couple of reasons: (1) $\alpha_1 \alpha_2$ is roughly proportional to the interfacial area per unit volume, $\frac{A_i}{V}$. and (2) better behavior results in the limit of single phase occurring due to disappearance of the other phase, i.e. $\alpha_1 \to 0 \left(\alpha_2 \to 1 \right)$ or $\alpha_2 \to 0 \left(\alpha_1 \to 1 \right)$.

In LANL's CFDLib code, [Kashiwa and Rauenzahn, 1994] take a different approach to the calculation of equilibration pressure. By enforcing that the saturation constraint is met:

$$1 - \sum_k \alpha_k = 0$$

or

$$1 - \sum_k \frac{m_k}{V} v_k \left(p, T_k \right) = 0$$

or

$$1 - \sum_k \frac{m_k}{V} \frac{1}{\rho_k^0 \left(p, T_k \right)} = 0$$

or, for two phases

$$1 - \frac{m_1}{V} \frac{1}{\rho_1^0 \left(p, T_1 \right)} - \frac{m_2}{V} \frac{1}{\rho_2^0 \left(p, T_2 \right)} = 0 \tag{14}$$

they seek a p (equilibration pressure) which will satisfy this equation. Material equations of state are used for $\rho_k^0\left(p,T_k\right)$. Additional terms are then added to account for differences between the individual phasic pressures and the equilibration pressure. A simple example of this approach will be given in the next section.

Recently, some French researchers, who originally had used Baer and Nunziato's model with some slight reformulation for similar applications, began to generalize it and apply it to other multiphase mixtures of interest in a fluid dynamics context. In 1998, Richard Saurel and Remi Abgrall [Saurel and Abgrall, 1999] published their 7-equation compressible multifluid/multiphase flow model (assuming no mass transfer between phases),

$$\frac{\partial\bar{\rho}_k}{\partial t}+\nabla\cdot\bar{\rho}_k\vec{u}_k=0 \tag{15}$$

$$\frac{\partial\bar{\rho}_k\vec{u}_k}{\partial t}+\nabla\cdot\left(\bar{\rho}_k\vec{u}_k\otimes\vec{u}_k\right)+\nabla\bar{p}_k=p_I\nabla\alpha_k+\lambda\left(\vec{u}_m-\vec{u}_k\right) \tag{16}$$

$$\frac{\partial\bar{\rho}_k E_k}{\partial t}+\nabla\cdot\left(\bar{\rho}_k E_k\vec{u}_k+\bar{p}_k\vec{u}_k\right)=p_I u_I\cdot\nabla\alpha_k+\lambda\left(\vec{u}_m-\vec{u}_k\right)u_I+\mu\left(p_k-p_m\right)p_I \tag{17}$$

$$\frac{\partial\alpha_k}{\partial t}+u_I\cdot\nabla\alpha_k=\mu\left(p_k-p_m\right) \tag{18}$$

where α_k, $\bar{\rho}_k=\alpha_k\rho_k$, $\vec{u}_k$, $\bar{p}_k=\alpha_k p_k$, and E_k represent the fluid phase k "volume fraction", mass density, velocity, pressure, and total energy, respectively. These equations, which represent the balance of mass, momentum, and total energy, and volume fraction evolution, respectively, with specific interphase transfer terms placed on the right-hand sides. In these equations, (for a two-phase flow) $k=1,2$ and correspond respectively with $m=2,1$; p_I and u_I represent the interfacial pressure and velocity. In the Baer-Nunziato model, these variables are chosen as $p_I=p_2$ and $u_I=\vec{u}_1$, while the Saurel model utilized the following interfacial values:

$$u_I=\frac{\sum\limits_{k=1,2}\alpha_k\rho_k u_k}{\sum\limits_{k=1,2}\alpha_k\rho_k}\qquad \textit{and}\qquad p_I=\sum_{k=1,2}\alpha_k p_k \tag{19}$$

This model contains relaxation parameters λ and μ that determine the rates at which the velocities and pressures of the two phases reach equilibrium. These equations are closed by two equations of state, the saturation constraint for the volume fractions and the stiffened gas equation of state (which holds approximately for a broad range of gases and liquids)

$$\alpha_1+\alpha_2=1 \tag{20}$$

$$p_k = (\gamma_k - 1)\rho_k e_k - \gamma_k \pi_k \quad (21)$$

where e_k is the internal energy and γ_k and π_k are constants, specific for each phase k. Their model is unconditionally hyperbolic and well-posed, and seems to be able to solve physical situations for which other models fail. In the original Baer and Nunziato model, which is now more popular in the literature and even has become known as the BN-model, u_i is taken equal to the velocity of the less compressible phase and p_i, the interphase pressure, is taken equal to the pressure of the most compressible phase. In Saurel and Abgrall, p_i is taken equal to the mixture pressure and u_i to the velocity of the center of mass. In [Lallemand and Saurel, 2000] new and enhanced pressure relaxation procedures are presented for this method.

New variants of this theory are appearing in the literature, or are in preparation. For example, [Chinnayya, Daniel, and Saurel, 2004] use a new homogenization method (DEM) to obtain explicit formulas for p_i and u_i that are symmetric, compatible with the second law of thermodynamics, and responsible for the fulfillment of interface conditions when dealing with contact/interface problems; they also provide a general explicit formula for μ. Other recent works with these models include [Andrianov, Saurel, and Warnecke, 2003] and [Andrianov and Warnecke, 2004]. Also of interest, [Guillard and Murrone, 2005] use asymptotic analysis, in the limit of zero relaxation time, to reduce the 7-equation two-phase equation model (which contains relaxation terms that drive the system toward pressure and velocity equilibrium) to a five equation reduced hyperbolic system.

This whole approach seems to be gaining momentum. It is important to get the correct wave behavior during transients. The methods discussed above seem to be headed in the right direction.

{Note: all equations given here are in a one-dimensional context, but extend directly to multidimensions. Also, though not discussed here, most of the above methods also include models for the difference between the mean phase and interface pressures, e.g. Hicks and Ransom as well as several recent papers by Moon-Sun Chung, Sung-Jae Lee and co-workers in South Korea; references available}

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Chapter 3: Two-Phase Example

Two Barotropic Fluids, No Phase Change

Consider the simple two-phase example of two barotropic fluids exhibiting no phase change, i.e. no mass exchange between the two fluids.

Continuity

$$\frac{\partial(\alpha_1\rho_1)}{\partial t}+\frac{\partial(\alpha_1\rho_1 u_1)}{\partial x}=0 \tag{1}$$

$$\frac{\partial(\alpha_2\rho_2)}{\partial t}+\frac{\partial(\alpha_2\rho_2 u_2)}{\partial x}=0 \tag{2}$$

Momentum (no surface tension)

$$\frac{\partial(\alpha_1\rho_1 u_1)}{\partial t}+\frac{\partial\left(\alpha_1\rho_1 u_1^2\right)}{\partial x}=-\frac{\partial(\alpha_1 p_1)}{\partial x}+p_{1i}\frac{\partial\alpha_1}{\partial x}+M_1 \tag{3}$$

$$\frac{\partial(\alpha_2\rho_2 u_2)}{\partial t}+\frac{\partial\left(\alpha_2\rho_2 u_2^2\right)}{\partial x}=-\frac{\partial(\alpha_2 p_2)}{\partial x}+p_{2i}\frac{\partial\alpha_2}{\partial x}+M_2 \tag{4}$$

$$\sum_{k=1}^{2}p_{ki}\frac{\partial\alpha_k}{\partial x}+M_k=0 \tag{5}$$

Volume Fraction Propagation (and saturation constraint)

$$\frac{\partial\alpha_1}{\partial t}+u_i\frac{\partial\alpha_1}{\partial x}=\frac{\alpha_1\alpha_2}{\mu_c}(p_1-p_2) \tag{6}$$

$$\sum_{k=1}^{2}\alpha_k=1 \tag{7}$$

where (a couple of choices)

$$u_i=\frac{\sum_k\alpha_k\rho_k u_k}{\sum_k\alpha_k\rho_k}\quad or\quad u_i=u_k \tag{8}$$

is an *interface velocity*.

Constitutive

$$p_1=p_{01}+c_1^2(\rho_1-\rho_{01})\qquad (p_{01},c_1,\rho_{01}\ constants) \tag{9}$$

$$p_2=p_{02}+c_2^2(\rho_2-\rho_{02})\qquad (p_{02},c_2,\rho_{02}\ constants) \tag{10}$$

$$\textit{Relationships for } p_{ki} \tag{11}$$

$$\textit{Relationships for } M_k \tag{12}$$

Now consider that at longer times the phasic pressures may tend toward a common *equilibrium* or *equilibration pressure*, p^* . Toward this end let us rewrite the right hand side (RHS) of (3) and (4)

$$\begin{aligned}
-\frac{\partial(\alpha_k p_k)}{\partial x} + p_{ki}\frac{\partial \alpha_k}{\partial x} + M_k &= -\frac{\partial(\alpha_k p_k)}{\partial x} + \frac{\partial(\alpha_k p^*)}{\partial x} + p_{ki}\frac{\partial \alpha_k}{\partial x} - \frac{\partial(\alpha_k p^*)}{\partial x} + M_k \\
&= -\frac{\partial}{\partial x}\left[\alpha_k\left(p_k - p^*\right)\right] + p_{ki}\frac{\partial \alpha_k}{\partial x} - p^*\frac{\partial \alpha_k}{\partial x} - \alpha_k\frac{\partial p^*}{\partial x} + M_k \\
&= -\underbrace{\alpha_k\frac{\partial p^*}{\partial x}}_{\substack{\textit{acceleration by}\\ \textit{equilibration pressure}}} + \underbrace{\left(p_{ki} - p^*\right)\frac{\partial \alpha_k}{\partial x}}_{\substack{\textit{momentum exchange by}\\ \textit{pressure difference between}\\ \textit{equilibration pressure and}\\ \textit{local phasic interface}\\ \textit{pressure (acceleration force)}}} - \underbrace{\frac{\partial}{\partial x}\left[\alpha_k\left(p_k - p^*\right)\right]}_{\substack{\textit{acceleration by nonequilibrium}\\ \textit{phase pressure (pressure difference}\\ \textit{between phase and equilibration}\\ \textit{pressures)}}} + M_k
\end{aligned} \tag{13}$$

Traditional two-phase models (i.e. 1-pressure models) have only the first term on the RHS of (13) . The second and third terms can be very important. Even if we had the case of interface pressures being equal to the phasic pressures, $p_{ki} = p_k$, the RHS of (13) would be

$$= -\alpha_k\frac{\partial p^*}{\partial x} - \alpha_k\frac{\partial\left(p_k - p^*\right)}{\partial x} + M_k \tag{14}$$

and it is seen that the second term only disappears as $p_k \to p^*$ which almost certainly does not occur in wave propagation.

Let us assume that the interface pressures are equal for the two phases, i.e. $p_{1i} = p_{2i} = p_i$, and that separate phase pressures exist. Then (5) and (7) give

$$M_2 = -M_1 = -M \tag{15}$$

and the momentum equations (3) and (4) can be written

$$\frac{\partial(\alpha_1\rho_1 u_1)}{\partial t} + \frac{\partial\left(\alpha_1\rho_1 u_1^2\right)}{\partial x} = -\frac{\partial(\alpha_1 p_1)}{\partial x} + p_i\frac{\partial \alpha_1}{\partial x} + M \tag{16}$$

$$\frac{\partial(\alpha_2\rho_2 u_2)}{\partial t} + \frac{\partial\left(\alpha_2\rho_2 u_2^2\right)}{\partial x} = -\frac{\partial(\alpha_2 p_2)}{\partial x} + p_i\frac{\partial \alpha_2}{\partial x} - M \tag{17}$$

Now if we introduce equilibration pressure as in (13) the momentum equations can be written as

$$\frac{\partial(\alpha_1\rho_1u_1)}{\partial t}+\frac{\partial(\alpha_1\rho_1u_1^2)}{\partial x}=-\alpha_1\frac{\partial p^*}{\partial x}-\frac{\partial}{\partial x}\left[\alpha_1\left(p_1-p^*\right)\right]+\left(p_i-p^*\right)\frac{\partial\alpha_1}{\partial x}+M \tag{18}$$

$$\frac{\partial(\alpha_2\rho_2u_2)}{\partial t}+\frac{\partial(\alpha_2\rho_2u_2^2)}{\partial x}=-\alpha_2\frac{\partial p^*}{\partial x}-\frac{\partial}{\partial x}\left[\alpha_2\left(p_2-p^*\right)\right]+\left(p_i-p^*\right)\frac{\partial\alpha_2}{\partial x}-M \tag{19}$$

Again it is seen that this model reduces to the traditional, single pressure model only as $p_1, p_2, p_i \to p^*$.

It would appear that the definition of mean or equilibration pressure, p^*, is arbitrary. By physical reasoning alone the equilibration pressure can be defined as the pressure that enables specified masses of separate materials to fill an entire volume with no ongoing compression or expansion of the materials. Using (7), this mathematical statement is

$$1-\sum_{k=1}^{2}\frac{\alpha_k\rho_k}{\rho_k\left(p^*\right)}=0 \tag{20}$$

in which $\frac{1}{\rho_k\left(p^*\right)}$ is the volume occupied by a unit mass of pure material k at the equilibration pressure p^* . This can be thought of as the asymptotic value of mixture pressure, as time becomes large, after packing arbitrary or specified amounts of multiple materials into a box or cell, and allowing them to expand or contract isentropically.

Notice that the term $\frac{\alpha_k\rho_k}{\rho_k\left(p^*\right)}$ has units of material k volume per unit total volume, suggesting an obvious definition for the *equilibrium volume fraction* α_k^*

$$\alpha_k^*=\frac{\alpha_k\rho_k}{\rho_k\left(p^*\right)} \tag{21}$$

which provides the most popular closure for this part of the equations, namely $\alpha_k=\alpha_k^*$. This is called the *equilibrium pressure model*. In this model, the term involving the pressure difference $\alpha_k\left(p_k-p^*\right)$ vanishes in the momentum equations (18) and (19) as does also the p_i-p^* term.

The pressure of a component (phase) of a barotropic fluid is given by (9) and (10). At equilibrium

$$\rho_k\left(p^*\right)=\frac{\left(c_k^2\rho_{0k}-p_{0k}\right)+p^*}{c_k^2} \tag{22}$$

Substitution of (22) into (20) allows us to obtain p^* and substitution of (22) into (21) provides α_k^* .

To summarize, the equilibrium pressure model is

$$\frac{\partial(\alpha_1\rho_1)}{\partial t}+\frac{\partial(\alpha_1\rho_1u_1)}{\partial x}=0 \tag{23}$$

$$\frac{\partial(\alpha_2\rho_2)}{\partial t}+\frac{\partial(\alpha_2\rho_2u_2)}{\partial x}=0 \tag{24}$$

$$\frac{\partial(\alpha_1\rho_1u_1)}{\partial t}+\frac{\partial(\alpha_1\rho_1u_1^2)}{\partial x}=-\alpha_1\frac{\partial p^*}{\partial x}+M \tag{25}$$

$$\frac{\partial(\alpha_2\rho_2u_2)}{\partial t}+\frac{\partial(\alpha_2\rho_2u_2^2)}{\partial x}=-\alpha_2\frac{\partial p^*}{\partial x}-M \tag{26}$$

$$1-\frac{(\alpha_1\rho_1)c_1^2}{(c_1^2\rho_{01}-p_{01})+p^*}-\frac{(\alpha_2\rho_2)c_2^2}{(c_2^2\rho_{02}-p_{02})+p^*}=0 \tag{27}$$

$$\alpha_1=\frac{(\alpha_1\rho_1)c_1^2}{(c_1^2\rho_{01}-p_{01})+p^*} \tag{28}$$

$$\alpha_2=1-\alpha_1 \tag{29}$$

Another useful relation can be developed for $\dot{p}^*$. Recall that p^* was defined to be the pressure satisfying (20). Differentiating (20) in time (denoted by the subscript t),

$$\sum_{k=1}^{2}\frac{1}{\rho_k}(\alpha_k\rho_k)_t-\frac{(\alpha_k\rho_k)}{\rho_k^2}(\rho_k)_t=0 \tag{30}$$

Applying (1) and (2) , and noting from (9) and (10) that $(p^*)_t=c_k^2(\rho_k)_t$ we get

$$\sum_{k=1}^{2}\frac{1}{\rho_k}\left(-\frac{\partial(\alpha_k\rho_ku_k)}{\partial x}\right)-\sum_{k=1}^{2}\frac{(\alpha_k\rho_k)}{(\rho_kc_k)^2}(p^*)_t=0 \tag{31}$$

But using $(p^*)_x=c_k^2(\rho_k)_x$

$$\begin{aligned}-\sum_{k=1}^{2}\frac{1}{\rho_k}\left(\frac{\partial(\alpha_k\rho_ku_k)}{\partial x}\right)&=-\sum_{k=1}^{2}\frac{1}{\rho_k}\left[\rho_k\frac{\partial(\alpha_ku_k)}{\partial x}+(\alpha_ku_k)\frac{\partial(\rho_k)}{\partial x}\right]\\&=-\sum_{k=1}^{2}\frac{\partial(\alpha_ku_k)}{\partial x}-\sum_{k=1}^{2}\frac{\alpha_ku_k}{\rho_kc_k^2}\frac{\partial p^*}{\partial x}\end{aligned} \tag{32}$$

and

$$\sum_{k=1}^{2}\frac{\left(\alpha_k\rho_k\right)}{\left(\rho_k c_k\right)^2}=\sum_{k=1}^{2}\frac{\alpha_k}{\rho_k c_k^2} \tag{33}$$

equation (31) becomes

$$\left(-\sum_{k=1}^{2}\frac{\alpha_k}{\rho_k c_k^2}\right)\left(p^*\right)_t-\left(\sum_{k=1}^{2}\frac{\alpha_k u_k}{\rho_k c_k^2}\right)\frac{\partial p^*}{\partial x}-\sum_{k=1}^{2}\frac{\partial\left(\alpha_k u_k\right)}{\partial x}=0 \tag{34}$$

This equation can be rewritten in the illustrative form

$$\dot{p}^*=\left(p^*\right)_t+u_p\frac{\partial p^*}{\partial x}=\frac{-\sum_{k=1}^{2}\frac{\partial\left(\alpha_k u_k\right)}{\partial x}}{\sum_{k=1}^{2}\frac{\alpha_k}{\rho_k c_k^2}} \tag{35}$$

where

$$u_p=\frac{\sum_{k=1}^{2}\frac{\alpha_k u_k}{\rho_k c_k^2}}{\sum_{k=1}^{2}\frac{\alpha_k}{\rho_k c_k^2}} \tag{36}$$

Equations (35)-(36) are referred to as the *pressure equation*; it has a nice form. It says if the volume of one material displaces another due to flow in and/or out of the volume, the equilibration pressure must respond, and does so in proportion to the sound speeds of the various materials present.

Note two limiting cases for (35)-(36). For a single-phase, $\alpha_k=1$ and we have

$$\dot{p}^*=\rho c^2\frac{\partial u}{\partial x} \tag{37}$$

which is an identity. The second limiting case is for a single fluid having $c\to\infty$,corresponding to the incompressible fluid; then this just says

$$\frac{\partial u}{\partial x}=0 \tag{38}$$

An alternative derivation of the pressure equation could be as follows. Beginning with the continuity equations (1)-(2)

$$\frac{\partial\left(\alpha_k\rho_k\right)}{\partial t}+\frac{\partial\left(\alpha_k\rho_k u_k\right)}{\partial x}=0 \tag{39}$$

or

$$\alpha_k \frac{\partial \rho_k}{\partial t} + \rho_k \frac{\partial \alpha_k}{\partial t} + \alpha_k u_k \frac{\partial \rho_k}{\partial x} + \rho_k \frac{\partial \alpha_k u_k}{\partial x} = 0 \tag{40}$$

Using the previous identities

$$\left(p^*\right)_t = c_k^2 \left(\rho_k\right)_t \tag{41}$$

$$\left(p^*\right)_x = c_k^2 \left(\rho_k\right)_x \tag{42}$$

equation (40) can be written

$$\frac{\alpha_k}{c_k^2} \frac{\partial p^*}{\partial t} + \rho_k \frac{\partial \alpha_k}{\partial t} + \frac{\alpha_k u_k}{c_k^2} \frac{\partial p^*}{\partial x} + \rho_k \frac{\partial \alpha_k u_k}{\partial x} = 0 \tag{43}$$

Dividing by ρ_k gives

$$\frac{\alpha_k}{\rho_k c_k^2} \frac{\partial p^*}{\partial t} + \frac{\partial \alpha_k}{\partial t} + \frac{\alpha_k u_k}{\rho_k c_k^2} \frac{\partial p^*}{\partial x} + \frac{\partial \alpha_k u_k}{\partial x} = 0 \tag{44}$$

Summing over the k phases

$$\left(\sum_k \frac{\alpha_k}{\rho_k c_k^2} \right) \frac{\partial p^*}{\partial t} + \underbrace{\frac{\partial}{\partial t} \left(\sum_k \alpha_k \right)}_{=0} + \left(\sum_k \frac{\alpha_k u_k}{\rho_k c_k^2} \right) \frac{\partial p^*}{\partial x} + \frac{\partial}{\partial x} \left(\sum_k \alpha_k u_k \right) = 0 \tag{45}$$

or

$$\frac{\partial p^*}{\partial t} + \left(\frac{\displaystyle\sum_k \frac{\alpha_k u_k}{\rho_k c_k^2}}{\displaystyle\sum_k \frac{\alpha_k}{\rho_k c_k^2}} \right) \frac{\partial p^*}{\partial x} + \frac{\displaystyle\frac{\partial}{\partial x} \sum_k \alpha_k u_k}{\displaystyle\sum_k \frac{\alpha_k}{\rho_k c_k^2}} = 0 \tag{46}$$