Resolution Matters: Issues in Computational Simulation of Detailed Kinetics Gas Phase Combustion [1]

Joseph M. Powers and Samuel Paolucci
Department of Aerospace and Mechanical Engineering,
University of Notre Dame,
Notre Dame, Indiana 46556-5637
powers@nd.edu, paolucci@nd.edu

A robust method is employed to provide rational estimates of fine scale reaction zone thicknesses in one-dimensional steady gas phase detonations in mixtures of inviscid ideal reacting gases described by detailed kinetics models. The equations for the evolution of N species mass fractions $\mathbf{Y}$ are formulated as a standard dynamical system of the form $d\mathbf{Y}/dx = \mathbf{f}(\mathbf{Y})$. These equations are integrated from a shock to an equilibrium end state. The eigenvalues of the Jacobian of $\mathbf{f}$ are calculated at every point in space, and their reciprocals give robust estimates of all length scales. Our main conclusion is that most computational results using detailed kinetics are not properly resolved. The finest physical length scale intrinsic to such models, $\sim 1 \times 10^{-5}$ cm, is much smaller than the discretization scale typically employed, $\sim 1 \times 10^{-3}$ cm. The finest physical scale is consistent with that provided by the molecular collision theory. Predictions of under-resolved numerical simulations are being artificially stabilized by numerical viscosity. While our conclusion has been drawn in the context of a detonation problem, we speculate that similar conclusions can be drawn for a wide range of reactive flow simulations which employ detailed kinetics.

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