Simulations of Shock-Induced Mixing & Combustion of an Acetylene Cloud in a Chamber

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In this paper we present numerical simulations of the interaction of a blast wave with an acetylene bubble in a closed chamber. We model the system using the inviscid Euler equations for a mixture of ideal gases. The formulation specifies the thermodynamic behavior of the system using a Chemkin [4] interface and includes the capability to model combustion as the ambient air mixes with the acetylene. The simulations are performed using a three-dimensional adaptive mesh refinement algorithm based on a second-order Godunov integration scheme. Simulations are compared with experimental measurements for the same configuration.

Experiments

Explosion experiments were conducted in a rectangular chamber (cross-section: 101.5*mm* x 101.5*mm*, & length = 386*mm*) equipped with Macrolon windows and a shadow photography system for flow visualization. A 0.3-*g* spherical PETN charge was placed at x = 96.5*mm*, and a spherical soap bubble (d = 55*mm*) containing acetylene was located at x = 268*mm*. Detonation of the charge created a spherical blast wave that reflected from the side walls, leading to complex Mach structures (Fig. 1: $t = 152ms$). The Mach fronts crush the soap bubble and deposit vorticity which causes turbulent mixing of the acetylene with air (Fig. 1: $165ms < t < 312ms$). This mixture is subsequently ignited by the arrival of the hot detonation products gases. The gas dynamics of this system were studied via numerical simulations.

Model

If we ignore viscosity, thermal conductivity and species diffusion, a multi-component mixture of gases satisfies the conservation equations for mass, momentum and total energy:

$$\partial_t r + \nabla\cdot(r\mathbf{u}) = 0 \tag{1}$$

$$\partial_t r\mathbf{u} + \nabla\cdot(r\mathbf{uu}) + \nabla p = 0 \tag{2}$$

$$\partial_t r(e + \mathbf{u}\cdot\mathbf{u}/2) + \nabla\cdot r(e + \mathbf{u}\cdot\mathbf{u}/2)\mathbf{u} + \nabla\cdot(p\mathbf{u}) = 0 \tag{3}$$

where r, e, p and $\mathbf{u}$ denote the mixture density, specific internal energy, pressure and velocity of the mixture, respectively. The system is augmented with equations for transport of the chemical species making up the mixture:

$$\partial_t rY_k + \nabla\cdot(rY_k\mathbf{u}) = \dot{w}_k \tag{4}$$

where Y_k is the mass fraction of the k^{th} species and $\dot{w}_k$ is the chemical production rate of the k^{th} species. We then have that $\sum Y_k = 1$ and that $\sum \dot{w}_k = 0$. For ideal gases:

$$e(T, Y_k) = \sum e_k(T)Y_k \tag{5}$$

where $e_k(T)$ is the internal energy of species k as a function of temperature. The mixture equation of state is given by

$$p = rRT\sum Y_k / W_k \qquad (6)$$

where W_k is the molecular weight of species k.

We solve the resulting system using a parallel adaptive mesh refinement algorithm based on an operator-split second-order Godunov integration scheme. The Godunov methodology is described in Colella and Glaz [2]; the adaptive refinement approach is discussed in Bell *et al.* [1]; and the approach to parallelization is described in Rendleman *et al.* [3].

Results

Here, we consider only the interaction of the initial blast wave with the acetylene bubble. The configuration we consider is analogous to the experimental conditions depicted in Fig. 1. For this case, experimental data indicates that ignition of the acetylene occurs at approximately 2.4 milliseconds; however, we will only present data for the computation up to approximately 0.7 milliseconds. The computational domain is discretized with a 152x40x40 base grid, with one level of refinement by a factor of two in regions of high density gradient and around the acetylene bubble.

In Fig. 2, we present color raster images of the density field in a slice down the center of the computational domain at times comparable to the frames in Fig 1. The figure uses a rainbow palette with red indicating higher densities and blue indicating lower densities. (The bubble is not very visible in the computational results because the density contrast between air and acetylene is not large, while in the experiment, imaging of the bubble is enhanced by the soap film). We note that the shock structure from the blast wave is well resolved and the computations provide an excellent match to experimental results as the leading shock wave traverses the bubble.

In Fig. 3, we explore the subsequent dynamics of the acetylene cloud after the shock has passed through the cloud and accelerated it toward the end wall. Volume-rendered (false color) images of the acetylene cloud are presented to illustrate the cloud shape from $0.325\,ms$ to $0.719\,ms$. The reflected blasted waves from the top, bottom and side walls of the chamber further deform the bubble, inducing an approximate four-fold symmetry in the bubble shape. The computations also reveal that acetylene is transported to the end wall and then reflected—thereby enhancing the dispersion of the acetylene through the domain.

Conclusions

We have presented calculations showing the initial phase of the interaction of a blast wave with a spherical bubble of acetylene. Comparison with experiment shows that the computations accurately depict the initial transit of the blast wave through the bubble. In the presentation we will present later time results that include ignition and combustion of the acetylene.

References

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[3] C. A. Rendleman, V. E. Beckner, M. Lijewski, W. Y. Crutchfield, J. B. Bell, "Parallelization of structured, hierarchical adaptive mesh refinement algorithms", *Computing and Visualization in Science*, **3**, 2000.

[4] R. J. Kee, F. M. Ruply, E. Meeks and J. A. Miller, "CHEMKIN-III: A FORTRAN chemical kinetics package for the analysis of gas-phase chemical and plasma kinetics," Sandia National Laboratories Report **SAND96-8216**.

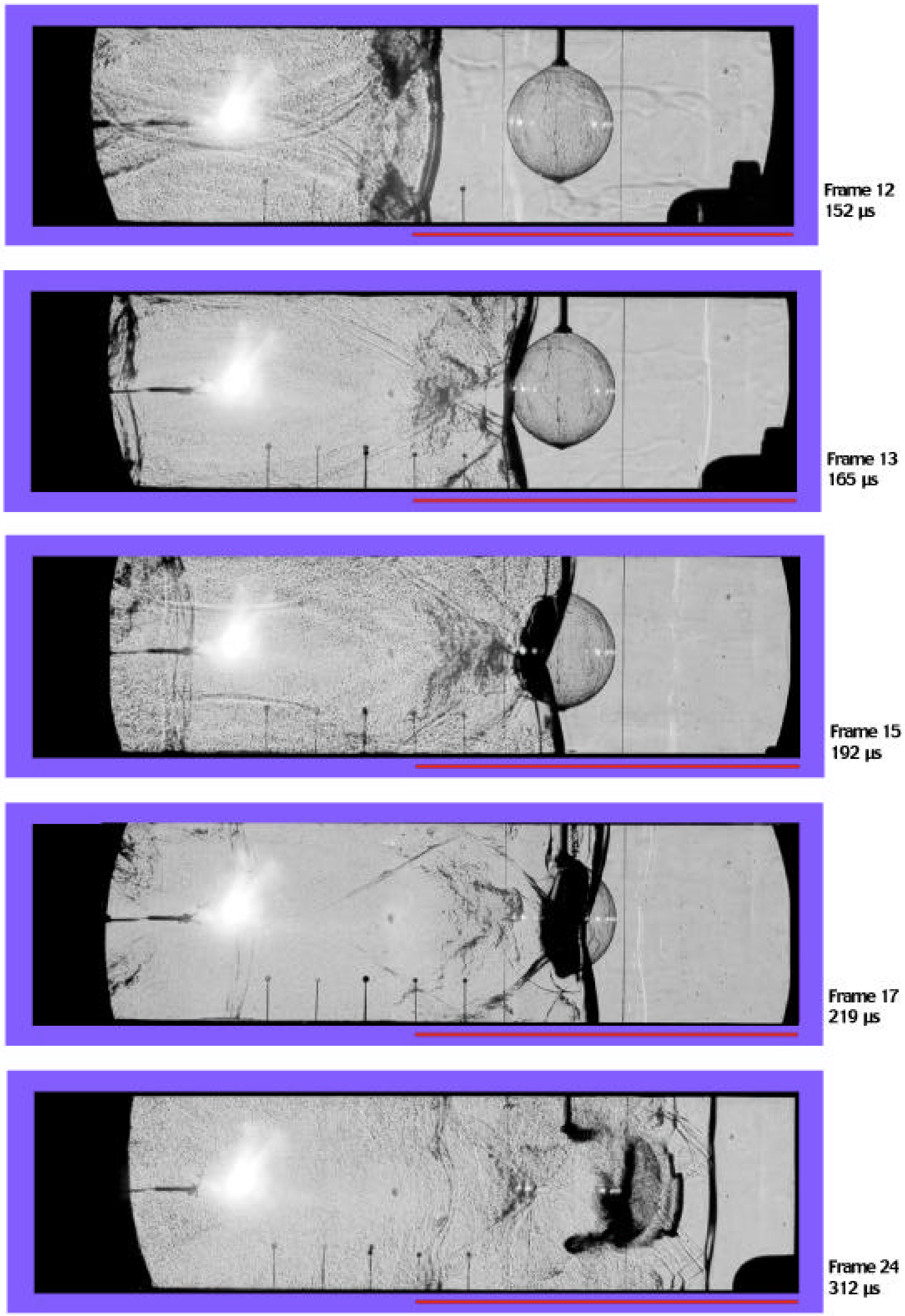

Figure 1. Shadow photographs showing the evolution of a blast wave from a 0.3-g PETN charge, and its interaction with a 55-mm soap bubble containing air.

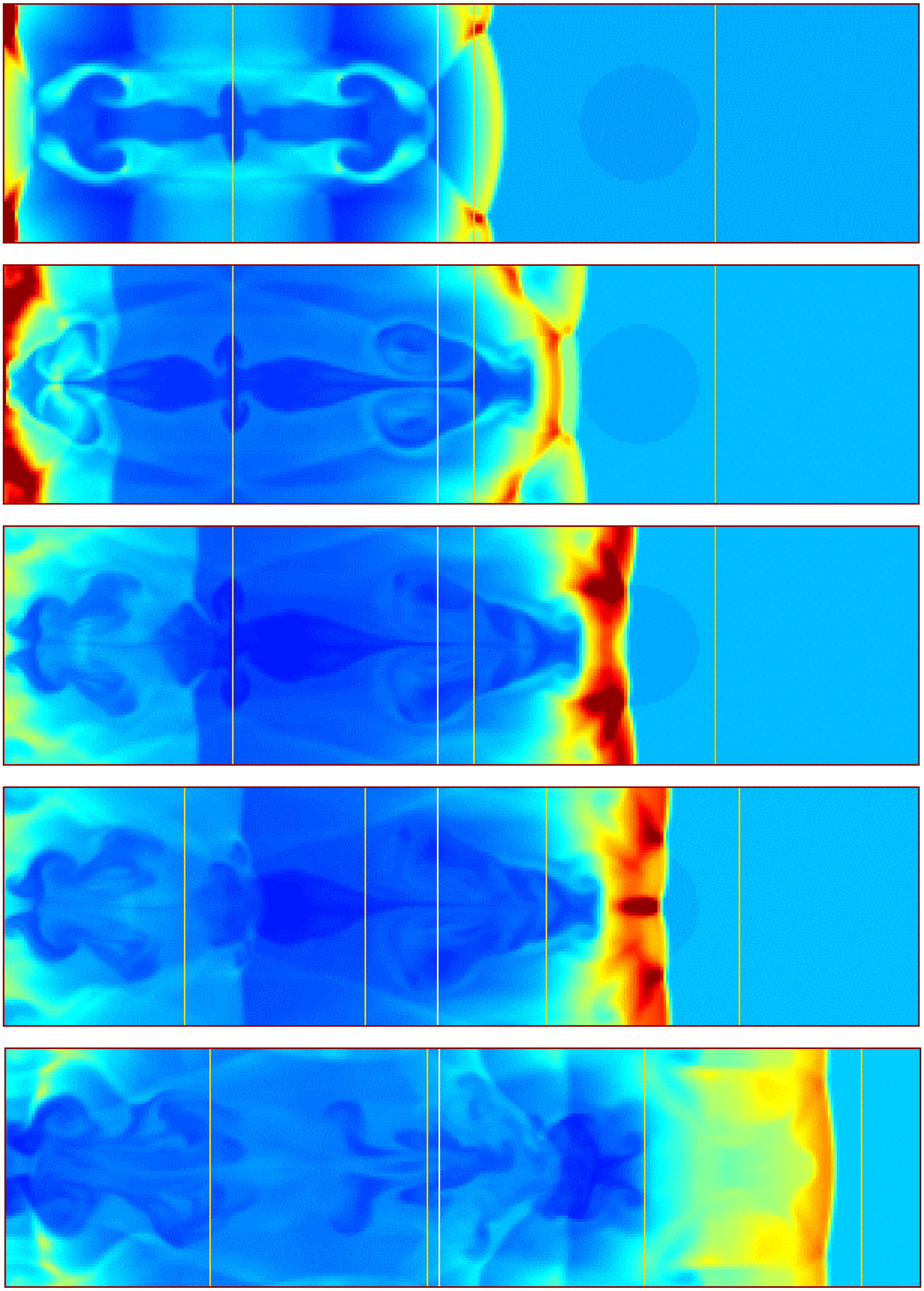

Figure 2. 3D-AMR simulation of blast interaction with acetylene cloud; color representation of the density field at the centerline.

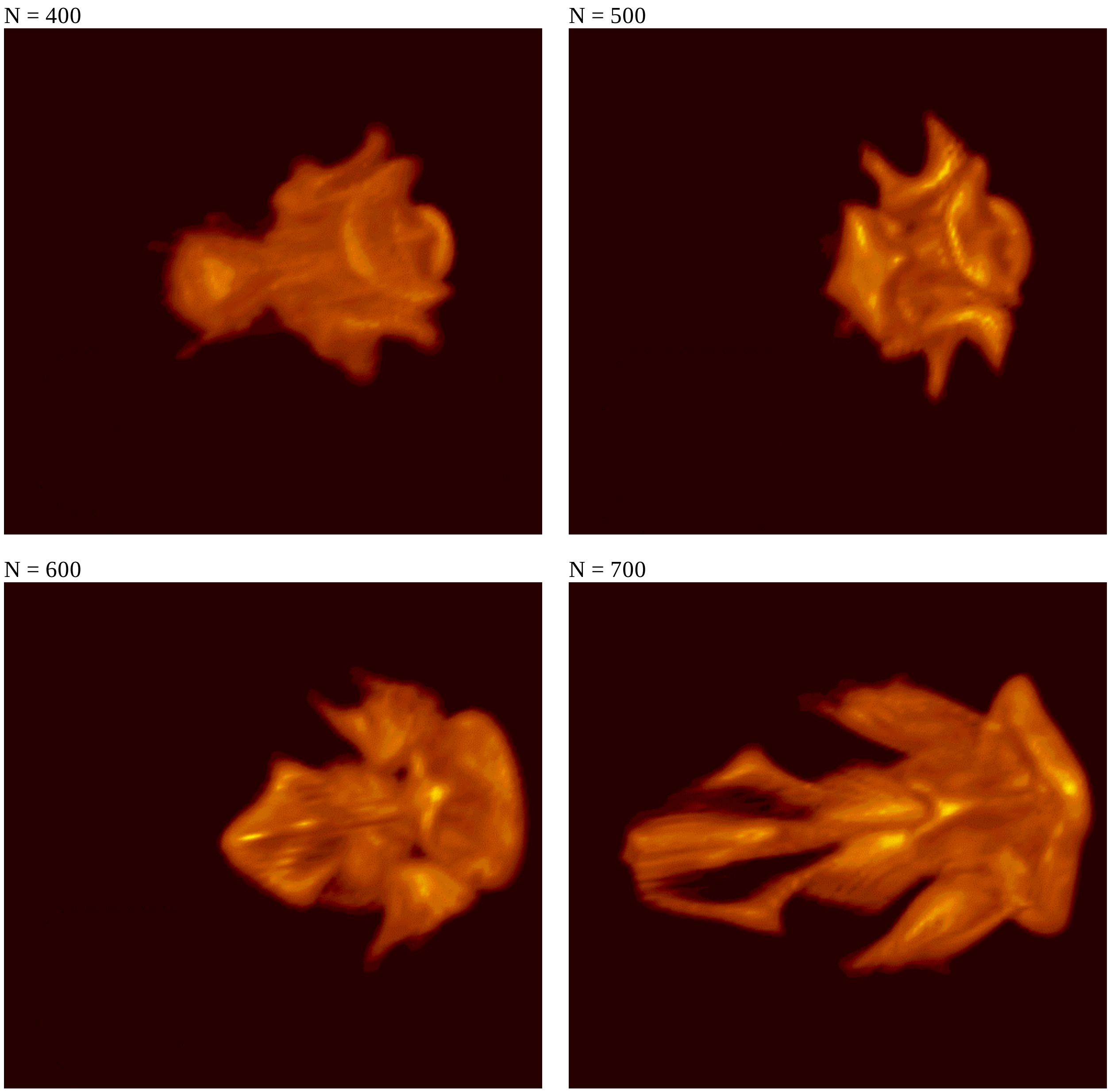

Figure 3. Volume rendering of acetylene cloud dynamics and impact on the end wall.