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Reactive Flow Modeling of Liquid Explosives via ALE3D/Cheetah Simulations

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Abstract. We carried out reactive flow simulations of liquid explosives such as nitromethane using the hydrodynamic code ALE3D coupled with equations of state and reaction kinetics modeled by the thermochemical code Cheetah. The simulation set-up was chosen to mimic cylinder experiments. For pure unconfined nitromethane we find that the failure diameter and detonation velocity dependence on charge diameter are in agreement with available experimental results. Such simulations are likely to be useful for determining detonability and failure behavior for a wide range of experimental conditions and explosive compounds.

Introduction

The chemical reactions that accompany the detonation of high explosives proceed at a very fast rate, typically reaching completion on times of order microseconds.[2-4] As a result, standard explosives properties such as detonation velocities and pressures can be accurately calculated for large charges by simply assuming that the reactions are instantaneous, the shock fronts are planar and infinitely thin, e.g. the Chapman-Jouguet theory, and by employing accurate equations of state for the detonation products. As the charge size is decreased however such assumptions start breaking down and the reaction rates play a larger role, determining for example the minimum steady detonation diameter (critical diameter) of any explosive. Thus, the detonability and detonation failure behavior of an explosive compound due to a decrease in the charge size, composition change (e.g. dilution) or confinement change is determined by the interplay between hydrodynamics and reaction kinetics. The theoretical study of these types of problems is difficult due to its complexity and typically requires that numerous simplifying assumptions need to be made to compare with experimental results. We explore the extent to which modern approaches that couple direct hydrodynamic simulations with accurate detonation products equations of state and kinetics can be employed to predict the detonability and failure mechanisms of liquid explosives. Here we present simulation results for the dependence of the detonation velocity on charge diameter for unconfined

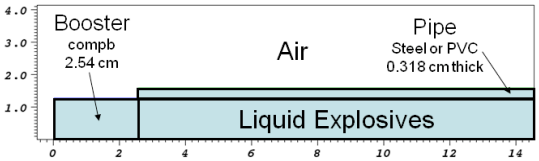

Fig 1. Schematic diagram of the 2D ALE3D/Cheetah simulations set-up mimicking a cylinder test.

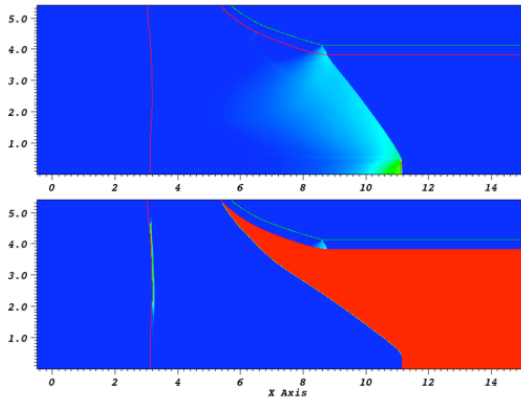

Fig. 2. An instantaneous snapshot from an ALE3D/Cheetah simulation after 16 μs showing the shock front pressure profile (top) and material composition (bottom); reactants shown in red and products in blue. Note the unstable shock front with decreasing curvature (top) and residual unburned energetic material behind the shock front (bottom).

nitromethane. We chose liquid nitromethane since it is a fairly well understood homogenous explosive, and it has been extensively studied both experimentally and theoretically[6-9].

The simulations were carried out in 2D, using the hydrodynamic code ALE3D coupled with equations of state and reaction kinetics modeled by the thermochemical code Cheetah.[10,11] The set-up (*see* Fig. 1) was chosen to mimic a standard cylinder test,[10,11] and enables well controlled initiation while providing simple boundary conditions.

The detonation kinetics of liquid explosives such as nitromethane is assumed to be well described by Arrhenius laws.[7,8] Here we employ a single nitromethane decomposition reaction:

$$CH_3NO_2 \rightarrow CO_2 + \tfrac{3}{2}H_2 + \tfrac{1}{2}N_2 \qquad (1)$$

With rate

$$k = A\exp(-\Delta H_r / RT)$$

The activation energy barrier is $\Delta H_r/R=12000K$ with a prefactor of $A=30000\ cc/(mol\ \mu s)$. We note

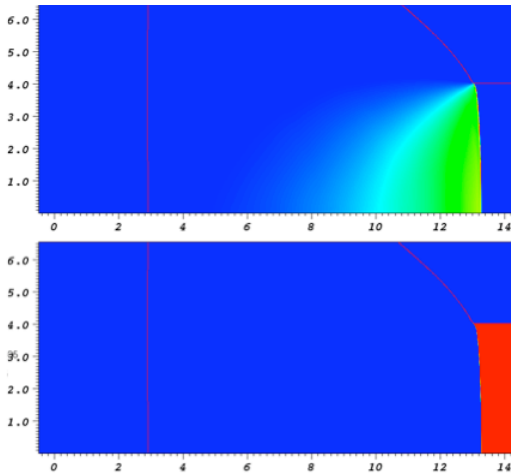

Fig. 3. An instantaneous snapshot showing the shock front (top) and material composition (bottom). Same coloring scheme are used as in Fig. 2. Note stable shock front across entire charge diameter (top) and complete decomposition of energetic material after the shock front (bottom).

that the value of the energy barrier is in line with modern estimates that place it approximately between 5000K and 16000K [6-9], and much smaller than the one originally assumed for nitromethane decomposition[1]. The above parameters were selected by matching the published detonation/failure characteristics for nitromethane under weak confinement.[5]

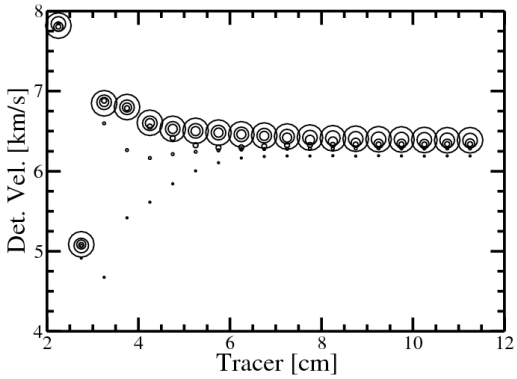

Fig. 4. Computed instantaneous shock velocity at various points within the simulation cell for unconfined/weakly confined NM. The size of the symbol shown is proportional to the charge diameter of the simulation.

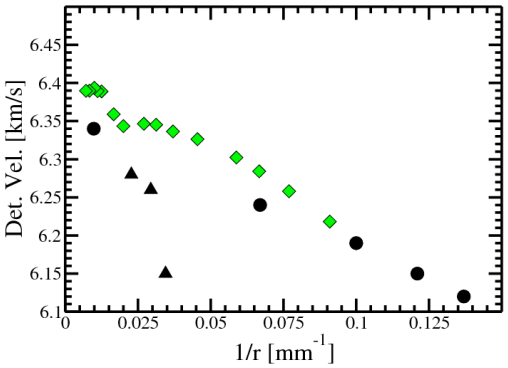

Fig. 5. Detonation velocity versus inverse charge radius for unconfined nitromethane. Green diamonds are ALE3D/Cheetah simulation results, while triangles and circles are data taken from Ref. 1 and Ref. 5

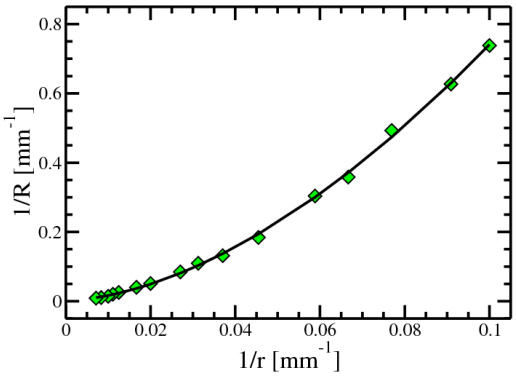

Fig. 6. Curvature of the shock front plotted as a function of the inverse charge radius for unconfined nitromethane. The results have been fitted to a power law shown in black.

Results

We performed simulations of pure nitromethane at different charge diameters with the goal of determining the detonation velocities and the shock front radius of curvature for steady detonations. We studied two criteria for successful detonation: 1) complete decomposition of the reactant behind the shock front, and 2) steady state detonation (shock front) velocity. We show for example in Fig. 2, a case where incomplete decomposition of the nitromethane leads to an extremely curved shock front, unsteady behavior and ultimately detonation failure. This simulation of a charge diameter of 80mm was performed with an Arrhenius prefactor one order of magnitude smaller than the optimal one for nitromethane; we show it for illustrative purposes. We note however that even much smaller changes in the rate lead to large effects in failure diameter. For comparison purposes we also show in Fig. 3 an example of a stable, steady detonation, with complete decomposition of the explosive behind the detonation front.

Detonation criteria based on the amount of material consumed are useful since often in simulations and/or experiments the samples are not long enough to unambiguously determine that the detonation is steady or is failing. We also studied however the standard detonation criteria, based on the shock front velocity. For this purpose we estimate the instantaneous velocity of the shock front at various positions in the simulation cell by placing numerical markers that monitor the steep rise in pressure associated with the arrival of the detonation wave; this is largely similar to the pins setup typically employed in experimental cylinder tests. The calculated shock front velocity is then plotted against the position along the cylinder axis to ascertain whether steady state detonation has been achieved. We show in Fig. 4 plots for a large set of diameters. We find that for nitromethane steady detonation velocity is achieved once the shock front passes a distance of approximately 6 cm in the simulation cell, irrespective of the charge diameter.

It is well known that starting from a very large charge the detonation velocity of any explosive will typically decrease as the charge radius decreases, until eventually no steady shock front propagation is possible at a small enough, critical diameter. We observe this behavior in our simulations of unconfined nitromethane. We show in Fig. 5 the detonation velocities from the ALE3D/Cheetah simulations as a function of the inverse charge radius. The dependence is approximately linear, as postulated by Eyring et al.[2] The results are in good agreement with the experimental data available, particularly those of Ref. 5 which correspond to very weak confinement.

Using the shock front structure information from the simulations we also determined the curvature of the detonation front for the different charge sizes. The detonation kinetics theory of

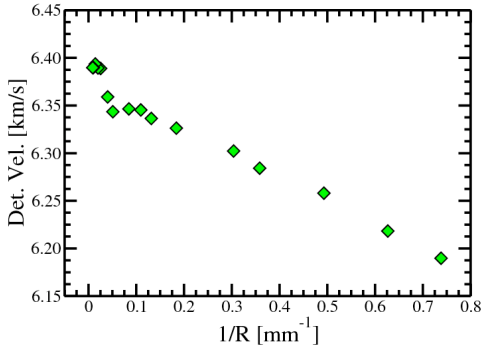

Fig. 7. Detonation velocity as a function shock front curvature for unconfined nitromethane.

Wood and Kirkwood predicts (under certain approximations that should hold well for homogenous explosives like nitromethane) a simple linear relation between the detonation velocity and shock front curvature.[4] We find that such a relation holds for the present simulations better than the one proposed by Eyring and coworkers.[2] (*see* Fig. 6) The relationship between the shock front curvature and charge radius is also shown in Fig. 7, and we find that the dependence is well represented by a power law fit (y=38.0$x^{1.7}$).

Conclusions

Reactive flow simulations of unconfined liquid nitromethane were performed using the ALE3D/Cheetah aggregate code to determine Arrhenius reaction kinetics parameters that match available experimental detonation. As expected, the failure diameter is found to be highly sensitive to the reaction rates. The optimal kinetic parameters yield a detonation velocity dependence on charge size that is in good agreement with experiments. By directly determining the shock front curvature we also find that the Wood-Kirkwood predicted linear dependence between detonation velocity and curvature holds well for nitromethane.[4] We expect that such simulations can be successfully employed to determine the detonation and failure behavior dependence on charge size, composition and confinement for a wide range of energetic compounds.

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