DEVELOPMENT OF COMPREHENSIVE REDUCED KINETIC MODELS FOR SUPERSONIC REACTING SHEAR LAYER SIMULATIONS

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Large-scale simulations of multi-dimensional unsteady turbulent reacting flows with detailed chemistry and transport can be computationally extremely intensive even on distributed computing architectures. With the development of suitable reduced chemical kinetic models, the number of scalar variables to be integrated can be decreased, leading to a significant reduction in the computational time required for the simulation with limited loss of accuracy in the results.

A general MATLAB-based automated mechanism reduction procedure is presented to reduce any complex starting mechanism (detailed or skeletal) with minimal human intervention. Based on the application of the quasi steady-state (QSS) approximation for certain chemical species and on the elimination of the fast reaction rates in the mechanism, several comprehensive reduced models, capable of handling different fuels such as C_2H_4, CH_4 and H_2, have been developed and thoroughly tested for several combustion problems (ignition, propagation and extinction) and physical conditions (reactant compositions, temperatures, and pressures). A key feature of the present reduction procedure is the explicit solution of the concentrations of the QSS species, needed for the evaluation of the elementary reaction rates. In contrast, previous approaches relied on an implicit solution due to the strong coupling between QSS species, requiring computationally expensive inner iterations. A novel algorithm, based on the definition of a QSS species coupling matrix, is presented to (i) introduce appropriate truncations to the QSS algebraic relations and (ii) identify the optimal sequence for the explicit solution of the concentration of the QSS species. With the automatic generation of the relevant source code, the resulting reduced models can be readily implemented into numerical codes.

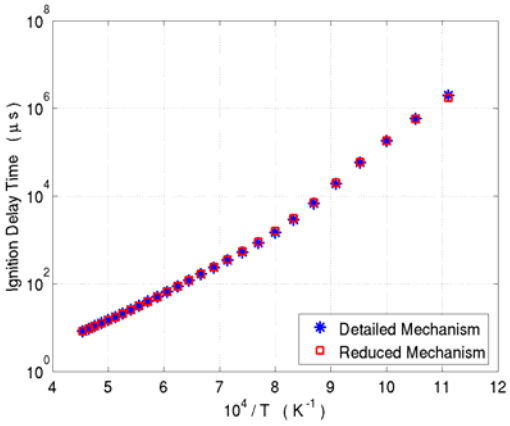

Fig. 1: Comparison of predicted ignition delay of ethylene/air using the detailed vs. reduced model.

Starting with a skeletal mechanism derived for ethylene from the detailed mechanism by Wang et al., an explicit 18-step reduced model (based on ignition – see Fig. 1) and a 15-step reduced model (based on flame propagation) are developed for C_2H_4 and an explicit 13-step model for CH_4. The implementation of the reduced models for a supersonic coaxial reacting shear layer problem with fuel delivered from the inner jet and air from the outer jet is pursued (see Fig. 2), where the determination of the flame stand-off distance is critical and strongly depends on the inflow parametric conditions and choice of finite-rate chemical kinetic and transport models. Here only laminar chemical kinetic models are evaluated. Future work with other collaborators will include turbulent-chemistry interactions as well as variable transport coefficient effects.

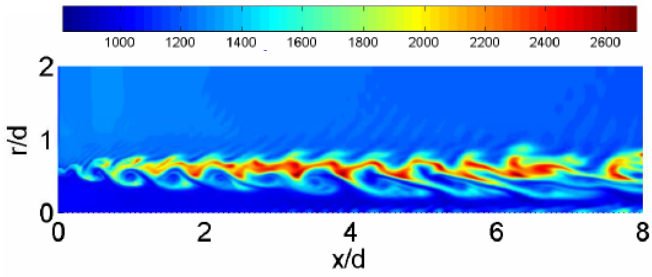

Fig. 2: Typical temperature contours of a co-axial supersonic shear layer using laminar chemistry indicating a detached reaction.