Modeling enhanced blast explosives using a multiphase mixture approach

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Abstract

In this overview we present a reactive multiphase flow model to describe the physical processes associated with enhanced blast. This model is incorporated into CTH, a shock physics code, using a variant of the Baer and Nunziato nonequilibrium multiphase mixture to describe shock-driven reactive flow including the effects of interphase mass exchange, particulate drag, heat transfer and secondary combustion of multiphase mixtures. This approach is applied to address the various aspects of the reactive behavior of enhanced blast including detonation and the subsequent expansion of reactive products. The latter stage of reactive explosion involves shock-driven multiphase flow that produces instabilities which are the prelude to the generation of turbulence and subsequent mixing of surrounding air to cause secondary combustion. Turbulent flow is modeled in the context of Large Eddy Simulation (LES) with the formalism of multiphase PDF theory including a mechanistic model of metal combustion.
Keywords: shock physics, blast waves, two-phase flow, combustion.

1 Introduction

Enhanced blast explosives (EBX) consist of energetic materials that are capable of producing high temperatures and high pressures over extended periods of time to greatly enhance the impulse and thermal output delivered by a blast. Whereas conventional high explosives produce extremely high pressures due to the full energy release at a shock front, the high pressure persists for only a short time. Enhanced blast explosives, on the other hand, produce lower pressures in the near field but sustain higher pressures and temperatures at a greater range over a longer duration

of time. The sustained long duration pressure is due to the entrainment and interaction of surrounding environmental oxidizer to supplement the energy release.

In this work modeling and experiments are combined to unravel the relevant physics and scaling laws that are critical in developing practical systems. A science-based predictive capability for assessment of blast performance must include the aspects of detonics and secondary combustion in turbulent reactive two-phase mixtures. Key to this understanding is a determination of the explosive dispersal of reactive mixtures and associated energy release enhancing impulse and overpressure. The important aspect of blast physics to resolve is determining how reactive waves are reinforced to achieve the ideal heat of combustion by secondary combustion.

In the sections to follow, we provide an overview of the Sandia National Laboratories modeling approach based on the shock physics code, CTH, with the implementation of the nonequilibrium multiphase mixture model. An example porous flow shock tube problem is shown to illustrate the dispersion and phase separation encountered in shock driven multiphase flow. As an example blast simulation, a 20 Kg EBX charge is modeled, including detonation and case breakup, to illustrate the onset of unstable multiphase flow prior to secondary combustion. A brief overview of the PDF formalism for the secondary combustion is then discussed. To model target lethality an effort is underway to couple this reactive multiphase modeling with Sandia's structural analysis capabilities.

2 Overview of CTH

CTH [1] was developed at Sandia National Laboratories to model complex multi-dimensional, multi-material problems that are characterized by large deformations and/or strong shocks. A two-step, second-order accurate Eulerian solution algorithm is used to solve the mass, momentum, and energy conservation equations. CTH includes a full stress/strain tensor formulation with models for material strength, fracture, porous materials, and high explosive detonation and initiation. CTH has a distributed data parallel capability and a block-based fully three-dimensional adaptive mesh refinement (AMR) scheme in parallel.

CTH uses staggered velocities with a mesh that is fixed in space and material flows through the mesh in response to boundary and initial conditions. The Lagrangian forms of the governing conservation equations are first integrated then a remap step is performed whereby distorted cells are remapped back to the initial fixed mesh. In this formulation the tensile state of a cell is monitored and tension is relieved by adding void. An explicit time step is taken as the minimum of a CFL or a cell-volume change limiting step to prevent excessive compression or expansion of a cell. AMR, with high resolution interface tracking, enhances the ability to resolve multiple scales and material interfaces to greatly minimize the effects of numerical diffusion. This is a critical requirement for developing a LES model of secondary combustion.

3 Multiphase mixture model

The multiphase mixture model of Baer and Nunziato [2] is used as the framework for the enhanced blast modeling; only the final forms of this model are given here. A two-phase system is modeled with each phase denoted with the subscript "a". Associated with each phase is the material partial density, $\rho_a = \phi_a \gamma_a$, true material density, γ_a, volume fraction, ϕ_a, particle velocity, $\vec{v_a}$, pressure, p_a, stress, $\boldsymbol{\sigma}_a$, temperature, T_a, and internal energy, e_a. The Eulerian form of these conservation equations are:

$$\textit{Mass:} \qquad \dot{\rho_a} = -\rho_a \nabla \cdot \vec{v_a} + c_a^\dagger \tag{1}$$

$$\textit{Momentum:} \qquad \rho_a \dot{\vec{v_a}} = \nabla \cdot \boldsymbol{\sigma}_a + \vec{m}_a^\dagger - c_a^\dagger \vec{v_a} \tag{2}$$

$$\textit{Energy:} \qquad \rho_a \dot{e_a} = \boldsymbol{\sigma}_a : \vec{\nabla} \vec{v_a} + e_a^\dagger - (\vec{m}_a^\dagger + c_a^\dagger \vec{v_a}/2) \cdot \vec{v_a} - c_a^\dagger E_a \tag{3}$$

where the material derivative for each phase is defined as $\dot{f}_a = \partial f_a / \partial t + \vec{v_a} \cdot \vec{\nabla} f_a$, the stress tensor is defined as $\boldsymbol{\sigma}_a = -\phi_a p_a \mathbf{I} + \boldsymbol{\tau}_a$ and the total energy for each phase is $E_a = e_a + \vec{v_a} \cdot \vec{v_a}/2$. The "†" superscript denotes a phase exchange quantity for mass, $c_a^\dagger$, momentum, $\vec{m}_a^\dagger$ and energy, $e_a^\dagger$.

Consistent with the derivations of mixture theory, summation of each balance equation over all phases yields the response of the total mixture corresponding to the well known equations of motion for a single phase material. The Second Law of Thermodynamics constraint suggests addmissible forms of the phase interaction quantities and the following final forms are defined:

$$\vec{m}_a^\dagger - c_a^\dagger (\vec{v_a} + \vec{v_i})/2 + p_i \vec{\nabla} \phi_a = \sum_j \delta_{j,a} (\vec{v_j} - \vec{v_a}) \tag{4}$$

$$e_a^\dagger - \vec{m}_a^\dagger \cdot \vec{v_a} - (e_a - \vec{v_a} \cdot \vec{v_a}/2) c_a^\dagger - W_i = \sum_j H_{j,a} (T_j - T_a) \tag{5}$$

$$\dot{\phi_a} - c_a^\dagger / \gamma_a = \sum_j \mu_{j,a} (p_a - \beta_a - p_j + \beta_j) \tag{6}$$

where $\delta_{j,a}$, $H_{j,a}$ and $\mu_{j,a}$ are exchange coefficients of the positive-definite symmetric tensors reflecting the interactions of phases. Interface quantities are denoted with the subscript "i". The configurational stress, β_a, is the stress associated with contact forces between phases and represents a different stress state than can be associated with material compressibility. The interfacial compaction work, W_i, is negligible at highly distended states. Model closure is obtained upon specifying independent equations of state and appropriate constitutive relationships for the exchange coefficients. Details of this derivation are given in [2].

Having established the general equations of motion the conservation equations are recast into integral form consistent with the finite volume formulation of CTH. Overall conservation relationships are preserved and relative flow effects are defined by a phase diffusion velocity, u_a. Phase interactions such as mass exchange,

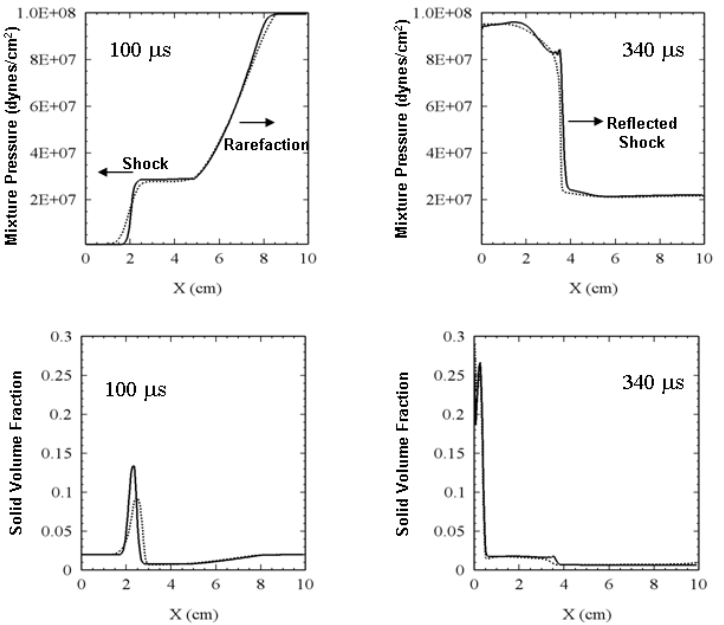

Figure 1: Multiphase shock tube problem comparing CTH and EDEN.

drag and heat transfer appear as cell-averaged quantities. The phase conservation equations have a common mathematical structure:

$$\frac{d}{dt}\int_V f_a dV = \int_V R_a dV - \oint_{\partial V} F_a \cdot \vec{n} dS - \oint_{\partial V} f_a(\vec{u_a} \cdot \vec{n}) dS. \qquad (7)$$

The first two terms on the right side correspond to conservation sources and cell-surface quantities that are solved during the Lagrangian step and the remaining phase diffusion term is incorporated during the remap step using operator splitting.

One of the preliminary steps in this development includes benchmarking and comparing the multiphase model in CTH to other shock physics codes. Several shock tube problems have been formulated in CTH and EDEN [3] to validate the multiphase model with particular emphasis at the dilute limit similar to conditions associated with far field particulate dispersal and secondary combustion. The initial condition for this example test problem corresponds to a uniform, stationary multiphase mixture at a temperature of 293 K and a solid volume fraction of 2%. A low pressure section (0 to 5 cm) at $1x10^6$ dynes/cm^2 is adjacent to a high-pressure section (5-10 cm) at $1x10^8$ dynes/cm^2.

Numerical results calculated with CTH (solid lines) for the mixture pressure and solid volume fraction are cross plotted with EDEN (dashed lines) in Figure 1. At 100 μs, the initial disperse shock wave propagates into the low pressure region creating a pressure jump state of approximately $2.9 \text{x} 10^7$ dynes/cm^2. The solid volume fraction evolves as a dispersive wave and consolidation of the solid phase occurs near the shock front. At 340 μs, the shock wave reflects from the rigid wall and interacts with the rarefaction fan from the high pressure driver section. The mixture pressure at the wall almost triples compared to the initial shock jump state and the solid volume fraction reaches a peak value of 0.26 at the wall. The CTH and EDEN results are in good agreement with each other for the wave speed and amplitudes.

4 An example of multiphase enhanced blast

Typical enhanced blast explosive formulations that are being formulated consist of blends of monopropellants and/or polycrystalline explosives, binders and metal additives. In this work, a representative enhanced blast explosive considers a mixture of 53% isopropyl nitrate, 29% RDX, 14.5% aluminum flake, and 3.5% cabo-sil (by weight). In typical charge configurations, these nonideal energetic materials are shock initiated using a booster charge that is nominally 10% by weight. This mixture has been shown to explosively disperses reactive particulate that can trigger secondary combustion by reflected shocks [4].

In determining the nature of the detonation dispersal process detailed mesoscale simulations have been conducted to provide insight into the shocked fields of a heterogeneous mixture of energetic constituents. The formalism of mesoscale modeling is given in [5]. A representative volume element is an assemblage of material representing the energetic mixture at the mesoscale. In this example, RDX crystals are represented as a distribution of cuboids of 50μm and 100μm sizes randomly mixed with 200μm by 200μm by 10μm aluminum platelets (representing agglomerated material) to create a packing configuration that conforms to the volume fractions of the mixture. IPN liquid fills the remaining interstitial regions. A C-4 booster explosive is used to shock initiate the RDX and IPN of the mixture; aluminum is considered inert. Appropriate equations of state and constitutive models are defined for the shock physics analysis (CTH) and details of this simulation (select time planes are displayed in Figure 2) indicate that much deformation of the metal additive occurs during the shock loading process. It is suggested that the aluminum and its passivated coating likely breaks up during detonation and thus the ignition and combustion characteristics of the dispersed aluminum should be expected to be greatly different than conditions encountered during propellant combustion.

To model the shock initiation process at the explosive charge scale the traditional approach of a continuum level detonation model is used to describe the initial expansion of the particulate and detonation products. As seen in the mesoscale simulation, the constituents have insufficient time to mix at the shock time scales and that relatively little aluminum is expected to participate in the detonation

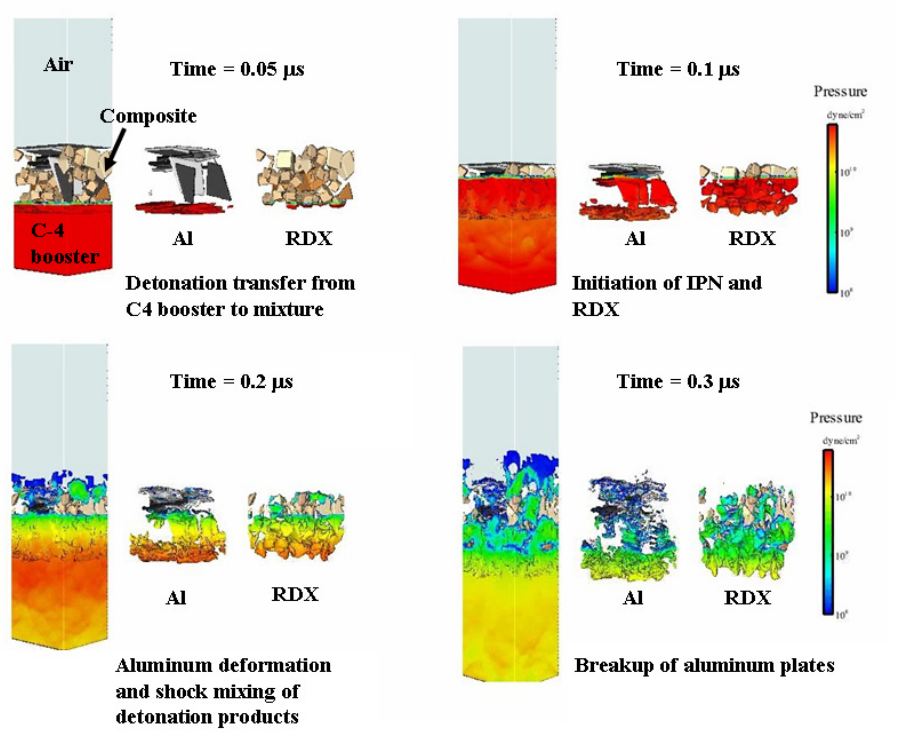

Figure 2: A mesoscale simulation of explosively shocked EBX mixture.

process. Thus, a tabular EOS was generated for the reactive mixture (excluding aluminum reactions) using the CHEETAH thermochemical equilibrium code [6]. Impact tests on thin layers of the explosive paste have been conducted to determine parameters for a phenomenological model for the reactive flow. Details of this test configuration and parameter estimations are given in [7] and not repeated here.

Having establishing a reactive flow model, the near field regions of an enhanced blast charge was then modeled. A blast assessment of the spherical ternary charge was modeled to resolve blast wave and reflected wave characteristics in tests conducted at Sandia National Laboratories [4]. Numerical modeling of the tests serves to guide the experimental studies and helps in interpreting pressure measurements.

Modeling has been applied to design free field tests of 20 Kg spherical charges, as illustrated in Figure 3. Of most interest is the determination of the charge standoff distance and instrumentation locations to best monitor booster rebound and ground reflection effects. In Figure 3 several time planes are shown of the evolution of material and wave fronts produced by a 20 Kg spherical ternary mixture charge at a standoff of 3 meters. A center booster charge has initiated and detonation products begin to emerge from the spherical charge at 1.0 ms and mixed phase dispersal

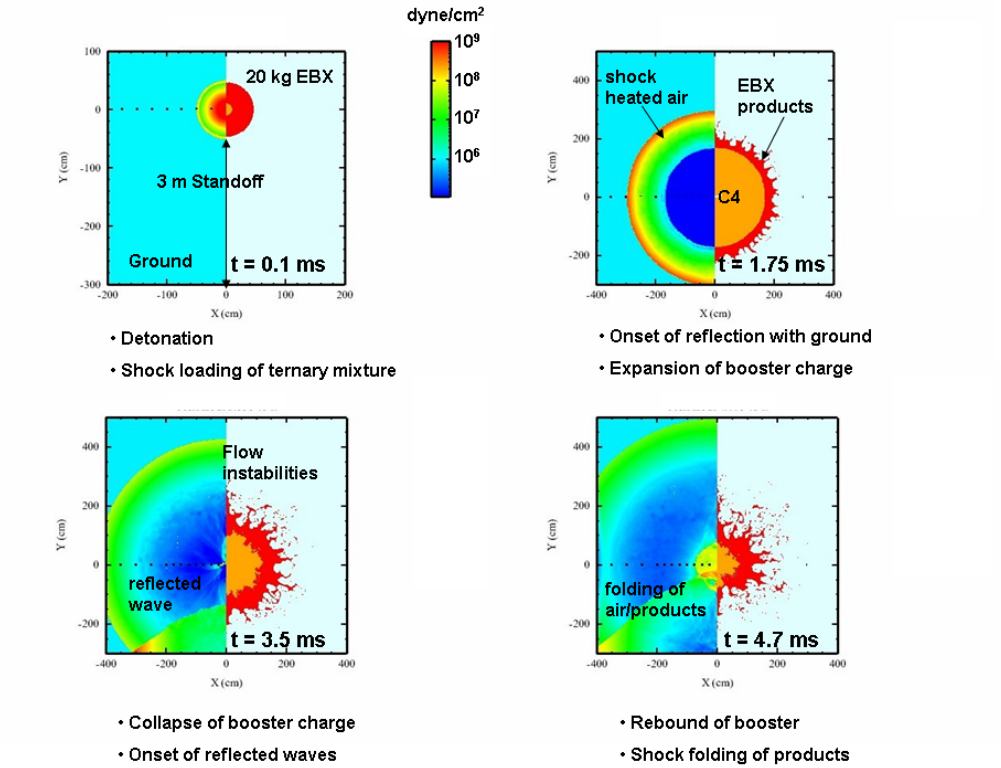

Figure 3: A simulation of a 20 Kg spherical EBX charge.

takes place. At 1.75 ms (top right image) a spherical air shock moves ahead of the contact surface. The expansion of the center booster charge accelerates the particulate laden detonation products and Rayleigh-Taylor instabilities form at the edge of the dispersed phase layer. The air shock encounters the ground and a reflected wave is produced. At 3.5 ms the center booster charge contact surface rebounds back toward the charge center and long filaments of dispersed products are produced as high local shear strains the two-phase mixture. At this time the reflected wave enhances the large scale mixing with ambient shock heated air. At 4.5 ms considerable folding of material has taken place and the effects of secondary combustion with ambient air should occur.

5 Modeling secondary combustion using PDF formalism

One of the challenges for modeling the pressure response from an enhanced blast is predicting the local turbulent mixing environment of the multiphase flow in the far-field. The range in turbulent time and mixing length scales quickly out scales

the ability to compute all the relevant physics from first principals, the approach taken in this effort is based on the use of Large Eddy Simulation (LES). In LES, the turbulent mixing processes are partitioned into length and time scale information that can be resolved using a CFD grid and information that falls below the grid requires a subgrid scale (SGS) model. For most flow conditions the main role of the SGS model is to dissipate turbulent kinetic energy [8]. For reacting flows, the role of the SGS model is much more important for predicting overall flow development. The combustion processes of highly energetic materials occur in very thin flame reaction fronts that are often much smaller than the CFD grid. The heat release at the small scales of motion defines the rate of gas expansion, and hence, the extent of enhanced blast from secondary combustion processes. Accurately accounting for the effects of these unresolved combustion processes is therefore paramount to developing a reliable modeling capability.

In the statistical modeling approach, the information regarding the spatial variations of the gas, liquid and solid phases are reduced to a single point joint probability density function (PDF). The PDF distribution defines the probability of finding the composition over an entire range of thermo-physical states [9]. The outstanding challenge in PDF approaches is determining the functional form of the PDF as a function of time and space in the computational domain. The simplest approach is to assume a functional form of the PDF and then parameterize its evolution using transport equations for the mean and RMS of the composition. As an improvement to an assumed PDF model, the full PDF approach is also being explored. The major benefit of this approach is that the PDF is determined through an evolution equation that can be derived from first principles. In this work PDF transport equations for multiphase flow are derived starting from the instantaneous separated two-phase conservation equations[10]. The PDF equations are then represented as a statistically equivalent system of stochastic differential equation (SDE's) that can be solved directly via Monte Carlo methods. Current efforts are in development to extend this approach to include the ignition and burning of aluminum particles using a recently developed particle ignition model [11] to include the effects of turbulent mixing and combustion environment of enhanced blast.

6 Summary

A goal of this effort is to develop a better understanding and advance modeling methodologies for enhanced blast munitions. The specific model development includes fundamental studies of turbulent mixing and combustion of metalized energetic materials. The Sandia program is purposely well-coordinated with experimental studies to first understand, and then devise and implement models that can be used to address several key elements for enhanced-blast applications. Although the development of modeling will eventually incorporate the statistical aspects turbulent secondary combustion effects, preliminary modeling has been successfully applied to design enclosed and free-field blast tests. Comparison of experimental results with model predictions is still in progress, but preliminary analysis shows good correlation to predictions of conditions of shock reflection and conditions

leading to secondary combustion ignition. A long-term goal remains to develop a predictive model for enhanced blast and other volumetric explosive performance, including lethality to targets, by coupling this shock physics analysis to Sandia's structural finite element analysis capabilities.

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