

# Theory of Two-Phase Detonation—Part I: Modeling

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A new, one-dimensional, two-phase model appropriate for describing the detonation of granulated solid propellants or explosives is presented. The model satisfies the principle that the mixture mass, momentum, and energy are conserved, is strictly hyperbolic, and is frame indifferent. Conditions are presented for satisfying the second law of thermodynamics. It is shown that this and previous models do not satisfy the second law under all circumstances. It is shown that in the limit of no chemical reaction or gas phase effects that inclusion of compaction work is in violation of the energy conservation principle. It is also shown that a complete two-phase particle combustion model with constitutive functions dependent on particle radius requires an equation specifying the variation of particle radius; such a relation can be given by a number evolution equation. The model equations are solved in a subsequent study which follows as a separate article.

## NOMENCLATURE

|          |   |
|----------|---|
| $a_i$    | interphase mass transfer                  |
| $A_{ij}$ | general matrix                            |
| $b$      | virial gas coefficient                    |
| $b_i$    | interphase momentum transfer              |
| $B$      | strictly positive drag function           |
| $B_{ij}$ | general matrix                            |
| $c_i$    | interphase energy transfer                |
| $c_v$    | specific heat at constant volume          |
| $C$      | strictly positive heat transfer function  |
| $C_i$    | general vector                            |
| $D$      | steady wave speed                         |
| $e$      | internal energy                           |
| $f$      | configurational stress                    |
| $F$      | number density forcing function           |
| $h$      | heat transfer constant                    |
| $i$      | subscript, $i = 1$ , gas; $i = 2$ , solid |
| ig       | ignition                                  |
| $l_i$    | eigenvector                               |
| $L$      | tube length                               |
| $m$      | burn exponent                             |
| $n$      | number density                            |
| $P$      | pressure                                  |
| $q$      | chemical energy                           |
| $r$      | particle radius                           |

|       |                |
|-------|----------------|
| $R$   | gas constant   |
| $s$   | entropy        |
| $t$   | time           |
| $u$   | velocity       |
| $u_j$ | general vector |
| $x$   | distance       |
| $X$   | distance       |

## Greek Symbols

|            |                                     |
|------------|-------------------------------------|
| $\alpha$   | burn constant                       |
| $\beta$    | drag constant                       |
| $\gamma$   | Gruneisen coefficient + 1           |
| $\Gamma$   | general variable                    |
| $\delta_a$ | momentum transfer switch (= 0, 1)   |
| $\delta_b$ | compaction work switch (= 0, 1)     |
| $\delta_c$ | number conservation switch (= 0, 1) |
| $\lambda$  | characteristic velocity             |
| $\mu_c$    | compaction viscosity                |
| $\xi$      | wave frame distance                 |
| $\rho$     | density                             |
| $\sigma$   | non-ideal solid parameter           |
| $\phi$     | volume fraction                     |
| $\psi$     | Helmholtz free energy               |
| $\omega$   | sound speed                         |

## INTRODUCTION

One-dimensional, two-phase continuum mixture models have been extensively used to model reactive gas dynamics in heterogeneous mixtures. Examples of the use of these models in combus-

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tion theory are found in the studies of Gough and Zwarts [1], Kuo and Summerfield [2], Butler et al. [3], Butler and Krier [4], Powers et al. [5], Drew [6], Akhatov and Vainshtein [7], Baer and Nunziato [8], and Baer et al. [9]. The models have been used to describe combustion wave dynamics in systems such as mixtures of granulated solid propellants and product gases in which it is possible to identify two components with distinct material properties. The work of Gough and Zwarts [1] and Kuo and Summerfield [2] is among the first to use two-phase models in reactive gas dynamics. The models were used to describe flame spreading and steady combustion in porous materials. These studies considered low-speed, low-pressure deflagration waves. Recently, Drew [6] has further studied low-speed, constant pressure combustion waves in two-phase materials. The study of Butler et al. [3] was the first reported in the archival open literature to exhibit a detonation wave in a two-phase material. Baer and Nunziato [8] have also used a two-phase model to describe a detonation in a two-phase reactive system. Using a similar model, Akhatov and Vainshtein [7] studied high-speed, high-pressure waves in two-phase materials. The results of Butler, et al. [3], Butler and Krier [4], Baer and Nunziato [8], Baer et al. [9], and Akhatov and Vainshtein [7] were obtained by numerical solution of time-dependent systems of two-phase reactive flow equations. Their models predict the transition from a low-pressure combustion to a high pressure regime associated with detonations.

A basic premise of two-phase mixture theory is that the mixture can be separated into discrete components. Each of these components behaves as a single material except when interacting with another component. In most two-phase models, the hypothesis of phase separation is employed [10]. This hypothesis holds that the internal state of one phase is not related to the internal state of another phase. In other words the thermodynamic state of a particular phase depends only on the properties of that phase. Mass, momentum, and energy equations resembling one-phase equations are written for each component. Each mass, momentum, and energy equation contains terms, not present in one-phase models, that are known as

phase interaction terms. These terms model the transfer of mass, momentum, and energy from one phase to another.

The particular form of the phase interaction terms is a source of much controversy. Mixture conservation principles and frame invariance provide restrictions on the functional forms of these terms but still allow for a wide variety of models. Beyond these rather loose restrictions, there are several, sometimes conflicting, rationales for choosing phase interaction terms. Because steady detonations have been observed in granular materials, the primary rationale for choosing phase interaction terms in this article is to pick them so that a two-phase model can predict a steady detonation. It is thus implicitly assumed that two-phase models are appropriate for describing detonations in granular materials.

Other secondary motivations for the form of phase interaction terms exist. The entropy inequality provides one such motivation. It is possible to determine an expression for the growth of mixture entropy. This expression suggests functional forms for the individual phase interaction terms such that the entropy inequality is always satisfied. This technique may be overly restrictive as the entropy inequality only requires that for the mixture, entropy must increase. Experiments that measure certain phase interactions can also be used as a justification for phase interaction models. Also examining the two-phase equations in the dilute limit can suggest how phase interaction terms must behave in this limit.

In choosing phase interaction terms it is difficult to simultaneously satisfy all the above criteria. As such certain compromises have been made in this article. Namely, the phase interaction terms chosen are not guaranteed under all circumstances to satisfy the entropy inequality. Also the functional form of these terms has not been shown to precisely match either experimental data or the dilute limit equations. This model, however, is intended to describe a two-phase detonation in a granular material far from the dilute limit. For solid explosives and propellants there are no experiments to measure phase interactions under detonation conditions, and for the bulk of the detonation process the dilute limit is not appropriate.

The goal of this article is to present a general two-phase model that satisfies the basic continuum mechanics principles and is appropriate for describing detonation and the transition from deflagration to detonation (DDT) in granulated propellants or explosives. This article examines how to construct a two-phase model that is consistent with these principles while remaining within the general framework provided by other two-phase models. This article does not address more basic issues such as the microstructural justification of these models. In presenting this model, some of the disparity among two-phase models is discussed.

The required principles are as follows. First it is required that, for the mixture, mass, momentum, and energy are conserved. The mass, momentum, and energy of the constituents are allowed to grow or decay as dictated by the forcing functions of the balance equations. When the constituent mass, momentum, and energy equations are added, the forcing functions must cancel to yield conservative mixture equations. Next, the model equations must be well-posed for the class of problems to be considered, which in this case is the initial value problem. A sufficient condition for the initial value problem to be well-posed is that the system of partial differential equations in two independent variables is strictly hyperbolic. To satisfy the second law of thermodynamics for a thermally isolated system, it is required that for any process, the entropy of the mixture remain constant or increase. It is also required that the model predicts an equilibrium condition for the material in the ambient state. Finally, it is required that the two-phase equations are invariant under a Galilean transformation.

The discussion here is mainly limited to the details of two models: the model of Baer and Nunziato (Eqs. 53–60 of Ref. 8, designated as the BN model) [8, 9] and the model of Powers, Stewart, and Krier (designated as the PSK model) [5]. To include a discussion of the many other two-phase models with the necessary detail is beyond the scope of this article. The BN and PSK models have been chosen for study because both are models for describing DDT in granulated solid propellants and thus share many assumptions. Also,

both are constructed explicitly to conform with the principles described above.

The model of this study is presented as a generalized model that incorporates most of the features of the BN and PSK models. The generalized model is examined to see how it conforms to the above-mentioned principles. In so doing, certain problems in both the BN and PSK model are identified. These problems include the issue of whether or not an evolutionary equation for particle number should be included, the failure of both the BN and PSK models to universally satisfy the entropy inequality, and the inability to satisfy energy conservation in the inert, all-solid limit when compaction work is included. Finally, for completeness and because many two-phase combustion models have been presented that have been shown not to be hyperbolic under all circumstances [12–14], a discussion of the characteristics of the two-phase equations is given.

## GENERAL TWO-PHASE MODEL

A two-phase model that is a generalization of the BN model and the PSK model is given. The governing equations in conservative form are given below:

$$\frac{\partial}{\partial t}(\rho_1\phi_1) + \frac{\partial}{\partial x}(\rho_1\phi_1u_1) = a_1, \quad (1)$$

$$\frac{\partial}{\partial t}(\rho_2\phi_2) + \frac{\partial}{\partial x}(\rho_2\phi_2u_2) = a_2, \quad (2)$$

$$\begin{aligned} &\frac{\partial}{\partial t}(\rho_1\phi_1u_1) + \frac{\partial}{\partial x}(\rho_1\phi_1u_1^2 + P_1\phi_1) \\ &= a_1u_2 + b_1 + \delta_a P_1 \frac{\partial\phi_1}{\partial x}, \end{aligned} \quad (3)$$

$$\begin{aligned} &\frac{\partial}{\partial t}(\rho_2\phi_2u_2) + \frac{\partial}{\partial x}(\rho_2\phi_2u_2^2 + P_2\phi_2) \\ &= a_2u_2 + b_2 - \delta_a P_1 \frac{\partial\phi_1}{\partial x}, \end{aligned} \quad (4)$$

$$\begin{aligned}
& \frac{\partial}{\partial t}(\rho_1 \phi_1 (e_1 + u_1^2/2)) \\
& + \frac{\partial}{\partial x}(\rho_1 \phi_1 u_1 (e_1 + u_1^2/2 + P_1/\rho_1)) \\
& = a_1(e_2 + u_2^2/2) + b_1 u_2 + c_1 + \delta_a P_1 u_2 \frac{\partial \phi_1}{\partial x} \\
& + \delta_b [(P_2 - f_2)(P_2 - f_2 - (P_1 - f_1))] \frac{\phi_1 \phi_2}{\mu_c}, \quad (5)
\end{aligned}$$

$$\begin{aligned}
& \frac{\partial}{\partial t}(\rho_2 \phi_2 (e_2 + u_2^2/2)) \\
& + \frac{\partial}{\partial x}(\rho_2 \phi_2 u_2 (e_2 + u_2^2/2 + P_2/\rho_2)) \\
& = a_2(e_2 + u_2^2/2) + b_2 u_2 + c_2 - \delta_a P_1 u_2 \frac{\partial \phi_1}{\partial x} \\
& - \delta_b (P_2 - f_2) [P_2 - f_2 - (P_1 - f_1)] \frac{\phi_1 \phi_2}{\mu_c}, \quad (6)
\end{aligned}$$

$$\begin{aligned}
& \frac{\partial \phi_2}{\partial t} + u_2 \frac{\partial \phi_2}{\partial x} \\
& = \frac{\phi_1 \phi_2}{\mu_c} [P_2 - f_2 - (P_1 - f_1)] + a_2/\rho_2, \quad (7)
\end{aligned}$$

$$\begin{aligned}
& (1 - \delta_c) \left[ \frac{\partial n}{\partial t} + \frac{\partial}{\partial x}(u_2 n) \right] \\
& = (1 - \delta_c) F(P_1, \rho_1, P_2, \rho_2, \phi_2), \quad (8)
\end{aligned}$$

$$n = \frac{3\phi_2}{4\pi r^3}, \quad (9)$$

$$\phi_1 + \phi_2 = 1, \quad (10)$$

$$e_1 = e_1(P_1, \rho_1, \phi_1), \quad (11)$$

$$e_2 = e_2(P_2, \rho_2, \phi_2), \quad (12)$$

$$P_1 = P_1(\rho_1, T_1, \phi_1), \quad (13)$$

$$P_2 = P_2(\rho_2, T_2, \phi_2). \quad (14)$$

In these equations, the subscripts “1” and “2” denote the gas and solid phase, respectively. The variable  $\rho$  represents the material density, that is, the mass of an individual phase divided by the volume occupied by that phase. The variable  $\phi$  represents the volume fraction of each phase, that is, the volume of an individual phase divided by the total volume. Velocities are denoted by the variable  $u$ , pressure by  $P$ , internal energy by  $e$ , temperature by  $T$ , number density by  $n$ , and particle radius by  $r$ . In Eqs. 1–8, some generality has been sacrificed so that differences in the BN and PSK model are highlighted. In these equations the variable  $\delta$  is used to describe either the BN formulation ( $\delta_a = \delta_b = \delta_c = 1$ ) or the PSK formulation ( $\delta_a = \delta_b = \delta_c = 0$ ). For  $\delta_a = 1$ , an additional term proportional to the product of gas pressure and volume fraction gradient is included as a phase interaction term in the momentum and energy equations. For  $\delta_b = 1$  a work term, known as compaction work, is included as an energy phase interaction. The compaction work term is constructed such that it is equal to the term

$$\delta_b (P_2 - f_2) \left( \frac{\partial \phi_2}{\partial t} + u_2 \frac{\partial \phi_2}{\partial x} - a_2/\rho_2 \right). \quad (15)$$

For  $\delta_c = 0$  a number evolution relation is enforced; for  $\delta_c = 1$  such a relation is not enforced. The term  $f$  represents the configurational stress as used by Baer and Nunziato. As defined in Ref. 8, the configurational stress is

$$f_i = \rho_i \phi_i \frac{\partial \psi_i}{\partial \phi_i}, \quad (16)$$

where the Helmholtz free energy of phase  $i$ ,  $\psi_i$ , is defined as

$$\psi_i = e_i - T_i s_i. \quad (17)$$

In Eq. 17  $s_i$  is defined as the entropy of phase  $i$ .

Here an inconsistency in Ref. 8 is noted. In developing the entropy inequality in Ref. 8, the definition in Eq. 16 is used; however, in practice,

in Ref. 8, and most other two-phase studies, the Helmholtz free energy is not a function of volume fraction, rendering the configurational stress to be zero. In practice, in Ref. 8 and other studies the configurational stress is estimated from experimental data and not required to satisfy the definition given by Eq. 16. These experiments suggest that the configurational stress  $f_2$  is a function of solid volume fraction  $\phi_2$  only. The functional form of  $f_2$  is determined experimentally by measuring the equilibrium stress required to compress a granular material to a specified volume fraction. It is found that the equilibrium stress  $f_2$  increases as a function of solid volume fraction  $\phi_2$ .

The definition of compaction viscosity  $\mu_c$  of the BN model is adopted here. Compaction viscosity is a constant that determines the relaxation time to the equilibrium solid stress and volume fraction in a granular material compaction process. The terms  $a_i$ ,  $b_i$ , and  $c_i$  are constitutive functions representing the interphase mass, momentum, and energy transport, respectively. The combustion model is contained in the term  $a_i$ , which specifies the rate of mass transfer per unit time per unit volume. It is assumed that  $a_i$ ,  $b_i$ , and  $c_i$  can be functions of all of the flow variables.

Equations 1 and 2 are the gas and solid mass equations, respectively, Eqs. 3 and 4 the gas and solid momentum equations, and Eqs. 5 and 6 the gas and solid energy equations. Equation 7 is the dynamic compaction equation. The use of such an equation is not standard. Passman et al. [15] argue that this equation allows volume fractions to change without affecting the bulk motion of the mixture and thus is able to model microstructural details in some way. For this model it is assumed that the particles are spherical. This assumption is probably not valid under all circumstances, especially when local deformation due to solid compaction is considered. Equation 8 is the number evolution equation and Eq. 9 is a definition of number density for spherical particles. Equation 8 allows for the total number of particles to change in response to the general forcing function  $F$ . For  $F < 0$ , particle agglomeration is predicted, and for  $F > 0$  particle breakup is predicted. For  $F = 0$ , the number of particles is conserved.

It is assumed that the mixture is saturated, that

is, all the volume is occupied by either gas or solid. This is stated in Eq. 10. Equations 11–14 are generalized caloric and thermal state equations for the gas and solid phase. In Eqs. 11–14 it is assumed that the pressure and internal energy of each constituent can be expressed as functions of that constituent's density, temperature, and volume fraction. These state equations are written as functions of volume fraction for generality in accordance with the assumptions of the BN model. In invoking specific constitutive theory, the volume fraction dependence is removed.

By applying the Galilean transformation  $\xi = x - Dt$ ,  $v_i = u_i - D$  to Eqs. 1–8 where  $D$  is a constant velocity, it can easily be shown that the equations are frame indifferent. This holds whether the BN or PSK formulations are adopted.

In examining Eqs. 1–6, it is noted that the mass, momentum, and energy of each constituent are not conserved but change in response to the forcing functions  $a_i$ ,  $b_i$ , and  $c_i$ . It is required, however, for the mixture that mass, momentum, and energy be conserved. To ensure that this holds, Truesdell's axioms of balance for mixtures [16] require that

$$a_1 + a_2 = 0, \quad b_1 + b_2 = 0, \quad c_1 + c_2 = 0. \quad (18)$$

With the adoption of Eq. 18, the following conservative mixture mass, momentum, and energy equations are obtained when Eqs. 1 and 2, 3 and 4, and 5 and 6 are added, respectively:

$$\frac{\partial}{\partial t}(\rho_1\phi_1 + \rho_2\phi_2) + \frac{\partial}{\partial x}(\rho_1\phi_1u_1 + \rho_2\phi_2u_2) = 0, \quad (19)$$

$$\begin{aligned} \frac{\partial}{\partial t}(\rho_1\phi_1u_1 + \rho_2\phi_2u_2) + \frac{\partial}{\partial x}(\rho_1\phi_1u_1^2 \\ + \rho_2\phi_2u_2^2 + P_1\phi_1 + P_2\phi_2) = 0, \end{aligned} \quad (20)$$

$$\begin{aligned} \frac{\partial}{\partial t}(\rho_1\phi_1(e_1 + u_1^2/2) + \rho_2\phi_2(e_2 + u_2^2/2)) \\ + \frac{\partial}{\partial x}(\rho_1\phi_1u_1(e_1 + u_1^2/2 + P_1/\rho_1) \\ + \rho_2\phi_2u_2(e_2 + u_2^2/2 + P_2/\rho_2)) = 0. \end{aligned} \quad (21)$$

Equations 19–21 predict that for an isolated system composed of a two-phase mixture the total mass, momentum, and energy of that system remains constant regardless of the processes that occur within the system boundaries. Though the constituent momentum and energy equations of the BN and PSK models differ, both models predict identical mixture equations.

Equations 3–6 can also be rewritten in non-conservative form, as is common practice in the two-phase literature. The following definition is adopted for the material derivative of the general variable  $\Gamma$ :

$$\Gamma'_i = \frac{\partial \Gamma_i}{\partial t} + u_i \frac{\partial \Gamma_i}{\partial x}. \tag{22}$$

The momentum and energy equations in nonconservative form are

$$\begin{aligned} \rho_1 \phi_1 u'_1 + \frac{\partial}{\partial x}(P_1 \phi_1) \\ = a_1(u_2 - u_1) + b_1 + \delta_a P_1 \frac{\partial \phi_1}{\partial x}, \end{aligned} \tag{23}$$

$$\rho_2 \phi_2 u'_2 + \frac{\partial}{\partial x}(P_2 \phi_2) = -b_1 - \delta_a P_1 \frac{\partial \phi_1}{\partial x}, \tag{24}$$

$$\begin{aligned} \rho_1 \phi_1 e'_1 + P_1 \phi_1 \frac{\partial u_1}{\partial x} \\ = \delta_a P_1 (u_2 - u_1) \frac{\partial \phi_1}{\partial x} \\ + a_1(e_2 - e_1 + (u_2 - u_1)^2/2) \\ + b_1(u_2 - u_1) + c_1 \\ + \delta_b (P_2 - f_2)[P_2 - f_2 - (P_1 - f_1)] \frac{\phi_1 \phi_2}{\mu_c}, \end{aligned} \tag{25}$$

$$\begin{aligned} \rho_2 \phi_2 e'_2 + P_2 \phi_2 \frac{\partial u_2}{\partial x} \\ = -c_1 - \delta_b (P_2 - f_2) \\ \times [P_2 - f_2 - (P_1 - f_1)] \frac{\phi_1 \phi_2}{\mu_c}. \end{aligned} \tag{26}$$

Equations 1–14 with  $\delta_a = \delta_b = \delta_c = 1$  are now compared to the BN model equations (Eqs. 53–60 of Ref. 8). A few minor differences exist. First, in the momentum equations (Eqs. 3 and 4), the term  $a_i u_2$  ( $i = 1, 2$ ) is included to account for momentum introduced by chemical reaction. This form assumes that as particles burn, the gas phase gains momentum at a rate equal to the product of the mass burning rate and the particle velocity. However in Refs. 8 and 9, it can be deduced that the rate of momentum change attributable to chemical reaction is assumed to be equal to the product of the particle mass burn rate and the average velocity  $[a_i(u_1 + u_2)/2]$ . Likewise in the energy equations (Eqs. 5 and 6) the rate of kinetic energy exchanged due to chemical reaction is taken to be  $a_1 u_2^2/2$ , proportional to the particle kinetic energy, whereas it can be deduced that a different term,  $a_1 u_1 u_2/2$ , is used in Refs. 8 and 9. For the one-step irreversible reaction of particles reacting to form gas, the formulation of Eqs. 3–6 is adopted because as the particles react, all their momentum and kinetic energy, determined by the particle velocity, is transferred to the gas phase. Which formulation should be adopted is to a certain degree arbitrary, as neither violates the frame indifference principle or, as will be seen, is suggested by the entropy inequality. The remaining differences are trivial. The BN model of Refs. 8 and 9 includes conductive heat transfer, which is not modeled in Eqs. 1–6. It is assumed that the time scales for conductive heat transfer to be important are much larger than the time scales of chemical reaction. Finally it is noted that the functions  $a_i$ ,  $b_i$ , and  $c_i$  are able to accommodate the more specific form of interphase transport terms given in Refs. 8 and 9.

## SECOND LAW OF THERMODYNAMICS

The second law of thermodynamics requires that the total entropy of a mixture thermally isolated from its surroundings remains constant or increases for any thermodynamic process within the volume occupied by the mixture. Accordingly, following Truesdell [16] and Baer and Nunziato [8], the second law of thermodynamics for a two-phase

mixture with no conductive or radiative heat exchange with its surroundings is as follows

$$\frac{\partial}{\partial t}(\rho_1\phi_1s_1 + \rho_2\phi_2s_2) + \frac{\partial}{\partial x}(\rho_1\phi_1u_1s_1 + \rho_2\phi_2u_2s_2) \geq 0. \quad (27)$$

To determine if the two phase model satisfies the entropy inequality (Eq. 27) requires a definition of entropy. In one-phase flows this can be accomplished by using the Gibbs equation  $T ds = de - P/\rho^2 d\rho$  to eliminate energy in favor of energy. An equivalent Gibbs equation for a component of a mixture is adopted identical to that of Ref. 8:

$$T_i ds_i = de_i - \frac{P_i}{\rho_i^2} d\rho_i - \frac{f_i}{\rho_i\phi_i} d\phi_i. \quad (28)$$

In writing Eq. 28, the definitions of configurational pressure (Eq. 16) and Helmholtz free energy (Eq. 17) are also adopted. With this two-phase Gibbs relation, the entropy change of a phase is a function of the change in volume fraction in addition to changes in internal energy and density. With this assumed form of the Gibbs relation, the energy equation can be rewritten in terms of entropy to evaluate the entropy inequality. However, as used in practice by Baer and Nunziato in Ref. 8 and by most other two-phase modelers, the thermodynamic state equations for each phase are independent of volume fraction, rendering the term  $f_i$  to be zero. In practice, as stated in Ref. 8 the gas phase configuration pressure is taken to be zero and the solid phase configuration pressure is estimated from experiment and not required to satisfy the definition  $f_i = \rho_i\phi_i \partial\psi_i/\partial\phi_i$ . This results in two entropy inequalities, one that employs the definition of  $f$  and assumes the state is a function of volume fraction and another that assumes that the state is not a function of volume fraction and that the configurational stress can be determined from experiment. In the following section the entropy inequality will be developed using both Eq. 28 and the Gibbs relation for the models as they are actually used. It will be seen that regardless of which Gibbs relation is used both PSK and BN models cannot absolutely guarantee the entropy inequality is satisfied.

In determining the entropy inequality, several restrictive sufficient conditions are developed, which, if satisfied, guarantee that the second law is satisfied. It should not be regarded that these conditions must always hold, but rather the more fundamental requirement is that the entropy inequality (Eq. 27) always hold. Thus if one of the sufficient conditions is not met in a particular calculation, the second law is not necessarily violated as long as other processes exist that are able to counteract the process which predicts an entropy decrease.

By using the two-phase Gibbs relation (Eq. 28) to eliminate the energy  $e_i$ , the energy equations (Eqs. 25 and 26) can be written as follows:

$$\begin{aligned} & \frac{\partial}{\partial t}(\rho_1\phi_1s_1) + \frac{\partial}{\partial x}(\rho_1\phi_1u_1s_1) \\ &= \frac{a_1}{T_1} \left( e_2 - e_1 + \frac{1}{2}(u_2 - u_1)^2 - \frac{P_1}{\rho_1} \right. \\ & \quad \left. + \frac{P_1 - f_1}{\rho_2} + T_1s_1 \right) + \frac{b_1}{T_1}(u_2 - u_1) \\ & \quad + \frac{c_1}{T_1} + \frac{u_2 - u_1}{T_1} \frac{\partial\phi_1}{\partial x} [\delta_a P_1 - (P_1 - f_1)] \\ & \quad + \frac{[P_2 - f_2 - (P_1 - f_1)] \phi_1\phi_2}{T_1 \mu_c} \\ & \quad \times [\delta_b(P_2 - f_2) - (P_1 - f_1)], \quad (29) \end{aligned}$$

$$\begin{aligned} & \frac{\partial}{\partial t}(\rho_2\phi_2s_2) + \frac{\partial}{\partial x}(\rho_2\phi_2u_2s_2) \\ &= \frac{a_1}{T_2} \left( \frac{f_2}{\rho_2} - T_2s_2 \right) - \frac{c_1}{T_2} \\ & \quad + \frac{(1 - \delta_b)}{T_2} [(P_2 - f_2)(P_2 - f_2 \\ & \quad - (P_1 - f_1))] \frac{\phi_1\phi_2}{\mu_c}. \quad (30) \end{aligned}$$

By adding the energy equations (Eqs. 29 and 30) and using the definition of Helmholtz free energy to eliminate internal energy, an expression can be

determined for the growth of total entropy:

$$\begin{aligned}
 & \frac{\partial}{\partial t} (\rho_1 \phi_1 s_1 + \rho_2 \phi_2 s_2) \\
 & + \frac{\partial}{\partial x} (\rho_1 \phi_1 u_1 s_1 + \rho_2 \phi_2 u_2 s_2) \\
 = & \frac{a_1}{T_1} \left( \psi_2 - \psi_1 + s_2(T_2 - T_1) + \frac{1}{2}(u_2 - u_1)^2 \right. \\
 & + P_1(1/\rho_2 - 1/\rho_1) + \left. \left( \frac{T_1}{T_2} f_2 - f_1 \right) \frac{1}{\rho_2} \right) \quad \text{mass transfer} \\
 & + \frac{b_1}{T_1} (u_2 - u_1) \quad \text{momentum transfer} \\
 & + c_1 \left( \frac{1}{T_1} - \frac{1}{T_2} \right) \quad \text{energy transfer} \\
 & + \frac{u_2 - u_1}{T_1} (\delta_a P_1 - (P_1 - f_1)) \frac{\partial \phi_1}{\partial x} \\
 & + \frac{(1 - \delta_b)}{T_2} (P_2 - f_2) \\
 & \times (P_2 - f_2 - (P_1 - f_1)) \frac{\phi_1 \phi_2}{\mu_c} \\
 & + \frac{P_2 - f_2 - (P_1 - f_1)}{T_1} \frac{\phi_1 \phi_2}{\mu_c} \\
 & \times (\delta_b (P_2 - f_2) - (P_1 - f_1)). \quad \text{compaction}
 \end{aligned} \tag{31}$$

In the Eq. 31, the contribution of each thermodynamic process, mass transfer, momentum transfer, energy transfer, and compaction, to the mixture entropy change has been isolated and labeled. A sufficient but not necessary condition for satisfying the second law is to require that each individual thermodynamic process yields an increase in the mixture entropy. In other words the sufficient condition is that each term on the right side of Eq. 31, representing mass transfer, momentum trans-

fer, energy transfer, and compaction, be strictly positive.

For the irreversible mass transfer process of solid to gas ( $a_1 > 0$ ), a positive contribution to the entropy change is predicted if the following inequality is satisfied:

$$\begin{aligned}
 & \psi_2 - \psi_1 + s_2(T_2 - T_1) + \frac{1}{2}(u_2 - u_1)^2 \\
 & + P_1(1/\rho_2 - 1/\rho_1) \\
 & + \left( \frac{T_1}{T_2} f_2 - f_1 \right) \frac{1}{\rho_2} \geq 0.
 \end{aligned} \tag{32}$$

Because  $(u_2 - u_1)^2/2$  is strictly positive it is sufficient to require that

$$\begin{aligned}
 & \psi_2 - \psi_1 + s_2(T_2 - T_1) + P_1(1/\rho_2 - 1/\rho_1) \\
 & + \left( \frac{T_1}{T_2} f_2 - f_1 \right) \frac{1}{\rho_2} \geq 0.
 \end{aligned} \tag{33}$$

In contrast to this model, Baer and Nunziato do not assume that  $a_1$  is strictly positive. Instead they postulate a form for the mass transfer term  $a_1$  that is designed to guarantee a positive contribution to the entropy change for the mass transfer process. Here a strictly positive form for  $a_1$  is chosen. This form can be calibrated at low pressure by experiments. In so doing a sacrifice is made because the sufficient condition (33) could potentially be violated in an arbitrary process. If the solid Helmholtz free energy is sufficiently larger than the gas energy, which is generally the case for an exothermic reaction, the condition can be met. If, however, the condition is not met, the more fundamental inequality (Eq. 27) can still be checked to determine if the second law is satisfied. To calculate if the entropy inequality (Eq. 27) holds at any given point and time, one checks if at that point and time the right-hand side of Eq. 31 is greater than or equal to zero.

For momentum transfer if it is assumed that  $b_1$  is of the form

$$b_1 = B(u_2 - u_1), \tag{34}$$

where  $B$  is a strictly positive function of the flow variables, then the contribution of the momentum



transfer terms to the entropy change is also strictly positive and is given by the expression

$$B(u_2 - u_1)^2. \quad (35)$$

Equation 34 has the form of a drag law. It states that the momentum transfer is proportional to the velocity difference between phases. Equation 34 holds that the momentum of the gas phase increases and solid phase decreases if the velocity of the solid is greater than that of the gas.

For energy transfer, if it is assumed that  $c_1$  is of the form

$$c_1 = C(T_2 - T_1), \quad (36)$$

where  $C$  is a strictly positive function of the flow variables, then the entropy change due to energy transfer is assured to be strictly positive and is given by the expression

$$C \frac{(T_2 - T_1)^2}{T_1 T_2}. \quad (37)$$

Equation 36 holds that the energy of the gas phase increases and solid phase decreases when the temperature of the solid is higher than that of the gas.

For a compaction process a positive contribution to the entropy change is predicted if the following inequality holds:

$$\begin{aligned} & \frac{u_2 - u_1}{T_1} (\delta_a P_1 - (P_1 - f_1)) \frac{\partial \phi_1}{\partial x} \\ & + \frac{(1 - \delta_b)}{T_2} (P_2 - f_2) \\ & \times (P_2 - f_2 - (P_1 - f_1)) \frac{\phi_1 \phi_2}{\mu_c} \\ & + \frac{P_2 - f_2 - (P_1 - f_1)}{T_1} \frac{\phi_1 \phi_2}{\mu_c} \\ & \times (\delta_b (P_2 - f_2) - (P_1 - f_1)) \geq 0. \quad (38) \end{aligned}$$

For both models the entropy change is dependent on the gradient of gas phase volume fraction. It is possible to construct a situation in which the gas volume fraction gradient has an arbitrarily large

value so that this inequality is not satisfied for either model formulation. Thus in order to ensure the second law is satisfied, one must restrict the magnitude of this derivative. It is noted that when the BN formulation is adopted with  $f_1 = 0$ , the term on the left-hand side of Eq. 38 is a perfect square and guaranteed to be positive. In this case the contribution of compaction processes to the entropy increase is guaranteed to be positive. Again if Eq. 38 is not satisfied for a particular process, the more fundamental inequality (Eq. 27) should be examined.

When the entropy inequality for the BN and PSK models are examined as those models are used in practice, a different entropy inequality is obtained. In practice, the state is independent of the volume fraction; thus  $\partial \psi_i / \partial \phi_i = 0$ , and a Gibbs equation analogous to the Gibbs equation from classical thermodynamics is used:

$$T_i ds_i = de_i - \frac{P_i}{\rho_i^2} d\rho_i. \quad (39)$$

In practice it is assumed that the definition of  $f_i$  (Eq. 15) does not apply and  $f$  is estimated from experiment. In practice it is assumed that  $f_1 = 0$  and that  $f_2$  is a known function of volume fraction. With these modifications the mixture energy equation in terms of entropy is slightly modified so that the change in entropy predicted by the model is

$$\begin{aligned} & \frac{\partial}{\partial t} (\rho_1 \phi_1 s_1 + \rho_2 \phi_2 s_2) \\ & + \frac{\partial}{\partial x} (\rho_1 \phi_1 u_1 s_1 + \rho_2 \phi_2 u_2 s_2) \\ & = \frac{a_1}{T_1} \left( \psi_2 - \psi_1 + s_2 (T_2 - T_1) \right. \\ & \left. + \frac{1}{2} (u_2 - u_1)^2 + P_1 (1/\rho_2 - 1/\rho_1) \right) \end{aligned}$$

mass transfer

$$+ \frac{b_1}{T_1} (u_2 - u_1) \quad \text{momentum transfer}$$

$$\begin{aligned}
 &+c_1 \left( \frac{1}{T_1} - \frac{1}{T_2} \right) \quad \text{energy transfer} \\
 &+ \frac{\phi_1 \phi_2 (P_2 - f_2 - P_1)}{\mu_c T_1 T_2} \\
 &\times \{ [(1 - \delta_b)P_2 + \delta_b f_2]T_1 \\
 &+ (\delta_b(P_2 - f_2) - P_1)T_2 \} \\
 &+ \frac{P_1}{T_1} (\delta_a - 1)(u_2 - u_1) \frac{\partial \phi_1}{\partial x}. \quad \text{compaction}
 \end{aligned}
 \tag{40}$$

As for Eq. 31 a sufficient condition for satisfying the entropy inequality (Eq. 27) is to require each term in the right-hand side of Eq. 40 to be positive. These conditions are quite similar to those yielded by Eq. 31. The conditions on the momentum transfer and energy transfer terms are identical. Slightly different expressions are obtained for the mass transfer and compaction conditions. As with Eq. 38, the entropy change predicted by a compaction process from Eq. 40 can be negative for both formulations.

**COMPACTION WORK**

In this section an argument is presented for not including the compaction work term of the BN model (present when  $\delta_b = 1$ ). It is shown that when  $\delta_b = 1$  for an inert material when gas phase effects are negligible that the compaction work term leads to a violation of the mixture energy conservation principle. Material compaction is predicted by the compaction equation (Eq. 7). For the limit of an inert solid ( $a_i = 0$ ) and negligible gas phase effects, this equation predicts that the volume fraction of solid changes if the instantaneous stress  $P_2$  differs from its equilibrium value  $f_2$ , where  $f_2$  is an experimentally determined function of equilibrium solid volume fraction  $\phi_2$ . The compaction equation predicts that the material is driven to a volume fraction where the instantaneous stress equals the equilibrium stress. To model hypothesized hot spot formation [17], the BN energy equations have been constructed

such that there is an exchange of energy between the solid and gas whenever material compaction is predicted. This energy exchange due to the compaction process is called compaction work. When gas phase effects are included, there is no violation of the mixture energy conservation principle.

When gas phase effects are neglected, however, energy conservation is violated because the model still predicts an energy loss due to compaction work. With no gas phase to absorb the energy of compaction work, the energy of compaction work necessarily leaves the system. This can be seen by examining Baer's form of the solid energy equation [11] when gas phase effects are negligible and for no chemical reaction. It is argued in Ref. 11 that in this limit drag and heat transfer effects can be ignored; this is essentially the limit where there is no gas present in the voids, and thus there can be no momentum or energy transfer to the voids. The unsteady form of the energy equation in this limit is

$$\begin{aligned}
 &\frac{\partial}{\partial t} (\rho_2 \phi_2 (e_2 + u_2^2/2)) \\
 &+ \frac{\partial}{\partial x} (\rho_2 \phi_2 u_2 (e_2 + u_2^2/2 + P_2/\rho_2)) \\
 &= -\delta_b (P_2 - f_2)^2 \frac{\phi_1 \phi_2}{\mu_c}.
 \end{aligned}
 \tag{41}$$

By considering the following problem, sketched in Fig. 1, it is clear that compaction work leads to violation of energy conservation in this limit. Consider a tube of length  $L$  closed at both ends filled with a granular material. The voids contain no gas mass. If one drives a piston into the granular material and then brings it to rest, the static equilibrium will be disturbed so that  $P_2 - f_2 \neq 0$ . In other words the tube is in an initial state where the instantaneous pressure  $P_2$  has not yet relaxed to its equilibrium value  $f_2$ . Both ends of the tube are stationary; consequently, a boundary condition for this problem is that  $u_2 = 0$  at  $x = 0$  and  $x = L$ . If the energy equation (Eq. 41) is integrated in space from  $x = 0$  to  $x = L$ , an expression can be written for the time rate of change of total energy (internal plus kinetic) contained in the tube. The spatially integrated energy equation

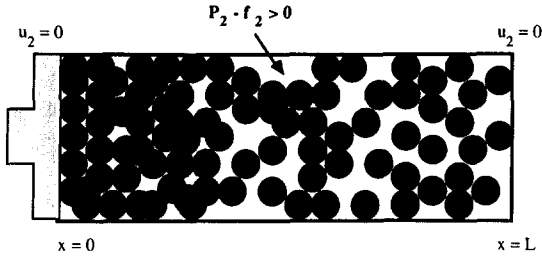


Fig. 1. Sketch of compaction problem.

is

$$\begin{aligned} \frac{\partial}{\partial t} \int_0^L \rho_2 \phi_2 (e_2 + u_2^2/2) dx \\ = -\delta_b \int_0^L (P_2 - f_2)^2 \frac{\phi_1 \phi_2}{\mu_c} dx. \end{aligned} \quad (42)$$

This equation shows that the time rate of change of total energy in the tube is zero if there is no compaction work ( $\delta_b = 0$ ) and negative if compaction work is included ( $\delta_b = 1$ ). By integrating Eq. 42 with respect to time, one would conclude that for no compaction work, the energy in the tube remains constant and when compaction work is included, the energy in the tube decreases. Thus in the limits considered, inclusion of compaction work violates the principle of energy conservation. This analysis suggests that an alternative to compaction work to describe hot spots should be considered.

## CONSTITUTIVE RELATIONS

A set of specific constitutive relations is introduced to model the combustion of granular explosives or propellants. As discussed in the introduction, these relations are to a certain extent arbitrary. Their choice is motivated with varying degrees by a desire to predict a steady detonation structure, satisfy the entropy inequality, maintain some consistency with other models, match some limited experimental data, and, insofar as possible, retain a simple algebraic form. These constitutive relations are also used in Refs. 5 and 18. The constitutive relations are

$$a_1 = \left(\frac{3}{r}\right) \rho_2 \phi_2 \alpha P_1^m H(T_2 - T_{ig}), \quad (43)$$

$$B = \beta \frac{\phi_1 \phi_2}{r}, \quad (44)$$

$$C = h \frac{\phi_1 \phi_2}{r^{1/3}}, \quad (45)$$

$$f_1 = 0, \quad (46)$$

$$f_2 = \frac{P_{20} - P_{10}}{\phi_{20}} \phi_2, \quad (47)$$

$$e_1 = c_{v1} T_1, \quad (48)$$

$$e_2 = c_{v2} T_2 + \frac{\rho_{20} \sigma}{\gamma_2 \rho_2} + q, \quad (49)$$

$$P_1 = \rho_1 R T_1 (1 + b \rho_1), \quad (50)$$

$$P_2 = (\gamma_2 - 1) c_{v2} \rho_2 T_2 - \frac{\rho_{20} \sigma}{\gamma_2}, \quad (51)$$

$$\omega_1^2 = R T_1 [1 + 2b \rho_1 + (R/c_{v1})(1 + b \rho_1)^2], \quad (52)$$

$$\omega_2^2 = \gamma_2 (\gamma_2 - 1) c_{v2} T_2, \quad (53)$$

$$\begin{aligned} s_1 = c_{v1} \ln \left( \frac{T_1}{T_{10}} \right) - R \ln \left( \frac{\rho_1}{\rho_{10}} \right) \\ - R b (\rho_1 - \rho_{10}) + s_{10}. \end{aligned} \quad (54)$$

$$\begin{aligned} s_2 = c_{v2} \ln \left( \frac{T_2}{T_{20}} \right) - (\gamma_2 - 1) c_{v2} \ln \left( \frac{\rho_2}{\rho_{20}} \right) + s_{20}, \\ (55) \end{aligned}$$

$$F = 0. \quad (56)$$

Equation 43 is the combustion model. It assumes that the mass transfer rate to the gas phase is a function of the particle radius, solid volume fraction, solid density, and gas phase pressure. The unit step function  $H(T_2 - T_{ig})$  is included in the combustion model to prevent combustion from being predicted until an ignition temperature  $T_{ig}$  is reached. The function  $a_1$  is strictly positive for  $r, \rho_2, \phi_2, \alpha, P_1 > 0$ , and thus an irreversible reaction of solid to gas is modeled. This combustion model has been constructed such that empir-

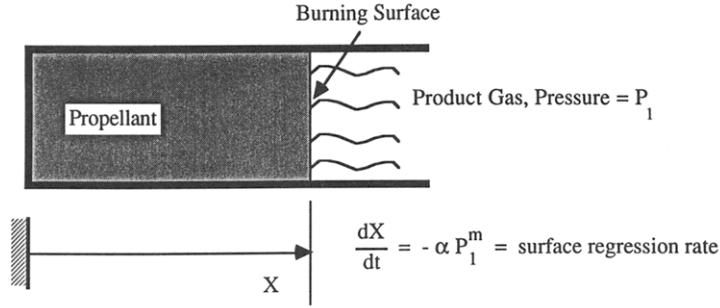


Fig. 2. Sketch of strand burning experiment used to determine combustion rate.

ical data that describe the rate of burning of a strand of propellant can be used to fix the coefficients  $\alpha$  and  $m$ . It is found from experiment that when a linear strand of propellant is burned, the rate of regression of the strand is proportional to the gas pressure raised to some power. That is,  $dX/dt = -\alpha P_1^m$ , where  $X$  is defined as the position of the burning surface. A sketch of such an experiment is shown in Fig. 2.

Here it is assumed this experimental burning relation can be adopted to describe the combustion of compressible propellant spheres. With  $a_1$  of Eq. 43 substituted into Eq. 2 and with use of the number equation (Eq. 8) (with number conservation implied by Eq. 56) and number density definition (Eq. 9) to eliminate the derivative of volume fraction from Eq. 2, an expression can be derived for the variation of particle radius:

$$\frac{\partial r}{\partial t} + u_2 \frac{\partial r}{\partial x} = -\alpha P_1^m H(T_2 - T_{ig}) - \frac{r}{3\rho_2} \left( \frac{\partial \rho_2}{\partial t} + u_2 \frac{\partial \rho_2}{\partial x} \right). \quad (57)$$

The model predicts that the particle radius can change in response to either combustion or density changes. As seen from Eq. 57 the experimental result  $dX/dt = -\alpha P_1^m$  is incorporated in the combustion model. However, Eq. 57 has more generality, as it also accounts for compressibility and convective effects. This has not been emphasized in many studies. If number is to be conserved and a compressible solid is assumed, then the model must necessarily predict that the particle radius changes in response to a change in particle density.

Because the BN model does not include an equation for variation of particle radius or number evolution, it has no counterpart to Eq. 57; thus, one is unable to determine how the radius varies as combustion or density changes occur. The combustion model of Butler and Krier [4] does include a relation for change in particle radius, which as implemented in the numerical model is given by the relation  $\partial r/\partial t = -\alpha P_1^m H(T_2 - T_{ig})$ . This equation is inconsistent with Eq. 57. It can thus be concluded that the number of particles is not conserved in the model of Ref. 4; that is, particles are allowed to split or coalesce without an apparent rationale for such an action.

The drag function  $B$  and heat transfer function  $C$  have been defined as functions of volume fraction and particle radius. The positive constants  $\beta$  and  $h$  have been introduced. These functions are somewhat arbitrary but when appropriate values for  $\beta$  and  $h$  are chosen can be shown to roughly correlate to particle gas drag and heat transfer data [18]. The configurational stress  $f_2$  is taken in Eq. 47 to be a linear function of solid volume fraction. The function  $f_2$  is constructed such that in the absence of combustion ( $a_i = 0$ ), no volume fraction change is predicted in the ambient state. This function is chosen for its simplicity and because it follows the same trend as experiments, that is, the equilibrium pressure is found to increase as the granular material is pressed to higher solid volume fraction. In the BN model a curve fit of the actual data is used.

For the gas, a virial state relation has been chosen; a caloric state equation, thermal state equation, sound speed definition, and entropy definition are given in Eqs. 48, 50, 52, and 54, respectively.

It is assumed that the specific heat at constant volume  $c_{v1}$  is a constant. The variables  $\omega$ ,  $R$ , and  $b$  are the sound speed, gas constant, and virial coefficient, respectively. For the solid, a Tait equation of state has been chosen; a caloric state equation, thermal state equation, sound speed definition, and entropy definition are given in Eqs. 49, 51, 53, and 55, respectively. The specific heat at constant volume  $c_{v2}$  is assumed to be a constant. The constant  $\gamma_2$  is defined as the Tait parameter, analogous to the ideal gas ratio of specific heats. The constant  $\sigma$  is defined as the nonideal solid parameter. Numerical values for the gas and solid state parameters can be chosen to match detonation wave speed data for the gas and shock impact data for the solid [5]. The subscript "0" denotes the initial state.

For these constitutive relations, sufficient conditions for the model equations to predict equilibrium in the ambient state are  $\phi_2(x, 0) = \text{constant}$ ,  $u_1(x, 0) = u_2(x, 0) = 0$ ,  $T_1(x, 0) = T_2(x, 0) = \text{constant} < T_{ig}$ ,  $\rho_1(x, 0) = \text{constant}$ , and  $\rho_2(x, 0) = \text{constant}$ .

**CHARACTERISTIC FORM OF TWO-PHASE EQUATIONS**

Following Whitham [19] for a system of partial differential equations of the form

$$A_{ij} \frac{\partial u_j}{\partial t} + B_{ij} \frac{\partial u_j}{\partial x} = C_i, \tag{58}$$

the characteristic velocities  $\lambda$  are found by solving the linear algebra problem

$$|\lambda A_{ij} - B_{ij}| = 0. \tag{59}$$

For each  $\lambda$ , a vector  $l_i$  is determined such that

$$l_i(\lambda A_{ij} - B_{ij}) = 0. \tag{60}$$

The characteristic equations are then given by the equation

$$l_i A_{ij} \frac{du_j}{dt} = l_i C_i, \tag{61}$$

which is valid on the curves specified by

$$\frac{dx}{dt} = \lambda. \tag{62}$$

The PSK model equations are written here in a form suitable for determining the characteristics. In these equations, the solid is assumed to be a Tait solid and the gas assumed to be an ideal gas ( $b = 0$ ). This analysis could also be performed for more general state equations; however, by making these assumptions, the results can be easily compared with well-known one-phase results.

The vector  $u_j$  for the eight partial differential equations of the PSK model is chosen to be  $u_j = (\rho_1, \rho_2, u_1, u_2, s_1, s_2, r, \phi_2)$ . As the momentum equations contain derivatives of pressure, it is necessary to express the derivatives in terms of  $u_j$  in order to find the characteristics. For both the ideal gas and Tait solid the pressure derivative can be written in terms of entropy and density derivatives as

$$dP_i = \frac{\rho_i \omega_i^2}{\gamma_i c_{vi}} ds_i + \omega_i^2 d\rho_i, \tag{63}$$

where  $\gamma_1 \equiv 1 + R/c_{v1}$ .

The unsteady two-phase equations in the form of Eq. 58 are given below:

$$\begin{aligned} \rho_i \frac{\partial \phi_i}{\partial t} + \phi_i \frac{\partial \rho_i}{\partial t} + \rho_i \phi_i \frac{\partial u_i}{\partial x} \\ + \rho_i u_i \frac{\partial \phi_i}{\partial x} + u_i \phi_i \frac{\partial \rho_i}{\partial x} = a_i, \end{aligned} \tag{64}$$

$$\begin{aligned} \rho_i \phi_i \frac{\partial u_i}{\partial t} + \rho_i \phi_i u_i \frac{\partial u_i}{\partial x} + \phi_i \omega_i^2 \frac{\partial \rho_i}{\partial x} \\ + \frac{\rho_i \phi_i \omega_i^2}{\gamma_i c_{vi}} \frac{\partial s_i}{\partial x} + P_i \frac{\partial \phi_i}{\partial x} \\ = (2 - i)a_1(u_2 - u_1) + b_i, \end{aligned} \tag{65}$$

$$\begin{aligned} \rho_i \phi_i T_i \frac{\partial s_i}{\partial t} + \rho_i \phi_i T_i u_i \frac{\partial s_i}{\partial x} - P_i \frac{\partial \phi_i}{\partial t} - P_i u_i \frac{\partial \phi_i}{\partial x} \\ = (2 - i) \left[ a_1 \left( e_2 - e_1 + \frac{1}{2} (u_2 - u_1)^2 \right) \right. \\ \left. + b_1 (u_2 - u_1) \right] - a_i \frac{P_i}{\rho_i} + c_i, \end{aligned} \tag{66}$$

$$\frac{\partial r}{\partial t} + u_2 \frac{\partial r}{\partial x} = -\alpha P_1^m - \frac{r}{3\rho_2} \left( \frac{\partial \rho_2}{\partial t} + u_2 \frac{\partial \rho_2}{\partial x} \right), \quad \frac{dr}{dt_{20}} + \frac{r}{3\rho_2} \frac{d\rho_2}{dt_{20}} = -\alpha P_1^m, \quad (71)$$

$$\frac{\partial \phi_2}{\partial t} + u_2 \frac{\partial \phi_2}{\partial x} = \frac{\phi_1 \phi_2}{\mu_c} (P_2 - f_2 - P_1) + a_2 / \rho_2. \quad \text{where} \quad \frac{d}{dt_{i\pm}} = \frac{\partial}{\partial t} + (u_i \pm \omega_i) \frac{\partial}{\partial x} \quad \text{on} \quad (67)$$

By solving Eq. 59 for the system of Eqs. 64–68, six characteristic velocities  $\lambda$  are found:  $\lambda = u_1, u_2, u_1 \pm \omega_1, u_2 \pm \omega_2$ . A detailed calculation shows that the characteristic ordinary differential equations of the form of Eq. 61 are given by

$$\begin{aligned} & \frac{1}{\rho_i \phi_i \omega_i^2} \frac{d(P_i \phi_i)}{dt_{i\pm}} \pm \frac{1}{\omega_i} \frac{du_i}{dt_{i\pm}} \\ &= \frac{1}{\rho_i \phi_i} \left\{ a_i \pm \frac{(2-i)a_1(u_2 - u_1) + b_i}{\omega_i} \right\} \\ &+ \frac{1}{\gamma_i c_{vi} \rho_i \phi_i T_i} \left\{ -a_i \frac{P_i}{\rho_i} + c_i + (2-i) \right. \\ &\times \left[ a_1 \left( e_2 - e_1 + \frac{1}{2}(u_2 - u_1)^2 \right) \right. \\ &\left. \left. + b_1(u_2 - u_1) \right] \right\} \\ &+ \frac{(i-1)}{\rho_2 \phi_2} \left( \gamma_2 \frac{P_2}{\omega_2^2} - \rho_2 \right) \\ &\times \left( \frac{\phi_1 \phi_2}{\mu_c} (P_2 - f_2 - P_1) + \frac{a_2}{\rho_2} \right), \quad (69) \end{aligned}$$

$$\begin{aligned} & \rho_i \phi_i T_i \frac{ds_i}{dt_{i0}} - P_i \frac{d\phi_i}{dt_{i0}} \\ &= -a_i \frac{P_i}{\rho_i} + c_i + (2-i) \left[ a_1 \left( e_2 - e_1 \right. \right. \\ &\left. \left. + \frac{1}{2}(u_2 - u_1)^2 \right) + b_1(u_2 - u_1) \right], \quad (70) \end{aligned}$$

$$\frac{d\phi_2}{dt_{20}} = (P_2 - f_2 - P_1) \frac{\phi_1 \phi_2}{\mu_c} + \frac{a_2}{\rho_2}, \quad (72)$$

$$\frac{d}{dt_{i\pm}} = \frac{\partial}{\partial t} + (u_i \pm \omega_i) \frac{\partial}{\partial x} \quad \text{on}$$

$$\frac{dx}{dt} = u_i \pm \omega_i$$

and

$$\frac{d}{dt_{i0}} = \frac{\partial}{\partial t} + u_i \frac{\partial}{\partial x} \quad \text{on}$$

$$\frac{dx}{dt} = u_i.$$

Equation 69 applies under the condition  $u_2 \pm \omega_2 \neq u_1 + \omega_1$  and  $u_1 \pm \omega_1 \neq u_2 + \omega_2$ .

In the one phase limit ( $\phi_2$  or  $\phi_1 = 0$ ) the characteristic equations properly reduce to the one-phase characteristic equations found for example in Courant and Friedrichs [20]:

$$\frac{1}{\rho \omega^2} \frac{dP}{dt_{\pm}} \pm \frac{1}{\omega} \frac{du}{dt_{\pm}} = 0, \quad (73)$$

$$\frac{ds}{dt_0} = 0. \quad (74)$$

Here the  $i$  subscripts have been dropped to indicate the one-phase equations.

### DISCUSSION

A two-phase model has been presented that meets most basic requirements of any fluid flow model. The model equations conserve mass, momentum, and energy for the mixture and are frame indifferent. These conditions are not really controversial and satisfied by most current two-phase models.

In other respects, the model presented here has certain advantages over other two-phase detonation models and some weaknesses. First, since the model equations are hyperbolic, there can be

no question that the initial value problem is well-posed. In many other two-phase combustion and detonation models, the characteristics are shown to be imaginary in some circumstances or simply are not discussed. In many of these studies the conditions for a well-posed problem are not well-defined. If not studied carefully, this could lead to inherent instabilities in the solution of these equations. Ermolaev et al. [12] take the cautious, but proper, step of checking the characteristics at each point in their calculations. If imaginary characteristics are found, they cease calculating the solution.

A distinguishing feature of both the BN and PSK models that guarantees the hyperbolicity of the equations and makes such attention to detail unnecessary is the dynamic compaction equation. None of the two-phase models that exhibit flow regimes with imaginary characteristics contains a dynamic compaction equation. Instead for closure it is generally assumed that the instantaneous particle stress equals the sum of the gas phase pressure and equilibrium configurational stress. Thus, it is suggested that the dynamic compaction equation is responsible for guaranteeing real characteristics.

However, the dynamic compaction equation is one of the most uncertain aspects of the present model. One of the most important parameters of this model, the compaction viscosity, has never been measured. Also, there is no clear reason why a mass transfer term must appear as a forcing term in the dynamic compaction equation. Nevertheless, the use of this equation significantly clarifies many issues in two-phase modeling. In addition to hyperbolicity, use of this equation results in easily interpreted shock discontinuity equations. The shock relations are essential in describing detonations in two-phase systems. As discussed in Ref. 5, the dynamic compaction equation holds that the volume fraction does not change through a shock jump. As a result, the gas shock state is independent of both the solid state and volume fraction. Likewise, the solid shock state is independent of the gas state and volume fraction. Both shock states are precisely the same as predicted by a single phase analysis. Consequently, this equation is viewed as a modeling convenience that, though it has some desirable features that lead to simple

interpretations, still needs further theoretical and experimental justification.

The PSK model contains an evolutionary equation for particle number. For models that describe the burning of moving particles, it would seem that such an equation is a necessity. However, this idea is not universally found in two-phase combustion models. For instance a number conservation equation is included in Refs. 5-7, whereas no comparable relation is found in Refs. 2, 8, and 9. In other studies [3, 4, 12], expressions for the evolution of particle radius are given. However, in these studies number is not conserved, and it is not clear what physical process is responsible for the breakup or agglomeration of particles.

A weakness of the PSK model is that it is not always guaranteed to satisfy the entropy inequality. The same can be said for the BN model, although the BN model is in general less restrictive than the PSK model. Most other two-phase detonation studies do not examine the implications of the second law. The idea of constructing a model to satisfy the entropy inequality is appealing but has led to very complicated expressions for phase interaction terms that have no other real justification. As it stands two-phase theory still needs an justification founded on more fundamental theory.

A two-phase theory based on the microstructural flow details could potentially determine the proper form for phase interaction terms. This theory could make the physical meaning of such things as particle and gas temperature and pressure clear. The present interpretation is that these terms are equivalent to their one-phase counterparts; however, two-phase theory lacks the microstructural rigor that is used to define these one-phase variables. At this point it may be best to view the two-phase variables only as state variables defined by a theory that is consistent with certain modeling principles and to realize that the physical interpretation of these variables may or may not be the same as for one-phase theory.

Finally, an advantage of the model proposed here is the simplicity of the constitutive relations. Although the model is admittedly complicated, when compared to many other models, it is more compact. If one's goal is to match experimental data under a wide variety of flow conditions,

then this model is inadequate. Many of the choices made are arbitrary and have not been confirmed by experiment of microstructural theory. It should be emphasized again, however, that for detonation conditions, no constitutive models have been verified. If one's goal is to describe a detonation, it would seem that such simple constitutive relations are as likely to be as valid as more complicated relations. As shown in Ref. 21, this model is indeed capable of describing a detonation in a two-phase system.

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