



# On the consistency of mechanistic multidimensional modeling of gas/liquid two-phase flows

M.Z. Podowski

Rensselaer Polytechnic Institute, Troy, NY, USA

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## ABSTRACT

The purpose of this paper is to present an overview of selected aspects of the mathematical modeling of multiphase flows, including the formulation of governing equations, gas/liquid interfacial forces and bubble/bubble interactions. Links between the combined physical, mathematical and computational models are discussed, including the recent progress in, and the limitations of, computational multiphase fluid dynamics (CMFD). Major differences and similarities are analyzed between the interpenetrating-fluids multifield modeling concept and the model of dispersed two-phase flows. Conditions are formulated under which the multifield modeling framework is applicable to gas/liquid dispersed bubbly flows. Also, the interactions between the continuous and dispersed fields are discussed, including a new mechanistic modeling concept for the turbulence-induced interfacial forces between the continuous liquid and dispersed bubbles. Finally, a multigroup approach to the modeling of bubble coalescence and breakup is presented.

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## 1. Introduction

The multifield modeling concept has become a very popular approach to simulate multidimensional two- and multiphase flow and heat transfer. Although the multifield conservation equations seem to be a direct extension of those governing single-phase flows, it turns out that the averaging procedure introduces several constraints on the formulation of individual models.

One of the objectives of this paper is to present selected theoretical aspects of applying the multifield modeling framework to dispersed gas/liquid flows. The emphasis is given to a consistent formulation of ensemble-averaged conservation equations, and the associated models of interfacial phenomena between the continuous and disperse fields.

The accuracy of computational predictions of gas/liquid two-phase flow and heat transfer strongly depends on the proper physical formulation of the governing interfacial phenomena. Several models of the mechanisms governing interfacial interactions have been developed to date, in particular for dispersed particle flows (Drew and Passman, 1998; Tiwari et al., 2006), but also for slug flows (Anglart and Podowski, 2002) and annular flows (Antal et al., 2001). Whereas most theoretical/analytical models are based on mechanistic principles, they are normally complemented by additional phenomenologically-based closure laws and/or adjustable coefficients.

New mechanistic models of gas-bubble/liquid interfacial forces are discussed in this paper. In particular, a complete turbulence-induced interfacial force is formulated, which is defined uniquely (i.e., without using arbitrary adjustable coefficients). This force is responsible for driving bubbles away from the wall in the near-wall region, and flattening void fraction distribution the central flow area, although in each region a different force component plays the dominant role. Thus, the new force combines the roles of the commonly used turbulent-dispersion force and wall force.

## 2. Multifield modeling concept of two-phase flow

### 2.1. Generic ensemble-averaged conservation equations of multifield model of interpenetrating immiscible fluids

Assuming that the  $k$ -th ( $k = 1, 2, \dots, N$ ) component of the multifield flow can be modeled using the concept of continuum, the corresponding Eulerian conservation equations for mass, momentum and energy, respectively, become

$$\frac{\partial \rho_k}{\partial t} + \nabla \cdot (\rho_k \mathbf{v}_k) = 0 \quad (1)$$

$$\frac{\partial (\rho_k \mathbf{v}_k)}{\partial t} + \nabla \cdot (\rho_k \mathbf{v}_k \mathbf{v}_k) = -\nabla p_k + \nabla \cdot \underline{\underline{\tau}}_k + \rho_k \mathbf{g} \quad (2)$$

$$\frac{\partial (\rho_k e_k)}{\partial t} + \nabla \cdot (\rho_k \mathbf{v}_k e_k) = -\nabla \cdot [(-p_k \mathbf{I} + \underline{\underline{\tau}}_k) \cdot \mathbf{v}_k] - \nabla \cdot \mathbf{q}_k'' + \rho_k \mathbf{g} \cdot \mathbf{v}_k \quad (3)$$

E-mail address: [podowm@rpi.edu](mailto:podowm@rpi.edu).

These equations are valid only at locations that pertain to fluid-*k* at a given time instant. At the boundaries between the fluids or phases (which may vary with time), appropriate interfacial conditions must be formulated, such as those for the continuity of velocity, shear stress and heat flux. Note that if the interfaces are being modeled as sharp discontinuities in fluid density and other properties, parameters such as pressure and velocity and temperature gradients may also experience discontinuities.

The multifield modeling concept of interpenetrating fluids is based on applying the time and space, or, in general, ensemble (statistical) averaging techniques to instantaneous conservation equations for each fluid. The resultant equations are determined with respect to a common physical and computational domain, and include terms accounting for the various interfacial effects between the individual fields.

A typical form of conservation equations for mass, momentum and energy, obtained by applying the appropriate averaging procedure to Eqs. (1)–(3), respectively, can be written as

$$\frac{\partial(\alpha_k \rho_k)}{\partial t} + \nabla \cdot (\alpha_k \rho_k \bar{\mathbf{v}}_k) = \Gamma_k \quad (4)$$

$$\begin{aligned} \frac{\partial(\alpha_k \rho_k \bar{\mathbf{v}}_k)}{\partial t} + \nabla \cdot (\alpha_k \rho_k \bar{\mathbf{v}}_k \bar{\mathbf{v}}_k) \\ = -\nabla(\alpha_k \bar{p}_k) + \nabla \cdot (\alpha_k \bar{\boldsymbol{\tau}}_k^t) + \alpha_k \rho_k \mathbf{g} + \mathcal{M}_k^i \end{aligned} \quad (5)$$

$$\begin{aligned} \frac{\partial(\alpha_k \rho_k \bar{e}_k)}{\partial t} + \nabla \cdot (\alpha_k \rho_k \bar{\mathbf{v}}_k \bar{e}_k) \\ = -\nabla \cdot (\alpha_k \bar{\mathbf{q}}_k^t) + \nabla \cdot [\alpha_k (-\bar{p}_k \mathbf{I} + \bar{\boldsymbol{\tau}}_k^t) \cdot \bar{\mathbf{v}}_k] + \alpha_k \rho_k \mathbf{g} \cdot \bar{\mathbf{v}}_k + \mathcal{E}_k^i \end{aligned} \quad (6)$$

where  $\bar{\boldsymbol{\tau}}_k^t = \bar{\boldsymbol{\tau}}_k^\mu + \bar{\boldsymbol{\tau}}_k^{Re}$  is the total combined shear and turbulent shear stress,  $\bar{\mathbf{q}}_k^t = \bar{\mathbf{q}}_k^k + \bar{\mathbf{q}}_k^{Re}$  is the total heat flux,  $\mathcal{M}_k^i$  is the interfacial force per unit volume exerted on field-*k* by the other fields, and  $\mathcal{E}_k^i$  is the corresponding interfacial energy transfer rate. Whereas the interfacial mass transfer is directly related to the net heat transfer rate at the interface, the interfacial transfer of momentum and energy also involve the effects of interfacial pressure and shear stress.

For the sake of clarity, let us consider a two-field model of two interpenetrating immiscible fluids. In such case, the interfacial momentum and energy transfer terms can respectively, be rewritten as

$$\mathcal{M}_k^i = \mathbf{M}_k^i + \bar{p}_k^i \nabla \alpha_k - \bar{\boldsymbol{\tau}}_k^i \cdot \nabla \alpha_k + \Gamma_k \bar{\mathbf{v}}^i \quad (7)$$

$$\mathcal{E}_k^i = E_k^i - \left[ (-\bar{p}_k^i \mathbf{I} + \bar{\boldsymbol{\tau}}_k^i) \cdot \bar{\mathbf{v}}^i \right] \nabla \cdot \alpha_k + \bar{\mathbf{q}}_k^i \cdot \nabla \alpha_k + \Gamma_k e_k^i \quad (8)$$

for *k* = 1, 2, where  $\bar{p}_k^i$  is the interfacial pressure on field-*k*,  $\bar{\boldsymbol{\tau}}_k^i$  is the interfacial shear stress on field-*k*,  $\bar{\mathbf{v}}_k^i$  is the velocity at the interface between field-*k* and field-*j*,  $\bar{\mathbf{q}}_k^i$  is the average interfacial heat flux between field-*k* and the interface with field-*j*, and  $e_k^i$  is the interfacial specific energy of field-*k* at the interface between this field and field-*j*. Also,  $\mathbf{M}_k^i$  is the effective interfacial force on field-*k* per unit volume of the mixture, and  $E_k^i$  is the interfacial energy transfer rate to field-*k* per unit volume. Naturally,  $\alpha_1 + \alpha_2 = 1$  and  $\Gamma_1 + \Gamma_2 = 0$ .

Summing up Eq. (7) over both fields yields the momentum interfacial jump condition

$$\begin{aligned} \mathcal{M}_j^i = \mathcal{M}_1^i + \mathcal{M}_2^i = \mathbf{M}_1^i + \mathbf{M}_2^i + (\bar{p}_2^i - \bar{p}_1^i) \nabla \alpha_2 - (\bar{\boldsymbol{\tau}}_2^i - \bar{\boldsymbol{\tau}}_1^i) \cdot \nabla \alpha_2 \\ = \mathbf{M}_1^i + \mathbf{M}_2^i + (\bar{p}_1^i - \bar{p}_2^i) \nabla \alpha_1 - (\bar{\boldsymbol{\tau}}_1^i - \bar{\boldsymbol{\tau}}_2^i) \cdot \nabla \alpha_1 \end{aligned} \quad (9)$$

Similarly, the energy interfacial jump condition can be obtained from Eq. (8) as

$$\begin{aligned} \mathcal{E}_j^i = \mathcal{E}_1^i + \mathcal{E}_2^i = E_1^i + E_2^i - \left[ (-\bar{p}_2^i \mathbf{I} + \bar{\boldsymbol{\tau}}_2^i) \cdot \bar{\mathbf{v}}^i - (-\bar{p}_1^i \mathbf{I} + \bar{\boldsymbol{\tau}}_1^i) \cdot \bar{\mathbf{v}}^i \right] \cdot \nabla \alpha_2 \\ + (\bar{\mathbf{q}}_2^i - \bar{\mathbf{q}}_1^i) \cdot \nabla \alpha_2 + \Gamma_2 (\bar{h}_2^i - \bar{h}_1^i) \\ = E_1^i + E_2^i - \left[ (-\bar{p}_1^i \mathbf{I} + \bar{\boldsymbol{\tau}}_1^i) \cdot \bar{\mathbf{v}}^i - (-\bar{p}_2^i \mathbf{I} + \bar{\boldsymbol{\tau}}_2^i) \cdot \bar{\mathbf{v}}^i \right] \cdot \nabla \alpha_1 \\ + (\bar{\mathbf{q}}_1^i - \bar{\mathbf{q}}_2^i) \cdot \nabla \alpha_1 + \Gamma_1 (\bar{h}_1^i - \bar{h}_2^i) \end{aligned} \quad (10)$$

Let us sum-up each of the following equations: Eq. (4), Eq. (5) and (Eq. (6) over the individual components (*k* = 1, 2). Defining

$$\rho_m = \alpha_1 \rho_1 + \alpha_2 \rho_2 \quad (11)$$

$$\bar{\mathbf{v}}_m = \frac{\alpha_1 \rho_1 \bar{\mathbf{v}}_1 + \alpha_2 \rho_2 \bar{\mathbf{v}}_2}{\rho_m} \quad (12)$$

$$p_m = \alpha_1 p_1 + \alpha_2 p_2 \quad (13)$$

$$\bar{\boldsymbol{\tau}}_m^t = \alpha_1 \bar{\boldsymbol{\tau}}_1^t + \alpha_2 \bar{\boldsymbol{\tau}}_2^t \quad (14)$$

$$e_m = \frac{\alpha_1 \rho_1 e_1 + \alpha_2 \rho_2 e_2}{\rho_m} \quad (15)$$

$$\bar{\mathbf{q}}_m^t = \alpha_1 \bar{\mathbf{q}}_1^t + \alpha_2 \bar{\mathbf{q}}_2^t \quad (16)$$

we obtain a rigorous form of the mixture conservation equations. In particular, the mass conservation (continuity) equation becomes

$$\frac{\partial \rho_m}{\partial t} + \nabla \cdot (\rho_m \bar{\mathbf{v}}_m) = 0 \quad (17)$$

Similarly, the mixture momentum equation can be written as

$$\begin{aligned} \frac{\partial (\rho_m \bar{\mathbf{v}}_m)}{\partial t} + \nabla \cdot (\rho_m \bar{\mathbf{v}}_m \bar{\mathbf{v}}_m) \\ = -\nabla \bar{p}_m + \nabla \cdot (\bar{\boldsymbol{\tau}}_m^t + \bar{\boldsymbol{\tau}}_m^{pturb}) + \rho_m \mathbf{g} + \mathcal{M}_j^i \end{aligned} \quad (18)$$

where  $\mathcal{M}_j^i$  is the interfacial momentum jump, given by Eq. (9), and  $\bar{\boldsymbol{\tau}}_m^{pturb}$  is the phasic-slip-induced pseudo-turbulent stress given by

$$\bar{\boldsymbol{\tau}}_m^{pturb} = -\frac{\alpha_1 \rho_1 \alpha_2 \rho_2}{\rho_m} (\bar{\mathbf{v}}_2 - \bar{\mathbf{v}}_1)(\bar{\mathbf{v}}_2 - \bar{\mathbf{v}}_1) \quad (19)$$

The following mixture energy conservation equation can be derived in a similar manner

$$\begin{aligned} \frac{\partial (\rho_m \bar{e}_m)}{\partial t} + \nabla \cdot (\rho_m \bar{\mathbf{v}}_m \bar{e}_m) \\ = -\nabla \cdot (\bar{\mathbf{q}}_m^t + \bar{\mathbf{q}}_m^{pturb}) + \nabla \cdot [(-\bar{p}_m \mathbf{I} + \bar{\boldsymbol{\tau}}_m^t) \cdot \bar{\mathbf{v}}_m] + \rho_m \mathbf{g} \cdot \bar{\mathbf{v}}_m + \mathcal{E}_j^i \end{aligned} \quad (20)$$

where  $\mathcal{E}_j^i$  is the interfacial energy jump, given by Eq. (10), and  $\bar{\mathbf{q}}_m^{pturb}$  is the phasic-slip-induced pseudo-turbulent heat flux given by

$$\bar{\mathbf{q}}_m^{pturb} = \frac{\alpha_1 \rho_1 \alpha_2 \rho_2}{\rho_m} (\bar{e}_2 - \bar{e}_1)(\bar{\mathbf{v}}_2 - \bar{\mathbf{v}}_1) \quad (21)$$

For fully-developed flows in pipes and conduits of different shapes, the interfacial jump practically decreases to zero, so that Eq. (18) reduces to a typical form of momentum equation for an equivalent single-phase fluid. In the case of one-dimensional models, the slip-induced pseudo-turbulent stress term is normally obtained from the drift-flux model.

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