AN EIGENVALUE-BASED ESTIMATE OF REACTION ZONE THICKNESSES IN GAS PHASE DETONATIONS

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A robust method is developed to provide rational estimates of reaction zone thicknesses in one-dimensional steady gas phase detonations in mixtures of inviscid ideal reacting gases described by detailed kinetics models. The conservation principles are cast as a set of algebraic relations giving pressure, temperature, density, and velocity as functions of species mass fractions. These are used with the kinetics equations to formulate the system as a standard dynamic system of the form $dY_i/dt = f(Y_i)$, where Y_i are the species mass fractions. These equations are integrated from a shocked state to an equilibrium end state. The eigenvalues of the Jacobian of f are calculated at every point in space, and their reciprocals give estimates of all length scales. The finest scales are often at a sub-micron level. Such a method provides a quick, rigorous, and reliable technique for estimating the necessary spatial resolution that is required in detailed computational studies of compressible reacting flows. In fact when multidimensionality is introduced, it is likely that even finer resolution will be necessary, though the one-dimensional estimates can serve as a useful bound. In contrast, a wide variety of less rigorous estimation techniques are often employed in the literature; many of these are *ad hoc* and often result in under-resolved calculations. For example, simply capturing the gross features of the induction zone provides insufficient resolution of the finest scales necessary for a fully converged solution. Nevertheless, a few studies do show resolved results through the use of grid refinement studies; in these cases the grid sizes found necessary for numerical convergence are in full agreement with our estimates.

The method is illustrated using a thirty-seven step, nine species model, of a hydrogen-oxygen-argon mixture with an initial stoichiometric distribution of $2H_2+O_2+7Ar$ at *300 K* and 10^6 *dyne/cm²*. The mixture is subjected to a shock with speed *1.71* x 10^5 *cm/s*, near the *CJ* velocity. One can write a system of nine ordinary differential equations for the evolution of the molecular species; accounting for the conservation of three atomic species, the dimension of the system can be reduced to six. Figure 1a shows a plot of the evolution of the magnitudes of the resulting six length scales of the system; two are coincident for $x < 5$ x 10^{-3} *cm*, and the spike at $x = 7$ x 10^{-3} *cm* is a consequence of an eigenvalue evolving from a positive to negative value. The finest scale ranges from *7.4* x 10^{-5} to *1.4* x 10^{-5} *cm*. In the early stages of the induction zone, $x < 10^{-4}$ *cm*, there is a power law growth of minor species mass fractions, as seen in Figure 1b. The induction zone terminates near $x = 2$ x 10^{-3} *cm*. At this point, vigorous chain branching and subsequent recombination commence, and the system relaxes to equilibrium near $x = 1$ *cm*. The global length scale is well estimated by the longest length scale predicted by the eigenvalue analysis; this ranges from *2.57* to *0.16 cm*.

The disparity of the length scales predicted here places serious demands on existing computational methods and hardware; few calculations exist satisfying these requirements, while many employ resolutions orders of magnitude too high. However, if one wants to obtain rigorous, repeatable, grid-converged predictions from detailed models of reaction dynamics, one has no choice but to reduce the grid sizes below the scales predicted here.
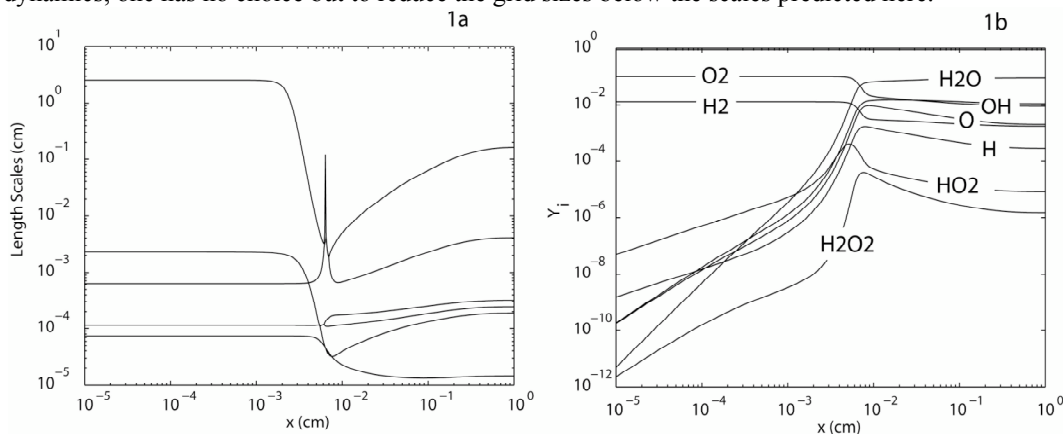

Figure 1. Reaction length scales and species mass fractions in hydrogen-oxygen-argon detonation, $T_o = 300$ K, $P_o = 10^6$ dyne/cm², $u_o = 1.71$ x 10^5 cm/s, $M_o = 4.88$, $2H_2+O_2+7Ar$, nine species, thirty-seven step kinetics.