

Al-Air Combustion in Unconfined SDF Explosions

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1 Introduction

Laboratory experiments have been performed with 1.5-gram Shock-Dispersed-Fuel (SDF) charges [1]. The charge consisted of a 0.5-g PETN booster surrounded by 1-g of flake Aluminum (Al) powder. The SDF charge was placed at the center of a bomb calorimeter. Detonation of the booster disperses the fuel, ignites it, and induces an exothermic energy release via a turbulent combustion process. Over-pressure histories in air were considerably larger than those measured in nitrogen atmospheres; impulses histories show factors of 2 to 4 increase due to Al-air combustion. At the 21st ICDERS we presented numerical simulations of those experiments [2].

Here we study the flow fields created by un-confined SDF explosions at the 10-kg scale. In particular, we consider an SDF charge consisting of 3.6-kg spherical C4 booster surrounded by 6.4-kg of flake Al powder. The charge was detonated 122 cm above a concrete pad instrumented with static pressure gages. Described here are numerical simulations of the explosion field performed with our three-dimensional (3D) Adaptive Mesh Refinement (AMR) code. The Combustion Model treats the flow field as a dilute heterogeneous continuum—with separate conservation laws each phase—and interaction terms that allow the phases to exchange mass, momentum and energy via phenomenological laws. A unique feature of the Model is that a high-order Godunov algorithm is used not only for the gas phase, but also for the particle phase. This provides an accurate solution of the governing hyperbolic conservation laws that is devoid of artificial effects of numerical diffusion. The system of equations is closed by a Quadratic EOS model [4] that specifies the thermodynamic states of the combustion fields. Results of the AMR code simulations of the 10 kg-SDF explosions will be described and compared with experimental results.

2 Model

Conservation Laws

The Model is based on the Eulerian multi-phase conservation laws for a dilute heterogeneous continuum, as formulated by Nigmatulin [3]. We model the evolution of the gas phase combustion fields in the limit of large Reynolds and Peclet numbers, where effects of molecular diffusion and heat conduction are negligible. The flow field is governed by the gas-dynamic conservation laws:

$$\text{Mass:} \quad \partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = \dot{\sigma}_s \quad (1)$$

$$\text{Momentum:} \quad \partial_t \rho \mathbf{u} + \nabla \cdot (\rho \mathbf{u} \mathbf{u} + p) = \dot{\sigma}_s \mathbf{v} - \dot{f}_s \quad (2)$$

$$\text{Energy:} \quad \partial_t \rho E + \nabla \cdot (\rho \mathbf{u} E + p \mathbf{u}) = -\dot{q}_s + \dot{\sigma}_s E_s - \dot{f}_s \cdot \mathbf{v} \quad (3)$$

where ρ, p, u represent the gas density, pressure and specific internal energy, \mathbf{u} is the gas velocity vector, and $E \equiv u + \mathbf{u} \cdot \mathbf{u}/2$ denotes the total energy of the gas phase. Source terms on the right hand side take into account: mass addition to gas phase due to particle burning ($\dot{\sigma}_s$), particle drag (\dot{f}_s), and heat losses (\dot{q}_s).

We treat the particle phase as a Eulerian continuum field [3]. We consider the dilute limit, devoid of particle-particle interactions, so that the pressure and sound speed of the particle phase are zero. We model the evolution of particle phase mass, momentum and energy fields by the conservation laws of continuum mechanics for heterogeneous media:

$$\text{Mass:} \quad \partial_t \sigma + \nabla \cdot \sigma \mathbf{v} = -\dot{\sigma}_s \quad (4)$$

$$\text{Momentum:} \quad \partial_t \sigma \mathbf{v} + \nabla \cdot \sigma \mathbf{v} \mathbf{v} = -\dot{\sigma}_s \mathbf{v} + \dot{f}_s \quad (5)$$

$$\text{Energy:} \quad \partial_t \sigma E_s + \nabla \cdot \sigma E_s \mathbf{v} = \dot{q}_s - \dot{\sigma}_s E_s + \dot{f}_s \cdot \mathbf{v} \quad (6)$$

$$\text{Particles:} \quad \partial_t n_s + \nabla \cdot n_s \mathbf{v} = 0 \quad (7)$$

where σ and \mathbf{v} represent the particle-phase density and velocity, n_s is the number of particles, and $E_s \equiv C_s T_s + \mathbf{v} \cdot \mathbf{v}/2$ denotes the total energy of the particle phase.

Interactions

The inter-phase interaction terms for mass, momentum, heat and particle burning law take the form as described by Khasainov et al. (2005):

$$\text{Mass Exchange:} \quad \dot{\sigma}_s = \begin{cases} 0 & T_s < T_{ign} \\ -3\sigma(1 + 0.276\sqrt{\text{Re}_s})/t_s & T_s \geq T_{ign} \end{cases} \quad (8)$$

$$\text{Momentum Exchange:} \quad \dot{f}_s = (3\rho\sigma/4\rho_s d_s) C_D (\mathbf{u} - \mathbf{v}) |\mathbf{u} - \mathbf{v}| \quad (9)$$

$$\text{where } C_D = 24/\text{Re}_s + 4.4/\sqrt{\text{Re}_s} + 0.42 \text{ and } \text{Re}_s = \rho d_s |\mathbf{u} - \mathbf{v}|/\mu \quad (10)$$

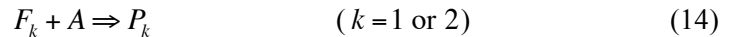
$$\text{Heat Exchange:} \quad \dot{q}_s = (6\sigma/\rho_s d_s) [Nu\lambda(T - T_s)/d_s + \varepsilon\sigma_{\text{Boltz}}(T^4 - T_s^4)] \quad (11)$$

$$\text{where } Nu = 2 + 0.6\text{Pr}\sqrt{\text{Re}_s} \quad (12)$$

$$\text{Ingignoli Burning Law (1999): } t_s = Kd_{s0}^n / \phi^{0.9} \quad (13)$$

Combustion

We consider two fuels: C4 detonation products (F_1) and Aluminum (F_2), along with their corresponding combustion products: C4-air (P_1) and Al-air (P_2). We consider the global combustion of fuel F_k with air (A) producing equilibrium combustion products P_k :



The mass fractions Y_k of the components are governed by the following conservation laws:

$$\text{Fuel-}k: \quad \partial_t \rho Y_{F_k} + \nabla \cdot \rho Y_{F_k} \mathbf{u} = -\dot{s}_k + \delta_{k2} \dot{\sigma}_k \quad (15)$$

$$\text{Air:} \quad \partial_t \rho Y_A + \nabla \cdot \rho Y_A \mathbf{u} = -\sum_k \alpha_k \dot{s}_k \quad (16)$$

$$\text{Products-}k: \quad \partial_t \rho Y_{P_k} + \nabla \cdot \rho Y_{P_k} \mathbf{u} = \sum_k (1 + \alpha_k) \dot{s}_k \quad (17)$$

Fuel and air are consumed in stoichiometric proportions: $\alpha_k = A/F_k$. In the above, \dot{s}_k represents the global kinetics sink term. In this work we use the fast-chemistry limit that is consistent with the inviscid gas-dynamic model (1)-(3), so whenever fuel and air enter a computational cell, they are consumed in one time step. Here δ_{k2} represents the Kronecker delta ($\delta_{k2} = 0$ if $k = 1$ and $\delta_{k2} = 1$ if $k = 2$) and takes into account the vaporization of Al fuel from the particle phase EQ. (4), which creates a source of Al fuel in the gas phase.

Equations of State

The thermodynamic states encountered during SDF explosions have been analyzed in by Kuhl and Khasainov [4]. The locus of states of component c in specific internal energy-temperature plane are fit with quadratic functions of temperature:

$$u_c(T) = a_c T^2 + b_c T + c_c \quad (18)$$

For cells containing a mixture of components, the mixture energy also satisfies a quadratic form:

$$u_m(T) = \sum_c Y_c u_c = a_m T^2 + b_m T + c_m \quad (19)$$

Given the mixture specific internal energy u_m , the mixture temperature can be evaluated by:

$$T_m = [-b_m + \sqrt{b_m^2 - 4a_m(c_m - u_m)}] / 2a_m \quad (20)$$

using mixture coefficients as defined by:

$$a_m = \sum_c Y_c a_c, \quad b_m = \sum_c Y_c b_c, \quad c_m = \sum_c Y_c c_c, \quad R_m = \sum_c Y_c R_c \quad (21)$$

For pure cells, the pressure of a component is calculated from the perfect gas relation $p_c = \rho_c R_c T_c$, or from the JWL function in the detonation products gases [4]. In mixed cells, the pressure is calculated from the mixture temperature by the ‘‘law of additive pressures’’:

$$P_m = \sum_c P_c(V_m, T_m) \quad (22)$$

where $P_c(V_m, T_m)$ denotes the pressure of component c if it existed alone at V_m and T_m .

Numerical Methods

The governing equations (1)-(7) and (15)-(17) are integrated with high-resolution upwind methods that represent high-order generalizations of Godunov’s method. The algorithm for gas phase conservation laws is based on an efficient Riemann solver for gas-dynamics first developed by Colella and Glaz [5]. The algorithm for the particle phase conservation laws is based on a Riemann solver for two-phase flows as developed by Collins et al. [6]. Source terms are treated with operator splitting methods. Being based on Riemann solvers, information propagates along characteristics at the correct wave speeds, and they incorporate nonlinear wave interactions within the cell during the time step.

These Godunov schemes have been incorporated into an adaptive mesh refinement (AMR) algorithm of Berger & Colella (1989) that allows us to focus computational effort in complex regions of the flow such as mixing layers and reaction zones. In this AMR approach, regions to be refined are organized into rectangular patches, with 100’s to 1,000’s of grid-points per patch. AMR is also used to refine turbulent mixing regions; by successive refinements we are able to capture the energy-bearing scales of the turbulence on the computational grid. In this way we are able to compute the effects of turbulent mixing without resorting to turbulence modeling (which is not applicable to this problem). This is consistent with the ‘‘MILES’’ approach of Boris et al. [7].

3 Results

Three-dimensional numerical simulations of a 10-kg SDF explosion at a height of burst of 122 cm were performed with our two-phase AMR code, based on the model described in §2. A cross-sectional view of the computed temperature field at 30 ms is presented in Fig. 1. Red corresponds to a temperature of 4,300 K, and illustrates where Al-air combustion is occurring within the explosion cloud. A variety of mixing scales are evident.

Figure 2 depicts blast wave pressure histories measured at ground zero (below the charge) for the SDF charge (red curve) versus the booster charge (blue curve); this comparison illustrates the reactive-blast-wave effect caused by ballistic mixing and combustion of Al particles with air during the initial blast wave (Fig. 2a). The black curve represents the 3D simulation with the two-phase AMR code; the computed waveform seems to be less dissipative than the experiment during the first blast wave. In Fig. 2b, waveforms for an SDF explosion in a vented chamber are shown. Multiple shocks arise from shock reflections from the walls. Computed and measured waveforms are in agreement.

References

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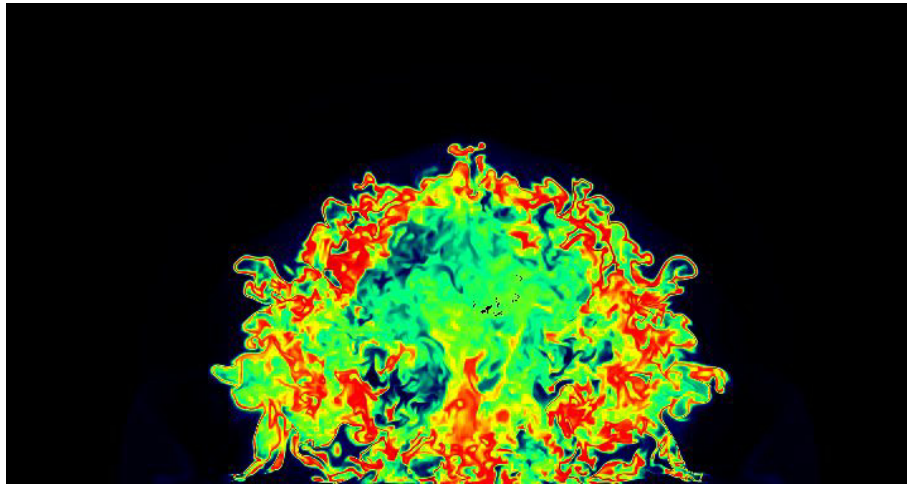


Figure 1. Temperature field illustrating Al-air combustion in an SDF explosion cloud ($t=30$ ms).

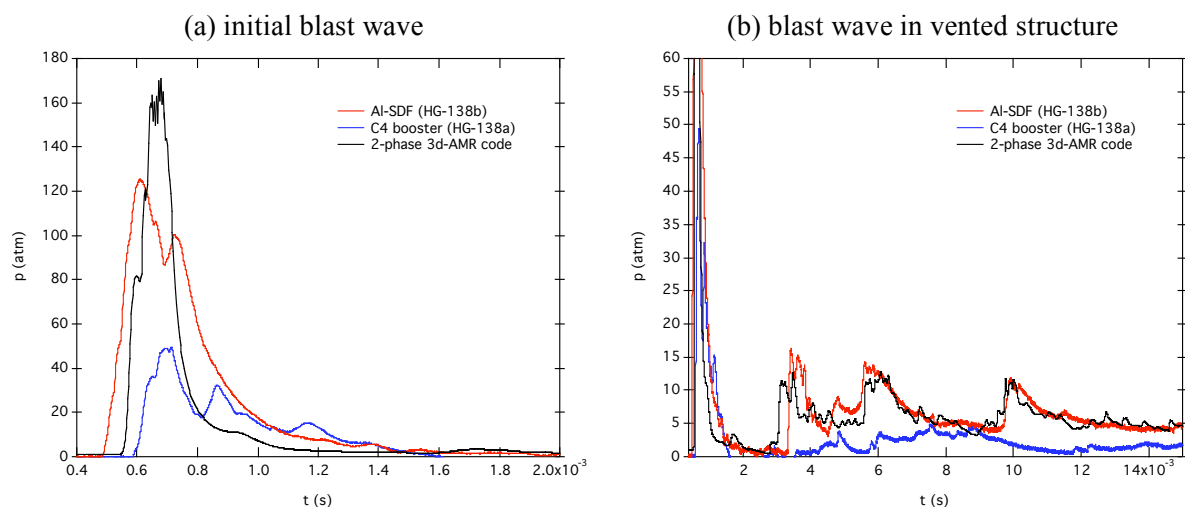


Figure 2. Blast wave pressure histories measured at ground zero (below the charge) for the SDF charge (red curve) versus the booster charge (blue curve) illustrating the reactive blast wave effect. Black curve represents the 3D simulation with the two-phase AMR code.