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 overall 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 \(\tau = \mu(\nabla U + \nabla U^t) + \lambda \nabla \cdot U\) where \(\mu\) and \(\lambda\) are the viscosity coefficients and \(\kappa\) is the thermal conductivity. For species transport, we will further assume unity Lewis number which implies that the species mass diffusion \(\rho D_k = \kappa/e_p\) where \(e_p\) is the specific heat of the mixture at constant pressure.

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

\[
p = \rho RT \sum \frac{Y_k}{W_k}
\]

\(^*_{\text{Compressible flow, shock waves, chemical mechanism}}\)
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 $\Delta t$ 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, explicit 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 $\ell$, $0 \leq \ell \leq \ell_{\text{max}}$ the following steps are taken:

- Advance level $\ell$ 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 $\ell < \ell_{\text{max}}$
  
  - Advance level $(\ell + 1)$ $r$ times with time step $\Delta t^{\ell+1} = \frac{1}{r^2} \Delta t^\ell$ using boundary conditions from level $\ell$, and from the physical domain boundaries.
  
  - Synchronize the data between levels $\ell$ and $\ell + 1$, interpolate corrections to higher levels if $\ell + 1 < \ell_{\text{max}}$.

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 two detailed mechanisms: GRI-Mech
1.2 [3], which contains 32 species and and 177 reactions; and, DRM-19 which contains 21 species and 84
reactions. DRM-19 was developed by Kazakov and Frenklach [4] by reducing 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 because 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.

As a second case we have preheated the ambient air and the methane bubble to 400K to reduce the
ignition delay and increased the size of the bubble to 1.0 cm in diameter. For this case we have run at
an effective resolution of 312.5 microns and considered only the two step mechanism and DRM-19. The
methane consumption as a function of time for this case is presented in Figure 3. Although the time scales
are dramatically reduced as a result of preheating, the two step mechanism still substantially underpredicts
the ignition delay compared to the more detailed mechanism. In the presentation we will present additional
results varying both the fluid dynamic conditions and the fuel to more fully compare the fidelity of simplified
kinetics to more realistic reaction models.
References


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