Numerical Simulations of Shock-Induced Mixing and Combustion *

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In this paper we use numerical simulation to investigate shock-induced ignition and combustion of a hydrocarbon gas. The focus of this paper is on quantifying the effect of fidelity in the chemical kinetics on the overal solution. We model the system using the compressible Navier Stokes equations for a reacting mixture. These equations express conservation of species mass, momentum, total energy. If we ignore radiative effects the system reduces to

$$\frac{\partial \rho Y_k}{\partial t} + \nabla \cdot (U \rho Y_k) = \nabla \cdot (\rho D_k \nabla Y_k) + \dot{\omega}_k$$

$$\frac{\partial \rho U}{\partial t} + \nabla \cdot (\rho U U) + \nabla p = \nabla \cdot \tau$$

$$\frac{\partial \rho E}{\partial t} + \nabla \cdot (\rho U E + p U) = \nabla \cdot (\kappa \nabla T) + \nabla \cdot (\tau U)$$

where U, p, T, and Y_k are velocity, pressure, temperature and mass fraction of species k, respectively. Here, the mass density, $\rho = \sum \rho Y_k$ and $E = e + U \cdot U/2$ with $e = \sum e_k(T) Y_k$. The stress tensor $\tau = \mu(\nabla U + \nabla U^t) + \lambda I \nabla \cdot U$ where μ and λ are the viscosity coefficients and κ is the thermal conductivity. For species transport, we will further assume unity Lewis number which implies that the species mass diffusion $\rho D_k = \kappa / c_p$ where c_p is the specific heat of the mixture at constant pressure.

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For the simulations presented here we assume an ideal gas equation of state for the mixture

$$p = \rho RT \sum \frac{Y_k}{W_k}$$

where W_k is the molecular weight of species k. We use standard fits to thermodynamic behavior and specify transport using TRANLIB which is part of the CHEMKIN package. We also include an interface for specification of reaction kinetics in a standard Chemkin form.

The basic discretization uses a symmetric operator split formula in which we first advance the chemistry in each zone by $\Delta t/2$, then advance the Navier-Stokes equations without the reaction term by Δt and finally advance the chemistry by $\Delta t/2$, again. The chemistry integration is performed using standard techniques for stiff ordinary differential equations. The integration algorithm for the Navier-Stokes equations combines an explicit second-order, unsplit Godunov method for the hyperbolic part of the operator with an second-order, explict Runge Kutta algorithm for the diffusive terms.

This integration algorithm is embedded in a hierarchical adaptive mesh refinement algorithm. In this approach, fine grids are formed by dividing coarse cells by a refinement ratio, r, in each direction. Increasingly finer grids are recursively embedded in coarse grids until the solution is adequately resolved with each level contained in the next coarser level. An error estimation procedure based on user-specified criteria evaluates where additional refinement is needed and grid generation procedures dynamically create or remove rectangular fine grid patches as resolution requirements change.

The adaptive time-step algorithm advances grids at different levels using time steps appropriate to that level based on CFL considerations. The time-step procedure can most easily be thought of as a recursive algorithm, in which to advance level ℓ, $0 \leq \ell \leq \ell_{max}$ the following steps are taken:

- Advance level ℓ in time as if it is the only level. Supply boundary conditions from level $\ell - 1$ if level $\ell > 0$, and from the physical domain boundaries.
- If $\ell < \ell_{max}$
  - Advance level $(\ell + 1)$ r times with time step $\Delta t^{\ell+1} = \frac{1}{r}\Delta t^{\ell}$ using boundary conditions from level ℓ, and from the physical domain boundaries.
  - Synchronize the data between levels ℓ and $\ell + 1$, interpolate corrections to higher levels if $\ell + 1 < \ell_{max}$.

The adaptive methodology is implemented for distributed memory parallel architectures using a message-passing model that exploits the coarse-grained parallelism inherent in the algorithms. The key elements of

the approach to parallelization are a dynamic load-balancing technique to distribute work to processors and a software methodology for managing data distribution and communications.

In order to evaluate the role of chemical fidelity on shock-induced combustion of a hydrocarbon bubble, we consider a 0.1 cm bubble of methane in air initially at atmospheric temperature and pressure interacting with a shock wave. Our goal is to examine the effects of fidelity in the chemical mechanism on the ignition and burning process for this type of flow. For all of the computations we use a base grid of 250 microns with two levels of refinement by a factor of two for an effective resolution of 62.5 microns.

In the initial conditions, the bubble is pure methane; hence, mixing of the methane with air resulting from the shock-bubble interaction is a prerequisite for combustion. To assess the degree to which mixing controls the combustion process in this setting we use, as our simplest approximation, a simple mixed-is-burned approximation in which methane and oxygen burn in stoichiometric proportion provided the temperature is above a prescribed ignition temperature which we set to be 900 degrees Kelvin. We also consider a single-step mechanism for methane-air combustion developed by Westbrook and Dryer [1] and a two-step mechanism developed by Zimont and Trushin [2]. Finally, we consider detailed kinetics mechansims GRI-Mech 1.2 [3], which contains 32 species and and 177 reactions as well as DRM-19 containing 21 species and 84 reactions that reduced by Kazakov and Frenklach [4] from GRI-Mech 1.2.

Our initial case is for a Mach 4 shock with the pre-shocked gas at ambient temperature and pressure. In Figure 1, we show early time images of the methane bubble being crushed by the shock and its subsequent evolution for the detailed mechanism, DRM-19. To assess the effect of the accuracy of the approximation to the chemical kinetics on the overall dynamics, we show in Figure 2, the mass of methane versus time for the three simplified mechanisms. We note that both the mixed-is-burned model and the single step chemistry exhibit essentially no induction delay before ignition, although the rate of fuel consumption for finite rate kinetics slows relative to the fast kinetics model. The 2-step mechanism delays ignition for approximately 40 micro-seconds and then burns fairly rapidly. We have not plotted either of the detailed mechanisms on this plot becauase for the time scale of the simulations, there is essentially no significant consumption of methane. For a range of stoichiometries the more detailed kinetic models predict an ignition delay of over one millisecond at the post-shock conditions in this example. We note that the post shock state for this example lies in a region of high variability in the ignition delay which accentuates the poor performance of the simplified kinetics models. In the presentation we will present additional results varying both the fluid dynamic conditions and the fuel to more fully compare the fidelity of simpified kinetics to more realistic reaction models.

References

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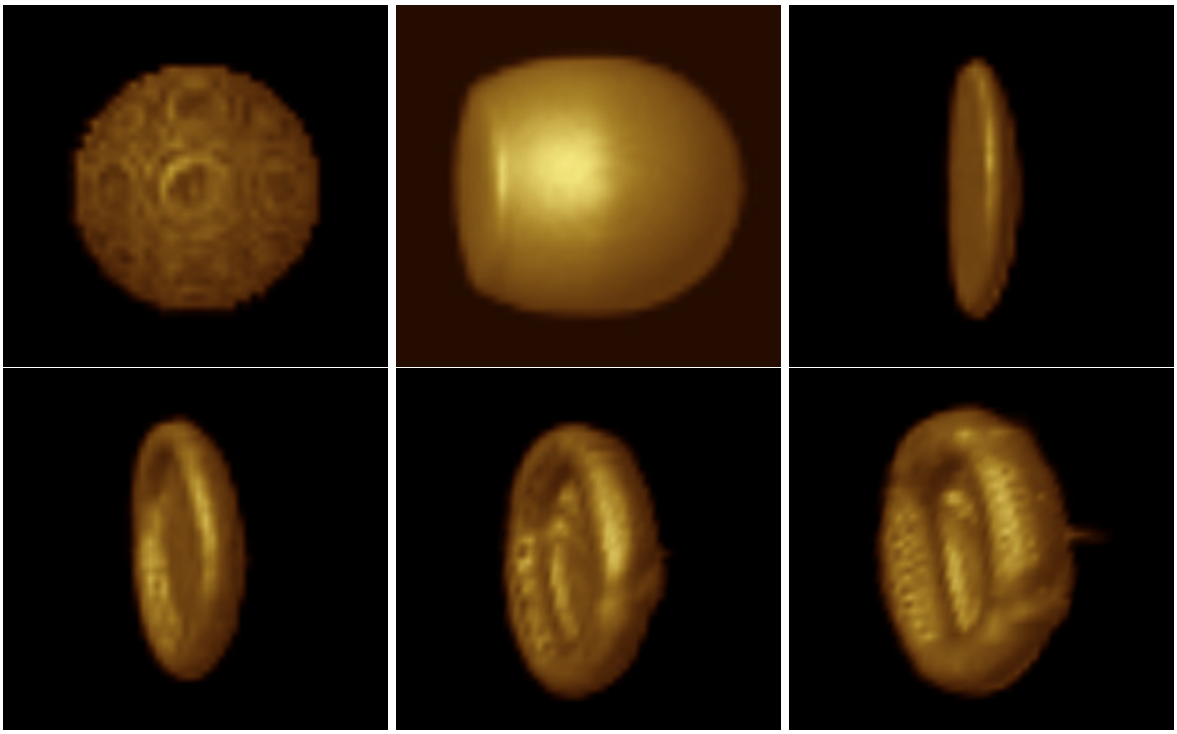

Figure 1. Early time dynamics of methane bubble crushed by a Mach 4 shock.