

Equilibrium-Chemistry Model for Multiphase Reactive Premixed and Nonpremixed Flows

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Introduction

Nikolaev and Fomin (1982, 1984) derived an approximate analytical equation for chemical equilibrium and used it to model the state of the flow of reactive gas-droplet mixture while calculating the velocity and structure of steady detonation. Based on the same idea the detonation of cryogenic hydrogen-oxygen mixtures was studied in the steady (Voronin 1984) and unsteady case (Voronin and Zhdan 1984). However, this approach does not consider all phase transitions and species one can encounter in the course of formation and expansion of reaction products. Therefore, to study detonation of aluminised high explosives (HE) the gas dynamic code was directly linked with the thermodynamic solver (Khasainov et al. 1995). Though such linking yields interesting results, the computation time seems to be too long for this technique to be applied in multi-dimensional gas dynamic simulations. The next logical step was to iterate on the pre-calculated equation of state in table form with 4 independent parameters (mixture volume V and internal energy E , and reaction progress variables x_{HE} and x_{Me}) and with about 10-20 output parameters (e.g., pressure, temperature, sound speed etc.) along with fractions of main species. Again, encouraging results were obtained, but this approach requires having a large tabulated equation of state with up to 10^6 lines for every new initial content of metal. Shifting from a two-component mixture to a ternary one with this approach is impractical.

Here we present a new model—based on equilibrium gas phase chemistry (Kuhl 2003)—which allows one to use for a given pair of components (i.e., HE and metal) the same two compact tables in a very wide range of metal content. An additional benefit is that the model can be extended to ternary mixtures. The predictive ability of the model is tested for two problems: (i) where concentration of metal is initially uniform; and (ii) the non-uniform case as combustion of Shock-Dispersed-Fuel (SDF) charges in confined explosions (Neuwald et al. 2003).

Numerical Model

The unsteady conservation equations for multiphase flows are coupled with equilibrium equation of state (EOS) pre-calculated in the form of two separate tables. The larger table describes the states of final reaction products using 3 independent variables (either T - V - x_o or E - V - x_o) where x_o is the *initial* mass fraction of metal in the mixture. The smaller table calculated at V =Const and x_o =0 describes the state of fresh gas (i.e. oxidiser or explosive mixture). Both tables are generated using the thermodynamic code TDS (Victorov 2002). The newly developed thermodynamic

solver is incorporated into the gas dynamic code to perform iterative procedure to find mixture pressure, temperature and composition for given values of mixture volume and energy and burnt fractions of HE and metal x_{HE} and x_{Me} found from solution of conservation and global kinetics equations. Below we apply the model to both premixed and non-premixed systems.

Detonation of a Premixed Hybrid System: Suspended Al Particles in a Gaseous Explosive

Fig. 1 presents pressure profiles, $p(x, t_k)$ during the detonation build-up process for a hybrid system: hydrogen/air gaseous explosive $[0.87\text{H}_2 + 0.5(\text{O}_2 + 3.76 \text{N}_2)]$ with uniformly suspended aluminium particles of 2 or 5 μm diameters. Simulations were one-dimensional and used the same booster charge; the flow was assumed to be adiabatic, so heat losses to the walls were neglected. One can see that delayed reaction of particles with gaseous detonation products results, at first, in the formation of secondary compression wave, that transforms over time into a secondary detonation which overtakes the leading front. The transition is faster for smaller particles. Calculated results agree with earlier ones (Khasainov 1996), however, the model proposed here gives in addition valuable information on chemical and physical transformations of species behind the leading front. In particular, Fig. 2 shows that water vapour formed in a pure gas case, is completely consumed in the combustion process of metal particles—which results in formation of liquid aluminium oxide. Moreover, there is an optimum aluminium concentration (between 15 and 30 %) that maximizes the detonation velocity and pressure.

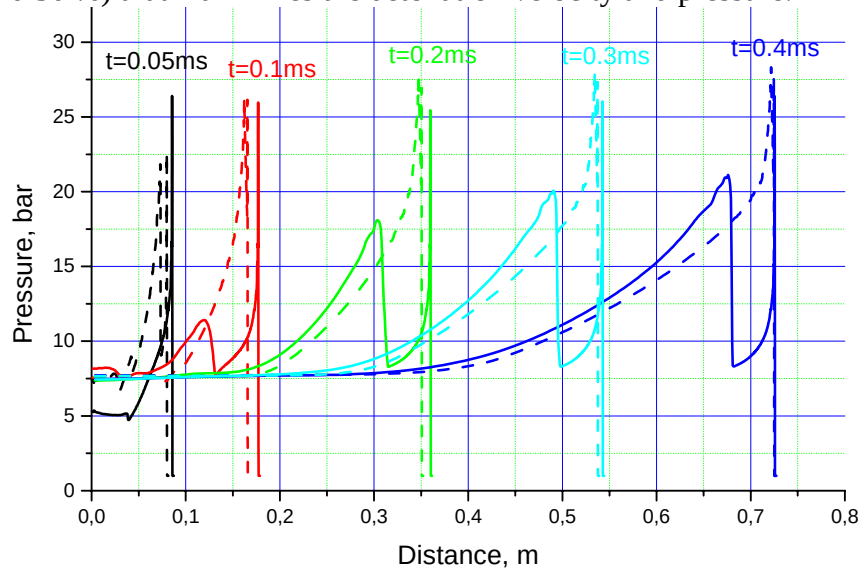


Figure 1. Effect of particle diameter d_{po} on detonation build-up at particle concentration 0.36 kg/m^3 and $d_{po} = 2 \text{ \& } 5 \mu\text{m}$ (dash and solid lines respectively).

Non-premixed Two-Phase Mixture

Here we use the model to simulate the experimental problem of explosive dissemination of 1 g of flake aluminium powder in a closed cylindrical 6.6-litre bomb; shock dissemination is induced by

the detonation of a 0.5 g spherical PETN booster (Neuwalde et al. 2003). Initial apparent densities of PETN and Al are about 1000 kg/m^3 . Final pressure in the bomb can be estimated by means of thermodynamic code but the interest is to simulate temporal evolution of the process. For simplicity we assume that the bomb is spherical and apply a 1D approximation taking into account thermal and velocity relaxation effects between the particles and the gas. Fig. 3 shows calculated time records of pressure at the bomb wall. Red curve corresponds to 6.6-litre bomb. One can see that blast wave generated by the booster gives rise to a multiple reverberations of the shock (experimental record is qualitatively similar but much more irregular). Mean residual pressure of nearly 10 bars is obtained after about 1 ms in agreement with experiments. Fig. 3 shows that the larger the bomb volume, the smaller the residual pressure (as in the experiment). No attempts were done to adjust burning rate parameters of flake Al (multi-dimensional AMR calculations, with turbulent transport taken into account, are needed to capture this effect)

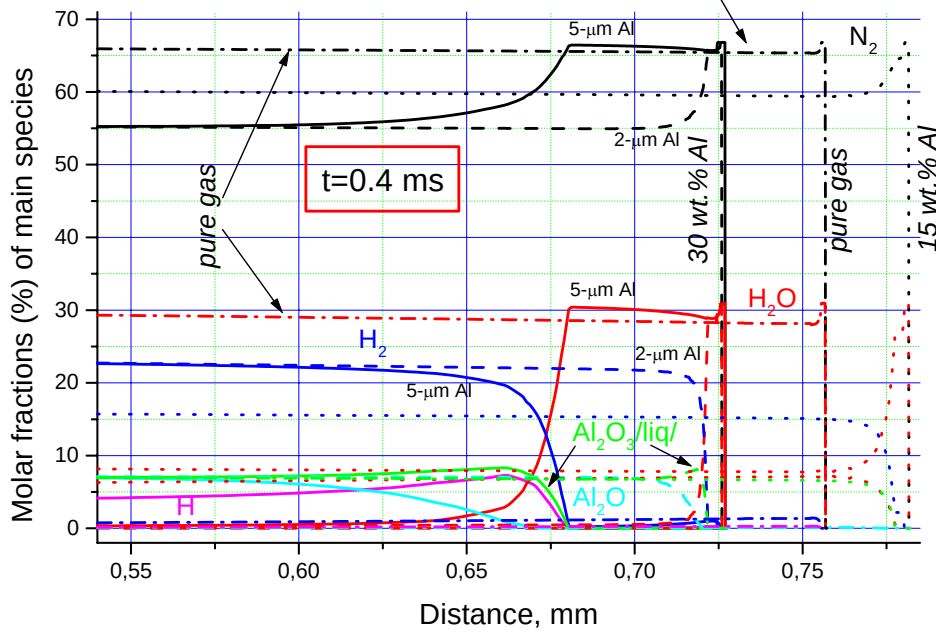


Figure 2. Molar fraction profiles of some species at $t=0.4 \text{ ms}$ for pure gas (dash-dot lines) and for hybrid mixtures at $x_o=0.3$: solid and dash lines correspond to 5-μm and 2-μm Al particles respectively. Dotted lines show results for finer particles with $x_o=0.15$.

Conclusion

A new approach is developed for using pre-calculated thermodynamic equilibrium states for heterogeneous explosives, and tabulated as EOS tables. Good agreement with available data is obtained for a suspension of aluminium particles in gaseous explosive. The non-premixed case is also considered for the problem of shock-dispersed metal particles in a closed bomb. One-dimensional simulations yield correct order of magnitude for the pressure rise when compared with experimental data.

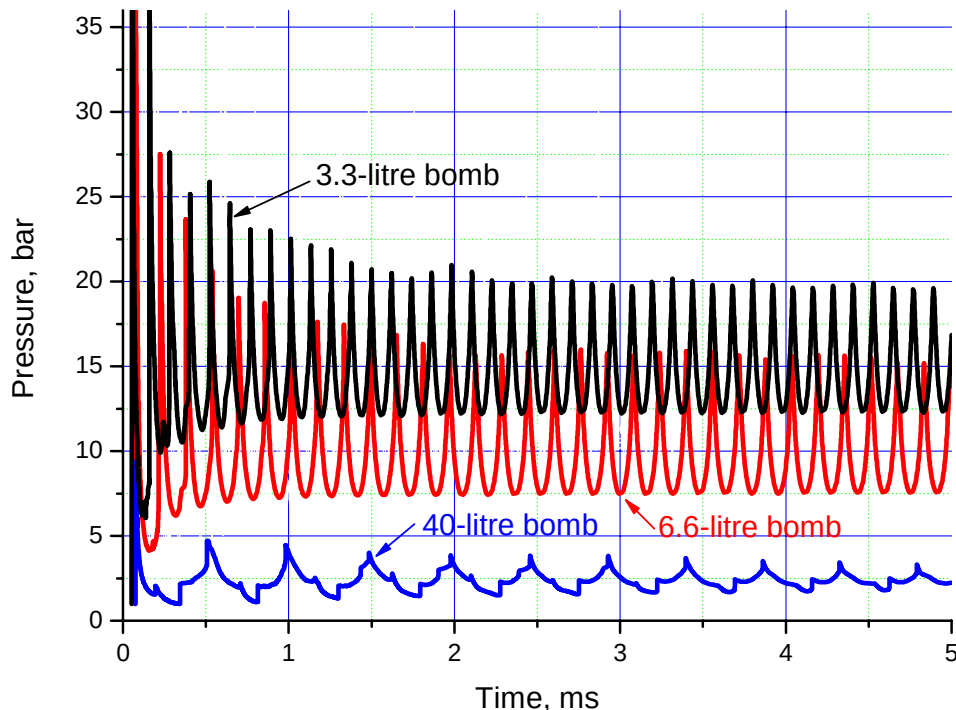


Figure 3. Effect of bomb volume on wall pressure – time records.

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