## ON INERTIAL COUPLING IN DYNAMIC EQUATIONS OF COMPONENTS IN A MIXTURE

## **B. T. CHAO,<sup>†</sup> W. T. SHA‡ and S. L. Soo†**

Argonne National Laboratory, 9700 South Cass Avenue, Argonne, IL 60439, U.S.A.

## *(Received* 27 *June* 1977)

**Abstract--The** existence and uniqueness of partition of the inertial coupling terms in the momentum and energy equations of a component in a mixture have been derived when disparate mass velocities and static temperatures exist. Evidences based on one dimensional analyses include reducing to the case of a dilute suspension, exhibiting consistently hyperbolic nature of both the mixture and the component equations, and giving real characteristics of the system equations.

Further comments on the existence of the inertial coupling terms (Soo 1976) and the "uniqueness" of splitting will help clarify the formulation of a mixture in terms of components. A general discussion of the philosophical difference in the formulation of conservation equations for multiphase systems seems appropriate. Most of the formulation of the conservation equations for multiphase systems begins with a consideration of the individual phases (Barenblatt 1953; Solbrig & Hughes 1975; lshii 1975; Harlow & Amsden 1975; Wallis 1969). The conservation equations for the mixture are deduced by combining those for the individual phases. This might be considered a natural approach which appears feasible in principle. In practice, however, it often leads to errors due to investigators' inability to include all relevant physical effects into the formulation. An example is the conspicuous absence of the inertial coupling forces in the momentum equation for the individual phases. This pitfall is recognized in the references (Soo 1976a; Sha & Soo 1977) and the view (Soo 1967) has been adopted that the formulation of the field equations should begin with the mixture. The basic reasoning for such a choice stems from the observation that all experimental evidence supports the use of Navier-Stokes equation for describing air motion despite the fact that air is a mixture of nitrogen and oxygen. Consequently, the authors believe that the global momentum and energy equation for the mixture of a multiphase system assume the same form as those for a homogeneous medium, when viewed within the context of continuum mechanics. The foregoing statement has been adopted by us as a fundamental postulate which we shall not abandon unless evidence of the contrary can be demonstrated. Rigorous derivation of basic equations was carried out (Sha & Soo 1977).

To illustrate our viewpoint, and for simplicity, we present in the following derivation of the momentum and energy equation for a one-dimensional, two-phase system. The results can be readily generalized for three-dimensional, multiphase systems. Our line of reasoning leads to the inertial coupling force in the momentum equation for the individual phases. However, such a contribution, conspicuously, has not been correctly accounted for in all other published equations. It is interesting to note that the use of the momentum equation without the inertial coupling term gives rise to imaginary characteristics in transient flow (Lyczkowski *et al.*  1975), while the equation of the mixture gives real characteristics. Experimental verifications of the latter are well known.

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

$$
\rho_1 \frac{dU_1}{dt_1} = \rho_1 \frac{\partial U_1}{\partial t} + \rho_1 U_1 \frac{\partial U_1}{\partial x} = -\frac{\partial P_1}{\partial x} + I_{12} + V_{12};
$$
\n[1a]

\*University of Illinois at Urbana-Champaign, IL 61801, U.S.A. \*Argonne National Laboratory, IL 60439, U.S.A.

$$
\rho_2 \frac{\mathrm{d}U_2}{\mathrm{d}t_2} = \rho_2 \frac{\partial U_2}{\partial t} + \rho_2 U_2 \frac{\partial U_2}{\partial x} = -\frac{\partial P_2}{\partial x} + I_{21} + V_{21}.
$$
 [1b]

Where  $\rho_1$ ,  $\rho_2$  are the densities of species 1 and 2 in the mixture respectively;  $U_1$ ,  $U_2$  are their respective velocities, and t is the time, x is the position coordinate; we use partial pressures  $P_1$ and *P2* because [la] and [Ib] are applicable to continuum as well as multiphase mechanisms. The inertial interaction forces  $I_{12}$  and  $I_{21}$  are to include the contribution resulting from phase change. A consideration of the physical origin of the viscous interaction forces leads to the simple relation  $V_{12} = -V_{21}$ . The evaluation of  $I_{12}$  and  $I_{21}$  is made possible via the mixture momentum equation for which we write

$$
\rho_m \frac{\mathrm{d}U_m}{\mathrm{d}t_m} = \rho_m \frac{\partial U_m}{\partial t} + \rho_m U_m \frac{\partial U_m}{\partial x} = -\frac{\partial P}{\partial x} \tag{2}
$$

where the mixture density, mixture momentum and system pressure are defined as  $\rho_m = \rho_1 + \rho_2$ and  $\rho_m U_m = \rho_1 U_1 + \rho_2 U_2$  and  $P = P_1 + P_2$  respectively. Thus, the mixture velocity,  $U_m$  is seen to be the mass center velocity. In [2] the viscosity of the mixture is purposely dropped since we wish to focus our attention to the nature of  $I_{12}$  and  $I_{21}$ , which are independent of the viscosities of the media.

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

$$
\frac{\partial \rho_1}{\partial t} + \frac{\partial \rho_1 U_1}{\partial x} = \Gamma_1,
$$
 [3a]

$$
\frac{\partial \rho_2}{\partial t} + \frac{\partial \rho_2 U_2}{\partial x} = \Gamma_2 \tag{3b}
$$

where  $\Gamma_1$ ,  $\Gamma_2$  are rates of generation per unit volume and  $\Gamma_1 + \Gamma_2 = 0$ , and the continuity equation for the mixture:

$$
\frac{\partial \rho_m}{\partial t} + \frac{\partial \rho_m U_m}{\partial x} = 0, \tag{4}
$$

we find after a straightforward calculation that [2] can be written as

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

Since

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

it follows then from a comparison of [5] with the sum of [la] and [lb] that

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

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

Note that the above *l's* are redefined in the momentum flux form.

From [7] and [8], one sees that the inertial coupling force originates from the difference in the velocity of individual phase and that of the mass center of the mixture. The inertial coupling force is the drag due to relative motion of particles in an ideal fluid (nonviscous) for the density

of a phase defined according to the multiphase mechanics (Soo 1976b). This term in the momentum equation also distinguishes a fixed particle in the system from a free particle at zero velocity. The existence of this force and its effect on the dynamics of the individual phase have not been recognized by other investigators. It was hinted by some investigators (Ishii 1975; Lyczkowski *et al.* 1975; Drew 1971), but not rigorously accounted for. As a matter of fact, it is unlikely that these inertial coupling terms could be overlooked, had one tried to derive the equation rigorously. If one denotes the viscous interaction force  $V_{12}$  by  $\rho_1F_{12}(U_2-U_1)$ , where  $F_{12}$  is the inverse relaxation time, then the momentum equation for phase 1 becomes,

$$
\rho_1 \frac{d U_1}{d t_1} - \frac{\partial}{\partial x} [\rho_1 (U_1 - U_m)^2] + \Gamma_1 (U_1 - U_m) = -\frac{\partial \phi_1 P}{\partial x} + \rho_1 F_{12} (U_2 - U_1),
$$
 [9]

where  $\phi_1$  is the volume fraction of phase 1. Note that partial pressure  $P_1$  in [1a] and [1b] is only pertinent to a gaseous mixture,  $\phi_1P$  is identified here because each phase in a multiphase mixture is under the pressure *P.*  $\phi_1 \partial P / \partial x$  is the force acting on phase 1 by the pressure gradient, while  $P\partial\phi_1/\partial x$  represents a diffusive force; its modification for particular physical systems is given in Sha & Soo (1977). Equivalently, in flux form, it becomes

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

The momentum equation for phase 2 can be obtained by an obvious modification of the subscripts.

We now turn our attention to the energy equation. Denoting the sum of the internal and kinetic energy per unit mass by  $E$ , the energy equations for adiabatic flow of the mixture, in the absence of heat source and dissipation are (in terms of total enthalpy *H, H = E + (P|p)*).

$$
\rho_1 \frac{dH_1}{dt_1} = \frac{\partial P_1}{\partial t} + L_{12} + Q_{12},
$$
 [11a]

$$
\rho_2 \frac{dH_2}{dt_2} = \frac{\partial P_2}{\partial t} + L_{21} + Q_{21}
$$
 [11b]

for the individual phases, and

$$
\rho_m \frac{\mathrm{d}H_m}{\mathrm{d}t_m} = \frac{\partial P}{\partial t} \tag{12}
$$

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

Following a procedure completely analogous to that used for the momentum equations, we find that [12] can be rewritten as

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

By comparing with [11a] and [11b], we readily identify

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

and

$$
L_{21} = \frac{\partial}{\partial x} \left[ \frac{\rho_1^2 \rho_2}{(\rho_1 + \rho_2)} (U_2 - U_1)(H_2 - H_1) \right] - \Gamma_2 (H_2 - H_1) \frac{\rho_1}{\rho_1 + \rho_2}
$$
  
=  $\frac{\partial}{\partial x} [\rho_2 (U_2 - U_m)(H_2 - H_m)] - \Gamma_2 (H_2 - H_m).$  [15]

As is the case of the inertial coupling force in the momentum equation for the individual phases, energy exchange associated with inertial effects,  $L_{12}$  and  $L_{21}$ , has not been recognized by other investigators.

In summary, the momentum and energy exchange between phases arising from their unequal velocities and associated with inertial effects can only be recognized through simultaneous consideration of the corresponding conservation equation for the mixture and for the individual phases as demonstrated here. This, then, is the basic difference between our formulation and others. Arguments favoring our line of thinking have been given; additional supporting evidence will be cited.

Experimental evidence is always the ultimate means for validating a formulation or resolving a controversy. In the present case, a proof of [2] is by weighing a bucket of water in which sand is settling and note that the total weight does not change. Additional evidences favoring the inclusion of inertial coupling terms in the above forms are:

(a) *Uniqueness of inertial coupling terms.* The desirability of such a split is evidenced by the fact that, for a dilute suspension of particle phase 1 in continuous phase 2,  $\rho_2 \gg \rho_1$  and, in, the limit, the presence of 1 does not affect the motion of 2. The momentum equation then gives

$$
\rho_1 \frac{dU_1}{dt_1} - \frac{\partial}{\partial x} [\rho_1 (U_2 - U_1)^2] = -\frac{\partial P \phi_1}{\partial x} + \rho_1 F_{12} (U_2 - U_1) + \Gamma_1 (U_2 - U_1),
$$
 [16a]

$$
\rho_2 \frac{dU_2}{dt_2} = -\frac{\partial P(1-\phi_1)}{\partial x} - \rho_1 F_{12}(U_2 - U_1)
$$
 [16b]

as expected, where the last term has negligible contribution to the second equation.  $F_{12}$  is the inverse relaxation time constant for momentum transfer and  $\Gamma_1$  is the mass generation rate per unit volume.

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

$$
\rho_1 \frac{dH_1}{dt_1} = \frac{\partial P\phi_1}{\partial t} + \frac{\partial}{\partial x} [\rho_1 (U_2 - U_1)(H_2 - H_1)] + \Gamma_1 (H_2 - H_1) + Q_{12},
$$
\n[17a]

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

that is the thermal state of 2 is not affected by the presence of 1 when  $Q_{12}$  is small compared to other terms in the second equation.

(b) *Transient flow.* The Newton's law is applicable to the mixture with disparate motion of phases and gives real characteristics. With the above split, the equations of the phases also gives real characteristics as they should. In as much as we could write in terms of the components of air and expect the unsteady motion to give real characteristics, this point was demonstrated as an example in Soo (1976b). The example is, of course, not the limit of the scope of the present study. The wave phenomenon in this case arises from  $\bar{\rho}_1\phi_1 + \bar{\rho}_2(1 - \phi_1)$  with  $\phi_1$  as a variable, and  $\bar{\rho}_1$ ,  $\bar{\rho}_2$  are the densities of materials constituting the species or phases.

It was shown (Soo 1976b) rigorously that without the inertial coupling effect properly accounted for, momentum equations of components give imaginary characteristics when the momentum equation of this mixture gives real characteristics. Such a result is contradictory to the experimental evidence which have been observed in the case of air. When the flow phenomenon is such that the mixture has real characteristics, no physical reasons are available for the equations for oxygen and nitrogen to have imaginary characteristics.

(c) *Stability of computation of transient flow.* Worth mentioning is that the stability of computation of transient flow is significantly improved when the inertial coupling terms are properly accounted for. This was found independently by Krier & Gonkale (1976) and Lyczkowski *et al.* (1975). The reason is that similar stability to that of the mixture momentum equation is retained via the inertial coupling terms. It is further noted that both the terms due to virtual mass and unsteady motion do not always stabilize the computation (Soo 1976b).

*Acknowledgement--The* work was done under the auspices of the office of Nuclear Regulatory Research, United States Nuclear Regulatory Commission (Contract No. A2045).

## REFERENCES

- BARENBLATT, G. I. 1953 On motion of suspended particles in turbulent flow. *Prikl. Mat. Mekh.* 17, 261-274.
- DREW, D. A. 1971 Average field equations for two-phase media. *Stud. Appl. Math.* L2, 133-166:
- HARLOW, F. H. & AMSDEN, A. A. 1975 Numerical calculation of multiphase flow. *J. Comp. Phys.* 17, 19-52.

Isml, M. 1975 *Thermo-Fluid Dynamic Theory on Two-Phase Flow.* Eyrolles. Paris.

KRIER, H. & GONKALE, S. S. 1976 Predictions of vigorous ignition dynamics in a packed bed of solid propellant grains. *Int. J. Heat. Mass. Transfer* 19, 915-923.

LYCZKOWSKI, R. W., SOLBRIG, C. W., GIDASPOW, D. & HUGHES, E. D. 1975 Characteristics and stability analysis of transient one-dimensional two-phase flow equations and their finite difference approximations. ASME Paper No. 75-WA/HT-23.

LYCZKOWSKI, R. W. 1976 Discussion at the Two-phase and Heat Transfer Conference, NSF and University of Miami.

- SHA, W. T. & Soo, S. L. 1977 Multidomain multiphase fluid mechanics. ANL-CT-77-3.
- SOLBRIG, C. W. & HUGHES, E. D. 1975 Governing equations for a seriated continuum: an unequal velocity model for two-phase flow. ANCR-1193.
- Soo, S. L. 1967 Fluid dynamics of multiphase systems, pp. 250–253, 259. Blaisdell, Waltham, MA.
- Soo, S. L. 1976a On one-dimensional motion of a single component in two-phases. *Int. J. Multiphase Flow* 3, 79-82.
- Soo, S. L. 1976b Multiphase mechanics and distinctions from continuum mechanics. Two-Phase Flow and Heat Transfer Symposium-Workshop, NSF and University of Miami, Fort Lauderdale, FL.
- WALLIS, G. B. 1969 *One Dimensional Two-Phase Flow.* McGraw-Hill, New York.