

## BRIEF COMMUNICATION

### ON THE EFFECT OF $P\nabla\alpha$ TERM IN MULTIPHASE MECHANICS

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#### 1. INTRODUCTION

Investigators in multiphase mechanics often do not agree on the formulation of the force due the interaction of static pressure  $P$  and volume fraction  $\alpha_k$  of phase  $k$ . Discussions of the  $P\nabla\alpha_k$  term in the momentum equation of multiphase mechanics were given in various publications in the past few years.

The present study takes into account various views on this matter with the aim of clarifying and resolving the differences via basic considerations.

#### 2. BACKGROUND

When dealing with a component  $k$  of a molecular mixture of  $\nu$  components with disparate mass motion, the equation of its  $i$ -th component of momentum takes the form (neglecting mass transfer and field forces):

$$\begin{aligned} \rho_k \frac{\partial U_{ki}}{\partial t} + \rho_k U_{kj} \frac{\partial U_{ki}}{\partial x_j} = & -\frac{\partial P_k}{\partial x_i} + \frac{\partial}{\partial x_j} (\tau_{mk})_{ji} \\ & + \rho_k \sum_{\substack{l=1 \\ (l \neq k)}}^{\nu} F_{lk} (U_{li} - U_{ki}) + \frac{\partial}{\partial x_i} [\rho_k (U_{kj} - U_{mj})(U_{ki} - U_{mi})], \end{aligned} \quad [1]$$

where  $t$  is the time and  $x_j$  is the  $j$ -th cartesian coordinate,  $\rho_k$ ,  $U_{ki}$  are the density and the  $i$ -th component of velocity of species  $k$  respectively,  $\tau_{mk}$  is the viscous stress of component  $k$  in the mixture (subscript  $m$ ) and  $F_{lk}$  is the inverse relaxation time for momentum transfer from other components  $l$  to  $k$ . The last term of [1] is the inertial coupling force (Soo 1967, 1976; Chao, Sha & Soo 1977),  $U_{mi}$  the mean velocity of mass motion is defined by:

$$\rho_m U_{mj} = \sum_{k=1}^{\nu} \rho_k U_{kj} \quad [2]$$

and  $P_k$  is the partial pressure of molecular component  $k$ . When summed over all the components, [1] gives:

$$\rho_m \frac{\partial U_{mi}}{\partial t} + \rho_m U_{mj} \frac{\partial U_{mi}}{\partial x_j} = -\frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j} (\tau_m)_{ji} \quad [3]$$

where  $P$  is the static pressure of the mixture and the last two terms in [1] cancel out for the overall mixture, because they are internal actions and reactions. Equation [3] is, of course, a consequence of the Newton's law of motion when applied to a dispersed multiphase system (Soo 1967, 1967a).

When formulating in terms of multiphase mechanics (Soo 1977), the above partial pressure  $P_k$  loses its meaning; clearly for stationary bubbles in a liquid, other than the effect of surface tension, the static pressure in the inside of each bubble is equal to that of the liquid in its vicinity. Considering the mutual exclusion of phases in a given space, multiphase mechanics (Soo 1976, 1977) gives (still neglecting mass transfer):

$$\begin{aligned} \rho_k \frac{\partial U_{ki}}{\partial t} + \rho_k U_{kj} \frac{\partial U_{ki}}{\partial x_j} = & - \frac{\partial P \alpha_k}{\partial x_i} + \frac{\partial}{\partial x_j} (\tau_{mk})_{ji} \\ & + \rho_k \sum_{(l \neq k)} F_{kl} (U_{li} - U_{ki}) + \frac{\partial}{\partial x_j} \rho_k [(U_{kj} - U_{mj})(U_{ki} - U_{mi})] + I'_{kj} + V'_{kj}. \end{aligned} \quad [4]$$

The last two terms are the forces due to the effect of virtual mass and unsteady flow field; these details (Soo 1967; Sha & Soo 1977) are not repeated here, so also the effectiveness of momentum transfer since they do not concern the present discussion directly. Note that in formulating [4], discrete bubbles  $k$  can be represented by a distributed density  $\rho_k$ , large numbers of bubbles must exist in the control volume as compared to the number of those at the boundary of that volume. When bubbles become large as compared to the characteristic dimension of a flow system, each bubble should be treated as a domain, with the interaction at the boundary of a bubble treated in detail (Sha & Soo 1977).

In order to explore fully the implication of the term  $\nabla P \alpha_k$  in the above, it is also useful to spell out the energy equation of phases which are derived corresponding to [4]. We also take note of the fact that the kinetic energy of the dispersed phase derived from the kinetic energy of the fluid in continuum phase (Soo 1967). For dispersed phase  $k$ , we have:

$$\begin{aligned} \rho_k \frac{\partial u_k}{\partial t} + \rho U_{kj} \frac{\partial u_k}{\partial x_j} = & - \frac{\partial U_{mj} P \alpha_k}{\partial x_j} + q_k + w_k \\ & + \frac{\partial}{\partial x_j} \rho_k (U_{kj} - U_{mj})(u_k - u_m), \end{aligned} \quad [5]$$

where  $u_k$  is the internal energy,  $q_k$ ,  $w_k$  are the rate of heat transfer and the dissipation of work per unit volume respectively,  $-U_{mj} P (\partial \alpha_k / \partial x_j)$  is the work of compression of bubbles  $k$ , the displacement work  $-\alpha_k (\partial U_{mj} P / \partial x_j)$  is part of the work of the fluid (Sha & Soo 1977).

### 3. AN OVERVIEW

An overview of the term  $\nabla P \alpha = \alpha \nabla P + P \nabla \alpha$  in [4] includes those who favor (1) dropping  $P \nabla \alpha$  for reasons of making computation easier or from consideration of an interfacial source force, (2) retaining part of it as a stabilizing force and (3) retaining  $P \nabla \alpha$  for the reason of an extension of the continuum mechanics, as a compressive (or expansive) force and validity of the laws of thermodynamics. While details of these view are given below, it suffices to say that an all encompassing formulation for multiphase mechanics will be to replace, in the momentum equation, the term  $\nabla P \alpha_k$  by

$$\nabla P \alpha_k - B_k P \nabla \alpha_k = \alpha_k \nabla P + (1 - B_k) P \nabla \alpha_k, \quad [6]$$

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

arises from a concentration gradient and the effect of diffusion is well known.  $B_k = 1$  for the case of  $\nabla\alpha_k$  arising from a liquid layer of varying depth which will not produce diffusion.  $B_k$  therefore accounts for the influence of flow configurations which is not accounted for by  $\nabla\alpha_k$  alone.

#### 4. VIEWS FAVORING THE CHOICE OF $B_k \sim 1$

(i) A derivation toward eliminating the  $P\nabla\alpha$  term from the momentum equation was given by Ishii (1975). He defines  $\alpha$  as a time (void) fraction and suggested that the term  $P\nabla\alpha$  is cancelled out via the interfacial source term when the bulk mean pressure is nearly equal to the interfacial mean pressure. His interfacial momentum source has corresponding terms of  $\Gamma_k U_m$  and  $V_k$  terms in our derivations (Chao, Sha & Soo 1978). Vernier (1975) suggested that the coefficient to  $\nabla\alpha$  in Ishii's derivation should be zero and should not have an effect on the  $P\nabla\alpha$  term via  $\nabla\alpha P$ .

(ii) The concern of Gidaspow & Solbrig (1976) is how to get real characteristics. We have shown that the imaginary characteristics has arisen solely from omission of inertial coupling term and there is no need to drop  $P\nabla\alpha$  for the sake of stabilizing the solution (Soo 1976a, Sha & Soo 1977). They suggest that "since unreasonably high pressures are obtained, the partial pressure model without compensating large relative forces must be regarded as unrealistic in general".

#### 5. VIEWS FAVORING THE CHOICE OF $0 < B_k < 1$

(i) A review was given by Gidaspow & Solbrig (1976). They attributed  $P\nabla\alpha$  as an "extra type diffusive force". They cited Roberts & Donnelly (1974) as having "such force in their equations." They also cited Wallis and others and pointed out that "although there exist forces that depend upon gradients of volume fraction, the coefficient should not be simply the thermodynamic pressure  $P$ ".

(ii) Jackson *et al.* (1971) and Medlin *et al.* (1974) use a force in their momentum equation  $P\nabla\alpha$ , calling  $P\nabla\alpha$  an "effective force without giving an exact value". Gidaspow and Solbrig had expected that  $P\Delta\alpha$  contributes to "reduce the region of imaginary characteristics, but alone is not sufficient to give a system of partial equations that can be solved by stable finite difference techniques". They also called

$$(P - P_{\text{interface}})\nabla\alpha \quad [7]$$

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

(iii) G. B. Wallis (Gidaspow 1974) confirmed the above and suggested that  $P\nabla\alpha$  might be dropped for the case of stratified flow, but not in suspensions. He suggested "careful experiments".

#### 6. EVIDENCE THAT FAVORS $B_k = 0$

(i) The characteristic analysis in Soo (1976a) and Sha & Soo (1977) shows that the term  $P\nabla\alpha$  gives rise to a wave velocity in transient flow as in the case of transient one-dimensional single phase flow.

(ii) A thermodynamic and therefore a basic evidence for the existence of the  $P\nabla\alpha$  term is seen in the physical case of adiabatic compression of a bubble, when the  $P\nabla\alpha$  term is carried into the energy equation in the form of [5]. When this is reduced to a single particle in a liquid at zero velocity of both phases and with negligible heat transfer or heat source, and  $dx_j/U_j \rightarrow dt$ , [5] in terms of internal energy  $u$  reduces, with the continuity equation, to

$$\alpha \bar{\rho}_1 \frac{du_1}{dt} = -P \frac{d\alpha}{dt} \quad [8]$$

For a bubble which can be approximated as that of a perfect gas,  $P/\bar{\rho}_1 = RT$ ,  $du_1 = c_{v1} dT$ ,

$d\alpha/\alpha = dV/V$ ,  $V$  being the volume of the bubble and  $u$  is the internal energy

$$\frac{c_v}{R} \frac{dT}{T} + \frac{dV}{V} = 0 \quad [9]$$

or for ratios of specific heats  $\gamma$ , we get

$$TV^{\gamma-1} = \text{constant}, \quad [10]$$

the well known adiabatic relation when dissipation is absent. It is believed that resolution of a dilemma of this kind should be made in favor of the validity of the laws of thermodynamics.

(iii) Extension from continuum mechanics to multiphase mechanics. In the case of a continuum gas mixture of species 2 with a trace of species 1, the one-dimensional momentum equation of species 1 can be written as:

$$\frac{\partial \rho_1 U_1}{\partial t} + \frac{\partial \rho_1 U_1^2}{\partial x} - \frac{\partial}{\partial x} \rho_1 (U_1 - U_2)^2 = -\frac{\partial P_1}{\partial x} + \rho_1 F_1 (U_2 - U_1). \quad [11]$$

For the case of  $U_2 = 0$ ,  $P = \text{constant}$  and with concentration gradient  $\partial\alpha_1/\partial x$  initially, [11] becomes

$$\frac{\partial \rho_1 U_1}{\partial t} = -P \frac{\partial \alpha_1}{\partial x} - F \rho_1 U_1. \quad [12]$$

For a constant  $P$  and  $T$  (a stipulation which simplifies the problem but not a necessary condition), [12] can be written as:

$$\frac{\partial \rho_1 U_1}{\partial t} + F \rho_1 U_1 = -\frac{P}{\bar{\rho}_1} \frac{\partial \rho_1}{\partial x}. \quad [13]$$

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

$$\frac{\partial \rho_1}{\partial t} = -\frac{\partial \rho_1 U_1}{\partial x}. \quad [14]$$

We take the derivative of [13] with respect to  $x$  to give:

$$\frac{\partial}{\partial t} \frac{\partial \rho_1 U_1}{\partial x} + F \frac{\partial \rho_1 U_1}{\partial x} = -\frac{P}{\bar{\rho}_1} \frac{\partial^2 \rho_1}{\partial x^2}. \quad [15]$$

$U_1$  can be eliminated by combining [14] and [15] to give

$$\frac{\partial^2 \rho_1}{\partial t^2} + F \frac{\partial \rho_1}{\partial t} = \frac{P}{\bar{\rho}_1} \frac{\partial^2 \rho_1}{\partial x^2}. \quad [16]$$

Equation [16] is a diffusion equation with the inertial term  $\partial^2 \rho_1 / \partial t^2$ , which by itself gives a wave equation with RHS.  $\partial^2 \rho_1 / \partial t^2$  is negligible for large viscous resistance, and the resulting diffusion equation has a diffusivity of  $P/(\bar{\rho}_1 F)$ . For a perfect gas, the diffusivity becomes  $RT/(\bar{U}\lambda)$ , where  $\bar{U}$  is the mean molecular speed of  $\sqrt{8RT/\pi}$  and  $\lambda$  is the mean free path of species 1 in 2, i.e. this diffusivity is nearly  $\bar{U}\lambda$ .

Hence,  $P\nabla\alpha_1$  term contributes to the spread of species 1 which has an initial concentration

gradient. The velocity  $U_1$  can be determined then from [14] or by expressing [16] in flux form

$$\frac{\partial^2(\rho_1 U_1)}{\partial t^2} + F \frac{\partial(P_1 U_1)}{\partial t} = \frac{P}{\bar{\rho}_1} \frac{\partial^2(\rho_1 U_1)}{\partial x^2}. \quad [17]$$

Now we apply this to a multiphase mixture of fine particles of neutral buoyancy in water in a tube. If we apply [16] and [17] then  $P/(\bar{\rho}_1 F)$  corresponds to a Brownian diffusivity. If we have solid spheres of neutral buoyancy in water in a tube, in the absence of field forces and adhesion and if we started out with a concentration gradient of these spheres, over a long time the mixture will become homogenous in the concentration of these spheres. This is because of the diffusion mechanism inherent in the continuum approximation via the continuity and the momentum equations of the trace species. Velocity  $U_1$  becomes zero, once  $\partial\alpha_1/\partial x$  becomes zero. The  $P\nabla\alpha_1$  exists in this case in view of the mechanism embodied in [16].

## 7. DISCUSSION

The range of  $0 \leq B \leq 1$  covers the whole range from dispersed to pure drift flux flow. Thus, the effects of  $BP\nabla\alpha$  term on system behavior under various conditions can be investigated.  $B = 0$  for small particles has been rigorously demonstrated.  $P\nabla\alpha_k$  term is not the source of imaginary characteristics if the inertial coupling force is correctly accounted for.

Both the continuity equation and the momentum equation of continuum mechanics are derivable from the kinetic transport equation (Chapman-Enskog—re: Hirschfelder, Curtis, & Bird 1954) via setting Enskog general function  $\psi$  as molecular mass  $m$  to get the continuity equation and to set  $\psi$  as molecular momentum  $mv$  to get the momentum equation. When one applies the kinetic equation to two molecular species, he gets the diffusion equation. Therefore this background information suggests that the diffusion equation, while obtainable from molecular considerations, must be obtainable from the continuity and momentum equations of each species. The diffusivity in [16] gives, for  $P/\bar{\rho}_1 = (k/m_1)T$ ,  $F = 9\mu/2a^2 \bar{\rho}_1 = 9(\mu/m_1) (2\pi a/3)$ , a value of  $kT/6\pi\mu a$ , which is identical to the Brownian diffusivity.

Of course, the above molecular theory does not account for wakes and turbulence directly.  $B_k$  empirically extends Brownian diffusion to turbulent diffusion.

It is further interesting to note that for a system including a continuous phase of fluid  $f$  with several dispersed phases  $k$  (such as bubbles of different equivalent radii), mutual interaction among phases  $k$  are negligible and we have

$$\sum B_k d\alpha_k + B_f d\alpha_f = 0.$$

Since  $\alpha_f = 1 - \sum \alpha_k$ , we get for constant values of  $B_k$ 's

$$B_f = \sum B_k \alpha_k / \sum \alpha_k. \quad [19]$$

as the relation between the displacement factors of dispersed phases  $k$  with fluid  $f$  depending on flow configurations.

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