APPLICATION OF A MULTIPHASE MIXTURE THEORY WITH COUPLED DAMAGE AND REACTION TO ENERGETIC MATERIAL RESPONSE

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A multiphase continuum mixture theory is presented that couples the mechanical response, damage evolution, and combustion of energetic materials. The model is demonstrated to capture shock-to-detonation transition, deflagration-to-detonation transition and response due to low velocity impact. The modeling approach has also been demonstrated to simulate delayed detonation for rocket propellants and to investigate the violence of reaction in thermal explosion experiments. The model described here is implemented into the Sandia National Laboratories shock physics code CTH. CTH is a multimaterial Eulerian code with tabular and analytic equation of state options and various strength models. Traditional models for shock-to-detonation transition are not appropriate when the processes that lead to initiation are not initiated directly by mechanical shock. Most shock-to-detonation models are empirically based with input parameters fit to POP-plot and other relevant data. Often, the fits are not unique and several sets of reaction rate parameters will yield similar results. These models are often applied in situations that may not be appropriate. One example is low velocity impact. In a low velocity impact, the stress wave from the impact propagates through the material multiple times before a violent reaction occurs. During this early phase of the impact the energetic material response involves mechanical response, damage evolution, and chemical reaction. A key aspect of the multiphase mixture model is that the dynamic damage evolution interacts with combustion and the resulting enhanced surface area burning will accelerate to shock induced reactions if sufficient damage develops. This paper focuses on the implementation of a level set interface tracking model into the multiphase mixture model framework. The level set model is then demonstrated in a series of calculations.

INTRODUCTION

The development of massively parallel platforms for performing modeling and simulation has led to the need for advanced constitutive response models for all classes of materials. The traditional constitutive response models have been capable of capturing continuum scale phenomenology that is observed in experiment. More advanced physics-based models are required to address the physical processes responsible for that phenomenology. The focus of this paper is the development of a multiphase continuum mixture theory (CMT) as a framework for the incorporation of advanced combustion, damage, and mechanical response models for energetic material response. This framework has been given the name coupled damage and reaction (CDAR) modeling.

CDAR modeling has been successfully applied to shock-to-detonation transition (SDT), deflagration-to-detonation transition (DDT), and delayed detonation transition (XDT). The CDAR model has also been applied to thermal explosion response[1].

Traditional SDT models are useful for analyzing response to single stimulus shock loading of energetic materials. These reactive flow models are designed to capture the response to large amplitude shock loading. However, when multidimensional effects become important or initiation is caused by shear, then SDT models should not be used. In this situation, a CDAR modeling paradigm is required to investigate the processes that lead to initiation and subsequent response. The CDAR model discussed here is a CMT formulation that provides a thermodynamically and mathematically consistent framework for coupling the mechanics of damage evolution, shear response, and chemistry. This paper focuses on the implementation of a level set algorithm for propagating "slow" combustion. This type of model is required because the processes that control flame/ignition spread occur at length and time scales that are currently not resolvable even with massively parallel computers and mesh adaptivity. That is, direct numerical simulation of the reactive flow processes including mechanics, chemistry, heat transfer, and porous flow occur at sub-micron length scales that require Courant limited time steps of about 10^{-14} s and accurate resolution of the stiff chemical kinetics (which are not known adequately) require even smaller time steps on the order of 10^{-16} s. The CDAR model is implemented in the Sandia National Laboratories multidimensional, multimaterial shock physics analysis package, CTH[2].

CONTINUUM MIXTURE THEORY FORMULATION

The multiphase continuum mixture theory discussed here is an extension of the Baer and Nunziato DDT model[3]. This extension uses the recent formulation developed by Drumheller to couple the volumetric, deviatoric, and damage states for a multiphase mixture in a mathematically and thermodynamically consistent fashion[4]. The current model was implemented by Matheson[5]. The conservation equations for each component in a multiphase mixture are represented in Lagrangian form as follows[6].

Component Conservation of Mass

$$\rho_a' = -\rho_a \nabla \cdot v_a + c_a^+ \tag{1}$$

Component Conservation of Momentum

$$\rho_a v_a' = \nabla \cdot T_a - c_a^+ v_a + m_a^+ + \rho_a b_a \tag{2}$$

Component Conservation of Energy

$$\begin{aligned} \rho_a e_a' &= T_a \cdot \nabla v_a - \nabla \cdot q_a \\ &- c_a^+ (e_a - \frac{1}{2} v_a \cdot v_a) - m_a^+ \cdot v_a + e_a^+ \\ &+ \rho_a s_a \end{aligned} \tag{3}$$

The subscript 'a' means this quantity applies to component a. The superscript '+' identifies the interphase source terms of mass, c, momentum, m, and energy, e. The variable ρ is the mass density, v is the velocity, T is the stress tensor, b is the body force, e is the energy, q is the heat flux vector, and s is the energy source. The component conservation equations when summed over all components yield the usual set of conservation equations for the mixture. These are obtained by removing the subscripts and superscripts from Eqs. (1-3) and removing the interphase source terms. The summation over each component yields the following definitions for mixture quantities,

Saturation (summation of volume fractions)

$$\sum \phi_a = 1 \tag{4}$$

Conservation/Phase Symmetry

$$\sum c_a^+ = 0 \quad \sum m_a^+ = 0 \quad \sum e_a^+ = 0 \tag{5}$$

Mixture Density

$$(6) \quad \rho = \sum \phi_a \gamma_a$$

Here, γ is the material true density and ϕ is the volume fraction. There are also definitions for mixture momentum, energy, stress, and work[7].

A key aspect of the multiphase mixture formulation is the specification of the interphase source terms. It has been demonstrated that the multiphase mixture formulation yields a system of equations that is completely hyperbolic with a set of eigenvalues and eigenvectors that are all real[8]. This implies that the equations can be solved by standard numerical methods without appealing to special algorithms to stabilize nonphysical solutions. The interphase source terms are determined by appealing to the second law of thermodynamics to place physically meaningful limiting conditions upon the admissible properties of the source terms. While some controversy still exists as to the necessity of appealing to the second law, it has been demonstrated as a useful technique that guarantees that the second law is **NOT** violated. Also the grouping of terms to define the interphase source terms often yields mathematical and physical insight into the nature of the governing equations. Equations for the interphase source terms are available in the literature[3,5,7].

LEVEL SET MODEL FOR IGNITION SPREAD

Many hazard scenarios involving mechanical insult to energetic materials are driven by low amplitude shock/stress wave phenomena. Under these conditions, the energetic materials' mechanical response and damage mechanics play important roles in the response to the stimulus. For example, the mechanical response of rocket propellants has been successfully described using a viscoelastic-viscoplastic constitutive model with tensile damage[5]. Unlike shock-to-detonation transition, a low amplitude mechanical stimulus may persist for several hundred microseconds prior to the onset of significant reaction and potential DDT- or XDT-like response[9]. Similarly, the response of energetic materials in thermal explosion scenarios involves the transition of combustion from a thermal ignition to flame spread, deflagration, and possible detonation[1]. The slow combustion processes may persist for hundreds of microseconds to milliseconds prior to either confinement failure or accelerated combustion and detonation transition behavior. To simulate these reactive processes, a level set flame or ignition spread model was incorporated into the multiphase mixture model framework. The level set equation has the following form[10],

$$(7) \quad \frac{\partial \lambda}{\partial t} + F_b \left|\nabla \lambda\right| + V \cdot \nabla \lambda = \varepsilon \kappa \left|\nabla \lambda\right|$$

Here, λ is the level set function, F_b is the velocity of ignition spread, V is the material velocity, $\varepsilon\kappa$ represents the propagation of the level set function with curvature dependent speed. The level set function, λ, is initialized as a signed distance function. The term in Eq. 7 containing the F_b velocity represents the evolution of the level set function with respect to ignition spread. The art of using the level set function to represent ignition spread is to assign an appropriate model for calculating the ignition spread velocity as a function of local conditions at the front. The third term on the left-hand side of the equation represents the advection of the level set field with the local material velocity. This equation can be descretized and solved using any number of techniques as discussed by Sethian[10]. Here, the level set function is propagated using first or second order schemes for convex speed functions.

Experimental results for convective combustion of powders and combustion in cracks correlate the flame spread or "ignition" locus with a velocity propagating proportional to the local pressure raised to a power[11]. This idea is used here to specify the ignition-spread velocity for the level set function. The velocity function used in this paper is,

$$(8) \quad F_b = A\left(\frac{T}{T_{ref}}\right)^{\sigma}\left(\frac{P}{P_{ref}}\right)^{n}$$

Here, A is the prefactor, T is temperature, P is pressure, σ is the temperature sensitivity exponent, and n is the pressure exponent. This equation is easily extended to include the effects of mechanical damage evolution, porosity, and multiphase flow[12]. The ignition locus is defined as the interior of the level set function ($\lambda < 0$). A straightforward interpolation is used to locate the zero level set. This determines which cells are burning and partially burning. The level set function is then used to calculate a mass source term in Eq. 1. The mass source term is calculated from a propellant burn rate expression similar to Eq. 8 and a calculated effective surface area. For this study, the effective surface area is specified as a constant. Future studies will incorporate the effects of porosity and mechanical damage on the effective surface area function and ignition spread velocity.

VISCOELASTIC-VISCOPLASTIC CONSTITUTIVE MODEL

The mechanical response model employed in this study was developed for analysis of rocket propellants. The model is represented as an elastic shear spring in parallel with up to five viscoelastic Maxwell elements. A Maxwell element is represented schematically as a spring in series with a dashpot[7]. The Maxwell elements are used to capture time-dependent material response over a wide range of strain rates. In addition, inelastic deformation is captured by a viscoplastic element in series with the composite elastic and Maxwell elements. This element defines a scalar plastic strain rate that is integrated to yield an equivalent plastic strain. This constitutive model also interacts with a mechanical damage model to modify the effective strength properties and the multiphase continuum mixture model can be employed to reduce the effective deviatoric stress in proportion to the porosity. The viscoelastic-plastic (VEP) model has been used to simulate the mechanical response of rocket propellants. The model was "calibrated" to wave profile data and mechanical testing data at quasi-static and dynamic strain rates. Further details of the model can be found in the literature[5,7,13].

DAMAGE MODEL

A model initially developed to simulate damage in rocket propellants was used in this study. The tensile damage and distention (TDD) model is built upon the multiphase continuum mixture theory originally developed by Baer and Nunziato[3] and extended by Drumheller[4]. The extension involves splitting the deformation of a multiphase mixture into a distention motion and a true deformation motion. The distention motion then provides a mathematically consistent treatment of a multiphase mixture that is deforming and undergoing chemical reactions. For an inert system, the distention is effectively the inverse of the volume fraction. However, when chemical reactions are considered, the distention ties the changes in volume fraction from deformation and reaction together. The use of distention allows a more consistent description of the multiphase mixture and ties the mechanical deformation, damage mechanics, and chemical reactions together in a mathematically and thermodynamically consistent fashion.

The TDD model is built upon the observation that bindered energetic material systems exhibit several modes of mechanical failure. These modes are represented by decohesion and scission damage. Decohesion damage describes the failure mode where the rubber binder detaches from the solid ingredients reducing the effective tensile strength of the material. However, this type of damage cannot go to completion because highly debonded materials will still support tension. Also, the recompacted material will still support shear stresses. Scission damage is an attempt to describe the failure modes that occur essentially in the binder at high stresses with low strain; and low stresses with high strains. The rates of decohesion and scission

damage are calculated from effective principal stress, strain rates, and strain. The effective properties are used to track a characteristic defect size. In addition the damage state interacts with combustion to increase or decrease the burning surface area. The TDD model is responsible for tracking distention and modifying damage variables that interact with the VEP and multiphase mixture models. For further details on the TDD model see Refs. 5 and 7.

CONFINEMENT GEOMETRY

The geometry used in this set of simulations is shown in Fig. 1. This geometry is a simplification of the Navy validation cookoff test geometry[14]. In this thermal explosion test, the steel cylinder is loaded with energetic material and heated slowly (approximately 0.1 K/min) until ignition. Following ignition the resulting combustion processes can lead to a pressure rupture or a detonation-like fragmentation and failure of the device[15]. It is hypothesized that the response of the energetic material is driven by the *effective* burning surface area. This surface area is proportional to mechanical damage, porosity, and extent of chemical reaction. Note that damage and porosity are used to calculate an effective burning surface area. The chemical reactions can either increase the surface area or decrease it depending upon the extent of reaction. Under this hypothesis, the "state" of the energetic material prior to ignition and the dynamic evolution of damage following ignition dictate the violence of reaction from the thermal explosion event.

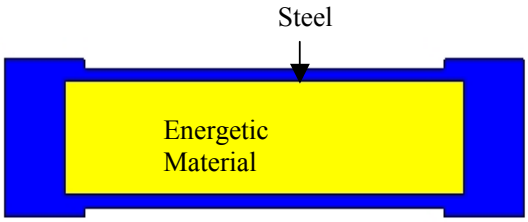

Figure 1. Schematic of the test geometry used for simulations. This is a simplification of the Navy validation geometry for thermal explosion experimentation.

DEFLAGRATION SIMULATION

A series of images depicting the mixture pressure (right), damage (left), and ignition locus (contour) at various times relative to the ignition event are shown in Fig. 2. The images shown in figure 2 are rotated 90 degrees from figure 1 and zoomed in to illustrate the level set propagation. The calculation is initiated by assuming a representative energetic material at 95% theoretical maximum density (TMD) with an initial ignition locus of a sphere with a radius of 2.5 mm. The pressure exponent in Eq. 8 was set equal to 1.0. The lower pressure exponent and the specific surface area at 95% TMD results in the inhibition of a deflagration-to-detonation transition. At 20 μs, the pressure in the burning region has reached 250 bars and the accumulated damage has risen to 60%. At 30 μs, the damage accumulation has progressed past the ignition front and the pressure at 2 cm from the ignition front has risen to 100 bars. At 50 μs, the damage within the ignition region is at almost 100% and the pressure in this region is 450 bars. The pressure and damage continue to rise through 70, 100, and 120 μs as the confinement starts to fail and lose structural integrity.

DEFLAGRATION-TO-DETONATION TRANSITION SIMULATION

A series of images depicting the mixture pressure (right), gas pressure (left), and ignition locus (contour) at various times relative to the ignition event are shown in Fig. 3. The calculation is initiated by assuming a representative energetic material at 90% theoretical maximum density (TMD) with an initial ignition locus of a sphere with a radius of 2.5 mm. The pressure exponent in Eq. 8 is set to 2.0. The higher pressure exponent and specific surface area at 90% TMD results in a deflagration-to-detonation transition. At 60 μs, the pressure in the mixture is 100 bars, at 80 μs, the pressure has risen to 800 bars. The onset of compressive combustion occurs at 100 μs. The reactive chemistry in the

continuum mixture model is activated and leads to deflagration-to-detonation transition at 104 μs. There are no direct experimental measurements of the time to DDT relative to the onset of combustion. Several experimental observations suggest that if a violent event is to occur it must occur within a few hundred microseconds. The calculations presented in Figs. 2 and 3 demonstrate that the porosity and specific surface area of the energetic material have strong influence on the system response.

SUMMARY AND CONCLUSIONS

The representation of an ignition locus following the onset of combustion was presented. The ignition locus was represented by a level set. The mathematical foundation for the model was built upon a continuum mixture theory for representing multiphase flow during mechanical deformation and combustion of energetic materials. The constitutive response model used was a viscoelastic-viscoplastic Maxwell element based model. The damage model used was a tensile damage and distention model. The coupled damage and reaction model was used to include the effects of dynamic mechanics and damage evolution upon the reaction chemistry. The dependence of the violence of reaction from variations in specific surface area was demonstrated. The computational results suggest that the state of the energetic material is the dominant factor for understanding the violence of reaction. This model represents an evolution in the ability to model violence of reaction initiated from either mechanical or thermal insult. This model is used to simulate the transient flame spread that occurs in the multiphase mixture. The subsequent response of the mixture is then dictated by the complex interactions between mechanics, damage, and chemistry.

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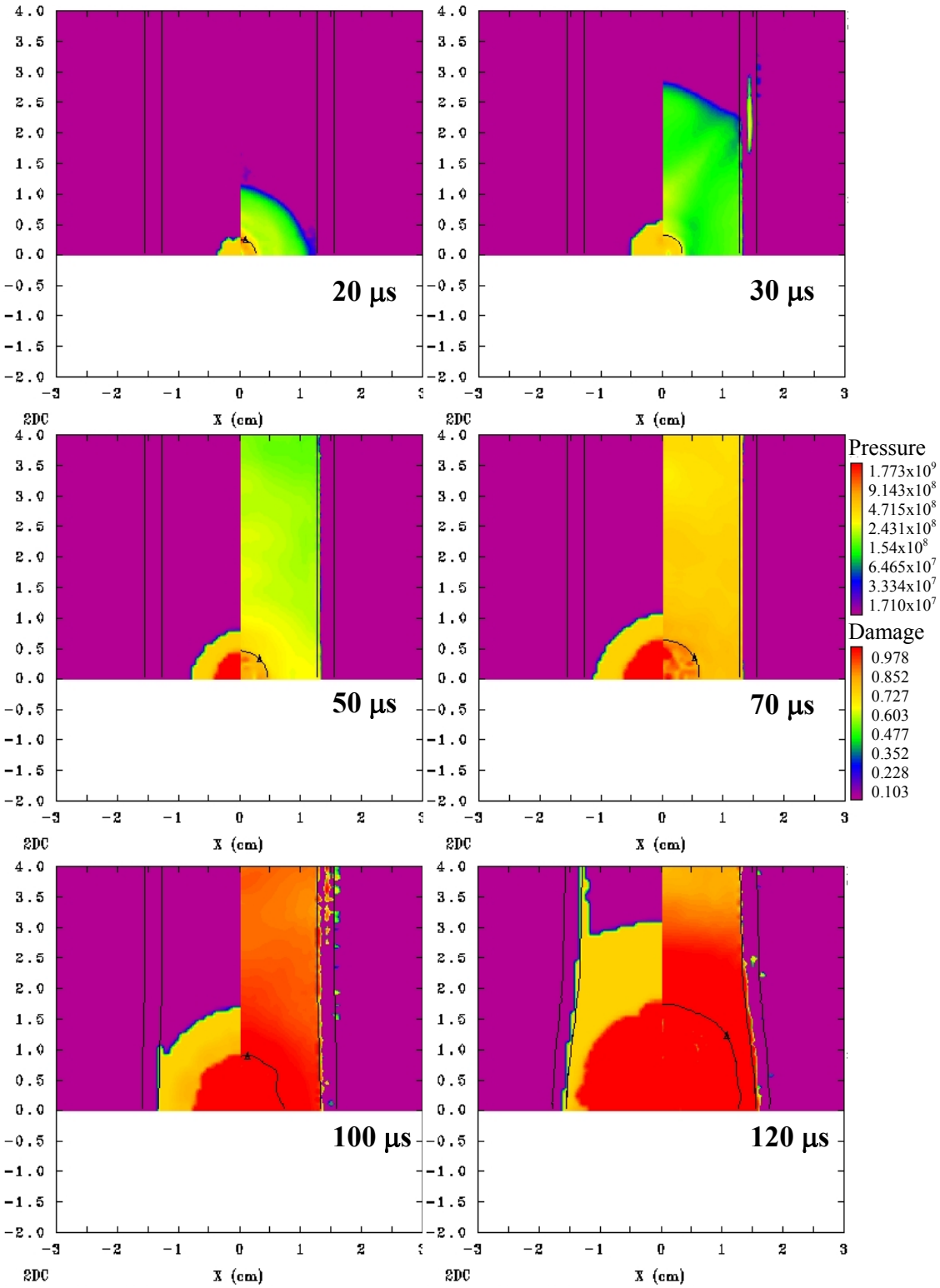

Figure 2. The mixture pressure (right) and damage (left) are shown at several times relative to ignition. This deflagration simulation uses the level set ignition front tracking model to propagate flame spread. The energetic material is initially at 95% TMD. The specific surface area is low and the burn rate exponent is such that transition to detonation is inhibited.

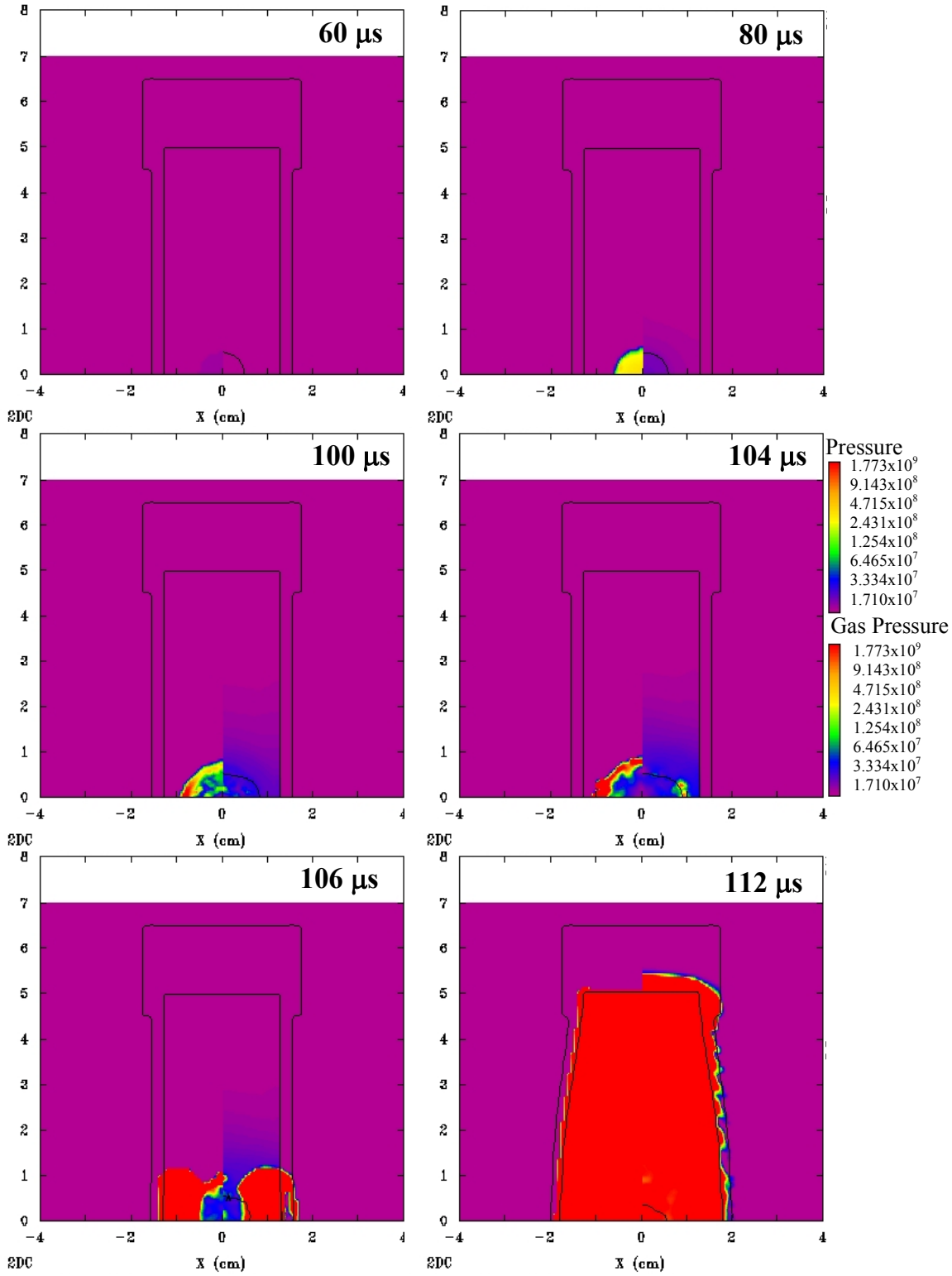

Figure 3. The mixture pressure (right) and the gas phase pressure (left) are shown at several times relative to ignition. Deflagration-to-detonation simulation uses the level set ignition front tracking model to propagate flame spread. The energetic material was initially at 90% TMD. The specific surface area evolution results in transition to detonation at 104 µs.