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Mechanistic Reactive Burn Modeling of Solid Explosives

This report is a sequel to LA-13794-MS, "A Unifying Framework for Hot Spots and the Ignition of Energetic Materials."

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Mechanistic Reactive Burn Modeling of Solid Explosives

by

Y. Horie, Y. Hamate, and D. Greening

Abstract

This report describes a computational framework for reactive burn modeling of solid explosives and the development of a test case where physical mechanisms represent RDX or RDX-based materials. The report is a sequel to LA-13794-MS, “A Unifying Framework for Hot Spots and the Ignition of Energetic Materials,” where we proposed a new approach to the building of a general purpose model that captures the essential features of the three primary origins of hot-spot formation: void collapse, shear banding, friction. The purpose of the present report is to describe the continuing task of coupling the unifying hot-spot model to hydrodynamic calculations to develop a mechanistic reactive burn model. The key components of the coupling include energy localization, the growth of hot spots, overall hot-spot behavior, and a phase-averaged mixture equation of state (EOS) in a Mie-Grüneisen form. The nucleation and growth of locally heated regions is modeled by a phenomenological treatment as well as a statistical model based on an exponential size distribution. The Mie-Grüneisen form of the EOS is one of many possible choices and is not a critical selection for implementing the model. In this report, model calculations are limited to proof-of-concept illustrations for shock loading. Results include (1) shock ignition and growth-to-detonation, (2) double shock ignition, and (3) quenching and reignition. A comparative study of Pop-plots is discussed based on the statistical model.

1. Introduction

Broadly speaking, three types of models are used to describe the shock-induced detonation of solid explosives. The first type, the most widely used approach, is built on the heuristic development of a progress variable such as reacted mass fraction and simplified equations of state for reactants and product mixture. In the simplest form, no distinction is even made between the reactant and the product. A single progress variable embedded in an equation of state and a hypothesized rate equation describe the entire transition from the initial to the terminal state (Fickett and Davis 1979). Often-referenced examples of this class are Forest Fire (Forest 1978), Lee-Tarver (Lee and Tarver 1980), and JTF (Johnson, Tang, and Forest 1985). Typically, these models do not discern hot spot mechanisms. If “hot spots” are mentioned in these models, they are used only empirically to reproduce certain characteristics such as shock-induced ignition temperature and induction time for global reactions. The second type, represented by Kang et al. (1992), Massoni et al. (1999), and Bennett et al. (1998), is an extension of the first type to include a microscopic description of the origin of hot spots, such as void collapse and frictional sliding. The evolution of reacted mass fraction is now modeled by simplified chemical kinetics occurring on the microscale. Our model in this report belongs to this class. The third class, the most complex existing model, is based on a multiphase continuum mixture theory (Baer and Nunziato 1987). In contrast, the first two types are designed for use with single-phase hydrodynamic equations. The complexity of the mixture theory is known to generate its own problems. Interested readers are referred to an excellent review article (Bdzil et al. 1999) for the discussions of the strength and weakness of models based on continuum mixture theory.

In our effort to develop a reactive burn model and its conceptual underpinnings, a conscious decision is made not to use a continuum mixture theory based on the first author’s experience during the early 1990s through his work on shock-induced inorganic powder mixtures (Horie 1993, 1993). A single-phase (phase-averaged) approach is chosen for two reasons. The first is the applicability of the model to existing codes that are based mostly on the single-phase hydrodynamic equations. The second is the desire to focus on a unifying hot-spot model in view of the fact that there is virtually no agreement as to the mechanism or mechanisms by which the macroscopic mechanical energy is localized (Field et al. 1992). As discussed in the first report (Yano et al. 2001), it is nearly inconceivable that any single mechanism, be it pore collapse, friction, shear banding, or jetting will be same over the wide-ranging loading conditions. Thus, attention is focused on the development of a unifying hot-spot model and a framework that incorporates key features of energy localization without introducing mechanism specific traits. In this approach, the kinematical issues of energy localization are transformed into the problem of finding appropriate parameter spaces that are consistent with mechanistic models. Details are referred to in the first report.

The primary objectives of the present work are (1) to build a conceptual framework to link the new hot-spot model and global, single-phase hydrodynamic calculations, (2) to develop a test model for the framework, and (3) to conduct proof-of-

concept calculations. The primary task is to develop a means to calculate the evolution of reacted mass fraction based on the unifying hot-spot model. This will require (1) a prescription for energy localization (hot-spot initiation and growth), (2) a means to aggregate a group of growing hot spots, (3) the calculation of reacted mass fraction, and (4) the overall mixture equations of state. A realization of the bridge described in this report is strongly dependent on the structure of the hot-spot model. In fact, the kinematically neutral feature of the model will play an important role.

The balance of the report is as follows. Section 2 discusses the basic concepts and assumptions involved in constructing the bridge. Section 3 describes the mathematical model based on the choice of RDX as a test case. The reason for this choice is nothing but historical, and HMX and other materials will be considered in the next phase of the work. Section 4 describes proof-of-concept calculations under the condition of symmetric impact.

2. Basic Concepts

We first review the conceptual structure of a single hot spot represented by the unifying model. Understanding of this structure, as illustrated in Fig. 1, is important in the subsequent discussion of connecting a group of hot spots to hydrodynamic calculations. However, details of the hot-spot model are referred to in the report, LA-13794-MS (Yano et al. 2001).

2.1 Structure of the Unifying Hot Spot

The structure of the unifying hot spot is planar and based on the abstraction of a representative unit section for the three primary origins of hot-spot formation: spherical void collapse, shear banding, and frictional sliding. Figure 1 is a schematic illustration of this structure. Key features of this ‘abstract’ model are a finite region of localized heating surrounded by material with a lower or zero heating rate; the existence or creation of a space within the heating zone that is occupied by gases; heat flow between the regions; and reaction chemistry within the gas, at the gas-solid interface, or both. We note that the same structure will result if a spherical pore model is made into a planar structure by splitting it into two halves and flattening them along the opened sections (Yano et al. 2001). The void space in this model could be viewed as a space in or between explosive grains or an unbonded interface between binder and explosive crystals. But, we will not interpret the space based on any specific situation in this first treatment. As is the case for the deformation mechanisms, we use the void as a mathematical entity rather than a physical one based on any specific geometry. What is important, if not the most important in this abstraction, is that attention is shifted from “hot spots (volume-like)” to “gas-producing, hot interfaces” of locally heated regions.

2.2 Framework of the Overall Linkage

In order to couple the above described hot-spot model to global hydrodynamic calculations, we need to develop three links (models). They are

- (a) A model of heterogeneous energy localization that converts the global energy dissipation into localized heating. The localization activates hot spots, and when sustained, the heating results in chemical ignition at the appropriate conditions of pressure and temperature.
- (b) A model of aggregating the effects of distributed hot spots (reacting surfaces) and capturing the essential features of their evolution. For most applications it is expected that computational volumes used for hydrodynamic calculations are larger than the typical size of a hot spot (on the order of 0.1 to 10 μm , Field et al. 1992). Therefore, it is essential to develop a means or a model to effectively describe the overall effects of distributed hot spots. It is not practical to keep track of individual hot spots and their history.
- (c) An equation of state (EOS) for the overall gas/solid mixture. Because hydrodynamics is based on the phase-averaged formulation, an EOS for the two-phase mixture is required to calculate the overall pressure. We adopt a simple approach in which velocity equilibrium is assumed between the product gas and the solid.

Figure 2 shows a schematic structure of the needed linkages in a modular form. The most difficult task in this chart is the micromechanical modeling of energy localization and reactive surface evolution. This difficulty is attributed in part to the fact that unlike the subject of EOS, there is not yet a definitive physical concept, nor a mathematical method that links the complex, heterogeneous microscopic events and the macroscopic hydrodynamic equations. They are path dependent on locally evolving structures as well as on state functions. The ultimate solution will probably require a new approach that does not belong to any of the existing methods. Models must be simple enough to be manageable for practical computer calculations, but complex enough to describe the collective essence of microscopic events. Existing micromechanical studies are often focused on the simulation of phenomenology at the grain level to gain insights into the nature of complex events (e.g., Menikoff and Kober 1999). They have not yet resulted in the development of explicit models that are based on the understanding gained through such studies. The sole exception to the above observation is Baer (2002). He proposes the use of stochastic dynamics involving probability distribution functions that are synthesized by image analysis of 3-D simulation results.

What we propose in this report is a simple, interim solution, taking the advantage of the structure of the new hot-spot model and the fact that energy localization is represented by a proper choice of parameter space. The new approach will include a statistical consideration of a distribution function for hot-spot size.

Fig. 1. Unifying hot-spot model for the three key mechanisms of energy localization. Idealized features are a finite region of localized heating surrounded by material with a lower or zero heating; the existence or creation of a space within the heating zone occupied by gases; heat flow between the regions; and reaction chemistry within the gas and at the gas-solid interface. Energy localization is modeled parametrically by the size of the heating region and a model for heating rate.

Fig. 2. Schematic diagram of modules for linking the new hot-spot model to a hydrodynamic code. The micromechanics of energy localization and evolving reactive surfaces control the evolution of the super (aggregated) hot-spot model. The latter in turn provides the fraction of mass reacted for hydrodynamic calculations. Given the reacted mass, the mixture equation of state calculates the pressure and the internal energy necessary for advancing an overall time step.

2.3 Energy Localization and Reacting Surface Evolution

In the new burn modeling, hot spots are parametrically specified in terms of global variables such as the rate of mechanical energy dissipation. We shall show two specific demonstrations of this prescription in the next section. The first is a heuristic model that specifies the mass (or volume) of locally heated regions, and the second is based on an assumed distribution of hot-spot size and its evolution.

The construction of a model depends critically on the idealization illustrated in Fig. 3 where we assume that hot spots can be aggregated without distinguishing the stages of individual evolution. This is a severe simplification, but we find it necessary at this stage of model development. Similar idealizations are used in other attempts where identical hot spots are multiplied by the density of identical hot spots to represent the whole (see for example, Massoni et al. 1999). There is, however, one important difference in that in our modeling, the aggregation of hot spots is imagined in terms of reacting surface areas. This difference will be described below.

Using the framework shown in Fig. 3, we first gather reacting hot regions into a mixture of gas and solid separated by locally heated thin regions. The area of this crimped surface (F_A) represents the sum total of reacting hot surfaces in an effective sense. This step is similar to one where crack volumes are summed to calculate the effect of distributed cracks on elastic properties (Addessio and Johnson 1990). Implicitly assumed in this step are (1) that once formed, hot spots are identical with a possible exception of size, (2) that intermediate steps in forming hot spots are not significant in burn calculations, and (3) gas-phase reactions in the reservoir are uniform and dependent only on the current state. If one must recognize the properties of individual hot spots, the modeling of their overall behavior becomes an exceedingly difficult task, to say the least.

Secondly, we map the curved, reacting surface onto a super hot spot having a unit (for one dimensional problems) cross section in such a way that the motion of unit plane section represents the “average” motion of the curved surface. Again, no distinction is made between old and new surfaces. This mapping (discussed later in mathematical terms) essentially defines the way we deal with the overall effects of distributed hot spots. It consists of two components. The first is the magnification of transport processes across the unit area to describe the overall effect. The second is an adjustment of the rate of energy deposition to account for the fact that the locally heated area is time dependent and that the unit section must represent the average behavior. These two scalings transform the motion of the flame front for the unit surface into the average motion of the crimped, collective surface.

Fig. 3. Schematic illustration of modeling the collective essence of distributed hot spots. The first step is to visualize the volume with hot spots as a two-phase medium separated by a single reactive area. Then we map the rate of localized heat deposition and other transport fluxes onto a unit cross section to create an effective, super hot-spot for the volume element. Hot areas are shown by their cross sections. Active areas are normal to the cross section.

The role of the area factor F_A is similar to that of the reacted mass fraction. We use it to represent an integrated effect of underlying complex heterogeneous events through a single variable. We may determine this variable through a system of rate equations, or we may simply hypothesize a function based on process parameters and/or local microstructure. This means that the effect of heterogeneities in starting materials may be dealt with by a proper selection of F_A and its parameters. However, in this report we shall not make any specific distinction of explosive compositions in terms of F_A . We shall develop the framework for burn modeling without specifying the microstructure of explosives: e.g., PBX, a porous explosive without binder, a solid explosive, etc. Although RDX will be used for a test case, it is best considered as a generic model explosive.

Obviously, the constitutive determination of F_A will ultimately require an approach that involves differential equations. In our first attempt, however, we will try an educated guess that F_A is an analytic function of such quantities as dissipated energy, its rate of deposition, and the volume fraction of mass reacted. Subsequently we will propose a statistical treatment of F_A involving a distribution function for hot-spot size and a hypothesized evolution equation. Specific expressions are discussed in the next section. We speculate that because F_A can be made to include the cell size for hydrocalculations, this parameter may be used to develop a reactive burn model that is independent of computational cell size.

In summary, a super hot-spot cell (and its multiples, if necessary) is created through the use of F_A , which is equivalent to a global hydrodynamic volume. The difference between a local hot-spot and the super hot-spot is the rate of localized heating and the mass and heat transfer across the unit cross section. The quantities for the super hot-spot signify those for the volume of global calculation, normalized to a unit cross section. The super hot-spot cell generates the overall degree of reaction for global calculations.

A prototype mathematical interpretation of both F_A and the localized heating is discussed in the next section. It will be done phenomenologically first and then through use of an exponential distribution function for hot-spot size.

2.4 Mixture Equations of State

The third task of developing the global mixture equations of state is no less easier than the first two, but there are many models available (compared with the first two) due in part to the fact that phase averaging and the assumption of local thermomechanical equilibrium provides a reasonable physical basis. If necessary, a tabular form of EOS may be used to improve model accuracy in a piecewise fashion.

In the current phase of our work, a standard treatment based on phase averaging is used to determine the mixture equations of state for the product gas and the solid. Details are seen in the next section through use of the form of Mie-Grüneisen equations of state.

3. Mathematical Model

In this section we discuss a prototype interpretation of the conceptual model of energy localization and the evolution of reacting surfaces that are illustrated in Fig. 3. It is important to note that within the framework shown in Fig. 2 there are other mathematical models one can construct without altering the structure of the hot-spot model, and what follows is the first attempt to assemble the entire module of the structure as shown in Fig. 2. Thus, the mathematical model of the hot-spot remains the same as that reported in Yano et al. (2001) and will not be discussed here. But, they are summarized in Appendix C for completeness.

3.1 Hydrodynamic Equations

In this report, hydrodynamic calculations are limited to solving the 1-D Lagrangian equations for the conservation of mass, momentum, and energy, using a standard artificial viscosity. We list them below in plane geometry for reference:

$$\frac{\partial u}{\partial t} = -\frac{1}{\rho_o} \frac{\partial}{\partial X} (P + Q), \quad (3.1)$$

$$\frac{\partial v}{\partial t} = \frac{1}{\rho_o} \frac{\partial u}{\partial X}, \text{ and} \quad (3.2)$$

$$\frac{\partial e}{\partial t} = -(P + Q) \frac{\partial v}{\partial t}, \quad (3.3)$$

where u is particle velocity, $v = 1/\rho(\text{density})$, P is normal stress, and Q is the artificial viscosity given by

$$Q = -\frac{k_1 c \Delta X}{v} \left(\frac{\partial u}{\partial X} \right) + \frac{k_2 (\Delta X)^2}{v} \frac{\partial u}{\partial X} \frac{\partial u}{\partial X}, \left(\frac{\partial u}{\partial X} \leq 0 \right), \quad (3.4)$$

$$= 0, \left(\frac{\partial u}{\partial X} \geq 0 \right).$$

If P is assumed to be hydrodynamic, then the above system of equations will be closed by specifying a thermodynamic equation of state. A simple example is the case where P is known as a function of density and internal energy: $P = f(\rho, e)$. The order of numerical computations proceeds from Eqs. (1.1) to (1.3) where Eq. (1.3) is solved with the equation of state. Similarly, the role of the new hot-spot model in this study will be viewed as that of an equation of state for the reason that will be explained in the next section. The function of the model is to provide new pressures to advance time in hydrodynamic calculations. More general cases where P contains a shear component will

not be considered in this phase of the work. It is felt that a selection of particular constitutive equations to describe the shear behavior will further complicate the burn modeling and may become a detraction from the main theme of the report.

3.2 Energy Localization and Normalized Heat Flux

We develop a model for the energy localization link by adopting a picture similar to that of shear bands that are often proposed for the formation of hot spots (Afanas'ev and Bobolev 1971, Heavens and Field 1974, Mader 1979, Frey 1981, Hayes 1983). In this treatment we closely follow the approach used by Kipp (1987) with one important difference discussed below.

The Kipp approach is phenomenological and involves several *ad hoc* assumptions. The first is that there is a single, representative hot region per hydrodynamic cell in some statistical sense and that all the mechanically dissipated energy at the macro level is channeled into this hot spot. In principle, one can partition the energy more precisely, but such a complication is not warranted in the initial, scoping attempt. The second is that the globally dissipated energy comes from the energy associated with the artificial viscosity (Q). This quantity is a computational artifact, but it has all the necessary attributes of energy dissipation occurring during shock compression. We adopt the same approach for expediency. Mathematically, the replacement of the energy associated with Q by other mechanisms is straightforward. The third is that the growth of the hot region is proportional to the dissipated energy.

The use of Q raises a well-recognized question about the cell size dependency of hydrodynamic calculations, but it will equally apply to other types of energy modeling. In our calculation, cell size will be chosen so that shock-wave calculations are considered physically resolved except for the question of Q . This aspect of reactive burn modeling will be examined in the next phase of the work when we consider a mechanics-based modeling of global energy dissipation.

Let $\dot{E}_d$ signify the total rate of energy dissipation per hydrodynamic cell based on the artificial viscosity. Then,

$$\dot{E}_d = \Delta x (\dot{\rho} / \rho) Q, \quad (3.5)$$

where Δx is the width of a hydrocell, ρ is the density of the cell, Q is the artificial viscosity force, and “ $\dot{}$ ” signifies the time derivative. Following Kipp, we assume that this energy is channeled into the hot region having an area F_A (the cross section of this area is shown in Fig. 3) and width δ . Then, the rate of energy channeled into the region of localized heating (Φ_{hs}) is

$$\Phi_{hs} = \dot{E}_d / (\delta F_A), \quad (3.6)$$

where the term (δF_A) is the volume of locally heated material. We emphasize again that this is a heuristic model that needs to be modified as we gain a better understanding of the dynamics of energy localization in heterogeneous materials. For strong shocks, however, it may be justified on the ground that the volume of localized heating becomes comparable to the size of the hydrodynamic cell, and there is little “cold” material left. Ultimately, this function may have to be replaced by differential equations involving constitutive behavior and microstructure parameters.

Although all the globally dissipated energy is channeled into the hot-spot region, the total rate of energy deposition cannot be used for the overall (super) hot-spot model. It needs to be “mapped” onto a unit cross section in proportion to the growth of the hot region (area). We show, in what follows, an energy argument for this mapping that is explicitly based on F_A .

Suppose now that the localized heating is adiabatic to the first approximation under shock loading. Then, the terminal temperature of the total hot region, T , may be approximated by

$$\rho_s \delta F_A C_v (T - T_o) = \int_0^t \delta F_A \Phi_{hs} d\tau , \quad (3.7)$$

where ρ_s is the density of the solid, C_v is its specific heat, T_o is the initial temperature, and ρ_s and C_v will be assumed constant. A similar equation holds for the hot region having a unit cross section.

$$\rho_s \delta C_v (\hat{T} - T_o) = \int_0^t \delta \hat{\Phi}_{hs} d\tau , \quad (3.8)$$

where the hat “ $\hat{}$ ” signifies the quantity associated with the hot sheet having a unit cross section. If the latter represents the average behavior of the arbitrarily shaped hot region, the terminal temperatures must be equal. Thus, equating Eqs. (3.7) and (3.8), one finds

$$\hat{\Phi}_{hs} = \frac{d}{dt} \left\{ \frac{\int_0^t \delta F_A \Phi_{hs} d\tau}{\delta F_A} \right\} . \quad (3.9)$$

Upon substituting Eq. (3.6) into Eq. (3.9), one obtains

$$\hat{\Phi}_{hs} = \frac{d}{dt} \left\{ \frac{E_d}{\delta F_A} \right\} , \quad (3.10)$$

where it is assumed that δ is constant. A more general derivation without the assumption of constant δ is given in Appendix A.

Another useful equation is obtained by the use of a specific quantity for the energy dissipation.

$$\hat{\Phi}_{hs} = \frac{d}{dt} \left\{ \frac{M \varepsilon_d}{\delta F_A} \right\} = M \frac{d}{dt} \left\{ \frac{\varepsilon_d}{\delta F_A} \right\} , \quad (3.11)$$

where ε_d is the energy dissipation per unit solid mass of the hydrodynamic cell and M is the total mass for the cell. Because δ is fixed, the above equation becomes

$$\hat{\Phi}_{hs} = \frac{M}{\delta} \frac{d}{dt} \left\{ \frac{\varepsilon_d}{F_A} \right\} . \quad (3.12)$$

An alternative expression of Eq. (3.12) that is similar in form to the equation Kipp used may be found by replacing δF_A with the mass fraction of the hot material. The resulting equation is

$$\hat{\Phi}_{hs} = \rho_s \frac{d}{dt} \left(\frac{\varepsilon_d}{\lambda_{hs}} \right) , \quad (3.13)$$

where λ_{hs} is the mass fraction of the hot material and is defined by

$$\lambda_{hs} = \rho_s F_A \delta / M = F_A / F_N , \quad \text{and} \quad (3.14)$$

$$F_N = M / \delta \rho_s .$$

Recalling the definition of M , one finds

$$F_N = \Delta x / \delta , \quad (3.15)$$

where Δx is the width of a hydrocell. Equations (3.14) and (3.16) suggest that the growth of reacting surfaces may be viewed as if ‘‘hot plates’’ are stacked in parallel in the thickness direction. F_N will then be the total cross-sectional area of the plates at which the whole cell will be subjected to localized heating. In general, however, F_N is influenced by such factors as microstructure and other material-related parameters.

3.3 Area Factor F_A

In the derivation of Eq. (3.13), emphasis is placed on the similarity of our analysis to that of Kipp. However, it is important to note one difference between the two models. That is, in the latter, thermochemistry is described primarily in terms of volumetric quantities such as λ_{hs} , and the burning rate does not involve the morphology of hot spots explicitly. In our model, the formulation of an overall combustion rate anticipates the introduction of such factors as hot-spot statistics as well as the morphology. Volume fraction varies from 0 to 1, but there is no such bound for reacting surface areas in any

given volume. Thus, disparate speeds between ordinary combustion and detonation are described in terms of the areal magnifying factor F_A . The density of hot spots will work in a similar fashion, but the focus is different. In what follows we shall illustrate the actual construction of F_A in two different ways: heuristic and statistical approaches.

3.3.1 Heuristic Model

A phenomenological construction is based on (1) the observation that the scaling factor F_N signifies the maximum area of “hot plates,” having width δ , that can be created in a hydro cell, and (2) the assumption (after Kipp 1987) that λ_{hs} is a monotonically increasing function of E_d bounded by the minimum energy required to initiate energy localization and the total dissipated energy at CJ pressure (or von Neumann peak-pressure). F_A assumes a minimum value at the initial state and the saturation value of $\Delta x / \delta$ at a maximum energy when the entire material becomes a hot region. We hypothesize that λ_{hs} is represented by

$$\lambda_{hs} = F_A / F_N = \frac{\lambda_m \frac{\epsilon_d}{\epsilon_N}}{1 - \lambda_m \left(1 - \frac{\epsilon_d}{\epsilon_N}\right)^n}, \quad (3.16)$$

where λ_m is a parameter that controls the maximum value of λ_{hs} . That is, not all of the solid needs to become hot spots at the maximum dissipated energy ϵ_N at which the mass fraction reaches the maximum value. The current choice of ϵ_N , again following Kipp, is the dissipated Hugoniot energy of the unreacted energetic material at CJ pressure.

Upon substitution of Eq. (3.16) into Eqs. (3.13) and (3.14), it is easily found that

$$\hat{\Phi}_{hs} = n \rho_s \left(1 - \frac{\epsilon_d}{\epsilon_N}\right)^{n-1} \dot{\epsilon}_d, \text{ and} \quad (3.18)$$

$$F_A = \frac{\lambda_m F_N}{1 - \lambda_m \left(1 - \frac{\epsilon_d}{\epsilon_N}\right)^n} \left(\frac{\epsilon_d}{\epsilon_N}\right). \quad (3.19)$$

Combining Eqs. (3.8), (3.13), and (3.16), one finds an analytical solution for the adiabatic heating of the hot material.

$$\Delta T = \Delta T_f \left[\left(\frac{\zeta}{\lambda_{hs}}\right) - \left(\frac{\zeta}{\lambda_{hs}_o}\right) \right] = 1 - \left(1 - \frac{\epsilon_d}{\epsilon_N}\right)^n, \quad (3.20)$$

where

$$\Delta T_f = \varepsilon_N / C_V , \quad (3.21)$$

$$\zeta = \varepsilon_d / \varepsilon_N ,$$

$$\left(\frac{\zeta}{\lambda_h} \right)_0 = \frac{1 - \lambda_m}{\lambda_m} . \quad (3.22)$$

If $(\varepsilon_d / \varepsilon_N) \ll 1$, then

$$\Delta T = \Delta T_f n \frac{\varepsilon_d}{\varepsilon_N} . \quad (3.23)$$

Equation (3.20) suggests a physical basis for the selection of ε_d . This equation is different from that of Kipp where the initial temperature of the hot material is shown to be independent of the loading strength. But as shown in Eq. (3.23), our model allows a finite rise time for the heating of hot spots.

In the current model, the area factor contains one additional parameter that controls a smooth termination of combustion. Physically it is similar to the change in the mode of combustion from burning in a cavity to grain burning in gas. Without such a control, a discontinuous change in $\dot{m}$ at the exhaustion of solid material is found to cause numerical problems. The current form of this factor, F_G , is given by

$$\begin{aligned} F_G &= 1 & (0 \leq \varphi_g \leq \varphi_1) , \\ &= 1 - a_1 (\varphi_g - a_2)^2 & (\varphi_1 < \varphi_g \leq \varphi_2) , \\ &= \left(\frac{1 - \varphi_g}{1 - \alpha} \right)^{2/3} & (\varphi_2 < \varphi_g \leq 1) , \end{aligned} \quad (3.22)$$

where φ_g is the volume fraction of product gas (see Appendix C), φ_1 signifies the onset of the switch, and φ_2 is the end of a smooth parabolic fit to a function that represents the volume fraction of spherical particles. Specifically, they are

$$\begin{aligned} \varphi_1 &= a_2 , \\ \varphi_2 &= 1 - (1 - \alpha) \beta^{3/2} , \\ a_1 &= [9(1 - \alpha)^2 \beta (1 - \beta)]^{-1} , \\ a_2 &= 1 - (1 - \alpha) (3 - 2\beta) \beta^{1/2} , \end{aligned} \quad (3.23)$$

where α and β are input parameters for F_G .

In summary, the overall mass production across the equivalent unit cross section is scaled by the following expression:

$$\dot{m}_{\text{all}} = F_A(\epsilon_d, \dots) F_G \dot{m}, \quad (3.24)$$

where $\dot{m}$ represents the mass production of gas due to intrinsic chemical reactions across the unit cross section of the super hot-spot. The symbol F_A is now a dimensionless magnitude of the area F_A . Heat conduction is only affected by the magnitude of F_A .

We emphasize again that Eq. (3.16) is an ad hoc function and needs to be modified for a better description of the physics of energy localization. Ultimately, the task may require a set of differential equations that describes the process in a stochastic fashion. As an interim solution, a statistical interpretation of F_A is given in the next section. A more advanced statistical treatment of energy localization and hot-spot growth remains a future challenge. Nevertheless, it is worth noting that Eqs.(3.5-3.24) are already in a form that can be readily manipulated for probabilistic analysis. In fact, they can be looked upon as those for an integrated distribution as shown in the next section.

3.3.2 Statistical Model

What follows is an attempt to improve the phenomenological treatment of energy localization by use of a distribution function for locally heated regions in the spirit of S. Cochran (1980). Following Cochran, we hypothesize a size distribution for energy localization along with the equations that evolve the distribution in time. However, in contrast to his model, the evolution equations do not contain hot-spot sinks resulting from thermal diffusion and the loss due to chemical explosion. In our model, these processes are treated mechanistically by the new, unifying hot-spot model. What we borrow from the Cochran approach is the handling of locally heated regions at “heterogeneities” that translate the globally dissipated energy into the locally heated sites. His notation is followed as closely as possible. The model consists of three basic components.

A. Size Distribution

We assume an exponential function,

$$f(r) = \frac{N_o}{r_o} \exp\left[-\frac{r}{r_o}\right], \quad (3.25)$$

where N_o is the total number of locally heated sites and r_o is the average size. This is an ad hoc assumption, but there are studies that suggest exponential functions as a reasonable choice. For example, the distribution of localized stress bridging in a granular material is found to follow an exponential distribution (Bardenhagen et al. 2000). Also, the distribution of microcracks seems to follow a similar pattern (Curren et al. 1987 and Margolin 1982).

B. Rate of Source Production

The rate of source production is thought to be a function of such parameters as r and hydrodynamic variables. But we have very little understanding of an actual rate in terms of process parameters as well as microstructure. So we follow Cochran again. But in our approach we prefer the rate of energy dissipation as the controlling parameter in place of the rate of relative compression used by Cochran.

Let $S(r, t)$ be the source of locally heated regions per cm^3 near size r at time t . Then, the rate of the source production is assumed to be

$$\dot{S} = \frac{\dot{\epsilon}_d}{\epsilon_d^0} f(r) \left(1 - \xi \frac{\frac{4\pi}{3} \langle S r^3 \rangle}{S_{\max}} \right), \quad (3.26)$$

where ϵ_d^0 is a normalizing constant, ξ is a parametric constant that controls growth, and the symbol $\langle \dots \rangle$ represents

$$\langle M r^n \rangle = \int_0^\infty M r^n dr, \quad (3.27)$$

and $S_{\max}$ represents the total volume of hot spots per unit volume and is given by

$$S_{\max} = \int_0^\infty \frac{4\pi}{3} f(r) r^3 dr = 8\pi N_o r_o^3. \quad (3.28)$$

We considered an exponential function for $\dot{S}$ that can be manipulated analytically, but results showed no qualitatively significant difference in behavior.

There is some indication that the production of locally heated regions is a function of strain rate (Hayes and Grady 1981). But in our initial attempt, the rate of energy dissipation is chosen to follow the formulation of Kipp (1987). The primary goal was to demonstrate a framework in which we can provide a statistical interpretation of the mass fraction λ_{hs} discussed in Section 3.3.1.

C. Closure of the Rate Equation

The closure to solve for S is given by the assumption that separates the variables.

$$\frac{d}{dt} \langle S r^3 \rangle = \langle \dot{S} r^3 \rangle. \quad (3.29)$$

This can be integrated to give the fraction of mass for hot spots per unit volume. But in observance of Eq. (3.16), we again introduce a parameter λ_m to specify the maximum fraction of hot spots. But its meaning is not identical to that for Eq. (3.16). Here λ_m is associated with unit volume,

$$\lambda_{hs} = \lambda_m \frac{\frac{4\pi}{3} \langle Sr^3 \rangle}{S_{max}} . \quad (3.30)$$

Then, (3.29) can be integrated to give

$$\lambda_{hs} = \frac{\lambda_m}{\xi} \left[1 - \alpha \exp \left(-\xi \frac{\epsilon_d}{\epsilon_d^o} \right) \right] , \quad (3.31)$$

where α is an integration constant. The boundary values that are useful for specifying the constants are

$$\lambda_{hs}(0) = \frac{\lambda_m}{\xi} (1 - \alpha) , \quad \text{and} \quad (3.32)$$

$$\lambda_{hs}(\epsilon_d^o) = \frac{\lambda_m}{\xi} (1 - \alpha \exp(-\xi)) . \quad (3.33)$$

A reasonable condition on the upper boundary is to impose

$$\lambda_{hs}(\epsilon_d^o) = \lambda_m , \quad (3.34)$$

where ϵ_d^o can again be interpreted as the energy associated with the CJ pressure or some such measure. Then, upon substitution of Eq. (3.34) into Eq. (3.33), one finds

$$\xi = 1 - \alpha \exp(-\xi) . \quad (3.35)$$

To further narrow the range of the constants, it is useful to evaluate the total deposited heat over time. That is,

$$H_{hs} = \int_0^t \bar{\Phi}_{hs} dt = \int_0^t d \left(\frac{\epsilon_d}{\lambda_{hs}} \right) = \rho_s \left[\left(\frac{\epsilon_d}{\lambda_{hs}} \right) - \left(\frac{\epsilon_d}{\lambda_{hs}} \right)_o \right] , \quad (3.36)$$

where the last expression is given by

$$\left(\frac{\varepsilon_d}{\lambda_{hs}} \right)_o = \frac{\varepsilon_d}{\frac{\lambda_m}{\xi} \left[1 - \alpha \exp \left(-\xi \frac{\varepsilon_d}{\varepsilon_d^o} \right) \right]} . \quad (3.37)$$

According to Eq. (3.32), there are two possible cases, depending on the value of α and the assumption about existing nucleation sites for hot spots. That is, if there are no preexisting sites (initiation sites), then $\alpha = 1$ and $\lambda_{hs}(0) = 0$. They in turn will imply by Los'pital's rule that

$$\left(\frac{\varepsilon_d}{\lambda_{hs}} \right)_o = \frac{\varepsilon_d^o}{\alpha \lambda_m} .$$

Upon substitution into Eq. (3.36), one finds

$$H_{hs} = \frac{\xi \rho_s}{\lambda_m} \frac{\varepsilon_d}{\left[1 - \alpha \exp \left(-\xi \frac{\varepsilon_d}{\varepsilon_d^o} \right) \right]} - \frac{\rho_s \varepsilon_d^o}{\alpha \lambda_m} .$$

Then, by use of Eq. (3.35), one obtains the condition

$$H_{hs}(\varepsilon_d^o) = 0 .$$

This is not physically admissible because it implies that there was negative flux during loading. On the other hand, if $\alpha < 1$, then

$$\left(\frac{\varepsilon_d}{\lambda_{hs}} \right)_o = 0 , \quad \text{and}$$

$$H_{hs} = \frac{\xi \rho_s}{\lambda_m} \frac{\varepsilon_d}{\left[1 - \alpha \exp \left(-\xi \frac{\varepsilon_d}{\varepsilon_d^o} \right) \right]} , \quad (3.38)$$

where the constants are interrelated by Eqs. (3.32) and (3.35). Now Eq. (3.32) implies that there are preexisting hot spots (nucleation sites). At the upper boundary where $\varepsilon_d = \varepsilon_d^o$, one finds

$$H_{hs}(\varepsilon_d^o) = \frac{\rho_s \varepsilon_d^o}{\lambda_m} . \quad (3.39)$$

Note that this expression produces a result similar to Eq. (3.20) under the adiabatic condition. However, the meaning of λ_m in the statistical interpretation is not identical to that for the heuristic model. The latter is just an adjusting parameter that fixes the upper boundary for λ_m . The former is a scaling parameter for energy localization and is required to satisfy the consistent upper boundary condition.

Finally, substituting Eq. (3.31) into Eq. (3.13), one obtains

$$\hat{\Phi}_{hs} = \frac{\rho_s \xi \dot{\epsilon}_d}{\lambda_m} \frac{1 - \alpha \left(1 + \frac{\xi \epsilon_d}{\epsilon_d^o} \right) \exp \left(-\xi \frac{\epsilon_d}{\epsilon_d^o} \right)}{\left[1 - \alpha \exp \left(-\xi \frac{\epsilon_d}{\epsilon_d^o} \right) \right]^2} . \quad (3.40)$$

For small ϵ_d/ϵ_d^o , it may be shown that

$$\hat{\Phi}_{hs} = \frac{\rho_s \dot{\epsilon}_d}{\lambda_o} ,$$

where $\lambda_o = \lambda_{hs}(0)$. This now explains why the constant ‘n’ in Eq. (3.16) required the magnitude on the order of 50 to 100 for shock ignition. Physically, the quantity $(1/\lambda_o)$ expresses the degree of localization. Therefore, the initiation sites of a few percents correspond to n of 50 to 100.

For F_A we will retain Eq. (3.13) with the understanding that F_N is no longer tied to the morphology used to obtain Eq. (3.16). At present it is considered a free parameter whose magnitude is comparable to that given by Eq. (3.16). Currently we are considering a model where F_A is calculated based on a statistical interpretation.

Numerically, the determination of the constants requires the estimates of $\lambda_{hs}(0)$ and λ_m , i.e., a measure of nucleation sites in the starting material, and a maximum volume fraction of hot spots at the CJ pressure or some such measure. Once we have the estimates, α and ξ are calculated from Eqs. (3.32) and (3.35).

3.4 Mixture Rule and Equations of State

The treatment of the mixture EOS is not as tentative as those for energy localization. Here we will follow the formulation by Massoni et al. (1999). We believe that their formulation will be useful in their basic form even for advanced models. Their formulation involves two assumptions. The first is that the mixing rule for mass, momentum, and internal energy is based on the mass fraction. For example, the mixture density ρ and internal energy e are related to those of constituents by

$$\rho = \phi_g \rho_g^{hy} + (1 - \phi_g) \rho_s^{hy} , \quad \text{and} \quad (3.41)$$

$$\rho e = \phi_g \rho_g^{\text{hy}} e_g + (1 - \phi_g) \rho_s^{\text{hy}} e_s , \quad (3.42)$$

where ϕ_g is the volume fraction of product gas, and the subscripts g and s denote gas and solid, respectively. Superscript “hy” is used to underline the need for a careful consideration of kinematics between the hot-spot model and the hydro code. If we impose the fact that the volume fraction in the above equation is the same as that of the super hot spot (defined by the ratio (a/c)), then mass conservation for each phase requires that

$$\rho_g^{\text{hy}} = (c / \Delta x) \rho_g^{\text{hs}} = (c / \Delta x) \overline{\rho_g} , \quad \text{and} \quad (3.43)$$

$$\rho_s^{\text{hy}} = (c / \Delta x) \rho_s (\text{hot spot}) = (c / \Delta x) \rho_s , \quad (3.44)$$

where ρ_s^{hs} for the hot spot is equated as that used in the previous section, $\overline{\rho_g}$ is the average gas density, and its derivation is given in Appendix B. We do not require the same distinction for the internal energies for the reason explained below.

The second assumption is that the EOS for each phase can be written in the Mie-Grüneisen form,

$$P = \Gamma \rho e + P^* , \quad (3.45)$$

where P^* is a function of density only. Then it is known that the assumption of partial pressure equilibrium leads to the mixture pressure in the same form (Massoni et al. 1999) in which Γ and P^* are related to constituent quantities by

$$1/\Gamma = \phi_g / \Gamma_g + (1 - \phi_g) / \Gamma_s , \quad \text{and} \quad (3.46)$$

$$P^* = \Gamma [\phi_g P_g^* / \Gamma_g + (1 - \phi_g) P_s^* / \Gamma_s] . \quad (3.47)$$

This means that because the internal energy is determined by the conservation equation (3.3), the mixture pressure is determined, if the volume fraction of the gas and the density of each phase are known. That is, a combination of Eqs. (3.43) and (3.44), and the definition that

$$\phi = a / c \quad (3.48)$$

closes the system equations.

What is not resolved at present is that the EOS for chemical processes in the hot-spot model is not the same as that for the overall equation of state. The former is used only to drive combustion in the hot-spot model. This disparity is created by the requirement that for the hot-spot, the equation of state for each individual chemical species is needed. On the other hand, hydrocalculations can be based on overall EOS.

In evaluating the mixture quantities, it is important to recognize that the hot-spot model supplies both ϕ_g and ρ_g^{hs} . These quantities are influenced primarily by $\dot{m}_{\text{all}}$, the motion of solid, and bulk reactions in the gas reservoir. The solid density is then determined by Eq. (3.41) in which the mixture density ρ is supplied by hydrodynamics. Similarly, the mixture internal energy in Eq. (2.29) is determined by hydrocalculations.

What follows is a discussion of EOSs that are currently used in the mixture calculation. Because e comes from hydrocalculations, what is required is P^* for each phase.

3.4.1 Solid EOS

We begin with the Mie-Grüneisen form,

$$P_s - P_r = \frac{\Gamma_s}{V_s} (e_s - e_r) , \quad (3.49)$$

where $V_s = 1/\rho_s^{\text{hy}}$, and introduce the Hugoniot state defined by a linear particle and shock-velocity relationship for the reference state. That is,

$$P_r = P_H = P_o + K_{\text{so}} \frac{\eta}{(1 - s\eta)^2} , \quad \text{and} \quad (3.50)$$

$$E_r = E_H = E_o + \frac{1}{2} (P_H + P_o)(V_o - V_s) , \quad (3.51)$$

where

$$\begin{aligned} \eta &= 1 - V_{\text{sb}}/V_o , \\ K_{\text{so}} &= \rho_{\text{so}} C_o^2 , \text{ and} \\ C_o^2 &= \text{the adiabatic sound speed at standard conditions.} \end{aligned} \quad (3.52)$$

Now comparing Eq. (3.45) and Eq. (3.51), and substituting Eqs. (3.49) and (3.50), one finds that

$$\begin{aligned} P_s^* &= P_H - \frac{\Gamma_s}{V_s} e_h \\ &= \left[P_o + K_{\text{so}} \frac{\eta}{(1 - s\eta)^2} \right] \left[1 - \frac{\Gamma_s}{2} \frac{\eta}{1 - \eta} \right] - \left[\frac{\Gamma_s}{1 - \eta} \right] \left[\frac{E_o}{V_o} + \frac{\eta}{2} P_o \right] . \end{aligned} \quad (3.53)$$

If, as commonly assumed, $\Gamma_s/V_s = (\Gamma_s/V_s)_o$, then

$$P_s^* = [P_o + K_{so} \frac{\eta}{(1-s\eta)^2}] [1 - \frac{\eta}{2} \Gamma_o] - \Gamma_o [\frac{E_o}{V_o} + \frac{1}{2} \eta P_o] . \quad (3.54)$$

3.4.2 EOS for the Product Gas

We adopt a high-temperature Mie-Grüneisen EOS discussed in Lemons and Lund (1999). If the composition is fixed and the specific heat were assumed constant, then in general

$$e = C_v T + E_o - C_v T_o , \text{ and} \quad (3.55)$$

$$P_g = \frac{\Gamma_g}{V_g} e_g + P_g^*(V_g) , \quad (3.56)$$

where C_v and E_o are mass-averaged quantities defined by

$$\begin{aligned} C_v &= \sum Y^k C_v^k , \\ E_o &= \sum Y^k E_o^k , \text{ and} \\ V_g &= 1 / \rho_g^{\text{hy}} . \end{aligned} \quad (3.57)$$

Then assuming the Mie-Grüneisen form shown in Eq. (3.49), one finds

$$P_g^* = P_r - \frac{\Gamma_g}{V_g} E_r = - \frac{P_r}{E_r - C_1} C_1 , \quad (3.58)$$

where

$$C_1 = E_o - C_v T_o . \quad (3.59)$$

Now following Fickett and Davis (1979), we adopt a polytropic EOS for the reference state. That is,

$$P_r = P_{CJ} \left(\frac{V_{CJ}}{V_g} \right)^\gamma , \text{ and} \quad (3.60)$$

$$E_r = \frac{P_r V_g}{\gamma - 1} . \quad (3.61)$$

Upon substitution, one obtains

$$P_g^* = \frac{\zeta^\gamma P_{CJ} C_2}{\zeta^{\gamma-1} P_{CJ} V_{CJ} + C_2} , \quad (3.62)$$

where

$$\zeta = V_{CJ} / V_g , \quad (3.63)$$

$$\begin{aligned} C_2 &= (\gamma - 1)(C_V T_o - E_o) = -(\gamma - 1) C_1 , \\ &= (\gamma - 1)(C_V T_o - \sum Y^k E_o^k) , \\ &= (\gamma - 1)(C_V T_o - P_o V_o - \sum Y^k \Delta H_f^k) , \\ &\approx (\gamma - 1)(-\sum Y^k \Delta H_f^k) . \end{aligned} \quad (3.64)$$

We note that after ignition, Y^k is nearly identical to that of the terminal composition (see Appendix B). Similarly, it may also be seen that

$$\Gamma_g^{-1} = \frac{1 + \frac{C_2}{P_{CJ} V_{CJ}^{\gamma-1}} V_g^{\gamma-1}}{\gamma - 1} . \quad (3.65)$$

This is Eq. (2.48) of Fickett and Davis (1979).

Empirically, the value of γ for explosive product gases is known to be on the order of 3. If we use empirical constants for RDX, then one finds

$$\Gamma_g = \frac{2}{1 + 3.83 V_g^2} ,$$

where it is assumed that $\gamma = 3$, $\sum (Y^k \Delta H_f^k) = -4.6$ kJ/g, $P_{CJ} = 34$ GPa, and $\rho_{CJ} (=V_{CJ}^{-1}) = 2.42$ g/cm³.

4. Model Calculations

In this section we present proof-of-concept calculations using the mathematical models discussed in Section 3. Because the energy dissipation is evaluated by use of an artificial viscosity, the primary purpose of this exercise is to gain qualitative understanding of the model behavior. Also, the model material continues to be RDX for expediency. Model parameters will not be optimized to match measurements. But parametric calculations of Pop-plots using the statistical model will be compared with known experimental data. Quantitative tests of the model capabilities are a task in themselves and will be carried out by the use of HMX and/or TATB-based materials in the future.

The hydrodynamic equations are solved using a standard leap-frog method (see for example, von Neumann and Richtmyer 1950 and Wilkins 1963). Materials parameters are those of RDX in Yano et al. (2001) and are tabulated in Tables 1–3. Parameters for energy localizations are listed in Table 4. Input shocks were created by symmetric impact where the flyer was solid RDX without chemical reactions. Figure 4 illustrates the

geometry of a typical setup for shock impact. A thin buffer was used to avoid the spurious ignition of chemical reactions at the impact end. The buffer creates in effect a smooth shock loading in the model specimen. All the calculations used the common cell size of 10 μm to resolve microscopic events. When necessary, subcycling in time is implemented to handle rapid chemical changes at detonation.

At first glance, one may develop the impression that there are too many parameters for either of our models. But if we set aside those associated with thermochemical data (these are necessary physical constants for detailed micromechanical modeling), there are only two that are guessed (or free parameters). They are δ (thickness of the hot region) and n or its equivalent λ_0 (a measure of initial nucleation sites). Other key parameters are calculated based on these two. F_N is based on Eq. (3.15), and ε_d° is calculated from the parametric simulation of ignition conditions (see the first report). We note that even these free parameters have specific physical significance as discussed earlier. The assumption of a fixed δ can be removed easily, if found important.

4.1 Heuristic Model

Figures 5–10 show results based on the heuristic model. Results of the statistical model are presented separately in the next section. The thickness of the hot region for these calculations is 0.2 μm unless otherwise noted. This selection is based on the parametric study of ignition reported earlier (Yano et al. 2001). Initial void space is found to have very little effect so long as its width is on the order of a few percent. This observation is also found to be true of other mechanical parameters that control the motion of void space in the early phase of collapse. Primary factors that affect chemical ignition and subsequent events are thermochemical data, including EOS, and parameters that are associated with energy localization. The value of ε_d° (1.528 kJ/g) is based on threshold energy calculations in the earlier study (see Fig. 24 on page 46) for a localization width of 0.2 μm . This energy is comparable to the dissipated energy of shock at a CJ pressure of 33 GPa (Gibbs and Popolate 1980) in inert RDX. F_N is based on Eq.(3.15). λ_m is one: that is, whole material can become a super hot spot near the CJ pressure. The selection of n ($=200$) was heuristic, but the statistical model offers a clue as to how we select this value.

Figure 5 depicts an early-time growth behavior observed at five locations that are separated by 2 mm from the impact end. We have not been able to find measured in situ profiles, but features of particle velocity histories shown in Fig. 5(b) are comparable to those seen for HMX-based explosives (Gustavsen et al. 1999 and Massoni et al. 1999). Similarly, Fig. 6 shows a buildup to steady detonation. The purpose of this figure is to show the heterogeneous nature of chemical ignition seen in Fig. 6(b). Chemical buildup begins not only at the impact end, but also near the shock front when its strength reaches a threshold value. Calculated detonation pressure and propagation speed are lower than those reported experimentally (Gibbs and Popolate 1980). But they are remarkably close in view of the fact that there were only two free parameters: F_N and

n. The rest were basic thermochemical data for RDX. It is also interesting to note that the steady detonation pressure and propagation velocity are independent of the energy localization model and are primarily controlled by the product EOS and mixture rules.

Figure 7 shows a double-shock calculation where no significant reaction was observed until the two shocks were merged to form a single shock of 4 GPa. Two consecutive jumps to the same terminal pressure of 4 GPa did not generate sufficient energy dissipation to ignite self-sustaining reactions. The required strength of a single shock is about 3.5 GPa to initiate ignition.

Figure 8 shows the quenching of the ignition by overtaking unloading waves that originate at the back of a thin flyer plate. We note that chemical ignition in this report is identified by the emergence of explosive reactions in the gas phase without sustained external heating. There is a natural delay in such an ignition due to the fact that gas-phase reactions are conditional on reactions at the interface. The thickness of the flyer was reduced to 0.3 mm to generate a sharp decaying shock. The initial shock of about 4 GPa ignites the materials in the vicinity of the impact end, but this shock rapidly decays as a result of the rarefaction from the back free surface. The reaction wave builds up to about 3.3 GPa, but it is not strong enough to initiate self-sustaining explosive reactions. The situation is similar to the double-shock calculation except that the second wave is not a shock, but a ramp wave. When the reaction wave catches up with the decaying precursor shock, the result is too weak to cause ignition. The lack of ignition is clearly seen in the volume fraction of product gas shown in Fig. 8 (b).

The above-described quenching mechanism suggests that if the merging of the two waves results in a shock that is strong enough to produce a sufficient amount of energy dissipation, the material will reignite at some distance down the stream. Such a scenario is illustrated in Fig. 9.

4.2 Statistical Model

Figures 10 to 13 show proof-of-concept calculations for the statistical model. Model parameters are the same as those for the heuristic model except those for energy localization. The latter for the statistical model are $F_N = 100$, $\lambda_m = 0.8$, and $\lambda_o = 0.1\%$.

Figure 10 shows a growth-to-detonation calculation comparable to Fig. 5 for the heuristic model. It is interesting to note that the calculated values of steady detonation pressure and velocity (30.5 GPa and 8 km/s respectively) are close to the reported values of 33.8 GPa and 8.6 km/s (Gibbs and Popolato 1980). No optimization of thermochemical data is attempted in the present work. It is remarkable that the results are obtained based solely on a combination of basic thermochemical data and the estimates of δ and λ_o . It is also worth noting that the steady detonation pressure and propagation velocity are not sensitive to the detail mechanisms of energy localization and subsequent chemical reactions. As expected, their primary controlling parameters are the product EOSs and mixture rules. Figure 11 shows early time behavior that is comparable to Fig.

6. Figure 11(b) displays pressure histories at five gauge locations. These features resemble those of other calculations and measurements for heterogeneous explosives.

Figure 12 is a demonstration of quenching as a result of rarefaction waves emanating from the back free surface of the flyer. Reaction waves induced by a weak shock of 2.5 GPa are obviously not as strong as those shown in Fig. 8 and cannot sustain reactions by themselves. As a result, ignition is limited to the region initiated by the decaying precursor shock. Also note that the P-x profile at 6 μ s clearly shows again the heterogeneous nature of chemical reactions that are initiated near the shock front as well as the impact interface.

Figure 13 is a parametric study of Pop-plots for the statistical model. In this study, we tested only those for the energy localization model: i.e., λ_m , λ_o , and F_N . A more comprehensive test of Pop-plots will be done in the future using other materials such as HMX- or TATB-based explosives. Experimental data for PBX 9504 were chosen because of the highest initial density that we could find in the literature for the explosives that contain RDX.

Computationally, time- and distance-to-detonation were determined using a least-square fitting of pressure profiles P-t (or P-x) based on the assumed function form,

$$P(t) = P_0 + (P_{cj} - P_0) \frac{1}{1 + e^{-a(t-b)}} .$$

DDT points are identified as those at which the pressure reaches the value of 0.999 ($P_{cj} - P_0$) first.

What follows is a summary of trends that were observed on the variation of the three statistical parameters.

1. Decreasing λ_o lowers the ignition threshold and steepens the slope of Pop plots. These trends are related to the fact that the total deposition of heat (H_{hs}) in the early stage is primarily controlled by the amount of preexisting initiation sites. A small λ_o increases H_{hs} rapidly over the existing sites and can initiate ignition under weak shock conditions and reduces ignition threshold pressures. The effects of both λ_o and λ_m on H_{hs} are shown in Fig. 14.

2. Increasing λ_m slows down the shock-to-detonation transition (SDT), but does not affect the ignition threshold nor the slope of Pop-plots (over the domain of simulation).

Increasing λ_m shifts the plot parallel toward the direction of a slower SDT. Because λ_m represents the mass fraction at the terminal condition ($\epsilon_d = \epsilon_d^o$), it affects deposition energy density for the hot spot. The smaller the λ_m , the smaller the volume into which energy is deposited. For a particular value of ϵ_d , a smaller volume fraction means higher energy density, which in turn results in faster SDT. Because $H_{hs} - \epsilon_d$ curves with different λ_m are self-similar, Pop-plots do not change their slopes, and they slide parallel to the vertical P-axis.

3. Decreasing F_N has an effect that is similar to increasing λ_m . Because F_N represents the maximum surface area of hot spots, a large F_N implies large energy and mass fluxes between the solid surface and the gas cavity. The larger the F_A , the more rapidly the void temperature increases. Thus, increasing F_N results in a rapid transition from shock to detonation.

Fig. 4. Geometry of test calculations. Both the impactor and the buffer are model RDX except for the lack of chemical reactions. The buffer is introduced to smooth the shock entering the target to avoid spurious ignition. Dimensions shown are for the calculations in Fig. 5. They are modified depending on the nature of the problem. For example, the quenching calculation shown in Fig. 7 used a thin impactor of 0.8 mm.

(a)

(b)

Fig. 5. Early-time behavior of the heuristic model observed by the pressure and particle velocity histories at five gauge locations that are separated by 2 mm from the impact end. A weak sign of heterogeneity is observed at the third gauge.

Fig. 6. Growth-to-detonation behavior of the heuristic model. The volume fraction of the product gas clearly shows the heterogeneous ignition behavior. Model parameters are not optimized to fit the observed detonation pressure and speed. The statistical model shows a closer match.

(a)

(b)

Fig. 7. A double-shock ignition in the heuristic model. The terminal pressure of double shock exceeds the threshold value, but the ignition does not occur until the two shocks merge into a single shock where the dissipation of energy satisfies the dissipated energy requirement.

(a)

(b)

Fig. 8. Quenching of ignition by an overtaking rarefaction wave. The initial shock is strong enough to ignite the material near the impact end (see [b]), but its decay is too rapid to sustain the reaction. When the reaction wave catches up with the decaying precursor shock, the combined wave is too weak to cause an ignition.

Fig. 9. Reignition will occur when the first reaction wave and the decaying precursor shock merge to produce a strong shock for reignition.

Fig. 10. Growth-to-detonation behavior of the statistical model. Steady detonation pressure and detonation velocity are close to the LASL values of 33.7 GPa and 8.6 km/s.

(a)

(b)

Fig. 11. Early time behavior of the statistical model. (a) Spatial profiles and (b) gauge histories. Cell 634 is very near the impact face. One – hundred cells are equivalent to 1 mm.

Fig. 12. An illustration of quenching behavior for the statistical model. Statistical parameters for this calculation are $F_N = 50$, $\lambda_o = 0.001$, and $\lambda_m = 0.8$. Growth of the reaction wave is not strong enough to sustain ignition. As a result, ignition is limited to the region initiated by the rapidly decaying precursor shock.

Fig. 13. A parametric comparison of calculated Pop-plots and measurements. Arrows indicate the increasing trend. Experimental data are those for PBX 9504 that contain 3.15 wt % nitrocellulose and 3.15 wt % chloroethylphosphate. It was picked for its initial density of 1.76 g/cm^3 . Calculations were made to show trends of parameter variation.

Fig. 14. Behavior of total energy deposition for the statistical model; λ_0 controls the early time characteristics; λ_m primarily affects the terminal values.

5. Conclusions

A computational framework for mechanistic reactive burn modeling of solid explosives has been developed based on the unifying hot-spot model proposed earlier. The key mechanistic features include thermochemical processes at the grain level, descriptions (both heuristic and statistical) of energy localization and growth of hot spots, and an effective method of aggregating hot spots. An exploratory model was created using RDX or RDX-based materials. The model contains two free parameters. They are the thickness of hot regions and initial nucleation sites for hot spots. Others are basic thermochemical data such as thermal conductivity, chemical kinetics, and equations of state.

Proof-of-concept calculations of shock-to-detonation show expected features for both homogeneous and heterogeneous behaviors. The calculations include early time behavior, shock-to-detonation, double-shock ignition, quenching by rarefaction waves, and Pop-plots. Steady detonation pressure and detonation velocity based on the model simulation of RDX with 1% void are 31 GPa and 8 km/s, respectively.

It is important to stress that all the computational features result from the same basic model and that the model is not manipulated to create any specific behavior. Results are based on the same mechanisms built into the model. A good example is the quenching that occurs as a result of a combined effect of wave interactions and chemical kinetics. The latter are based on an Arrhenius-type rate law, but the extinction occurs because the ignition of self-sustained reactions is sensitive not only to the hot-spot temperature, but also to the accumulation of reactant gas in the gas reservoir. The interaction of the precursor shock with the rarefaction waves creates the window of opportunity for the Arrhenius-type kinetics to be extinguished.

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Tables

Table 1. Material constants.

Variable (units)	Value	Variable (units)	Value
ρ_s (kg/m ³)	1.799×10^3	Δh_{fs}^R (J/kg)	2.773×10^5
κ_s (W/m/K)	0.2093	Δh_{fg}^R (J/kg)	8.64×10^5
κ_g (W/m/K)	8.33×10^{-2}	Δh_{fg}^{PI} (J/kg)	-1.048×10^6
C_{vs}, C_{ps} (J/kg/K)	1.465×10^3	Δh_{fg}^{P2} (J/kg)	-4.208×10^6
C_{pg}^I (J/kg/K)	1.0963×10^3	R_g^I (J/kg/K)	297.3
$C_{pg}^R, C_{pg}^{PI}, C_{pg}^{P2}$ (J/kg/K)	1.2571×10^3	$R_g^R, R_g^{PI}, R_g^{P2}$ (J/kg/K)	37.50

Table 2. Hot-spot model parameters

Variable (units)	Value	Variable (units)	Value
a_0 (m)	1.0×10^{-7}	A_g (s ^{1.44} /m ^{1.78} /kg ^{0.22})	1.07989×10^4
c_0 (m)	1.0×10^{-5}	E_g (J/mol)	1.36×10^5
w_{s0} (m/s)	0.0	r	1.22
ρ_{g0} (kg/m ³)	1.221	μ_s	0.0
T_{g0}, T_{s0} (K)	300	χ (m ³ /kg)	5.5461×10^{-4}
Y_{g0}^R	0.0	k_v (1/s) (compression)	2.223×10^{11}
Y_{g0}^I	1.0	k_v (1/s) (expansion)	3.335×10^{10}
$\delta(=b-a)$ (m)	2.0×10^{-7}	E_s (J/mol)	1.93×10^5
a_{min}/a_0	0.4	A_s (1/s)	5.0×10^{15}
n	3	q_s (J/kg)	1.51×10^6

Table 3. Hydrocode parameters

Variable (units)	Value	Variable (units)	Value
C_0 (m/s)	2.789×10^3	P_0 (Pa)	1.0×10^5
s	1.9	E_0 (J/kg)	2.772×10^{-5}
Γ_0	0.93	P_{CJ} (Pa)	3.4×10^{10}
k_1	3	V_{CJ} (m ³ /kg)	4.132×10^{-4}
k_2	0.4	γ	2.85

Table 4. Energy localization parameters

Variables (Units)	Value	Variables (Units)	Value
$\delta(=b-a)$ (m)	2.0×10^{-7}	ϵ_d^0 (J/kg)	1.528
n	200	λ_0	0.001, 0.01
F_N	50, 100	λ_m	0.6, 0.8, 1.0

Appendix A: Heat-Flux Calculation with a Variable Width for the Locally Heated Region

For a general derivation of the flux calculation for the unit cross-sectional hot shot, we introduce a new variable based on the unit mass rather than the unit volume. That is, define ε_d^1 by

$$\frac{d}{dt} \varepsilon_d^1 = (v_h^1 / m_h^1) \Phi_{hs}^1 = \rho_s^1 \Phi_{hs}^1, \quad (A-1)$$

where the superscript “1” signifies the quantity associated with the hot spot having the unit cross-sectional area. In terms of the new variables, the equivalence of adiabatic temperature becomes

$$\Delta T = \frac{1}{m_h^1 C_V} \int v_h^1 \Phi_{hs}^1 d\tau = \frac{M \varepsilon_d}{m_h C_V} = \frac{\varepsilon_d}{\lambda_{hs} C_V}, \quad (A-2)$$

where M is the mass in the hydro cell and m_h is the mass in the total hot-spot region. Taking the time derivative of (A-2), one finds

$$\Phi_{hs}^1 v_h^1 = m_h^1 \frac{d}{dt} \varepsilon_d = \frac{d}{dt} \left(\frac{m_h^1 \varepsilon_d}{\lambda_{hs}} \right). \quad (A-3)$$

Solving for Φ_{hs}^1 or ε_d^1 , one finds

$$\Phi_{hs}^1 = \rho_s^1 \frac{d}{dt} \left(\frac{\varepsilon_d}{\lambda_{hs}} \right) + \frac{\varepsilon_d}{\lambda_{hs} v_h^1} \frac{d}{dt} m_h^1, \quad \text{and} \quad (A-4)$$

$$\frac{d}{dt} \varepsilon_d^1 = \frac{1}{m_h^1} \frac{d}{dt} \left(\frac{m_h^1 \varepsilon_d}{\lambda_{hs}} \right). \quad (A-5)$$

In the derivation of these equations, no assumption has been made as to the width or the area. The area factor F_A is absorbed in the mass fraction of hot spots λ_{hs} . It may be easily seen that if m_h^1 is constant, that is, if the width of the unit hot spot is fixed, then the above formulas reduce to those seen in Section 3.2.

We also note one constraint that exists for the normalized flux calculation when m_h^1 (for the unit hot spot) is constant and the mass fraction is a function of only ε_d . That is, it can be shown that

$$\Phi_{hs}^1 = \rho_s \frac{d}{dt} \left(\frac{\varepsilon_d}{\lambda_{hs}} \right) = \rho_s \dot{\varepsilon}_d \frac{d}{dt} \left(\frac{\psi}{\lambda_{hs}(\psi)} \right) = \rho_s \dot{\varepsilon}_d \frac{\lambda_{hs} - \psi \lambda'_{hs}}{(\lambda_{hs})^2}, \quad (A-6)$$

where $\psi = \varepsilon_d / \varepsilon_d^0$, λ'_{hs} signifies the derivative of λ_{hs} with respect to ψ . Because the localized heat flux and global rate of energy dissipation are positive, the numerator of (A-6) must also be positive. That is,

$$\frac{d\lambda_{hs}}{d\psi} < \frac{\lambda_{hs}}{\psi} . \quad (A-7)$$

This inequality requires that at any point on the curve $\lambda_{hs} = \lambda_{hs}(\psi)$, the tangent at that point must be smaller than that of the polar line at that point. This means that no portion of the curve can lie in the domain where $\lambda_{hs} < \psi$. At present it is not clear whether this is unique to the assumption of adiabatic equivalence and the fixed hot-spot width.

Appendix B: Thermochemical Data for RDX

In this appendix, a summary is given of thermochemical data on RDX and the enthalpies used in our calculations for completeness of description. The data are taken from two sources: LASL Explosive Properties Data (Gibbs and Popolate 1980) and Kuo (1986).

Values for the heat of formation of solid RDX and latent heat of melting and evaporation are taken from the LASL Handbook. The units are kcal/mol. They are schematically illustrated in the insert.

Heat of formation of RDX (solid)	= 14.7 kcal/mol
Latent heat of melting	= 7.89
Latent heat of sublimation	= 31.1

Values of heat of formation for product gas species are taken from Kuo (1986).

H ₂ O (l)	= -68.315
H ₂ O (g)	= 31.83
CO ₂ (g)	= -94.051
CO (g)	= -26.42
H (g)	= 52.1
OH (g)	= 9.432
O (g)	= 59.559
NO (g)	= 21.58
CH ₂ O (g)	= -27.7
NO ₂ (g)	= 7.91
N ₂ O (g)	= 19.61

The stoichiometric relationships for products P₁ and P₂ described in the text are

Upon substitution, one obtains

$$\begin{aligned} \Delta h_f^{\text{P}_1} &= -55.58 \text{ kcal/mol} \\ Q_D^{\text{P}_1} &= \Delta h_f^{\text{RDX(s)}} - \Delta h_f^{\text{P}_1} = 1.33 \text{ kcal/mol} = 1.33 \text{ kJ/g} \\ \Delta h_f^{\text{P}_2} &= -244.017 \text{ kcal/mol} \\ Q_D^{\text{P}_2} &= \Delta h_f^{\text{RDX(g)}} - \Delta h_f^{\text{P}_2} = 289.8 \text{ kcal/mol} = 5.46 \text{ kJ/g} \end{aligned}$$

In comparison, values found in the literature are

$$Q_D^{\text{P}_1} = 1.51 \text{ kJ/g} \quad (\text{Kang et al. 1992})$$

$$Q_D^{p_2} = 5.76 \text{ kJ/g} \quad (\text{Mitani, T. and F.A. Williams 1986})$$

We also note that in the text, the following abbreviations are used.

$$\Delta h_f^{\text{RDX(g)}} = \Delta h_f^{\text{R}}$$

$$h_{\text{ga}}^{\text{R}} - h_{\text{sa}}^{\text{R}} = \Delta h_f^{\text{RDX(s)}} - \Delta h_f^{\text{RDX(s)}}$$

Appendix C: Hotspot Model

As sketched in Fig. 1, thermomechanically induced hot spots are envisioned as a thin, flat region (hot sheets) and resemble shear bands. The hot layer is bounded by a large “cold” mass that serves as a heat sink and a void or gas volume that serves as a repository of gas products. This particular idealization in plane geometry is chosen to represent multiple types of hot spots that are created by mechanisms such as spherical-void collapse (Kang et al. 1992), shear banding (Kipp 1987), and friction (Dienes 1984) in a unified fashion. The model is a framework in which various mechanisms at grain level are conceptualized in plane geometry to capture the essential features of hot-spot ignition and growth. In the new model, quantities such as the width of hot sheets, hot surface areas, and the rate of energy dissipation must be prescribed separately for the hypothesized mechanisms. Mathematically, there is a close parallel between the present mode and the model based on spherical-pore collapse.

As in the spherical-void model, an initially existing gas volume collapses under compressive loads and the interface follows the motion of the solid phase. The solid is assumed to be incompressible, but its motion is controlled by three forces: global pressure, pressure in the gas, and the configuration forces that are essentially contact forces across solid interfaces (Yano et al. 2001). External loads provide confinement to gas products and influence ignition behavior. It is important to recognize that in the new model, gas reservoirs are not closed-in cavities. In plane geometry there is no distinction between “inside” and “outside.” The motion of the solid phase defines the interface position and it in turn defines the volume fraction of the gas in the overall material.

The interface motion is described by three differential equations whose meaning can be understood intuitively,

$$\dot{a} = w_s + \frac{\dot{m}}{\rho_s} \quad , \quad (C.1)$$

$$\dot{c} = w_s \quad , \text{ and} \quad (C.2)$$

$$\dot{w}_s = \frac{1}{\rho_s(c-a)} [\bar{p}_g + p_N - p_B + m^2 (\frac{1}{\rho_g} - \frac{1}{\rho_s})] \quad , \quad (C.3)$$

where a is the interface position, w_s is the normal velocity of the solid phase, c specifies the external boundary of the solid phase where the global pressure p_B is exerted, and p_B is assumed to be the pressure calculated in the hydrocode. The bar above p_g and ρ_g emphasizes the fact that they are averages over the gas volume. The variable p_N is the configuration stress. Currently, it is modeled as follows:

$$\begin{aligned} p_N &= -k_v \rho_s (c-a) w_s + \frac{(a_{\min}/a_o)^n}{1 - (a_{\min}/a_o)^n} \frac{1 - (a/a_o)^n}{(a/a_o)^n} p_B, \quad (0 \leq c \leq c_o) \quad , \\ &= 0, \quad (c_o \leq c) \quad . \end{aligned} \quad (C.4)$$

This expression contains both viscous and position-dependent parameters, and

$\dot{m}$ is the rate of mass transfer across the gas-solid interface. We note that when the hot spot model is integrated into the new burn model, this quantity describes the intrinsic rate that is concerned only with local chemical kinetics. The global rate representing the mass flux for a collection of hot spots is modified by two additional functions that handle the statistics.

At present $\dot{m}$ is that of Kang et al. for RDX (1992) and is solely dependent on the surface temperature. Details are referred to in the original paper.

$$\dot{m}^2 = \rho_s \kappa_s T_{sa} \frac{R_u T_{sa}}{E_s} \frac{A_s \exp\left(\frac{-E_s}{R_u T_{sa}}\right)}{q_s (1-G) - [c_{ps}(T_{sa} - T_o) - q_s] \ln(1/G)} , \quad (C.5)$$

where G is a parameter that controls the proportion of evaporation and chemical reactions at the interface,

$$\begin{aligned} G &= 0.65 & (T_{sa} \leq 700 \text{ K}) , \\ &= 0.69 - 2 \times 10^{-4} T_{sa} + 4.1 \times 10^{-7} T_{sa}^2 & (700 < T_{sa} < 1150 \text{ K}) , \\ &= 0 & (1150 \text{ K} \leq T_{sa}) . \end{aligned} \quad (C.6)$$

The average density of the gas is determined by the mass flux $\dot{m}$ and the motion of the solid phase,

$$\bar{\rho}_g = \frac{1}{a} \left[\dot{m} \left(1 - \frac{\bar{\rho}_g}{\rho_s} \right) - \bar{\rho}_g w_s \right] . \quad (C.7)$$

The meaning again is intuitive.

As described above, the chemical response is initially governed by the solid surface temperature. When the temperature of a hot surface becomes high enough, first the solid undergoes both evaporation and surface chemical reactions as specified by Eq. (1.4). These gases then react uniformly in the bulk gas volume, following the specified kinetic equations. Current models for the latter are again based on the mechanisms discussed in Kang et al. (1992). We emphasize that the detail assignment of chemical reactions is open to change and needs to be modified, when available, by the model that better describes the transformation of solids into the final gas products.

The surface temperature is obtained by solving the heat-conduction equation for the solid phase subject to the boundary conditions at a and c ,

$$\frac{\partial T_s}{\partial t} = \alpha_s \frac{\partial^2 T_s}{\partial \chi^2} + \frac{\Phi_{hs}^1}{\rho_s c_{vs}} , \quad (C.8)$$

where Φ_{hs}^1 is the source term. The exterior boundary condition at c is assumed adiabatic, and the interior boundary condition at the solid-gas interface is the interface energy conservation equation given by

$$\kappa_s \left(\frac{\partial T_s}{\partial z} \right)_a = \kappa_g \frac{T_{sa} - \overline{T_g}}{\delta_g} - \mu_s \left(\frac{\partial u_s}{\partial z} \right) u_{sa} + m[h_{ga} - h_{sa} + a(w_s - w_{ga})] , \quad (C.9)$$

where h_{ga} and h_{sa} are enthalpies of the gas and the solid at the interface, respectively.

$$h_{ga} - h_{sa} = (h_{ga}^R - h_{sa}^R) + (1 - G)[\Delta]_f^{P_1} - \Delta h_f^R + (c_p^{P_1} - c_p^R)(T_{sa} - T_o) + \frac{1}{2}(w_{ga}^2 - w_s^2) , \quad (C.10)$$

$$w_{ga} = w_s + m \left(\frac{1}{\rho_s} - \frac{1}{\rho_g} \right) , \text{ and}$$

δ_g = thermal layer thickness = a function of “a” .

Calculations of the enthalpy and the heat of formation are discussed in Appendix B. The calculation of bulk gas temperature is fairly involved and is referred to in Yano et al. (2001). Only the result is listed here.

$$\overline{\rho_g c_{pg}} \frac{d}{dt} \overline{T_g} = \frac{1}{a} \left[\kappa_g \frac{T_{sa,a} - T_g}{\delta_g} + m c_{pg,a} (T_{s,a} - \overline{T_g}) \right] - \overline{\omega_g^R} [\Delta h_f^R - \Delta h_f^{P_2} + (c_{pg}^R - c_{pg}^{P_2})(\overline{T_g} - T_o)] + (1 - \eta \overline{\rho_g}) \frac{d}{dt} \overline{P_g} , \quad (C.11)$$

where c_p stands for heat capacity and $\overline{\omega_g^R}$ is the bulk reaction rate given by

$$\overline{\omega_g^R} = -A_g \overline{Y_g^R} \overline{p_g^r} \exp\left(-\frac{E_g}{R_u \overline{T_g}}\right) , \quad (C.12)$$

where A_g and E_g are a frequency factor, and an activation energy of gas-phase reaction and r is a parameter. The heat of formation Δh_f is discussed in Appendix B.

The kinetics of the bulk reactions are described by a set of three ordinary differential equations,

$$\overline{\rho_g} \frac{d}{dt} \overline{Y_g^R} = \overline{\omega_g^R} + \frac{1}{a} m (G - \overline{Y_g^R}) , \quad (C.13)$$

$$\overline{\rho_g Y_g^R} = -\overline{\omega_g^R} + \frac{1}{a} \dot{m}(1 - G - \overline{Y_g^P}) \quad , \text{ and} \quad (\text{C.14})$$

$$\overline{\rho_g Y_g^I} = -\frac{1}{a} \dot{m}(\overline{Y_g^I}) \quad , \quad (\text{C.15})$$

where superscripts R, P, and I represent reactant, product, and inert components, respectively. Stoichiometry of the reactions is given in Appendix B.

The equation of state of the product gas is that of a modified ideal gas law given by

$$\overline{p_g} = \frac{\overline{\rho_g}}{1 - \chi \overline{\rho_g}} R \overline{T_g} \quad . \quad (\text{C.16})$$

The onset of the surface reaction is not necessarily equivalent to the ignition of the solid material. There has to be a continuing energy supply until such a point where there will be a sufficient amount of high-temperature reactants in the gas reservoir and a high enough surface temperature to induce self-sustained reactions both in the gas and at the solid surface. The quenching of self-sustained reactions can take place for a variety of reasons. For instance, (1) there is not enough localized energy supply, (2) the rate of localized energy supply is too slow (conducted away from the hot spot) to induce self-sustained reactions, and (3) there is not enough reactant gas, etc.

In summary, the present hot-spot model is a planar, combustion model with a propagating hot, reacting surface that is initially heated by either localized mechanical heating or by other means of external heat supply.

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