

A two-phase model for compressible granular flows based on the theory of irreversible processes

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In this article we introduce a new two-phase model for compressible viscous flows of saturated mixtures consisting of a carrier fluid and a granular material. The mixture is treated as a multicomponent fluid, with a set of thermodynamic variables assigned to each of its constituents. The volume fraction occupied by the granular phase and its spatial gradient are introduced as additional degrees of freedom. Then, by applying the classical theory of irreversible processes we derive algebraic expressions for the viscous stresses and heat flux vectors, the momentum and energy exchanges between the two phases, as well as a parabolic partial differential equation for the volume fraction. In our model, thermal non-equilibrium between the two phases emerges as a source term of the evolution equation for the volume fraction, in contrast with earlier models.

1. Introduction

A two-phase model for compressible flows of gas-permeable viscous granular materials is derived in this article. Such flows are encountered in numerous industrial and technological applications, for example, power plants, chemical plants, solid rocket motors, deflagration-to-detonation transitions of granular explosives. Due to their wide applicability, modelling of these flows has attracted much attention over the years. Typically, models of such flows employ either an averaging approach or a mixture-theory approach. The averaging approach is based on modifying the equations of motion for a single component to account for the other components, and then averaging these equations over time or volume, see Drew & Passman (1999), and references therein.

On the other hand, mixture theories consider the mixture as a multicomponent fluid: the mixture is assumed to consist of two separate, identifiable and co-existing continua that are in thermodynamic non-equilibrium with each other. A set of balance equations is assigned to each phase separately, along with an entropy balance for the mixture. The challenging part is to supplement the balance equations with constitutive relations for the viscous stresses as well as suitable expressions for the phase interactions (i.e. the mass, momentum, and energy exchanges between the two phases). These expressions appear in the balance equations as source terms that drive the mixture to equilibrium. A standard approach, followed herein, for the derivation of such expressions is to make use of the constraints imposed by the entropy inequality.

The bibliography of mixture theories of granular materials is very extensive. More than 30 years ago Goodman & Cowin (1972) presented a model for dry granular

materials based on the thermodynamic theory of Coleman–Noll. Subsequently their model has been extended or modified by various authors; see, for example, Svendsen & Hutter (1995), Wang & Hutter (1999), as well as references therein for earlier models. Recently, variational approaches for two-phase modelling have also been employed; see, for example, Sciarra, Hutter & Maugin (2003). In all the above cited works, viscosity effects are taken into account and constitutive relations for the viscous stresses are derived.

Correctly or not, viscous stresses are typically ignored in proposed models for high-speed compressible flows of two-phase mixtures; see, for example, Baer & Nunziato (1986), Bdzil *et al.* (1999), Powers, Stewart & Krier (1990), Saurel & LeMetayer (2001). The well-known BN model of Baer & Nunziato (1986) is based on the formalism introduced by Passman *et al.* (1984) which, in turn, is based on the Coleman–Noll theory. An extension to the original BN model has been proposed by Bdzil *et al.* (1999) who identified and addressed some of its inconsistencies. More recently, Gavriluk & Saurel (2002), and Saurel, Gavriluk & Renaud (2003) derived compressible two-phase flow models that take into account microinertia by using a variational approach.

Here, we focus on compressible flows of granular mixtures and derive closure terms for the balance equations of each phase by applying the theory of irreversible processes (de Groot & Mazur 1984; Beris & Edwards 1994). This theory is well known and represents a standard approach for non-equilibrium processes. It has been previously applied to classical heterogeneous mixtures (Blokhin & Dorovsky 1995), but not to the granular mixtures of interest. Yet, as will be shown herein, this theory provides a straightforward way to properly take into account all the thermodynamic forces that appear in the balance equations of the mixture. Since it is well-known that granular materials can support shear in equilibrium, we take into account viscosity effects and provide suitable expressions for the shear viscous tensors as well as the bulk viscous pressures. However, in §3 we consider the inviscid limit of our model in order to draw comparisons between the phase interaction terms presented herein and those appearing in the models mentioned in the previous paragraph.

2. Derivation of the two-phase flow model

In this article we consider the flow of a mixture of an (isotropic) gas and an isotropic granular material in the absence of chemical reactions or phase transformations, i.e. there is no mass exchange between the two phases. The assumptions upon which our model is based are the following: (i) the mixture consists of two separate, coexisting continua, (ii) each phase of the mixture is in a local (equilibrium) state, (iii) the principle of phase separation holds (Passman, Nunziato & Walsh 1984), (iv) the momentum and energy exchanges between the two phases are assumed to be pure exchanges, i.e. their sum must vanish, (v) microinertia effects of the granular phase, such as grain vibration or rotation, are ignored.

Each phase is assigned a density ρ_α , temperature T_α , specific energy e_α , velocity vector \mathbf{u}_α , and a volume fraction ϕ_α , where $\alpha = \text{g, s}$, and g and s denote the gaseous phase and solid phase, respectively. Also, let p_α , η_α , and $\psi_\alpha = e_\alpha - T_\alpha \eta_\alpha$, denote the thermodynamic pressure, specific entropy, and specific Helmholtz free energy for each phase, respectively. The volume fractions represent the percentage of volume occupied by each constituent and satisfy the saturation condition

$$\phi_{\text{g}} + \phi_{\text{s}} = 1. \quad (1)$$

The properties of the mixture are weighted sums of the properties of its constituents. Therefore, the density, velocity, and specific entropy of the mixture are written as

$$\rho = \rho_g \phi_g + \rho_s \phi_s, \quad \mathbf{u} = \rho^{-1}(\rho_g \phi_g \mathbf{u}_g + \rho_s \phi_s \mathbf{u}_s), \quad \eta = \rho^{-1}(\rho_g \phi_g \eta_g + \rho_s \phi_s \eta_s), \quad (2)$$

respectively.

For a complete description of the state of the mixture we are required to introduce an additional variable, namely, the volume fraction ϕ_s . In fact, ϕ_s represents an additional degree of freedom and, therefore, must be considered as a new thermodynamic variable. On the other hand, it is well known that granular material can support shear in equilibrium. Since these forces depend on the intergranular surface area and the interfacial surface, the introduction of ϕ_s alone is not sufficient to yield expressions for the shear stresses on each phase at equilibrium. This necessitates the introduction of an additional variable related to the microstructure of the system. Inspired by Goodman & Cowin (1972), we therefore introduce the volume fraction gradient $\nabla\phi_s$, which is a measure of the interfacial area density, as an independent state variable.

Having augmented the state-variable vector, we then introduce the generalized Gibbs equations for each phase:

$$T_\alpha d\eta_\alpha = de_\alpha - \frac{p_\alpha}{\rho_\alpha^2} d\rho_\alpha - \frac{\beta_\alpha}{\rho_\alpha \phi_\alpha} d\phi_\alpha - \frac{1}{\rho_\alpha \phi_\alpha} \mathbf{h}_\alpha \cdot d\nabla\phi_\alpha, \quad \alpha = g, s, \quad (3)$$

where

$$\beta_\alpha = \rho_\alpha \phi_\alpha \frac{\partial \psi_\alpha}{\partial \phi_\alpha}, \quad \mathbf{h}_\alpha = \rho_\alpha \phi_\alpha \frac{\partial \psi_\alpha}{\partial \nabla\phi_\alpha}, \quad \alpha = g, s. \quad (4a, b)$$

It is straightforward to verify that the above definitions of β_α and \mathbf{h}_α satisfy the convexity requirements for intrinsic stability of thermodynamic equilibria. Further, β_α and \mathbf{h}_α do not necessarily vanish at equilibrium. Due to the presumed isotropy of the materials involved, the Helmholtz free energies of each phase are isotropic functions, i.e. $\psi_\alpha(\dots, \nabla\phi_\alpha) = \psi_\alpha(\dots, \nabla\phi_\alpha \cdot \nabla\phi_\alpha)$. In turn, this implies that relation (4b) can be written as

$$\mathbf{h}_\alpha = \gamma_\alpha \nabla\phi_\alpha, \quad \gamma_\alpha \equiv 2\rho_\alpha \phi_\alpha \frac{\partial \psi_\alpha}{\partial (\nabla\phi_\alpha \cdot \nabla\phi_\alpha)}, \quad \alpha = g, s. \quad (5)$$

The quantities $\beta_\alpha, \mathbf{h}_\alpha, \alpha = g, s$, are termed herein the *affinities* of ϕ_α and $\nabla\phi_\alpha$, respectively. Goodman & Cowin (1972) and Baer & Nunziato (1986) characterize β_α as the *configuration* pressure of each phase. These pressures are due to the volume distribution of the granular phase. More specifically, β_s represents the elastic, contact forces that are developed between grains under compaction. The work performed by β_s is the compaction energy of the granular phase. Since such forces are not expected to be developed in the gaseous phase, many authors set $\beta_g = 0$ (Bdzil *et al.* 1999).

Further, the stress vectors \mathbf{h}_α represent forces related to rearrangements in the distribution of interfacial area density. In other words, γ_α are coefficients related to dispersion effects. In the analysis of Goodman & Cowin (1972), \mathbf{h}_α plays the role of the *equilibrated* stress vector, according to the formalism of Coleman–Noll. The thermodynamic pressures $p_\alpha, \alpha = g, s$, are derived by appropriate equations of state. In accordance with the Gibbs equations above, the equation of state for each constituents should generally depend on the volume fraction and on its gradient, i.e. $e_\alpha = e_\alpha(p_\alpha, T_\alpha, \phi_\alpha, \nabla\phi_\alpha)$. Similarly, both β_α and γ_α are functions of all four independent state variables.

According to the standard description of multicomponent fluids (Drew & Passman 1999), the mass, momentum, and energy equations of each phase are written as

$$\frac{\partial \rho_\alpha \phi_\alpha}{\partial t} + \nabla \cdot (\rho_\alpha \phi_\alpha \mathbf{u}_\alpha) = 0, \quad (6)$$

$$\frac{\partial \rho_\alpha \phi_\alpha \mathbf{u}_\alpha}{\partial t} + \nabla \cdot (\rho_\alpha \phi_\alpha \mathbf{u}_\alpha \mathbf{u}_\alpha) + \nabla (p_\alpha \phi_\alpha) = -\nabla \cdot (\phi_\alpha \mathbf{P}_\alpha) + \mathbf{f}_\alpha, \quad (7)$$

$$\frac{\partial \rho_\alpha \phi_\alpha e_{T,\alpha}}{\partial t} + \nabla \cdot (\phi_\alpha \mathbf{u}_\alpha (\rho_\alpha e_{T,\alpha} + p_\alpha)) = -\nabla \cdot (\phi_\alpha \mathbf{P}_\alpha \cdot \mathbf{u}_\alpha) - \nabla \cdot \mathbf{q}_\alpha + \mathcal{E}_\alpha, \quad (8)$$

respectively. We have considered the multidimensional form of the balance equations and not their one-dimensional version, as in Baer & Nunziato (1986) and Bdzil *et al.* (1999), because the tensorial ranks of the various thermodynamic forces play an important role in the derivation of the flow model.

In (8), $e_{T,\alpha}$ is the sum of the specific internal and kinetic energies of each phase,

$$e_{T,\alpha} = e_\alpha + \frac{1}{2} \mathbf{u}_\alpha \cdot \mathbf{u}_\alpha, \quad (9)$$

while the vectorial quantities \mathbf{q}_α , $\alpha = \text{g, s}$, are the conductive heat fluxes inside each phase. The tensorial quantities \mathbf{P}_α , $\alpha = \text{g, s}$, are the viscous pressure tensors for each phase. By virtue of the isotropy of each constituent and the conservation of angular momentum, these tensors are symmetric, i.e. $\mathbf{P}_\alpha^T = \mathbf{P}_\alpha$. Then, as usual, each of these tensors is decomposed according to

$$\mathbf{P}_\alpha = p_\alpha^v \mathbf{I} + \mathbf{P}_\alpha^v, \quad p_\alpha^v = \frac{1}{3} \text{tr}(\mathbf{P}_\alpha), \quad \alpha = \text{g, s}, \quad (10)$$

where p_α^v are the bulk viscous pressures and \mathbf{P}_α^v are traceless deviatoric tensors. The terms \mathbf{f}_α in (7) represent the momentum exchanges (forces) between the two phases. As postulated above, the sum of the momentum exchange terms must vanish:

$$\sum_\alpha \mathbf{f}_\alpha = \mathbf{f}_g + \mathbf{f}_s = 0 \implies \mathbf{f}_s = -\mathbf{f}_g \equiv \mathbf{f}. \quad (11)$$

The terms \mathcal{E}_α in (8) represent the energy exchanges between the two phases. Each of these terms can be written as the sum of the contribution of the force \mathbf{f} plus a remaining part (Drew & Passman 1999),

$$\mathcal{E}_\alpha = E_\alpha + \mathbf{f}_\alpha \cdot \mathbf{u}_\alpha, \quad \alpha = \text{g, s}. \quad (12)$$

Further, as postulated above, the sum of these terms must vanish. Thus, from (11) and (12) we arrive at

$$\mathcal{E}_s = E + \mathbf{f} \cdot \mathbf{u}_s = -\mathcal{E}_g, \quad E \equiv E_s. \quad (13)$$

Using equations (6)–(11) and (13), we can write the balance equations for each phase as

$$\frac{d\rho_g \phi_g}{dt_g} + \rho_g \phi_g \nabla \cdot \mathbf{u}_g = 0, \quad (14a)$$

$$\rho_g \phi_g \frac{d\mathbf{u}_g}{dt_g} + \nabla (p_g \phi_g) = -\nabla (p_g^v \phi_g) - \nabla \cdot (\phi_g \mathbf{P}_g^v) - \mathbf{f}, \quad (14b)$$

$$\begin{aligned} \rho_g \phi_g \frac{de_g}{dt_g} + p_g \phi_g \nabla \cdot \mathbf{u}_g &= -p_g^v \phi_g \nabla \cdot \mathbf{u}_g - \phi_g \mathbf{P}_g^v : \mathbf{V}_g^v \\ &\quad - \nabla \cdot \mathbf{q}_g + \mathbf{f} \cdot (\mathbf{u}_g - \mathbf{u}_s) - E; \end{aligned} \quad (14c)$$

$$\frac{d\rho_s\phi_s}{dt_s} + \rho_s\phi_s\nabla\cdot\mathbf{u}_s = 0, \quad (15a)$$

$$\rho_s\phi_s\frac{d\mathbf{u}_s}{dt_s} + \nabla(p_s\phi_s) = -\nabla(p_s^v\phi_s) - \nabla\cdot(\phi_s\mathbf{P}_s^v) + \mathbf{f}, \quad (15b)$$

$$\rho_s\phi_s\frac{de_s}{dt_s} + p_s\phi_s\nabla\cdot\mathbf{u}_s = -p_s^v\phi_s\nabla\cdot\mathbf{u}_s - \phi_s\mathbf{P}_s^v:\mathbf{V}_s^v - \nabla\cdot\mathbf{q}_s + E, \quad (15c)$$

where the material derivatives are defined as $(d/dt_\alpha)(\) = (\partial/\partial t + \mathbf{u}_\alpha\cdot\nabla)(\)$, $\alpha = g, s$. Also \mathbf{V}_α^v are the deviatoric, traceless parts of the rate of deformation tensors \mathbf{V}_α , respectively. In other words, $\mathbf{V}_\alpha = \frac{1}{2}(\nabla\mathbf{u}_\alpha + (\nabla\mathbf{u}_\alpha)^T)$, and $\mathbf{V}_\alpha^v = \mathbf{V}_\alpha - \frac{1}{3}(\nabla\cdot\mathbf{u}_\alpha)\mathbf{I}$, $\alpha = g, s$, with \mathbf{I} being the identity matrix.

Summing the above equations over the constituents yields the usual balance equations for a single phase. The overall entropy of the mixture η satisfies an equation of the form (de Groot & Mazur 1984)

$$\rho\frac{d\eta}{dt} + \nabla\cdot\mathbf{J}_\eta = \sigma \geq 0. \quad (16)$$

where \mathbf{J}_η is the entropy flux and σ is the (non-negative) specific entropy production rate. On the other hand, by employing relations (2), (14a), and (15a) we obtain the following expression for the time derivative of the entropy of the mixture:

$$\rho\frac{d\eta}{dt} = \nabla\cdot(\rho_g\phi_g\eta_g(\mathbf{u} - \mathbf{u}_g) + \rho_s\phi_s\eta_s(\mathbf{u} - \mathbf{u}_s)) + \rho_g\phi_g\frac{d\eta_g}{dt_g} + \rho_s\phi_s\frac{d\eta_s}{dt_s}. \quad (17)$$

This equation can be expanded further by introducing the Gibbs equations (3) and the balance equations (14a, c), (15a, c), for each phase respectively. By doing so and by employing the identities

$$\frac{d\phi_g}{dt_g} = -\frac{d\phi_s}{dt_s} - (\mathbf{u}_g - \mathbf{u}_s)\cdot\nabla\phi_s, \quad (18)$$

$$\begin{aligned} \frac{1}{T_\alpha}\mathbf{h}_\alpha\cdot\frac{d\nabla\phi_\alpha}{dt_\alpha} &= \frac{\gamma_\alpha}{T_\alpha}\nabla\phi_\alpha\cdot\left(\nabla\frac{d\phi_\alpha}{dt_\alpha} - \nabla\phi_\alpha\cdot\nabla\mathbf{u}_\alpha\right) \\ &= \nabla\cdot\left(\frac{\gamma_\alpha}{T_\alpha}\frac{d\phi_\alpha}{dt_\alpha}\nabla\phi_\alpha\right) - \frac{d\phi_\alpha}{dt_\alpha}\nabla\cdot\left(\frac{\gamma_\alpha}{T_\alpha}\nabla\phi_\alpha\right) - \frac{\gamma_\alpha}{T_\alpha}(\nabla\phi_\alpha\nabla\phi_\alpha):\nabla\mathbf{u}_\alpha, \quad \alpha = g, s, \end{aligned} \quad (19)$$

we arrive at the balance equation for the mixture entropy. This equation has the form of (16) with the entropy flux given by

$$\mathbf{J}_\eta = \sum_{\alpha=g,s}\frac{\mathbf{q}_\alpha}{T_\alpha} + \frac{\gamma_\alpha}{T_\alpha}\frac{d\phi_\alpha}{dt_\alpha}\nabla\phi_\alpha + \rho_\alpha\phi_\alpha\eta_\alpha(\mathbf{u}_\alpha - \mathbf{u}), \quad (20)$$

and the entropy production rate given by

$$\begin{aligned} \sigma &= E\left(\frac{1}{T_s} - \frac{1}{T_g}\right) + \frac{d\phi_s}{dt_s}\left[\frac{p_s - \beta_s}{T_s} - \frac{p_g - \beta_g}{T_g} + \nabla\cdot\left(\left(\frac{\gamma_s}{T_s} + \frac{\gamma_g}{T_g}\right)\nabla\phi_s\right)\right] \\ &\quad - \left(p_g^v\phi_g - \frac{\gamma_g}{3}|\nabla\phi_s|^2\right)\frac{1}{T_g}\nabla\cdot\mathbf{u}_g - \left(p_s^v\phi_s - \frac{\gamma_s}{3}|\nabla\phi_s|^2\right)\frac{1}{T_s}\nabla\cdot\mathbf{u}_s \\ &\quad + \left[\mathbf{f} - \left(p_g - T_g\nabla\cdot\left(\frac{\gamma_g}{T_g}\nabla\phi_s\right)\right)\nabla\phi_s\right]\cdot\frac{1}{T_g}(\mathbf{u}_g - \mathbf{u}_s) + \mathbf{q}_g\cdot\nabla(T_g^{-1}) + \mathbf{q}_s\cdot\nabla(T_s^{-1}) \\ &\quad - (\phi_g\mathbf{P}_g^v - \gamma_s\phi_s^v):\frac{1}{T_s}\mathbf{V}_g^v - (\phi_s\mathbf{P}_s^v - \gamma_s\phi_s^v):\frac{1}{T_s}\mathbf{V}_s^v, \end{aligned} \quad (21)$$

where the dual product $\nabla\phi_s\nabla\phi_s$ has been decomposed into a diagonal part plus a traceless deviatoric tensor,

$$\nabla\phi_s\nabla\phi_s = \frac{1}{3}|\nabla\phi_s|^2\mathbf{I} + \Phi_s^v. \quad (22)$$

We see that the entropy production rate is the sum of products between nine independent generalized thermodynamic fluxes J_i , and nine independent generalized thermodynamic forces X_i . In other words,

$$\sigma = \sum_{i=1}^9 J_i X_i \geq 0, \quad (23)$$

with

$$J_i \in \left\{ E, \frac{d\phi_s}{dt_s}, \left(p_s^v \phi_s - \frac{\gamma_s}{3} |\nabla\phi_s|^2 \right), \left(p_g^v \phi_g - \frac{\gamma_g}{3} |\nabla\phi_s|^2 \right), \right. \\ \left. \left(\mathbf{f} - \left(p_g - T_g \nabla \cdot \left(\frac{\gamma_g}{T_g} \nabla\phi_s \right) \right) \nabla\phi_s \right), \mathbf{q}_g, \mathbf{q}_s, (\phi_g \mathbf{P}_g^v - \gamma_g \Phi_s^v), (\phi_s \mathbf{P}_s^v - \gamma_s \Phi_s^v) \right\}, \quad (24)$$

and

$$X_i \in \left\{ \frac{1}{T_s} - \frac{1}{T_g}, \left(\frac{p_s - \beta_s}{T_s} - \frac{p_g - \beta_g}{T_g} + \nabla \cdot \left(\frac{\gamma_s}{T_s} + \frac{\gamma_g}{T_g} \right) \nabla\phi_s \right), -\nabla \cdot \mathbf{u}_g, \right. \\ \left. -\nabla \cdot \mathbf{u}_g, \frac{1}{T_g} (\mathbf{u}_g - \mathbf{u}_s), \nabla T_g^{-1}, \nabla T_s^{-1}, -\frac{1}{T_g} \mathbf{V}_g^v, -\frac{1}{T_s} \mathbf{V}_s^v \right\}. \quad (25)$$

According to the theory of irreversible processes, linear constitutive relations exist between the fluxes and the forces. These relations can be obtained by Taylor expanding around the equilibrium values $J_{i,\text{eq}} = 0$ and $X_{i,\text{eq}} = 0$ and omitting second and higher order terms:

$$J_i = \sum_{j=1}^9 L_{ij} X_j, \quad i = 1, \dots, 9, \quad (26)$$

where the quantities L_{ij} are the phenomenological coefficients of the flow model and depend on material properties of the mixture.

The phenomenological coefficients are subject to four constraints. The first arises from the tensorial rank of the fluxes and forces. According to the representation theorem of isotropic tensors, linear or quasi-linear relations for fluxes and forces of different tensorial rank do not couple. (This statement is often referred to as the Curie principle).

The second constraint is imposed by the principle of phase separation. Expansion (26) permits couplings between the fluxes $\nabla\mathbf{q}_\alpha$, p_α^v , and \mathbf{P}_α^v , and thermodynamic forces X_i related to both phases. This is a consequence of the assumption that the two phases coexist, i.e. they occupy the same space. This assumption, however, is valid only on the macroscopic level and not on the mesoscopic (that is, at length scales equal to the grain diameters) or microscopic levels. For example, we expect that the conductive heat transfer inside each grain is independent of the gradient of the gas temperature. Therefore, the conductive heat fluxes and viscous fluxes can be coupled only to thermodynamic forces associated with the same phase. This is a restatement of the principle of phase separation.

The third constraint arises from the Onsager–Casimir reciprocal relations between the phenomenological coefficients, i.e.

$$L_{ij} = \epsilon_i \epsilon_j L_{ji}, \quad (27)$$

where ϵ_i, ϵ_j are equal to $+1$ or to -1 depending on whether the corresponding flux is even or odd under time reversal. Taking into account the above three constraints we finally arrive at the following constitutive relations:

$$E = L_{11} \left(\frac{1}{T_s} - \frac{1}{T_g} \right) + L_{12} \left(\frac{p_s - \beta_s}{T_s} - \frac{p_g - \beta_g}{T_g} + \nabla \cdot \left(\left(\frac{\gamma_s}{T_s} + \frac{\gamma_g}{T_g} \right) \nabla \phi_s \right) \right), \quad (28a)$$

$$\frac{d\phi_s}{dt_s} = L_{12} \left(\frac{1}{T_s} - \frac{1}{T_g} \right) + L_{22} \left(\frac{p_s - \beta_s}{T_s} - \frac{p_g - \beta_g}{T_g} + \nabla \cdot \left(\left(\frac{\gamma_s}{T_s} + \frac{\gamma_g}{T_g} \right) \nabla \phi_s \right) \right), \quad (28b)$$

$$p_g^v = \frac{\gamma_g}{3\phi_g} |\nabla \phi_s|^2 - L_{33} \frac{1}{\phi_g T_g} \nabla \cdot \mathbf{u}_g, \quad (28c)$$

$$p_s^v = \frac{\gamma_s}{3\phi_s} |\nabla \phi_s|^2 - L_{44} \frac{1}{\phi_s T_s} \nabla \cdot \mathbf{u}_s, \quad (28d)$$

$$\mathbf{q}_g = L_{55} \nabla (T_g^{-1}), \quad (28e)$$

$$\mathbf{q}_s = L_{66} \nabla (T_s^{-1}), \quad (28f)$$

$$\mathbf{f} = \left(p_g - T_g \nabla \cdot \left(\frac{\gamma_g}{T_g} \nabla \phi_s \right) \right) \nabla \phi_s + L_{77} \frac{1}{T_g} (\mathbf{u}_g - \mathbf{u}_s), \quad (28g)$$

$$\mathbf{P}_g^v = \frac{\gamma_g}{\phi_g} \Phi_s^v - L_{88} \frac{1}{\phi_g T_g} \mathbf{V}_g^v, \quad (28h)$$

$$\mathbf{P}_s^v = \frac{\gamma_s}{\phi_s} \Phi_s^v - L_{99} \frac{1}{\phi_s T_s} \mathbf{V}_s^v. \quad (28i)$$

All of the above coefficients are scalar quantities. $L_{33}, L_{44}, L_{55}, L_{66}, L_{88}, L_{99}$ are related to the usual transport coefficients of thermal conductivity λ_α , bulk viscosity ζ_α , and shear viscosity μ_α by

$$L_{33} = \lambda_g T_g^2, \quad L_{44} = \lambda_s T_s^2, \quad (29)$$

$$L_{55} = \zeta_g \phi_g T_g, \quad L_{66} = \zeta_s \phi_s T_s, \quad L_{88} = 2\mu_g \phi_g T_g, \quad L_{99} = 2\mu_s \phi_s T_s. \quad (30)$$

From (28b) we verify that the volume fraction obeys a parabolic partial differential equation which reduces to an advection equation in the limit $\gamma_\alpha \rightarrow 0, \alpha = g, s$. Further, from (28e, f) we observe that each constituent obeys Fourier's law of heat conduction. On the other hand, the bulk viscous forces and the shear stresses of each constituent are sums of a term that is linear to the deformation rates (i.e. a 'Newtonian' part) plus another term that involves the derivatives of the volume fraction. The existence of the latter demonstrates the ability of the mixture to support shear at equilibrium. Note also that the equilibrium values of the viscous stress tensors are the same as predicted by Goodman & Cowin (1972).

The fourth constraint on the phenomenological coefficients is imposed by the positivity of the entropy production rate. It is straightforward to verify that necessary and sufficient conditions for positive entropy production rate are

$$L_{ii} \geq 0, \quad i = 1, \dots, 9, \quad L_{12}^2 \leq L_{11} L_{22}. \quad (31)$$

This implies that $\lambda_\alpha, \zeta_\alpha$, and μ_α are non-negative quantities. Equations (14), (15), and (28), supplemented with appropriate equations of state for the two constituents and functional relations for β_α and γ_α , constitute a complete (closed) flow model for the mixtures of interest. In flows where heat conduction, viscous pressures, and

shear stresses have negligible effects (for example, flows with strong shocks) the model reduces to a non-conservative system of hyperbolic partial differential equations, i.e. it is evolutionary.

Assuming that the thermal conductivities (29) and viscosity coefficients (30) are known, the model introduces four additional coefficients, namely L_{11} , L_{12} , L_{22} , and L_{77} . These coefficients are related to the usual transport coefficients via

$$h_1 = \frac{L_{11}}{T_g T_s}, \quad h_2 = \frac{T_g T_s \phi_g \phi_s}{L_{12}}, \quad \mu_c = \frac{\phi_g \phi_s}{L_{22}}, \quad \delta = \frac{L_{77}}{T_g}. \quad (32)$$

In (32), h_1 is the interfacial heat transfer coefficient, δ is the interfacial drag coefficient, μ_c is the dynamic compaction coefficient, and h_2 is an additional compaction coefficient termed herein the *thermal compaction coefficient*. Empirical correlations for the heat transfer coefficient h_1 and the drag coefficient δ can readily be found in the literature; see for example Baer & Nunziato (1986), and Saurel & LeMetayer (2001). These correlations are traditionally based on the Nusselt and Reynolds numbers (for h_1 and δ respectively). On the other hand, we have no real basis on which to determine the coefficients μ_c and h_2 because the proposed equation for the volume fraction is new and has not yet been studied. Therefore, these two transport coefficients have to be measured experimentally.

3. The inviscid limit: comparison with earlier models

As regards comparisons with earlier models for high-speed flows (namely Baer & Nunziato 1986 and Bdzil *et al.* 1999), we first note that our analysis takes into account viscous effects. Such effects might be important in phenomena such as deflagration-to-detonation transition in granular explosives. Nonetheless, in order to compare the source terms in earlier models and the ones proposed herein, we now consider the ‘inviscid’ limit of our model by setting the shear stress tensors and the bulk viscous pressures equal to zero. In other words, we assume throughout this section that

$$\zeta_\alpha = 0, \quad \mu_\alpha = 0, \quad \gamma_\alpha = 0, \quad \alpha = g, s. \quad (33)$$

In this limit, expression (28g) for the momentum exchange between the two phases becomes the same as the one appearing in the BN model. The most important differences are that our model predicts a coupling between (i) the energy exchange between the two phases and the pressure non-equilibrium, cf: (28a), and (ii) the volume fraction evolution and thermal non-equilibrium between the two phases, cf. (28b). By contrast, in earlier models the evolution of the volume fraction ϕ_s was considered to be a function of $(p_g - p_s)$ only, while the energy exchange between the two phases was considered to be a function of $(T_g - T_s)$ only. Therefore, in earlier models, thermal non-equilibrium between the two phases influences the volume fraction evolution only in an indirect way, via the pressure–temperature dependence in the equations of state.

One might argue that these differences stem from the fact that in our analysis the term $(p_s - \beta_s)/T_s - (p_g - \beta_g)/T_g$ appears as an independent thermodynamic force. In the earlier models this term was decomposed in such a way that the pressure difference $(p_s - \beta_s) - (p_g - \beta_g)$ emerged as an independent thermodynamic force. However, we note that the choice of forces and fluxes is not in any way unique. Even if we had selected the same thermodynamic forces as in earlier works, the direct couplings predicted by our model would still be present due to the linear relations between thermodynamic fluxes and forces predicted by the theory of irreversible processes. Therefore, the assumption that these couplings do not exist cannot be justified on

purely thermodynamic grounds. These direct couplings have not been taken into account before and constitute the essential differences between the ‘inviscid’ version of our model and the earlier models.

The prediction of our model that there is a coupling between thermal non-equilibrium and the evolution of the volume fraction can be supported by the following physical argument. In compressible flows of granular mixtures, pressure equilibrium is typically attained much faster than temperature equilibrium; see relevant discussion in Kapila *et al.* (2001) and experimental results referenced therein. As an example, we may consider the propagation of a compression wave in a quiescent granular mixture. Then, behind the compression wave and a short zone at the end of which the pressures become almost equal, there is a long temperature relaxation zone where $p_s - \beta_s \simeq p_g - \beta_g$ and $T_g \neq T_s$. Inside this zone equation(28b) gives, to a first-order approximation for $p_s - \beta_s$,

$$\frac{d\phi_s}{dt_s} = (L_{12} + L_{22}(p_g - \beta_g)) \left(\frac{1}{T_s} - \frac{1}{T_g} \right). \quad (34)$$

We see that even if cross-coupling effects are ignored (i.e. $L_{12} = 0$), the source term of (34) does not vanish; the coefficient L_{22} cannot be zero (otherwise there would be no compaction at all) while the equilibrium value of the pressure behind the wave is typically large. Therefore, the source term that appears in (34) cannot be considered as small. The amplitude of this term increases with the strength of the compression wave because stronger waves result in higher equilibrium pressures. It is possible that there are cases where the new couplings introduced by the proposed model (i.e. between volume fraction evolution and thermal non-equilibrium and between interfacial energy exchange and pressure non-equilibrium) are not important and can be neglected. However, as indicated by the above physical argument, there are flows where these couplings can play a non-negligible role. Ultimately, whether these couplings are important or not should be determined separately for each case, based on the physical properties of the mixture and the initial conditions.

Finally, it is worth mentioning that the coupling between thermal non-equilibrium and volume fraction evolution cannot be ignored *a priori* even in cases where the temperature differences are relatively small. To this end, assume that $1/T_s$ is expanded in Taylor series around T_g and that $T_g - T_s$ is sufficiently small so that $T_s^{-1} - T_g^{-1} \simeq (T_g - T_s)/T_g^2$. Under this approximation, equations (28a,b) become

$$E = \frac{L_{11} + L_{12}(p_s - \beta_s)}{T_g^2} (T_g - T_s) + \frac{L_{12}}{T_g} (p_s - \beta_s - p_g + \beta_g), \quad (35a)$$

$$\frac{d\phi_s}{dt_s} = \frac{L_{12} + L_{22}(p_s - \beta_s)}{T_g^2} (T_g - T_s) + \frac{L_{22}}{T_g} (p_s - \beta_s - p_g + \beta_g). \quad (35b)$$

We observe that the pressure and temperature differences now act as independent thermodynamic forces. From equation (35b) we see that $d\phi_s/dt_s$ and $(T_g - T_s)$ decouple only if $p_s - \beta_s = -L_{12}/L_{22}$. However, this condition is not always valid for a mixture of arbitrary constituents at arbitrary concentrations.

4. Concluding remarks

In this article, a two-phase model for compressible flows of granular mixtures has been derived. Each phase is described as a continuum endowed with its own mass, momentum, angular momentum, and energy balance equations. The volume fraction

of the granular phase and its gradient are introduced as additional degrees of freedom. The model is derived by applying directly the classical theory of irreversible processes which is based on the local equilibrium hypothesis. The introduction of the gradient of the volume fraction as an additional degree of freedom leads to constitutive relations for the shear stresses that do not vanish at equilibrium, in accordance with physical observations. Further, our model includes a parabolic partial differential equation for the volume fraction and algebraic expressions for the momentum and energy exchanges between the two phases. The model proposed herein predicts, in contrast with earlier ones, that the volume fraction evolution and the energy exchange between the two phases depend directly on both mechanical and thermal non-equilibrium between the two phases.

Finally, it should be mentioned that there are cases where the hypothesis of the local equilibrium state is no longer valid; for example, flows with strong micro-inertial effects, such as grain vibration or rotation, etc. For such cases it is possible to extend the proposed model by applying, for example, the theory of extended irreversible thermodynamics, Jou *et al.* (2001). According to this theory, the dissipative fluxes are included in the set of state variables. This results in a set of evolutionary equations for the dissipative fluxes instead of the algebraic ones, cf. (26), that are predicted by the classical theory.

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