Reduction of Chemical Models under Uncertainty

HABIB NAJM, Sandia National Laboratories, Livermore, CA 94551, USA, RICCARDO MALPICA GALASSI, MAURO VALORANI, Sapienza University of Rome, Rome, Italy — We discuss recent developments for dynamical analysis and reduction of hydrocarbon fuel chemical kinetic models under uncertainty. We rely on computational singular perturbation analysis, allowing for uncertainties in reaction rate parameters. We outline a construction for representation of uncertain reduced chemical models, and estimation of probabilities for inclusion of sets of reactions in the reduced model. We demonstrate the approach in the context of homogeneous ignition of a hydrocarbon fuel-air mixture, illustrating the robustness of the reduced model under parametric uncertainty.

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