A CONTINUUM THEORY FOR THE FLOW OF PULVERIZED COAL IN A GASIFIER

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ABSTRACT

Multiphase flows have increasingly become the subject of considerable attention because of their importance in many industrial applications, such as fluidized beds, pneumatic transport of solids, coal combustion, etc. For example, coal conversion in an entrained flow reactor has received much attention as an important process for transforming coal into fuel gas [cf. Phuoc and Durbetaki (1987)]. In this work the behavior of coal particles in a down flow reactor is modeled using the theory of interacting continua (or mixture theory). The mixture is considered to be made up of saturated granular materials (coal particles) infused with a linearly viscous fluid (gas). Appropriate constitutive relations for stresses and interactive forces are motivated and proposed [Massoudi (1988)]. The conversion of coal particles is studied in terms of chemical kinetics, fluid dynamics flow of volatiles and the heat transfer mechanism at the interface.

INTRODUCTION

The flows of a mixture of solid particles and a fluid have relevance to several important technologies. Pneumatic transport of solid particles, fluidized bed combustors, and flow in a hydrocyclone are but a few examples. In many processes, such as coal conversion in an entrained flow reactor, coal is transformed into clean fuel gas. A fundamental understanding of the behavior of dense flow of coal particles and the interaction between the gas and the coal particles is extremely important.

In general, developing models capable of describing various multiphase flow regimes has attracted considerable attention due to their significant applications in many chemical and transport processes. These mathematical models or theories may be roughly classified into two categories. In one class, the basic conservation laws are postulated and the ideas in continuum mechanics are used to arrive at appropriate constitutive relations with proper restrictions. In the other class, averaging techniques are used to derive the fundamental balance laws. Whichever approach is used, constitutive relations are needed which would supply connections among kinematic, mechanical, and thermal fields which are compatible with the balance laws and which, in conjunction with them, provide a theory which can be solved for properly posed problems.

In this work the behavior of coal particles in a down flow reactor is modeled using the theory of interacting continua (or mixture theory). This theory is a means for the mathematical modeling of multicomponent systems by generalizing the equations and principles of the mechanics of a single continuum. This theory, which traces its origins to the work of Fick (1855), was first put into a rigorous mathematical format by Truesdell (1957). The theory is, in a sense, a homogenization approach in which each component is regarded as a single continuum and at each instant of time, every point in space is considered to be occupied by a particle belonging to each component of the mixture. That is, each component of the mixture is homogenized over the whole space occupied by the mixture. A historical development of the theory can be found in the review articles by Atkin and Craine (1976), Bowen (1976), and the book by Truesdell (1984). We assume the mixture is made up of saturated granular materials (coal particles) infused with a linearly viscous fluid (gas). Appropriate constitutive relations for stresses and interactive forces are motivated and proposed. The conversion of coal particles is studied in terms of chemical kinetics, fluid dynamics flow of volatiles and the heat transfer mechanism at the interface. The specific assumptions in the theory of interacting continua, and the constitutive models are presented in the next section.

MODELING

In almost all the modeling of solid particles and a fluid, the solid particles are assumed to behave like a linearly viscous fluid [for a review of this, see Rajagopal, et al. (1990)] with a viscosity μ_s and an associated pressure field p_s. A fundamental shortcoming of assuming a fluid-like behavior for the solid phase is that, theoretically, in one limit, as the volume fraction of solids becomes zero, the mixture of fluid and solid particles should behave as a fluid; in the other limit, as the volume fraction of fluid becomes small, the mixture should behave as a granular material. This second limiting case is not described if the particles are assumed to behave like a Newtonian fluid. Indeed, rheological behavior of granular materials is quite different from that of Newtonian fluids. For example, phenomena such as normal stress effects which are observed experimentally, in the shearing motion of dense flow of granular materials, cannot be predicted using a Newtonian model [Massoudi and Boyle (1987)]. Recently, Massoudi (1988) advocated the modeling of the stress in the solid constituent of the mixture by a constitutive expression appropriate to flowing granular solids, and the stress in the fluid constituent of the mixture by a linearly viscous fluid. Therefore, we assume that the stress tensors ${}^s\underset{\sim}{T}$ and ${}^f\underset{\sim}{T}$ of a granular material and a fluid are, respectively [cf. Rajagopal and Massoudi (1990)].

$$
\begin{aligned}
{}^s\underset{\sim}{T} &= [\beta_0(\rho_1) + \beta_1(\rho_1)\, \nabla\rho_1 \cdot \nabla\rho_1 + \beta_2(\rho_1)\, \mathrm{tr}\, {}^s\underset{\sim}{D}]\, \underset{\sim}{1} \\
&\quad + \beta_3(\rho_1)\, \nabla\rho_1 \otimes \nabla\rho_1 + \beta_4(\rho_1)\, {}^s\underset{\sim}{D} \ , \qquad (1)
\end{aligned}
$$

$$
{}^f\underset{\sim}{T} = (1-\nu)\ \{[-p_f + \lambda_f(\rho_2)\ \mathrm{tr}\ {}^f\underset{\sim}{D}]\ \underset{\sim}{1} + 2\mu_f(\rho_2)\ {}^f\underset{\sim}{D}\ \} \ , \qquad (2)
$$

where β_i's are material properties of the granular solid*, ν is the volume fraction of solid particles defined through

$$
\nu \equiv \rho_1/\rho_s \ , \qquad (3)
$$

in which ρ_s denotes the reference density for the granular solid. Notice that if the total stress tensor of the mixture is defined as the sum of the two stresses, ${}^s\underset{\sim}{T}$ and ${}^f\underset{\sim}{T}$, then indeed the two limiting cases (i.e., $\nu\to0$ and $\nu\to1$), mentioned earlier, are recovered with the present forumlation. In Equations (1) and (2) ${}^s\underset{\sim}{D}$ and ${}^f\underset{\sim}{D}$ denote the stretching tensor for the solid and fluid phases, respectively; λ_f and μ_f are coefficients of the viscosity of the fluid; p_f the pressure; ρ_2 the density of fluid; ∇ designates the gradient operator; $\otimes$ denotes the outer product; and $\underset{\sim}{1}$ is the identity tensor.

CONSERVATION EQUATIONS

A detailed description of the conservation laws for mixtures is given in the review articles by Bowen (1976), Atkin and Craine (1976), and the book by Truesdell (1984). Associated with each constituent is its mass supply $\hat{c}_a$, momentum supply $\underset{\sim}{m}_a$, and an energy supply e_a, where all these quantities are assumed to be continuous functions. The balance laws are then expressed as

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*For the meaning of material properties β_0 through β_4 and especially how they can be measured experimentally, we refer the reader to Rajagopal and Massoudi (1990).

$$\partial \rho_a / \partial t + \operatorname{div} (\rho_a \underset{\sim}{v}_a) = \hat{c}_a \tag{4}$$

$$\rho_a \underset{\sim}{v}_a' = \operatorname{div} \underset{\sim}{T}_a + \rho_a \underset{\sim}{b}_a + \hat{\underset{\sim}{m}}_a - \hat{c}_a \underset{\sim}{v}_a \tag{5}$$

$$\rho_a e_a' = \underset{\sim}{T}_a \cdot \operatorname{grad} \underset{\sim}{v}_a + \operatorname{div} \underset{\sim}{q}_a + \rho_a r_a - \hat{\underset{\sim}{m}}_a \underset{\sim}{v}_a$$

$$- \hat{c}_a (e_a - 1/2 \, v_a^2) + \hat{e}_a \quad , \tag{6}$$

$$a = 1, 2$$

where prime denotes material time derivative following the motion of the constituent a, $\underset{\sim}{v}_a$ is the velocity of the constituent a, $\underset{\sim}{T}_a$ the stress tensor, $\underset{\sim}{q}_a$ the heat flux vector, r_a external heat sources, and e_a is the specific internal energy. Equation (4) is a statement of conservation of mass, Equation (5) conservation of linear momentum, and Equation (6) conservation of energy.

The modeling of $\underset{\sim}{T}_a$ (a=1,2), was explained in the previous section. In addition, constitutive relations for $\hat{c}_a$, $\hat{\underset{\sim}{m}}_a$, and $\hat{e}_a$, would also have to be provided so that the system of Equations (4) - (6) can be used to study this problem.

In this problem, we will study the downflow of coal-gas mixtures in a gasifier. Specific models for $\hat{c}_a$, $\hat{\underset{\sim}{m}}_a$, and $\hat{e}_a$ will be proposed and motivated. Appropriate boundary conditions will be provided. The basic numerical scheme is that of Phuoc and Durbetaki (1987). Restrictions and assumptions concerning the material properties appearing in the constitutive relations will also be discussed. Quantities and fields of interest which will be calculated and plotted are velocity, temperature, density fields, and pressure distribution.

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