

# Modeling Heterogeneous Two-Phase Reacting Flow

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The balance equations for heterogeneous two-phase reacting flow are deduced by a formal averaging procedure. The equations are compared with alternatives which have been reported in the literature for the study of convective burning in porous beds. Errors in the latter are noted by reference to simple limiting case arguments. The empirical data required to support the balance equation are discussed. The balance equations are shown to be hyperbolic but not totally hyperbolic. Two methods of numerical solution of unsteady quasi-one-dimensional two-phase flow with discontinuous distributions of porosity are described.

## Nomenclature

$a$	=rate of propagation of intergranular disturbances
$B_1, B_2, B_3$	=parameters in burning rate law
$c$	=speed of sound in gas
$D_p$	=effective diameter of particles
$\dot{d}$	=rate of regression of surface of propellant
$e$	=internal energy of gas
$\langle F \rangle^i$	=interphase drag per unit area of solid phase
$f_s$	=steady-state drag per unit volume
$g$	=weighting function used to define average
$\vec{I}$	=unit tensor of rank 2
$k_f$	=thermal conductivity of gas at film temperature
$Nu_p$	=Nusselt number based on $D_p$
$n$	=normal to interface between phases
$Pr$	=Prandtl number
$p$	=pressure
$q$	=heat flux vector
$\vec{R}$	=granular stress tensor
$Re_p$	=Reynolds number based on $D_p$
$S_p$	=surface area of particle
$\vec{T}$	=stress tensor, positive in compression
$t$	=time
$u$	=velocity
$V_p$	=volume of a particle
$w$	=velocity of interface between media
$x$	=position vector
$\beta$	=virtual mass coefficient
$\gamma$	=ratio of specific heats
$\epsilon$	=porosity or fraction of unit volume occupied by gas phase
$\epsilon_0$	=settling porosity
$\epsilon_*$	=porosity above which $a(\epsilon) = 0$
$\theta$	=temperature
$\kappa$	=stress attenuation factor
$\mu$	=viscosity
$\rho$	=density
$\Sigma$	=region of integration defined by product of interphase surface and time
$\phi, \psi$	=dummy variables
$\langle \rangle$	=average of enclosed quantity

## Subscripts

$p$	=property of the solid phase
$m$	=a barycentric property

## Superscript

$( )'$	=fluctuation of a local property from the average
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## Introduction

THE work we describe herein was stimulated by the desire to model interior ballistic phenomena in a conventional medium-caliber solid propellant gun. The propelling charge for such a gun consists of an aggregate of randomly packed grains of solid propellant. Generally speaking the grains are all the same regular shape, typically a multiperforated cylinder. The charge is ignited by the venting of hot gas from a primer into the bed. The grains in the neighborhood of the primer are heated convectively and, due to their low thermal conductivity, their surface temperature rises rapidly to the point of self-sustained combustion. The combustion products combine with the primer gas and assist in spreading the flame through the bed. The penetration of the bed by the gas is strongly resisted by drag which in turn leads to motion and compaction of the solid phase.

Clearly, the theoretical basis for the study of such processes must be formulated in terms of the unsteady motion of two phases having unequal velocities and temperatures, coupled through drag, heat transfer, and combustion. It will also be apparent that the formulation must be content with a description of bulk, average, or macroscopic properties of the flow if results of practical interest are to be obtained. The results of our inquiries into this problem are contained in Refs. 1-5. In the present paper, we will summarize the more important of our findings, referring the reader to Refs. 1-5 for supporting details. We consider successively the formulation of the balance equations, their closure, their mathematical structure, and their numerical solution.

## Determination of the Balance Equations

A considerable body of literature exists with respect to the determination of the balance equations for the average properties of a two-phase flow. A review will not be attempted here. The reader may consult the dissertation of the first author<sup>3</sup> or the more recent work by Gidaspow.<sup>6</sup> We show that the balance equations may be obtained by formal averaging of the equations which govern the microflow together with the boundary conditions at the interface between the phases. Our approach follows that of Anderson and Jackson,<sup>7</sup> who introduced the concept of an average de-

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finned in terms of a weighting function. This approach has the benefit of great generality as the results are formally indifferent to the precise nature of the weighting function, except for certain broad conditions, and is moreover analytically convenient. Results have also been obtained by Pantón<sup>8</sup> using an area average. Most recently Wnek et al.<sup>9</sup> have reported results for the gas phase based upon the method of Slattery.<sup>10</sup> Anderson and Jackson provided statements of the averaged continuity and momentum equations for both the solid and the gas phases but did not consider an energy equation for either phase. There are, moreover, compensating errors in their derivation which we have noted previously.<sup>3</sup> Pantón produced results for both phases but did not separate the energy equation which was reported for the mixture alone. We extend the approach of Anderson and Jackson by taking the weighting function to depend on both time and position so that the theory of turbulence is formally included in the derivation. However, no discussion is given of the correlations among the fluctuations which are so important in turbulence. The corresponding terms, which have been referred to as representing pseudoturbulence by Buyevich,<sup>11</sup> are assumed to exert a negligible influence in the problems of interest.

We consider specifically the two-phase flow consisting of a compressible gas and an aggregate of incompressible but deformable particles. The Reynolds number is presumed to be high and the influence of viscosity and heat conduction is assumed to be confined to thin boundary layers. The balance equations necessarily include statements of conservation of mass, momentum, and energy of the gas and of mass and momentum of the solid phase. No energy equation is required for the solid phase, due to the assumption of incompressibility. This observation which has been contested by Krier<sup>12</sup> is intuitively obvious and has been demonstrated formally.<sup>3</sup>

#### Definition of the Average

We introduce a weighting function  $g(y-x, \tau-t)$  which reflects the influence of remote points  $(y, \tau)$  on the average value at  $(x, t)$  where  $x$  and  $y$  are understood to be three-dimensional vectors. Except for certain mild conditions which include any conceivable physically motivated average,  $g$  may be regarded as arbitrary. We require that  $g$  be nonnegative and that it approach zero sufficiently rapidly with distance from the point of collocation to insure the existence of its integral over all space and time. We may then assume  $g$  to be normalized so that

$$\int_{\substack{\text{all space} \\ \text{all time}}} g(r, t) dv d\tau = 1 \quad (1)$$

The void fraction, or porosity, may be defined in terms of  $g$  according to

$$\epsilon(x, t) = \int_{\substack{\text{region occupied} \\ \text{by gas}}} g(y-x, \tau-t) dv d\tau \quad (2)$$

and an average value of the gas property  $\psi$  is defined by

$$\langle \psi(x, t) \rangle = \frac{1}{\epsilon(x, t)} \int_{\substack{\text{region occupied} \\ \text{by gas}}} g(y-x, \tau-t) \psi(y, \tau) dv d\tau \quad (3)$$

The average properties of the solid phase are determined in a completely analogous manner. It is emphasized that the region of integration in Eqs. (2) and (3) extends over time as well as space.

Clearly, the definitions in Eqs. (2) and (3) are purely formal, since the regions of integration are only known in principle. In order to deduce governing equations for the average properties, we will refer to the microscopic balance equations which will involve derivatives of the state variables.

Evidently, therefore, we will require a commutation principle which describes the effect of the order in which differentiation and averaging are performed.

Let  $x_i$  be a component of  $x$ , the point at which the average is formed. Since the region of integration in Eq. (3) does not depend on  $x$  we have

$$\begin{aligned} \frac{\partial}{\partial x_i} \epsilon(x, t) \langle \psi(x, t) \rangle \\ = \int_{\substack{\text{region occupied} \\ \text{by gas}}} \frac{\partial}{\partial x_i} [g(y-x, \tau-t) \psi(y, \tau)] dv d\tau \end{aligned}$$

Now the integrand on the right-hand side may be written as

$$\begin{aligned} \frac{\partial}{\partial x_i} [g(y-x, \tau-t) \psi(y, \tau)] &= g(y-x, \tau-t) \frac{\partial \psi}{\partial y_i}(y, \tau) \\ &- \frac{\partial}{\partial y_i} [g(y-x, \tau-t) \psi(y, \tau)] \end{aligned}$$

Accordingly, an application of the divergence theorem<sup>13</sup> yields

$$\begin{aligned} \frac{\partial}{\partial x_i} \epsilon(x, t) \langle \psi(x, t) \rangle &= \epsilon(x, t) \left\langle \frac{\partial}{\partial x_i} \psi(x, t) \right\rangle \\ &- \int_{\Sigma} \psi(y, \tau) g(y-x, \tau-t) n_i dA \end{aligned} \quad (4)$$

where  $\Sigma$  is the region of integration defined by the interface between the media and all time,  $w$  is the velocity of the interface, and  $n$  is the normal to the interface taken positive out of the medium for which the average is being formed. Similarly we have

$$\begin{aligned} \frac{\partial}{\partial t} \epsilon(x, t) \langle \psi(x, t) \rangle &= \epsilon(x, t) \left\langle \frac{\partial}{\partial t} \psi(x, t) \right\rangle \\ &+ \int_{\Sigma} \psi(y, \tau) g(y-x, \tau-t) w \cdot n dA \end{aligned} \quad (5)$$

Equations (4) and (5) are the key to the formal replacement of the microequations by governing equations for the average properties. We may also anticipate that the bulk of the analytical task will relate to the formal manipulation and simplification of the surface integrals. The following observations may be made.

1) The expression  $\int_{\Sigma} g dA$  is, in effect, the average surface area per unit volume. Provided  $g$  is such as to sample many particles and provided these have locally similar volume ( $V_p$ ) and surface area ( $S_p$ ) one may show

$$\int_{\Sigma} g dA = (1 - \epsilon) S_p / V_p \quad (6)$$

2)  $\int_{\Sigma} g \psi dA$  is, in effect, a definition of the average of  $\psi$  over the interface, apart from the normalizing factor defined by Eq. (6). For some of the quantities which arise in the problems of convective burning, the surface average is the rational representation. Such quantities as the rate of regression of the propellant surface, the friction, and the heat transfer between the media are naturally expressed in this form.

We therefore introduce the surface average of  $\psi$  according to:

$$\langle \psi \rangle' = \int_{\Sigma} g \psi dA / \int_{\Sigma} g dA \quad (7)$$

3) For a quantity such as gas pressure or velocity, the surface average is likely to be quite different from the overall average. Therefore, the two must be distinguished in general. The only exception to this rule is the particle velocity, for which the surface average may be expected to be close to the overall average, provided that  $g$  is such as to sample many particles.

It is necessary, in general, to introduce the fluctuation field associated with the tensor  $\psi$  according to

$$\psi' = \psi - \langle \psi \rangle \quad (8)$$

Provided that we may assert  $\langle \langle \psi \rangle \rangle = \langle \psi \rangle$  it follows that  $\langle \psi' \rangle = 0$ . It should be understood that this assertion has the character of a postulate<sup>3</sup>; physically it corresponds to the embedding into the theory of only those characteristics of the flow whose scale is large in comparison with the domain of influence of the weighting function. When  $\langle \psi' \rangle = 0$  it follows that

$$\langle \phi \psi \rangle = \langle \phi \rangle \langle \psi \rangle + \langle \phi' \psi' \rangle \quad (9)$$

so that the correlation is introduced. In respect to the manipulation of the surface average we have

$$\int_{\Sigma} \langle \psi \rangle g dA = \langle \psi \rangle \int_{\Sigma} g dA \quad (10)$$

Finally, we need the identity

$$\int_{\text{region occupied by gas}} \langle \psi \rangle \nabla g dV d\tau = - \nabla \epsilon \langle \psi \rangle \quad (11)$$

and similarly for the case in which the integration extends over the solid phase.

#### Assumptions

Following Ref. 3 we state the assumptions required to establish the averaged form of the balance equations. We use  $\rho$ ,  $u$ ,  $p$ ,  $e$  to denote the density, velocity, pressure, and internal energy of the gas and add the subscript  $p$  to denote the corresponding properties of the solid phase. We use  $q$  to denote the heat flux and  $\vec{T}$ , positive in compression, to denote the stress tensor. Reference 3 considers the influence of an external source which we ignore herein for the sake of brevity. The balance equations for the gas phase are

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho u = 0 \quad (12)$$

$$\frac{\partial}{\partial t} \rho u + \nabla \cdot (\rho u u + \vec{T}) = 0 \quad (13)$$

$$\frac{\partial}{\partial t} \rho \left( e + \frac{u \cdot u}{2} \right) + \nabla \cdot \left[ \rho u \left( e + \frac{u \cdot u}{2} \right) + u \cdot \vec{T} + q \right] = 0 \quad (14)$$

Dyadic notation is followed, with the expression  $uu$  signifying an outer product of the vector  $u$  with itself, or a tensor of rank 2. The tensor  $\vec{T}$  is assumed to be symmetrical. Equations analogous to Eqs. (12) and (13) are assumed to govern the solid phase.

The boundary conditions at the interface between the phases may be expressed as

$$\rho(u - w) \cdot n = \rho_p(u_p - w) \cdot n \quad (15)$$

$$[\vec{T} + \rho u(u - w)] \cdot n = [\vec{T}_p + \rho_p u_p(u_p - w)] \cdot n \quad (16)$$

$$\begin{aligned} & \left[ \vec{T} \cdot u + q + \rho(u - w) \left( e + \frac{u \cdot u}{2} \right) \right] \cdot n \\ &= \left[ \vec{T}_p \cdot u_p + q_p + \rho_p(u_p - w) \left( e_p + \frac{u_p \cdot u_p}{2} \right) \right] \cdot n \end{aligned} \quad (17)$$

The velocity of the interface may be expressed as

$$w = u_p + n\dot{d} \quad (18)$$

The tangential components of velocity and traction are taken to be continuous and we may introduce the pressure jump as

$$(\vec{T}_p - \vec{T}) \cdot n = n\Delta p \quad (19)$$

We assume that the average stress in the gas is isotropic

$$\langle \vec{T} \rangle = \langle p \rangle \vec{I} \quad (20)$$

where  $\vec{I}$  is the unit tensor of rank 2. The average heat flux in each phase is zero.

$$\langle q \rangle = \langle q_p \rangle = 0 \quad (21)$$

The solid phase is taken to be incompressible so that  $\rho_p$  is constant. Moreover, we assume that Eq. (6) describes the surface area per unit volume. We also assume that the rate of regression of the surface  $\dot{d}$  is sufficiently smooth that fluctuations about the average  $\langle \dot{d} \rangle^i$  may be neglected and that the magnitude of  $\dot{d}$  is sufficiently small that the pressure jump  $\Delta p$  is negligible by comparison with  $\langle p \rangle$ . We also assume, ab initio, that the correlations of the fluctuations may be neglected whereas Ref. 3 deduces their formal influence. Reference 3 may also be consulted for a discussion of the significance of the assumptions.

Finally, we introduce a granular stress tensor  $\vec{R}$  according to the definition,

$$\langle \vec{T}_p \rangle = \vec{R} + \langle p \rangle \vec{I} \quad (22)$$

Evidently,  $\vec{R}$  reflects the difference between the average stress in the solid phase and that in the ambient gas.

#### Balance of Mass

Multiply Eq. (12) by  $g$  and integrate over the region occupied by the gas, use the commutation laws of Eqs. (4) and (5) to get

$$\frac{\partial}{\partial t} \epsilon \langle \rho \rangle + \nabla \cdot \epsilon \langle \rho u \rangle = - \int_{\Sigma} g \rho (u - w) \cdot n dA \quad (23)$$

Expand  $\langle \rho u \rangle$  according to Eq. (9) and neglect the correlation  $\langle \rho' u' \rangle$ . Use the jump condition of Eq. (15) and the identity in Eq. (18) in the right-hand side. Make use of Eq. (6) and we have

$$\frac{\partial}{\partial t} \epsilon \langle \rho \rangle + \nabla \cdot \epsilon \langle \rho \rangle \langle u \rangle = (1 - \epsilon) \frac{S_p \rho_p}{V_p} \langle \dot{d} \rangle^i \quad (24)$$

Proceeding analogously we find the mass balance for the solid phase as

$$\frac{\partial}{\partial t} \epsilon - \nabla \cdot (1 - \epsilon) \langle u_p \rangle = (1 - \epsilon) \frac{S_p}{V_p} \langle \dot{d} \rangle^i \quad (25)$$

Due to the assumption of incompressibility, this is a governing equation for the porosity.

#### Balance of Momentum

Let Eq. (13) be averaged, use the commutation laws of Eqs. (4) and (5), expand the terms involving the averages of

products, neglect the correlations and use Eq. (24) to get, for the gas phase

$$\epsilon \langle \rho \rangle \frac{D}{Dt} \langle u \rangle + \nabla \cdot \epsilon \langle \tilde{T} \rangle = \langle u \rangle \int_{\Sigma} g \rho (u - w) \cdot n dA - \int_{\Sigma} g (\tilde{T} + \rho u (u - w)) \cdot n dA \quad (26)$$

where

$$\frac{D}{Dt} \equiv \frac{\partial}{\partial t} + \langle u \rangle \cdot \nabla \quad (27)$$

We now use the jump conditions of Eqs. (15) and (16) to evaluate the surface integrals. We use  $\Delta p = 0$  and we take  $\langle u_p \rangle^i = \langle u_p \rangle$ . Moreover, using Eq. (20) and introducing:

$$(1 - \epsilon) \frac{S_p}{V_p} \langle F \rangle^i = \int_{\Sigma} g \tilde{T}^i \cdot n dA \quad (28)$$

we may deduce the averaged balance of momentum in the form

$$\epsilon \langle \rho \rangle \frac{D}{Dt} \langle u \rangle + \epsilon \nabla \langle p \rangle = - (1 - \epsilon) \frac{S_p}{V_p} \langle F \rangle^i + (1 - \epsilon) \frac{\rho_p S_p}{V_p} [\langle u_p \rangle - \langle u \rangle] \langle \dot{d} \rangle^i \quad (29)$$

Similarly, but making use of Eq. (22), we have the corresponding balance of momentum for the solid phase in the form

$$(1 - \epsilon) \rho_p \frac{D}{Dt} \langle u_p \rangle + (1 - \epsilon) \nabla \langle p \rangle + \nabla \cdot (1 - \epsilon) \tilde{R} = (1 - \epsilon) \frac{S_p}{V_p} \langle F \rangle^i \quad (30)$$

#### Balance of Energy for Gas Phase

The derivation of this equation follows the same series of steps that we have outlined in the preceding discussion. The only difficult step in the procedure relates to a work term which is to be averaged over the interface between the media. Referring to Ref. 3 for details we simply assert that, neglecting the correlation terms, we have

$$\int_{\Sigma} g u_p \cdot \tilde{T}_p \cdot n dA = - \langle p \rangle \langle u_p \rangle \cdot \nabla \epsilon + (1 - \epsilon) \frac{S_p}{V_p} \langle u_p \rangle \cdot \langle F \rangle^i + (1 - \epsilon) \langle p \rangle \nabla \cdot \langle u_p \rangle \quad (31)$$

The averaged balance of energy may then be stated as

$$\begin{aligned} \epsilon \langle \rho \rangle \frac{D}{Dt} \langle e \rangle + \epsilon \langle p \rangle \nabla \cdot \langle u \rangle + \langle p \rangle \frac{D\epsilon}{Dt} \\ = (1 - \epsilon) \frac{S_p}{V_p} [(\langle u \rangle - \langle u_p \rangle) \cdot \langle F \rangle^i - \langle q \rangle^i] \\ + (1 - \epsilon) \frac{\rho_p S_p}{V_p} \langle \dot{d} \rangle^i [\langle e_p \rangle^i + \frac{\langle p \rangle}{\rho_p} - \langle e \rangle \\ + \frac{1}{2} (\langle u \rangle - \langle u_p \rangle) \cdot (\langle u \rangle - \langle u_p \rangle)] \end{aligned} \quad (32)$$

and where

$$(1 - \epsilon) \frac{S_p}{V_p} \langle q \rangle^i = \int_{\Sigma} g q' \cdot n dA \quad (33)$$

#### Closure and the Constitutive Laws

An inspection of the five balance equations shows them to involve the 13 quantities  $\langle \rho \rangle$ ,  $\langle p \rangle$ ,  $\langle u \rangle$ ,  $\langle u_p \rangle$ ,  $\langle e \rangle$ ,  $\langle e_p \rangle$ ,  $\langle F \rangle^i$ ,  $\langle q \rangle^i$ ,  $\langle \dot{d} \rangle^i$ ,  $\epsilon$ ,  $\tilde{R}$ ,  $S_p$ , and  $V_p$ . Thus, we require eight constitutive laws to close the theory. A full discussion of the requirements for closure is given in Ref. 3. Here we confine ourselves to the following brief summary which describes the laws we have used in modeling convective burning.

#### Equation of State of Gas

We assume that the Noble-Abel equation of state governs the average properties according to

$$\langle e \rangle = \frac{\langle p \rangle}{(\gamma - 1) \langle \rho \rangle} (1 - b \langle \rho \rangle) \quad (34)$$

where  $\gamma$  is the ratio of specific heats and  $b$  is the covolume. We also consider the molecular weight and the ratio of specific heats to depend upon the composition of the gas, although not on its temperature.

#### Form Functions for Particles

We assume that  $V_p$  and  $S_p$  are known as algebraic functions of the total surface regression and the initial geometry. The functional relationships for cylinders and spheres are obvious and need not be stated here. Relationships for multiperforated cylinders of the type used in gun propelling charges may be found in the work of Krier.<sup>14</sup>

#### Rate of Surface Regression

We assume that the rate of surface regression can be related to the average gas pressure according to the well-known exponential law for steady burning:

$$\langle \dot{d} \rangle^i = B_1 + B_2 \langle p \rangle^{B_3} \quad (35)$$

At the same time, the value of  $\langle e_p \rangle^i$  may be taken to be the chemical energy released in combustion of the solid propellant.

Since initially the solid phase is expected to be at room temperature, it is necessary to determine the conditions under which combustion begins. We have taken the interphase heat transfer as a boundary condition for the unsteady heat conduction equation applied to the solid phase. In general, the depth of penetration of the thermal layer is small in comparison with the size of the grains and we have therefore taken the conduction to be one dimensional. Ignition of the solid phase is predicated on the value of the surface temperature.

#### Interphase Heat Transfer

The interphase heat transfer is related to the average flow properties according to existing correlations for packed and fluidized beds. Thus, for the packed bed we may use the correlation of Denton<sup>15</sup> as modified by Eckert and Drake<sup>16</sup> in the form,

$$Nu_p = 0.4 Re_p^{0.7} Pr^{1/3} \text{ if } \epsilon < \epsilon_0 \quad (36)$$

where  $Nu_p = h D_p / k_f$ ,  $h = \langle q' \rangle^i / (\langle \theta \rangle - \langle \theta_p \rangle^i)$ ,  $Re_p = \langle \rho \rangle |\langle u \rangle - \langle u_p \rangle| D_p / \mu_f$ ,  $Pr = 4\gamma / (9\gamma - 5)$ , and  $\epsilon_0$  is the settling porosity. The viscosity  $\mu_f$  is deduced according to a Sutherland-type law; the thermal conductivity  $k_f$  follows from the Prandtl number; and the subscript  $f$  indicates that the transport properties are computed at the film temperature  $\frac{1}{2}(\langle \theta \rangle + \langle \theta_p \rangle^i)$ . We discuss the particle diameter  $D_p$  in the following subsection. The representation of Eq. (36) differs from that of Kuo and Summerfield<sup>17</sup> who included a factor  $\epsilon^{0.7}$  on the right-hand side in order to convert Denton's results, based on the superficial velocity  $U = \epsilon \{ \langle u \rangle - \langle u_p \rangle \}$ ,

into a form based upon the average velocity. Since Denton's results were acquired for the single value of  $\epsilon = 0.370$ , the factor  $\epsilon^{0.7}$  is speculative and in fact runs counter to intuition according to which the influence of tortuosity would produce an increase in heat transfer with decreasing porosity. When the bed is dispersed we use the correlation of Gelperin-Einstein<sup>18</sup>

$$Nu_p = 0.4 Re_p^{2/3} Pr^{1/3} \quad (37)$$

which differs only slightly from that of Denton according to our interpretation.

#### Interphase Drag

The term  $\langle F \rangle^i$  may be interpreted as the interphase drag per unit wetted area and may be resolved, to a certain extent, by reference to existing data. However, care must be taken to use the data properly. We have used the data of Ergun<sup>19</sup> to describe the steady-state interphase drag in a packed bed, as have Kuo and Summerfield. However, our respective representations differ by a factor of  $\epsilon$ . In order to account for unsteady effects we incorporate a virtual mass effect in the following functional form

$$(1-\epsilon) \frac{S_p}{V_p} \langle F \rangle^i = f_s + \beta \langle \rho \rangle (1-\epsilon) \left\{ \frac{Du}{Dt} - \frac{Du_p}{Dt_p} \right\} \quad (38)$$

where  $\beta$ , the virtual mass coefficient, is known to be equal to  $1/2$  for an isolated sphere. Values for an aggregate of particles have been proposed by Buyevich<sup>11</sup> and Zuber<sup>20</sup> but must be regarded as speculative at the present time. The functional dependence of  $f_s$  on the flow conditions is assumed to be described by the data of Ergun when the bed is packed

$$f_s = \frac{1-\epsilon}{D_p} |\langle u \rangle - \langle u_p \rangle| (\langle u \rangle - \langle u_p \rangle) \langle \rho \rangle \left\{ 1.75 + 150 \frac{1-\epsilon}{\epsilon Re_p} \right\} \quad (39)$$

The effective diameter is defined as  $D_p = 6V_p/S_p$  which coincides with the true diameter for a sphere. The basis for the extrapolation of Ergun's law to multiperforated cylinders has not been clarified and is the subject of a current inquiry. For the interim we use Eq. (39) with  $D_p$  evaluated in terms of actual volume and total surface area. Calculations show that typically  $Re_p \sim 10^5$  so that the first term within the brackets of Eq. (39), which represents the base drag, exceeds the second term, which represents the viscous drag, by two or more orders of magnitude. Accordingly, we neglect the second term. If Eq. (39) is recast so as to enable the identification of the drag coefficient per particle, based on cross section, we find  $C_D = 2.333$ , which is much higher than the value for a sphere in isolation with  $Re_p \sim 10^5$ . The discrepancy may be interpreted as being due to tortuosity and the correlation of Anderssen<sup>21</sup> may be used to describe the manner in which the drag particle decreases as the bed becomes fluidized. Thus, we describe the interphase drag according to<sup>5</sup>

$$\frac{f_s}{\frac{1-\epsilon}{D_p} \langle \rho \rangle \{ \langle u \rangle - \langle u_p \rangle \}^2} = \begin{cases} 1.75 & \epsilon \leq \epsilon_0 \\ 1.75 \left[ \frac{1-\epsilon}{1-\epsilon_0} \frac{\epsilon_0}{\epsilon} \right]^{0.45} & \epsilon_0 < \epsilon \leq \epsilon_1 \\ 0.3 & \epsilon_1 < \epsilon \leq 1 \end{cases} \quad (40)$$

where

$$\epsilon_1 = \left[ 1 + 0.02 \left( \frac{1-\epsilon_0}{\epsilon_0} \right) \right]^{-1}$$

#### The Granular Stress

This topic is of particular interest not only because of the physical content of the constitutive law for the granular stress, but also because of its mathematical ramifications. As we have discussed elsewhere,<sup>3</sup> in the absence of the granular stress term the balance equations are only totally hyperbolic under special conditions which are obtained rarely in problems of convective burning. On the other hand, the presence of the granular stress usually results in the balance equations being totally hyperbolic. This observation, with its obvious implications in respect to the solution of initial and boundary value problems, has led us to consider constitutive laws whose formulation is motivated by mathematical as well as purely physical considerations.

Physically, the term  $\mathbf{R}$  represents the difference between the average stress in the solid phase and that in the gas phase. Clearly, when both media are at rest and the solid phase is dispersed we expect  $\mathbf{R} = 0$ . With both phases at rest, but the solid phase packed and responding to external loads applied through a gas permeable membrane, we may visualize the granular stress becoming quite large while the gas pressure remains fixed. Since the particles are presumed to be incompressible, it follows that the average dilatation of the solid phase, which arises in response to the external load, will be a function of the porosity alone. We may therefore postulate an isotropic stress law in the form  $\mathbf{R} = R(\epsilon) \mathbf{I}$ . It will also be evident that the relative motion of the phases will result in a contribution to  $\mathbf{R}$  due to the variation of gas pressure over the surface of each particle. However, calculations of interior ballistic problems show that the relative Mach number rarely exceeds 0.3, so that the stress distribution associated with relative motion may be neglected by comparison with the gas pressure. There will also be a contribution to  $\mathbf{R}$ , when the solid phase is dispersed, due to impacts among particles. However, the functional form of the stress associated with the random motion is unclear and we postulate that the granular stress becomes negligibly small when the solid phase is dispersed. It should be clearly understood therefore that when we subsequently consider a constitutive law for which the granular stress is not zero in the dispersed condition, we do so for purely mathematical reasons associated with the total hyperbolicity of the balance equations.

The functional form of the granular stress law is expressed in terms of the rate of propagation of infinitesimal granular disturbances<sup>3</sup>:

$$a(\epsilon) = \sqrt{-\frac{1}{\rho_p} \frac{d}{d\epsilon} (1-\epsilon) R(\epsilon)} \quad (41)$$

We define a reversible stress law according to:

$$a(\epsilon) = \begin{cases} a_1 (\epsilon_0/\epsilon) & \epsilon \leq \epsilon_0 \\ a_1 \exp[-\kappa(\epsilon - \epsilon_0)] & \epsilon_0 < \epsilon \leq \epsilon_* \\ 0 & \epsilon > \epsilon_* \end{cases} \quad (42)$$

where  $\epsilon_0$  is the settling porosity of the bed,  $\kappa$  is referred to as the stress attenuation factor, and  $\epsilon_*$  is introduced as the value of porosity above which  $a(\epsilon) = 0$ . Only the values of  $a_1$  and  $\epsilon_0$  are experimentally supported; measurements of Soper<sup>22</sup> show  $a_1 \sim 1400$  fps for NACO propellant. The nonlinear dependence in the packed regime is speculative. The exponential dependence in the dispersed regime is introduced for mathematical reasons; physically, we postulate  $\kappa = \infty$ . In the preparation of numerical results we have used both the reversible law in Eq. (42) and an irreversible law according to which  $a(\epsilon) = 0$  when  $D\epsilon/Dt_p > 0$ .

### Comparison with Some Alternative Systems of Balance Equations

It is beyond the scope of this paper to perform a complete comparison of our balance equations with all of the alternative systems which have been proposed in the literature at large. Even within the narrow field defined by applications to problems of interior ballistics, it was the case that four groups of investigators developed four different systems of balance equations, all purporting to describe the same physical phenomena! A discussion of these systems was given by Gough<sup>23</sup> and certain simple physical arguments were advanced to disqualify the alternative systems. Here we confine our attention to the systems of balance equations which have been proposed for the study of convective burning. A detailed comparison of our equations with the results of Anderson and Jackson<sup>7</sup> and of Panton<sup>8</sup> may be found in Ref. 3. Taking into account minor differences due to the applications of interest we may note that the balance equations presented here accord with those of Kraiko and Sternin,<sup>24</sup> Nigmatulin,<sup>25</sup> and of Harlow and Amsden.<sup>26</sup>

Here we wish to comment on certain differences between our equations and those of Krier<sup>12</sup> and of Kuo.<sup>27</sup> We delete from our equations the virtual mass effect, which has not been considered by the other authors, and the granular stress, whose neglect by Krier constitutes a serious omission, in our judgement. We further confine our attention to the differential terms since the differences which arise in the nonhomogeneous terms have already been commented upon in the previous section. As in Ref. 23 we show, by recourse to limiting case arguments, that certain of the equations of Kuo and of Krier cannot be correct.

There is no disagreement concerning the continuity equations. Moreover, our momentum equations agree with those of Kuo.<sup>27</sup> Krier<sup>12</sup> expresses the momentum equation for the gas as

$$\epsilon \rho \frac{Du}{Dt} + \frac{\partial}{\partial x} \epsilon p - \frac{\partial}{\partial x} \epsilon \rho (u - u_m)^2 = N.H. \quad (43)$$

while that for the solid phase is:

$$(1 - \epsilon) \rho_p \frac{Du_p}{Dt_p} - \frac{\partial}{\partial x} (1 - \epsilon) \rho_p (u - u_m)^2 = N.H. \quad (44)$$

Here we use the symbol  $N.H.$  to signify the nonhomogeneous or algebraic terms. We do not use an explicit average notation; however, the field quantities are assumed to represent macroscopic properties of each constituent. The quantity  $u_m$  represents the barycentric velocity of the mixture:

$$u_m = \frac{\epsilon \rho u + (1 - \epsilon) \rho_p u_p}{\epsilon \rho + (1 - \epsilon) \rho_p} \quad (45)$$

Both Krier and Kuo offer somewhat different statements of the gas phase energy from that which we have presented. Krier<sup>12</sup> has

$$\frac{De}{Dt} + \frac{p}{\rho} \nabla \cdot u + \text{mechanical diffusion terms} = N.H. \quad (46)$$

When the terms representing heat conduction and the normal viscous force are deleted from the one-dimensional energy equation of Kuo<sup>27</sup> we have

$$\epsilon \rho \frac{De}{Dt} + p \frac{D\epsilon}{Dt} + \epsilon p \frac{\partial u}{\partial x} - p u_p \frac{\partial \epsilon}{\partial x} = N.H. \quad (47)$$

The equations of Krier<sup>12</sup> are immediately distinguished by the presence of mechanical diffusion terms which we have written in extenso in Eqs. (43) and (44) and whose presence we

have simply indicated in Eq. (45). It is our position that these terms are unsupported by physical considerations; they belong in the balance equations for the mixture. Whereas Krier et al. cite Truesdell's principle that the behavior of the mixture should follow as a mathematical consequence of the behavior of the species, they effectively pursue the opposite course in their derivation. The mixture is first proposed to be a Newtonian fluid, a proposal entirely unsupported by experience and directly contradicted by some data.<sup>28</sup> Subsequently the mixture is taken to be ideal, an even stronger hypothesis and one without apparent foundation. Accordingly, the application of Truesdell's fundamental identity and the reasonable hypothesis of equipresence of terms in each of the species equations forces the diffusion terms into the balance equations for the separate species.

In order to assess the validity of these alternative sets of equations we propose the following limiting case arguments.

#### A. Equilibrium Solution with Variable Porosity

From a purely physical point of view it is clear that there exists an equilibrium solution with both media at rest and in which the porosity of the aggregate varies from point to point while the pressure is everywhere uniform. If we insert  $u = u_p = 0$  and  $p = \text{constant}$  into the various momentum equations and note that the nonhomogeneous terms vanish when  $u = u_p$ , we find that our momentum equations are reduced to identities. However, the gas momentum equation of Krier et al. can only be satisfied if the porosity is uniform and the correctness of this equation is therefore denied.

#### B. Symmetry of the Momentum Equation with Respect to Species

The momentum equations do not depend on any assumptions concerning the compressibility of the particles. Moreover, in a dispersed flow at low relative Mach number, the average pressure inside the particles is expected to be very nearly the same as that in the ambient gas. Accordingly, we expect the gas and particle momentum equations to be completely symmetrical when we put  $\epsilon \rightarrow (1 - \epsilon)$  and  $\rho \rightarrow \rho_p$ . This is not true of the equations of Krier et al.

This argument for symmetry can be reinforced and shown to be independent of the dispersed character of the particles by considering the limit in which the properties coincide with those of the ambient gas. Clearly, the balance equations must also coincide in this limit.

#### C. Analogy with Duct Flow

The form of the equations of motion for the gas should be independent of the microgeometry of the granular aggregate. We can therefore consider the limiting case in which this geometry is regularized into identical parallel ducts of varying area. Clearly the porosity will be proportional to the cross-sectional area of each of these ducts and the one-dimensional equations of motion of the gas should degenerate to those for the flow of a compressible fluid through a time-dependent duct. This test is only satisfied by our own equations.

#### D. Isentropic Behavior of the Energy Equation in the Absence of Irreversible Processes

If we consider the gas to be ideal so that the velocity dependent drag vanishes (d'Alembert's Paradox) and we further assume heat transfer and combustion to be absent, then the flow of the gas is thermodynamically reversible and the entropy of the gas is constant. This permits a strong test of the energy equation for the gas; by using the continuity equation and the first and second laws of thermodynamics, we may recast it as an equation for the entropy. This test is satisfied by neither the energy equation of Krier et al. nor that of Kuo. It is satisfied by our own.

### Classification of Balance Equations for One-Dimensional Unsteady Flow

It is of considerable interest to determine the classification of the balance equations as a system of partial differential equations. A knowledge of the characteristic directions and their associated conditions of compatibility is of fundamental value in respect to assessing the well-posedness of the initial and boundary value problem<sup>29</sup> and, moreover, provides a reliable basis for the determination of boundary values in numerical solutions.<sup>30</sup> As we have discussed elsewhere in detail<sup>2,3</sup> the five balance equations constitute a hyperbolic system of partial differential equations; however, they are not totally hyperbolic in general. There always exist at least three real characteristics corresponding to the gas material and the gas acoustic waves. However, the two remaining characteristics are only real under certain circumstances.

Generally speaking, when the solid phase is packed and the rate of propagation of granular disturbances,  $a(\epsilon)$ , is not too small in comparison with the speed of sound in the gas, the remaining pair of characteristics are real and correspond to the solid phase acoustic waves. When the solid phase is dispersed and  $a(\epsilon) = 0$ , the remaining pair are real only for  $\langle u \rangle = \langle u_p \rangle$  unless the relative Mach number  $|\langle u \rangle - \langle u_p \rangle|/c$  exceeds unity.<sup>3</sup> Similar conclusions have been reached by Lyckowski et al.<sup>31</sup> The earliest classification of the equations known to us is contained in the 1965 paper by Kraiko and Sternin<sup>24</sup> which is, however, confined to dispersed flow. The results which we present here neglect the influence of the virtual mass effect; Ref. 3 may be consulted for the influence of this term.

Proceeding in the usual manner<sup>3</sup> one finds that the direction  $dx/dt = \langle u \rangle$  is always a real characteristic direction. The remaining characteristics are given by the roots of the following quartic equation:

$$\left\{ \left( \frac{dx}{dt} - \langle u \rangle \right)^2 - c^2 \right\} \left\{ \left( \frac{dx}{dt} - \langle u_p \rangle \right)^2 - a^2 \right\} = \frac{1-\epsilon}{\epsilon} c^2 \left\{ a^2 + \frac{\rho}{\rho_p} \left( \frac{dx}{dt} - \langle u \rangle \right)^2 \right\} \quad (48)$$

It is easy to show by a graphical analysis that if  $a=0$  and  $|\langle u \rangle - \langle u_p \rangle|/c < 1$ , then Eq. (48) has just two real roots unless  $\langle u \rangle = \langle u_p \rangle$ . Introduce

$$y = \frac{1}{c} \left( \frac{dx}{dt} - \langle u \rangle \right) \quad (49)$$

and recast Eq. (48) as

$$\{y^2 - 1\} \left\{ \left( y + \frac{\langle u \rangle - \langle u_p \rangle}{c} \right)^2 - \frac{a^2}{c^2} \right\} = \frac{1-\epsilon}{\epsilon} \left\{ \frac{a^2}{c^2} + \frac{\rho}{\rho_p} y^2 \right\} \quad (50)$$

Now set  $a=0$  in Eq. (50) and view the left- and right-hand sides as each being functions of  $y$ , namely a quartic and a quadratic, respectively. The right-hand side is clearly non-negative. The left-hand side has roots at  $\pm 1$ , a double root at  $y = (\langle u_p \rangle - \langle u \rangle)/c$  and is positive as  $y \rightarrow \pm \infty$ . Thus, the left-hand side is never positive in the interval  $[-1, +1]$  and, if  $|\langle u \rangle - \langle u_p \rangle|/c < 1$ , increases monotonically with  $\pm y$  outside this interval. Therefore, the two sides may be equal in  $[-1, +1]$  if and only if  $\langle u_p \rangle = \langle u \rangle$ , and there will be at most two intersections outside this interval unless  $|\langle u \rangle - \langle u_p \rangle|/c > 1$ . A numerical study of the domain of total hyperbolicity of Eq. (48) was performed by Gough.<sup>4</sup>

The fact that the equations are not totally hyperbolic makes it difficult to assert that the physically reasonable initial and boundary value data will constitute both necessary and sufficient conditions to determine a unique solution of the balance equations. For this reason, Gough<sup>2</sup> initially proposed

that the equations be made totally hyperbolic by taking  $a(\epsilon)$  sufficiently large, for all values of porosity. This may be accomplished by choosing  $\epsilon_* = 1$  and  $\kappa$  sufficiently small in Eq. (42). Moreover, if  $a(\epsilon) \neq 0$  except for  $\epsilon = 1$ , there is established a one-to-one correspondence between the porosity and the granular stress with the result that a free surface of the aggregate is characterized by the condition  $\epsilon = 1$  in order to satisfy  $R = 0$ . Therefore, internal boundaries characterized by gas/mixture interfaces may be represented as small regions through which the porosity varies rapidly, but continuously, thereby enabling an implicit numerical representation. This approach is in close analogy to that of von Neumann and Richtmyer<sup>32</sup> for the implicit representation of a shock as a region of rapidly varying properties rather than as a discontinuity. In practice, however, we found difficulties in establishing indifference of our results to the value of  $\kappa$ ; so that the physically spurious term was unduly influential.<sup>4</sup>

Therefore, in subsequent work,<sup>5</sup> we dealt directly with the ill-posed problem for which  $a(\epsilon) = 0$  when the bed is either dispersed or unloading. It is assumed that if we specify initial distributions of  $\langle p \rangle$ ,  $\langle \rho \rangle$ ,  $\langle u \rangle$ ,  $\langle u_p \rangle$ , and  $\epsilon$  for a region occupied by the dispersed or unloading mixture, so that  $a(\epsilon) = 0$  and the balance equations are not totally hyperbolic, then the boundary values of  $\langle u_p \rangle$  and  $\epsilon$  are determined by the balance equations and cannot be specified independently without overdetermining the solution. This assumption, which we state without proof, may be supported by considering the dispersed aggregate in isolation. We have the simple balance equations:

$$\frac{D\epsilon}{Dt_p} - (1-\epsilon) \frac{\partial}{\partial x} \langle u_p \rangle = 0 \quad (51)$$

$$\frac{D}{Dt} \langle u_p \rangle = 0 \quad (52)$$

A characteristic analysis shows that  $dx/dt = \langle u_p \rangle$  is the only real characteristic and that the corresponding condition of compatibility is, of course,  $\langle u_p \rangle = \text{constant}$ . However, the porosity is not constrained by a condition of compatibility. Still, it is clear that if the initial distribution of  $\langle u_p \rangle$  is known, then the values at any future time may be determined without recourse to additional data. Then, given  $\langle u_p \rangle$  and the initial distribution of  $\epsilon$ , the future values of porosity may likewise be determined. The specification of boundary data for  $\epsilon$  is unnecessary and, in fact, would represent an overdetermination of the solution.

### Methods of Solution

It has been claimed by Gidaspo<sup>33</sup> and by Lyckowski<sup>31</sup> that, since the balance equations are not totally hyperbolic, it is not possible, in general, to determine stable numerical solutions. Therefore, the equations should be modified in some fashion to make them well posed. We take the position, also asserted by Harlow,<sup>26</sup> that the potential for instability is, in fact, an important piece of physics which is embedded in the partial differential equations. Therefore, the lack of total hyperbolicity means that we must proceed cautiously; certainly any unstable feature of a numerical solution would have to be examined scrupulously before it could be declared to be of purely physical origin. In practice, however, this difficulty does not arise when one determines solutions of interior ballistic problems. We have performed completely stable calculations using the so-called "ill-posed" equations over a wide range of both conventional and unconventional interior ballistic configurations. Instabilities and numerical wiggles have, in our experience, been due to careless coding, improper attention to the treatment of external and internal boundaries, and, finally, to the use of the finite-difference approximation for distributions which vary rapidly over a distance comparable with the mesh spacing.

We now describe briefly two methods which we have used. The first method involves an implicit representation of the internal boundaries defined by the gas/mixture interface. The second involves an explicit representation. Full details may be found elsewhere.<sup>4,5</sup> An explicit finite-difference scheme is used in both cases. We should also note that other internal boundaries may arise in interior ballistic calculations. In particular when the mixture, packed or dispersed, impacts on an external boundary there will be created a condensation or granular compaction wave.<sup>5</sup> This wave is treated implicitly in both methods.

#### Implicit Representation of Internal Boundaries

This method treats only the external boundaries explicitly. The balance equations are integrated at the interior points using an explicit two-step method due to MacCormack<sup>34</sup> with an allowance for the nonhomogeneous terms. The boundary values of the state variables are deduced from the conditions of compatibility on those characteristics which intersect both the boundary and the line bearing the current state of the solution. The balance equations are always totally hyperbolic near the boundaries because a reversible granular stress law is used with a sufficiently small value of  $\kappa$ . Initially, the mixture is in contact with the forward boundary. As the boundary moves, separation may occur and is determined by the condition  $\epsilon = 1$  at the boundary. The resulting gas/mixture interface is therefore represented implicitly.

#### Explicit Representation of Internal Boundaries Defined by Gas/Mixture Interfaces

In this method we recognize explicitly the gas/mixture interface as an internal boundary. The state variables at interior mesh points are again updated by means of the MacCormack scheme with an additional modification. The convective terms in the solid phase balance equations are represented by upwind differences in both the predictor and the corrector step.<sup>5</sup> Boundary values on each side of the gas/mixture interface are determined by means of the available conditions of compatibility together with the jump conditions and the solid phase balance equations. The gas regions which may exist between pairs of mixture regions or between the mixture and the external boundaries are represented as continua when large and, when small, according to a lumped parameter formulation which avoids undue restriction of the time step due to the stability requirement.

This method is in no way dependent upon having a totally hyperbolic system of equations; the ill-posed problem is attacked directly. Therefore, the constitutive law for the granular stress is taken to be irreversible in general. Moreover, there is no restriction on the value of  $\kappa$ .

We refer the reader elsewhere for a discussion of the merits of each approach and a comparison of their respective solutions.<sup>35</sup> Likewise, comparisons of theory and experiment may be found in other sources.<sup>3,23,36</sup>

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