ADAPTIVE HIGH-RESOLUTION METHODS FOR SIMULATING COMBUSTION IN EXPLOSIONS

A. L. Kuhl[1], J. B. Bell[2], V. E. Beckner[2]

[1] *Lawrence Livermore National Laboratory, 7000 East Ave, Livermore, CA 94551*
[2] *Lawrence Berkeley National Laboratory, 1 Cyclotron Rd, Berkeley, CA 94720*

Key words: TNT charges, Al-SDF charges, 2-phase flow, turbulent combustion modeling

We have developed adaptive high-resolution methods for numerical simulations of turbulent combustion explosions. The code is based on our AMR (Adaptive Mesh Refinement) technology that was used successfully to simulate distributed energy release in explosions, such as: afterburning in TNT explosions and turbulent combustion of Shock-Dispersed-Fuel (SDF) charges in confined explosions. Versions of the methodology specialized for low-Mach-number flows have also been developed and extensively validated on a number of laboratory-scale laminar and turbulent flames configurations. In our formulation, we model the gas phase by the multi-component form of the reacting gasdynamics equations, while the particle phase is modeled by continuum mechanics laws for 2-phase reacting flows, as formulated by Nigmatulin. Mass, momentum and energy interchange between phases are taken into account using Khasainov's model. Both the gas and particle-phase conservation laws are integrated with their own second-order Godunov algorithms that incorporate the non-linear wave structure associated with such hyperbolic systems. Specialized methods are used to integrate the stiff chemical kinetics equations and inter-phase terms. Adaptive grid methods are used to capture the energy-bearing scales of the turbulent flow (the MILES approach of J. Boris) without resorting to traditional turbulence models. The code is built on an AMR framework that manages the grid hierarchy. Our work-based load-balancing algorithm is designed to run efficiently on massively parallel computers. Gas-phase combustion in the explosion-products (EP) cloud is modeled in the fast-chemistry limit, while Aluminum particle combustion in the EP cloud is based on the finite-rate empirical burning law of Ingignoli and the physio-chemical kinetic model for the ignition of Al particle clouds recently introduced by Kuhl & Boiko (2010). The thermodynamic properties of the components are specified by the Cheetah code; the caloric equation of state $u(T)$ is fit with a quadratic function of temperature (thereby taking into account variations of specific heat with temperature), while the thermal equation of state is based on the perfect gas law (which has proven to be accurate in this combustion regime). These models were used to simulate the following problems:

- spherical combustion clouds from unconfined TNT and Al-SDF explosions-Fig. 1
- turbulent combustion of an Al-SDF charge in a 21-liter calorimeter-Fig. 2
- turbulent combustion of an Al-SDF charge in a 6.3-liter tunnel-Fig. 3
- turbulent combustion of an Al-SDF charge in 4-liter chamber-Fig. 4;
- turbulent combustion of an acetylene cloud-Fig. 5;
- turbulent combustion of a 10-kg Al-SDF charge in a vented chamber-Fig. 6, 7;
- turbulent combustion in a 10-kg Al-SDF explosion at a HOB = 122 cm-Fig. 8,9

Extensive validation of the modeling has been accomplished by comparisons of pressure histories with experimental data for 18 different cases; complete results are provided in the Appendix. Such numerical simulations will be used to elucidate the fundamental combustion mechanisms and the physical processes that control the energy release process in such explosions.