# Modeling of Convective Mode Combustion through Granulated Propellant to Predict Detonation Transition

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**An analysis of the transient reactive flow through highly loaded but mobile particles of solid propellant is presented in order to determine whether the high-speed flame front can provide a pressure wave that can interact with the flow to build up to a condition of detonation. Discussions are presented which deal with the various forms of the field balance conservation equations, as well as the significant number of additional constitutive relations required to model this flow. Results are presented which indicate the sensitivity of the most important parameters on the unsteady flame-spreading rate. Possible criteria for DDT (deflagration-to-detonation transition) are presented.**

## Nomenclature

$a$ = propellant burning rate constant
$B'$ = particle-particle interaction proportionality constant
$b$ = propellant burning rate proportionality constant
$C_v$ = specific heat at constant volume
$\mathfrak{D}$ = gas particle viscous interaction
$d_p$ = initial grain diameter
$e$ = total energy per unit mass
$\hat{e}$ = energy liberated due to combustion per unit mass
$f_{gs}$ = drag coefficient
$\bar{h}$ = convective heat-transfer coefficient
$K_g$ = gas conductivity
$m$ = particle-particle interaction exponent
$n$ = propellant burning rate index
$P_g$ = gas pressure
$Pr$ = Prandtl number
$P_s$ = particle phase pressure
$P$ = total stress of the mixture
$R$ = universal gas constant
$\dot{r}$ = burning rate
$r_p$ = instantaneous particle radius
$Re_p$ = Reynolds number based on particle radius
$T$ = temperature
$t$ = time
$u$ = velocity
$x$ = coordinate along propellant bed
$\alpha_1$ = gas porosity
$\alpha_2$ = solid volume fraction
$\Gamma_g$ = mass of gas generated per unit total flow volume
$\mu$ = gas viscosity
$\eta$ = covolume of propellant gas
$\zeta$ = ratio of specific heats at constant volume of gas and particle ($=C_{v_g}/C_{v_p}$)
$\rho$ = density
$\sigma$ = partial phase density
$\tau$ = partial stress
$\phi$ = void fraction ($=\alpha_1$ = gas volume/total volume)

*Subscripts*

$g$ = gas phase
$m$ = mixture
$p$ = particle phase

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## Introduction

THE ability to predict transition from a convectively driven deflagration wave to a detonation in a highly loaded bed of small-particle propellant or explosive requires an accurate ability to describe the reactive two-phase fluid mechanics of the system (see Fig. 1). In addition to the problem of the appropriate form of all conservation equations, one also must have an accurate description of such highly transient phenomena as the interphase viscous forces, the ignition criterion for the solid, the interphase heat transfer by convection to the solid from the hot propellant gases, and the burning rate dependencies on the ambient conditions of the flow.

Studies of the spontaneous deflagration-to-detonation transition (DDT) in gases indicate that in an accelerated deflagration a shock front runs ahead of the flame. The present paper is concerned with such dynamic behavior in granular propellant, with an attempt to elucidate the details of propagation of the flame (ignition) front, pressure fronts, and possible shock fronts before development of steady-state detonation. The experimental work of Bernecker and Price[1] with granular explosives and the work of Gipson and Maček[2] with DDT in solid explosives indicate clearly that, in the study of buildup to detonation, it is important to know the relationship of the pressure (shock or compression) fronts to the flame front.

In the problem of concern here, a fraction of the propellant grains is assumed ignited at one end of a closed chamber. The mass generated in the ignition region accelerates the flame

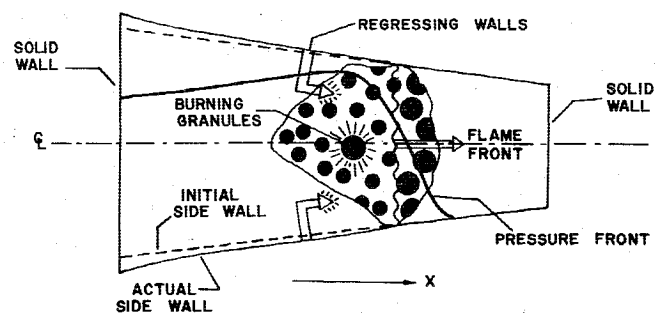


**Fig. 1 Schematic of bed packed with granular propellant.**

forward, with the region behind the flame rapidly increasing in pressure as more and more mass is being generated due to the pressure-sensitive burning rate. Calculations then show that a steep pressure front begins to accelerate and attempts to overtake the flame front. When this happens, there is an almost abrupt increase in the flame speed. A detonation can be said to have started when the pressure front precedes the flame front and they both attain about the same high speed. We are, of course, limited by our numerical differencing scheme to indicate a true shock front preceding the flame. But with a rapid transition of the flame front in conjunction with the interaction of the pressure fronts, one can suppose that DDT can occur. A discussion of a criterion for DDT is presented later.

## Formulation of Two-Phase Conservation Equations

Basic differences in the approach to deriving the field balance continuity, momentum, and energy conservation equations provide a continuing current controversy in the area of two-phase fluid mechanics. Although it is difficult to categorize all of the models published, one of the main differences stems from the assumptions that 1) the equations of motion be derived based on the center of mass of each phase vs 2) those derived based on the center of mass of the mixture. Then, in addition to that distinction, there are models that 3) attempt to define rigorous average-flow properties in which one phase does *not* constitute a continuum.

A brief review was prepared recently by Krier[3] which discusses the concepts that result in conservation equations based on assumption 1) vs those obtained by assumption 2). Derivations utilizing assumption 1 have been termed the "separated-flow" approach; those using assumption 2 are called the "continuum-mixture" approach. Some examples of those models that we term the separated-flow models would be the work of Anderson and Jackson,[4] Green and Naghdi,[5] Nigmatulin,[6] Kuo and Summerfield,[7] and Gough.[8] (There are, of course, many other multiphase models.)

The models using the continuum-mixture approach are those by Van Tassell and Krier,[9] Krier et al.,[10] and Soo.[11,12] Also, a recent report by Sha and Soo[13] presents details of why the continuum-mixture approach results in different forms of the conservation equations. Finally, under the broad definition of the averaging approach (assumption 3), one might place there the derivations of Panton,[14] Hughes,[15] and Crowe.[16]

## Continuum-Mixture Model

The continuum-mixture model assumes that the mixture momentum and energy equations describe a continuum fluid in terms of the mean mass-weighted mixture velocity and mixture energy. This concept is stated clearly in the paper by Soo.[11] Thus one should write for the two-phase mixture momentum that

$$\rho_m\left[\frac{\partial u_m}{\partial t}+u_m\frac{\partial u_m}{\partial x}\right]=-\frac{\partial P}{\partial x} \tag{1}$$

and, for the mixture energy,

$$\rho_m\left[\frac{\partial e_m}{\partial t}+u_m\frac{\partial e_m}{\partial x}\right]=-\frac{\partial (u_m P)}{\partial x}+\Gamma_g\hat{e}_m \tag{2}$$

where

$$\rho_m=\rho_g\alpha_1+\sigma_p\alpha_2\equiv\sigma_g+\sigma_p \quad \text{(density)} \tag{3}$$

$$u_m=(\rho_g\alpha_1 u_g+\rho_p\alpha_2 u_p)/\rho_m \quad \text{(velocity)} \tag{4}$$

$$\rho_m e_m=\sigma_g e_g+\sigma_p e_p+(\sigma_g u_g^2/2)+(\sigma_p u_p^2/2) \tag{5}$$

Here $e_i\equiv C_v T$, where an average but constant specific heat has been assumed. In general, $P$ represents the gas-phase pressure if one neglects solid-phase interaction. Also, $\alpha_1$ would represent the gas porosity, often termed $\phi$, which is the ratio of gas volume to the mixture volume. Thus $\alpha_2=1-\phi$, the solid volume fraction. Assuming a one-dimensional bed several centimeters long of small-particle propellant (diameters of the order of 100 to 400 $\mu$m), with a typical solids loading fraction of $\alpha_2=0.70$, a localized ignition source will, within a matter of time less than 1 ms, pressurize the closed system at extreme rates, often at pressures exceeding $0.5\times10^6$ psi (3.5 GPa). The ability to model this transient process requires solving two field balance continuity, two momentum, and two energy conservation equations. These equations follow in many ways those derived in Ref. 9, although some significant changes have been made and will be discussed below. The assumptions made to express these equations were discussed in Ref. 9, but additional ones also are enumerated following the stated equations. These would be as follows:

Mass Balances: Gas Phase

$$\frac{\partial}{\partial t}(\sigma_g)+\frac{\partial}{\partial x}(\sigma_g u_g)=\Gamma_g \tag{6}$$

Solid Phase

$$\frac{\partial}{\partial t}(\sigma_p)+\frac{\partial}{\partial x}(\sigma_p u_p)=-\Gamma_g \tag{7}$$

where

$\sigma_g$ = $\rho_g\alpha_1$, partial gas density, kg/m$^3$
$\sigma_p$ = $\rho_p\alpha_2$, partial solid density, kg/m$^3$
$\rho_i$ = actual phase density ($i=g, p$)
$\Gamma_g$ = mass of gas generated per unit total flow volume [e.g., if the particles are assumed to be spherical and are burning at a rate $\dot{r}$ (cm/s), then $\Gamma_g=(3/r_p)\alpha_2\dot{r}$, where $r_p$ is the particle radius]

Momentum Balances: Gas Phase

$$\sigma_g\left[\frac{\partial u_g}{\partial t}+u_g\frac{\partial u_g}{\partial x}\right]=-\frac{\partial}{\partial x}[\alpha_1\tau_g]-\mathfrak{D}-\Gamma_g(u_g-u_m)$$
$$+\frac{\partial}{\partial x}[\sigma_g(u_g-u_m)^2] \tag{8}$$

where generally $\tau_g$ = gas-phase pressure $P_g$ only. Note that the last term in Eq. (8) also can be expressed as

$$\frac{\partial}{\partial x}\left[\frac{\sigma_g\sigma_p^2}{(\sigma_g+\sigma_p)^2}(u_g-u_p)^2\right]$$

This term has been referred to as an "inertial coupling" term by Soo.[11] Also, Sha and Soo[13] give examples of some limiting two-phase flow situations which indicate that, without such inertial interaction forces per unit volume of the mixture, one cannot represent physically meaningful flow situations.

Solid Phase

$$\sigma_p\left(\frac{\partial u_p}{\partial t}+u_p\frac{\partial u_p}{\partial x}\right)=-\frac{\partial}{\partial x}[\alpha_2\tau_p]+\mathfrak{D}+\Gamma_g(u_p-u_m)$$
$$+\frac{\partial}{\partial x}[\sigma_p(u_p-u_m)^2] \tag{9}$$

It was assumed that the gas-particle viscous interaction $\mathfrak{D}=f_{sg}\cdot(u_g-u_p)$, where $f_{sg}$ defines a drag coefficient, dependent upon the solids loading fraction and some average flow speed. Such correlation for the drag would be the

classical Ergun relation for a packed bed.[17] It is easy to show that Eqs. (8) and (9) sum to Eq. (1) if $P$ includes both the gas pressure and axial solid-phase stress $\tau_p$. Interestingly enough, Soo[12] has shown that in Eqs. (6-9) for the limiting case of incompressible fluids and for $\sigma_p \gg \sigma_g$, all of the characteristics are real, and the problem is, in general, well posed.

Taking into account the criticisms made by Green and Naghdi[5] that in the derivation of two-phase flow conservation equations the "primitive" concepts be used for partial stresses and heat fluxes, the energy equations are modified somewhat from those given in Ref. 9. The energy balances are written here by assuming that $\tau_g = -P_g$, and not $\tau_g = -P_g + \rho_g (u_g - u_m)^2$:

Energy Balances: Gas Phase

$$\sigma_g \left( \frac{\partial e_g}{\partial t} + u_g \frac{\partial e_g}{\partial x} \right) = -\frac{\partial}{\partial x}[\alpha_1 P_g u_m] + \Gamma_g (\hat{e}_g - e_g) + \frac{\partial}{\partial x}[\sigma_g e_g (u_g - u_m)] - \frac{\bar{h} 3 \alpha_2}{r_p c_v} (e_g - \zeta e_p) \tag{10}$$

Here $\bar{h}$ is the heat-transfer coefficient for convective energy transport from the gas to the particles. Heat transfer by conduction, $\partial/\partial x(-K_g \partial T/\partial x)$, has been neglected. The energy liberated by combustion in the gas per unit mass is defined by the symbol $\hat{e}_g$. Also, $e_g = C_{v_g} T_g$.

Solid Phase

$$\sigma_p \left[ \frac{\partial e_p}{\partial t} + u_p \frac{\partial e_p}{\partial x} \right] = -\frac{\partial}{\partial x}[\alpha_2 \tau_p u_m] - \Gamma_g (\hat{e}_p - e_p) + \frac{\partial}{\partial x}[\sigma_p e_p (u_p - u_m)] + \frac{\bar{h} 3 \alpha_2}{r_p C_{v_g}} (e_g - \zeta e_p) \tag{11}$$

It can be shown that the sum of Eqs. (10) and (11) yields a mixture energy equation, which is

$$\rho_m \left[ \frac{\partial e_m}{\partial t} + u_m \frac{\partial e_m}{\partial x} \right] = -\frac{\partial}{\partial x}[P u_m] + \Gamma_g \hat{e}_m \tag{12}$$

where $\hat{e}_m = \hat{e}_g - \hat{e}_p$, the chemical content of the propellant, and $P$ includes the solid stress collision pressure.

Equations (6-12) are solved by a modified form of the explicit two-step Richtmyer variation of the Lax-Wendroff scheme, using artificial damping to insure stability. A short description of this technique and how boundary conditions are handled at the closed ends is given by Krier et al.[10] The text by Ames[18] discusses how artificial viscosity can be employed for "changing a shock from a discontinuity to a narrow region across which the fluid variables change rapidly but continuously." The appropriate space and time increments in the difference formulations were determined by trial and error, until one arrived at identical but stable results for the largest value of $\Delta x$ and $\Delta t$. Typically, $\Delta x = 0.05$ in., and $\Delta t$ was $0.01 \times 10^{-6}$ s.

## Constitutive Relations

In order to predict the pressure wave dynamics and the unsteady spreading of the ignition fronts due to the penetration of the hot gases, one must specify 1) an ignition criterion, in terms of the bulk temperature of the solid propellant, $T_p (= e_p / C_{v_p})$; 2) the interphase heat-transfer coefficient $\bar{h}$; 3) the interphase drag coefficient $f_{gs}$; 4) the rate of propellant burning $\dot{r}$ as a function of the impressed local pressure and the particle temperature $T_p$; and 5) the axial normal stress to account for the particle-particle interaction.

Some discussion concerning items 1-4 has been given in Ref. 9, with additional details presented in the report by Krier et al.[19] To represent item 5, we have utilized the concepts presented by Wallis[20] for the particle-particle forces by defining a particle-phase pressure $P_s = B' \alpha_2^m$, where $B'$ and $m$ are empirical constants obtained from flow studies through fibrous materials.[20] Thus the term

$$\alpha_2 \frac{\partial P_s}{\partial x} = m B' \alpha_2^m \frac{\partial \alpha_2}{\partial x} \tag{13}$$

is utilized in the solid-phase energy equation. The parameter $B'$ is updated as the flow progresses from information of the average total pressure drop in the bed and the average mean porosity.[19] Note that in Eq. (9) the stress $\tau_p$ then is set to $\tau_p = P_g + P_s$.

For the interphase heat-transfer coefficient, we assumed that Denton's correlation[21] can be applied at any instant, that is,

$$\bar{h} = 0.58 \frac{K_g}{2 r_p} \left[ \frac{2 \rho_g |u_p - u_g| \alpha_1 r_p}{\mu_g} \right]^{0.7} \cdot Pr^{0.3} \tag{14}$$

where $Pr$ is the gas-phase Prandtl number. After ignition, with hot gases being generated "at" the propellant surface, the heat-transfer coefficient $\bar{h}$ was reduced arbitrarily to 10% of the value given by the preceding equation, to simulate the "film cooling" reduction.

For the packed-bed condition, the drag correlation was based on Ergun's relation (see Wallis[20] for additional discussion). Thus,

$$f_{gs} = \frac{\alpha_2 \rho_g |u_g - u_p|}{2 r_p \alpha_1} \left\{ \frac{150 \alpha_2}{Re_p} + 1.75 \right\} \tag{15a}$$

where

$$Re_p = [2 \rho_g |u_g - u_p| \alpha_1 r_p] / \mu_g \tag{15b}$$

represents the appropriate Reynolds number.

Finally, the propellant burning rate (which is nonzero only when the solid-phase temperature exceeded an assumed ignition value ranging from 30° to 45°R) was assumed to be

$$\dot{r} = (a + b T_p) P_g^n \tag{16}$$

where $a$, $b$, and $n$ are assumed known constants.

Also, a gas-phase state equation is required, and, because of the resulting high pressure, a simple Noble-Abel relation, i.e.,

$$P_g = \rho_g R T_g / (1 - \rho_g \eta) \tag{17}$$

initially was employed. Here $\eta$ is the covolume factor. The solid density $\rho_p$ was assumed a constant equal to 1.9 g/cm$^3$. However, it soon was noticed that Eq. (17) was not valid at pressures greater than 50 to 100 kpsi. Hence a variable covolume was manufactured which attempted to match other nonideal equations of state valid at much higher pressures, e.g., $\eta = \eta(\rho_g)$.[22]

The initial conditions are as follows. The problem is specified after a time, chosen as $t = 0$, in which at one end of a closed bed an ignition stimulus is assumed by a step distribution of high-pressure, hot gases. This "ignition" region was taken to be about 15% of the total porous bed length. It also was assumed that in this portion the propellant already was ignited. It was determined essentially by the predicted results that the pressure and flow variables remained basically the same as time progressed, as long as the ignited region was less than approximately 15% of the total length of the bed. Results with both a 2- and 3-in.-long bed essentially predicted DDT at the same length when both beds had 15% of the bed initially ignited.

## Predictions Using the Continuum-Mixture Model

Figure 2 presents the predictions of the developing pressure distribution for a 2-in.-long bed of 200-$\mu$m-diam particles,

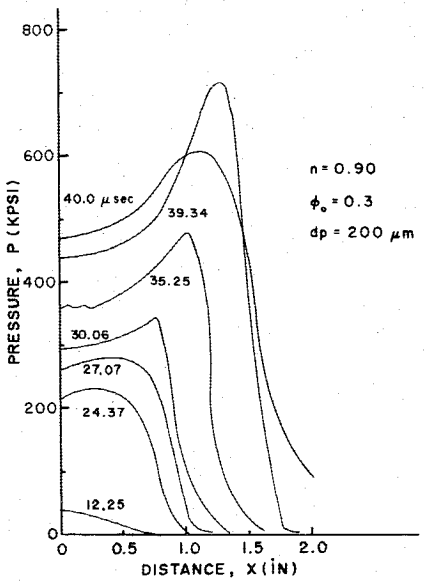


**Fig. 2 Pressure distribution history in a highly loaded bed of small-particle energetic solid propellant.**

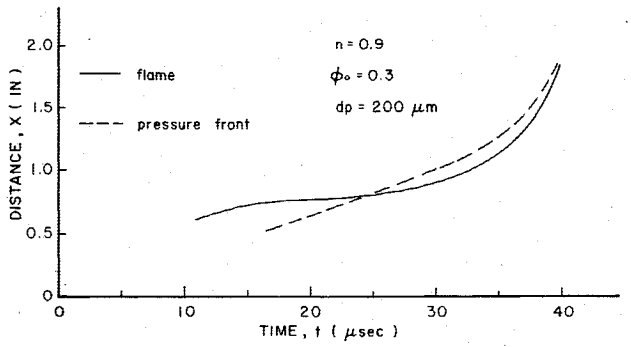


**Fig. 3 Locus of the flame (ignition) front and pressure front, complementary to conditions shown in Fig. 2.**

with an initial porosity of $\alpha_2 = 0.70$. The propellant is a rapid-burning type, with a pressure index of $n = 0.90$ and a heat of combustion $\hat{e}_m = 1300$ cal/g. The initial pressure in the region from $0 < x \leq 0.2$ in. was 1600 psi, with the initial gas temperature in that region fixed at 5900°R. Other pertinent inputs to the calculations are indicated in Table 1.

The predictions indicate a rapid buildup of pressure in the bed interior, leading to a "continental-divide" type of pressure distribution and steep pressure gradients forming a shocklike front. Notice that a peak pressure of 720 kpsia (5.03 GPa) is predicted. During this pressure buildup, the flame accelerates moderately at first and then much more rapidly, as shown in Fig. 3. A pressure front locus also is presented in Fig. 3, indicating the apparent merging of the pressure and flame front at a time of 39 μs. The pressure front can be calculated by first plotting pressure vs time at a given $x$ location and recording the time when the pressure there begins to increase abruptly. The flame speed (ignition front) accelerates, for example, from a velocity of 1.21 mm/μs at $x = 1$ in. (midpoint) to 4.32 mm/μs at $x = 1.4$ in.

It is, of course, not clear whether one should consider the results depicted in Figs. 2 and 3 to be a transition to a detonation. There appear in Fig. 3 to be many of the dynamic features of DDT as observed in the work of Bernecker and Price.[1] And predictions with less energetic propellant or a lower burning rate index $n$ do not show either the large continental-divide pressure fields or acceleration of the flame front to velocities approaching detonation speed. Some discussion of a DDT criterion is given later in this section.

One of the controversies when modeling the momentum conservation equations for a two-phase flow centers on the question of whether each phase is subject to its partial gradient of pressure, $-(\alpha_i\ \partial\tau_i/\partial x)$, rather than the gradient of the partial pressure, $-\partial/\partial x\ (\alpha_i\tau_i)$. Arguments for which form is correct are given in Refs. 8, 10, 13, and 16. Predictions with our model, for the various cases considered to date, indicate that results like those presented in Figs. 2 and 3 (and those figures following) essentially remain unchanged, regardless of which way the pressure gradient is expressed. Apparently, the nonlinear viscous drag terms and the other source/sink terms in the mathematical operators dominate the expected variations. That is, the term $-\tau_i\ \partial\alpha_i/\partial x$ is less important than those other terms.

However, the variations in the predicted results due to the changes in the form of the pressure gradient force per unit volume in the solid-phase momentum equation are significant. As mentioned previously, the pressure gradient term in Eq. (9) is expressed as

$$-\frac{\partial}{\partial x}(\alpha_2\tau_p)$$

where $\tau_p = P_g + P_s$, and $\alpha_2\partial P_s/\partial x$ is given by Eq. (13). Figure 4 shows the pressure distribution at a time of 30.5 μs as case 4 for the preceding standard form. When increasing the compaction constant $B'$ [Eq. (13)] by 20% and 100% (cases 2 and 3, respectively), much greater pressures are predicted, and the predicted flame front accelerates to greater velocities, often exceeding 10-15 mm/μs. Apparently, resistance to bed

**Table 1 Typical input data**

| Parameter | Value |
|---|---|
| Initial bed temperature $T_g$, $T_p$ | 530°R (294.0 K) |
| Ignition temperature $T_{ign}$ | 560°R (310.8 K) |
| Initial bed pressure $P_g$ | 14.7 lbf/in.$^2$ (0.103 MPa) |
| Propellant burning rate constant $a$ | 0.0 in./s (0.0 cm/s) |
| Propellant burning rate proportionality constant $b$ | 0.009 in/s (psi)$^n$ [0.2 cm/s (MPa)$^n$ for $n = 0.9$] |
| Propellant burning rate index $n$ | 0.9 |
| Propellant density $\rho_p$ | 0.0685 lbm/in.$^3$ (1.9 g/cm$^3$) |
| Initial grain diameter $d_p$ | 0.07874 in. (200 μm) |
| Chemical energy released $E_{chem}$ | 2360.9 Btu/lbm (5.48 MJ/kg) |
| Molecular weight of gas $MW$ | 24.09 lbm/lb-mole (24.09 kg/kg-mole) |
| Covolume of propellant gas $\eta$ [variable covolume $\eta = \eta(\rho_g)$] | 26.89 in.$^3$/lbm (0.973 cm$^3$/g) |
| Specific heat ratio $\gamma$ | 1.333 |
| Gas viscosity $\mu_g$ (temperature-sensitive) | $0.757 \times 10^{-3}$ lbm/in.-s ($1.35 \times 10^{-2}$ N-s/m$^2$) |
| Universal gas constant $R$ | 1.987 Btu/lb-mole-°R (1.987 cal/g-mole-K) |
| Total bed length $\ell_B$ | 2.0 in. (50.4 mm) |
| Particle-particle interaction proportionality constant $B'$ | $0.254\ \Delta P/(\bar{\alpha}_4)^4$ psi [$1.8\ \Delta P/(\bar{\alpha}_2)^4$ kPa] |
| Particle-particle iteration exponent $m$ | 4.0 |

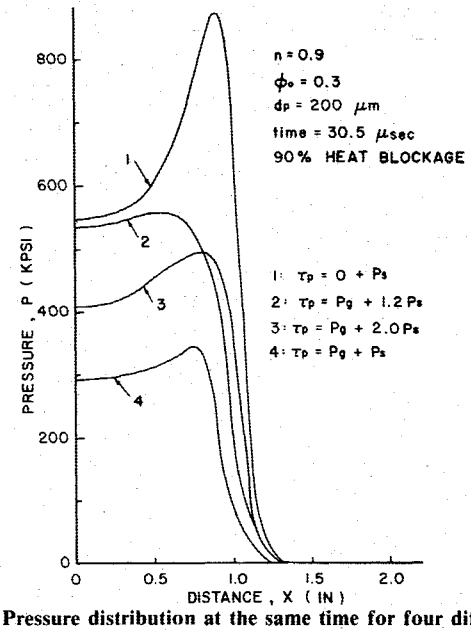


**Fig. 4 Pressure distribution at the same time for four different intragranular normal stress functions.**

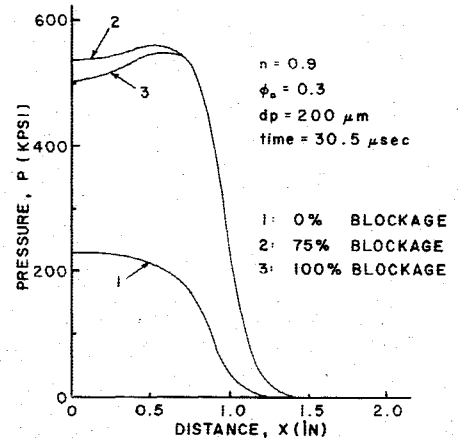


**Fig. 5 Pressure distribution at the same time for three cases of the postignition interphase heat-transfer rates.**

compaction has a prominent effect on the overall dynamic behavior of the bed. Dropping the gas-phase pressure $P_g$ as a component of $\tau_p$ results in the distribution, case 1 in Fig. 4, with extreme peak pressures.

Another important but actually unknown quantity is the relative amount of gas-particle heat transfer after the particles are ignited. With hot gases from the burning propellant now "blowing" into the thermal boundary layer surrounding the spherical grains, it makes sense that the heat-transfer coefficient [see Eq. (14)] should be reduced drastically. Figures 5-7 show the pressure distribution, the flame front locus, and the porosity distribution ($\alpha_I = \phi$), respectively, for three cases of the heat-transfer coefficient, changed after ignition. Case 1 assumes that Eq. (14) holds even after ignition; case 3 assumes that $\bar{h} = 0$. The typical standard case used in most of our calculations is case 2. Note that, as shown in Fig. 6, with heat blockage (cases 2 and 3) there is a predicted sudden jump in the flame front at $x = 1.45$ in. When reducing the energy loss by convection to the propellant (after ignition has been met), conditions for increased axial energy transport downstream into the unignited portion of the bed are more favorable, and transition to steeper fronts occurs sooner.

## DDT Criterion

At this point in our research, we have yet to define an acceptable criterion that indicates deflagration-to-detonation

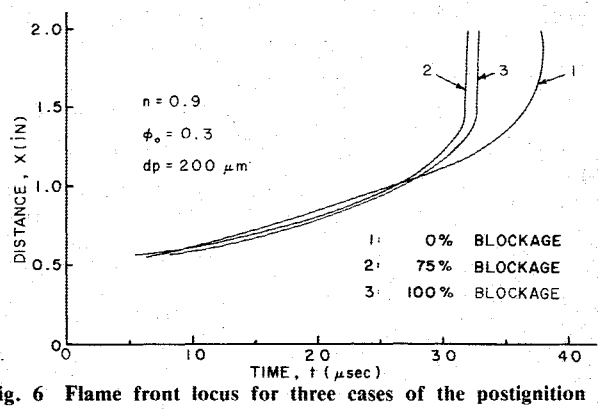


**Fig. 6 Flame front locus for three cases of the postignition interphase heat-transfer rates.**

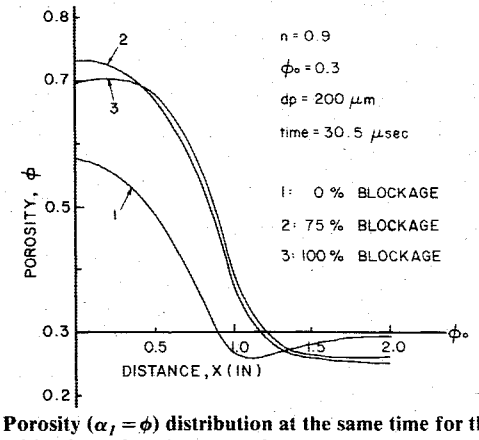


**Fig. 7 Porosity ($\alpha_I = \phi$) distribution at the same time for three cases of postignition interphase heat-transfer rates.**

transition. The model itself cannot differentiate between a deflagration or a detonation, chiefly because numerical predictions of shock fronts in a continuous-wave transition would be smeared out by the differencing scheme presently employed.

Nevertheless, we have made some key observations in the predicted results of the pressure wave front locus which indicate that conditions for a detonation would be feasible. One of these concerns the motion of the peak pressure (peak of the continental divide) in the bed, relative to the flame front. Figure 8 presents, for a typical case that we might say would exhibit DDT, the time history of the separation distance, called $\xi$, between the continental divide and the flame front. For a small, initially ignited portion of the bed, the flame front accelerates slowly into the bed while for some time the peak pressure remains at the ignited end, near $x = 0$. This is depicted (by the dotted lines) in Fig. 8.

However, at some point in time the pressure front begins to move into the bed and accelerates rapidly toward the flame. A minimum separation distance is predicted in which the pressure front and flame front accelerate at approximately the same speed. This minimum, for the case shown in Fig. 8 first occurs at $x = 1.30$ in. One therefore might define DDT to occur at $x = 1.30$ in. or at least before the flame reaches 1.75 in. Near that latter point, the peak pressure begins to reduce, and the continental divide actually moves backward toward $x = 0$. The result, as shown in Fig. 8, is that the separation distance $\xi$ between the flame and peak pressure begins to grow. Results almost identical to those shown in Fig. 8 were predicted when the initial bed length was increased by 50% to a length of 3 in. Hence this phenomenon is not a consequence of the reflected pressure waves of the back end wall but might be termed a "property" of a system that gives DDT. If an actual shock front were to be predicted one would expect that the separation distance should approach zero, and the pressure wave should lead the flame front. In conclusion, one

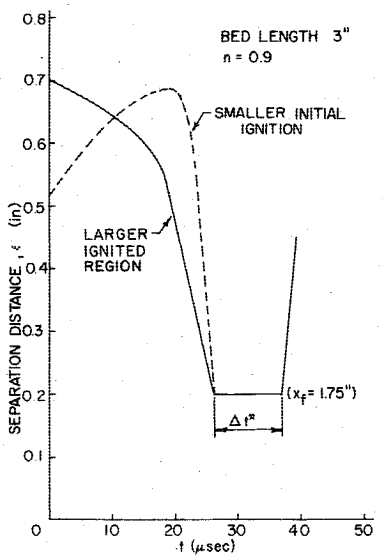


**Fig. 8 Development of the separation distance between the peak pressure in the bed and the flame front, indicating possible DDT conditions.**

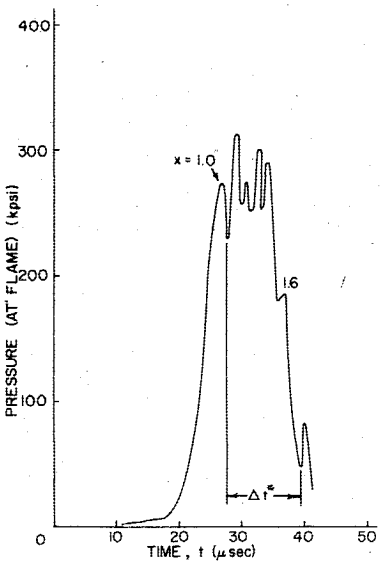


**Fig. 9 Pressure history at the flame front showing wave interaction previous to assumed DDT.**

might define a time to detonation somewhere within the time noted as $\Delta t^*$ on the figure.

The actual pressure history at the flame front as it accelerates in the bed is shown in Fig. 9. Note the appearance of wave structure in the time period when we have termed DDT to have occurred. The same $\Delta t^*$ also is shown on this figure to compare to time scale shown in Fig. 8.

An attempt to fix a clear definition of the condition for transition to detonation was proposed by Beckstead et al.[23] at Hercules, Inc. There, use was made of the concept of a "critical energy" for initiation to detonation, as originally proposed by Walker and Wasley[24] for the shock initiation of a solid explosive. As stated by Beckstead, "...detonation is assumed to be initiated when and where the gas reaches a pressure which would cause detonation, and then maintains (or exceeds) that pressure for a period,... specified by the condition that $p^2t$ = constant, $C$." It is not obvious what one should use for the constant $C$ for a granulated propellant or explosive. A recent analysis of shock initiation discusses limits of the critical energy concept.[25]

The detonation run-up length predictions are given in the following. Figure 10 shows the flame front speed at two locations in the bed, $x = 1.0$ and 1.4 in., as a function of the burning rate index $n$. It appears that detonation-like speeds are not predicted if the index is lower than 0.85, for the other properties assumed fixed. And, in fact, below this value one thus cannot predict the general peak pressure/flame front

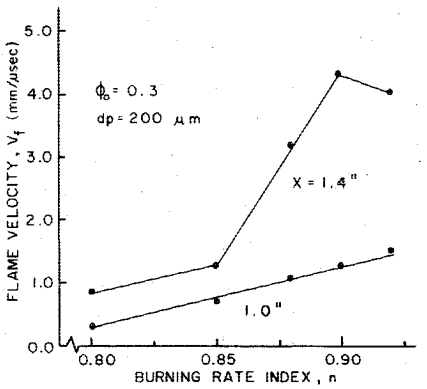


**Fig. 10 Convectively driven flame velocity as a function of the propellant burning rate index $n$.**

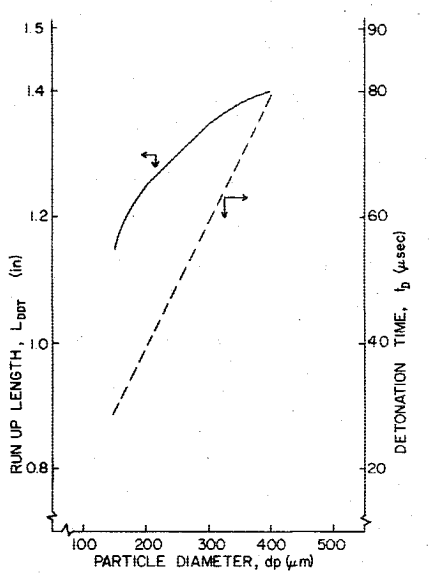


**Fig. 11 Predictions of run-up length to detonation (and time to detonation) as a function of propellant size.**

separation minimum as presented in Fig. 8. Thus, as intuitively expected, only high-energy, high-burning-rate propellants would have DDT.

Figures 11 and 12 present the predicted run-up length to detonation (and the time to detonation) as a function of the initial propellent size and the burning rate index $n$. For the range of particle sizes studied, $150\ \mu m \leq d_p \leq 400\ \mu m$, the run-up length $L_{DDT}$ is proportional to $d_p^{1/4}$. It is expected that the exponent ¼ would be larger for spheres of less than 100 $\mu$m. The variation in $L_{DDT}$ vs $n$, given by the simple equation shown on Fig. 12, was not tested beyond $n = 0.925$. The linear relation would predict a zero run-up length at $n = 1.15$, which is, of course, physically incorrect. And, finally, our results would predict no detonation (infinite run-up length) if the burning rate exponent is less than 0.80, assuming that all other variables were fixed.

## Conclusions

A model has been developed which utilizes continuum mechanics, two-phase flow conservation equations, and a series of constitutive relations for the interphase heat transfer and momentum (viscous) transfer, for propellant axial compressive forces, and for propellant ignition and burning rate, which predicts transient flow behavior exhibiting conditions of possible transition to detonation. Because these constitutive formulations generally were not developed for the extremely transient, high-pressure, and temperature flow conditions of interest here, and because the numerical integration scheme cannot handle the description of a strong shock wave, the results presented here cannot as yet be termed

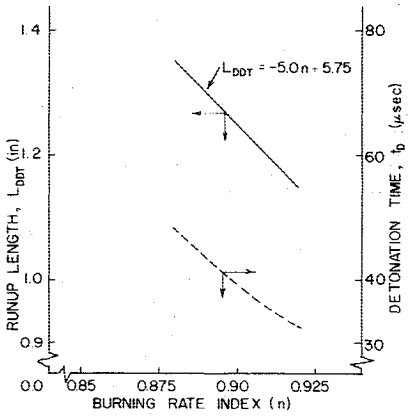


**Fig. 12 Predictions of run-up length to detonation (and time to detonation) as a function of the propellant burning rate index $n$.**

as quantitative predictions of actual conditions of deflagration-to-detonation transition. However, the results indicate that, as expected, only high-energy, rapid-burning-rate propellant, with a large solids loading, exhibits trends for transition to detonation. Flame (ignition) fronts are predicted to accelerate from deflagration speeds of the order of 0.1 mm/μs to "detonation speeds" exceeding 5-10 mm/μs. Extreme bed interior pressures approaching $7\times10^9$ N/m$^2$ ($10^6$ psi) are predicted, assuming that the walls confining the granulated bed remain rigid.

Work also is in progress to determine whether similar DDT trends are predicted if, instead, the momentum and energy field balance equations were of the separated-flow type, i.e., those of Refs. 4-8. Preliminary results indicate that, in general, for the problem being analyzed here in which substantial gas generation occurs and with the fairly large gas-particle viscous and heat-transfer interactions, there really are no major differences.[26]

There are three primary tasks that should be completed in order to provide rigorously a prediction for transition from deflagration to detonation:

1) The numerical integration scheme should be modified to incorporate the analysis of an embedded shock wave. It appears that with our present technique this will not be feasible, even if the space-domain step size $\Delta x$ were to be reduced further.

2) Sensitivity studies related to the various equations used as the constitutive relations should be continued. For example, we have found that, if one reduces the viscous gas-particle drag coefficient to 1/10 of the value calculated at all conditions when using Eq. (15), the predicted gas velocities are so large that eventually numerical computation broke down. Similar numerical instability occurred if the particle-particle stress coefficient $B'$ [Eq. (13)], was increased arbitrarily by more than five times the nominal value reported by Wallis.[20]

3) A rigorous criterion for DDT must be developed which incorporates the formation of an actual detonation (shock) wave.

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