Abstract Submitted for the DFD16 Meeting of The American Physical Society

Reduction of Chemical Models under Uncertainty¹ 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.

¹Support provided by the US Dept. of Energy, Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences, Biosciences.

Habib Najm Sandia National Laboratories, Livermore, CA 94551, USA

Date submitted: 01 Aug 2016 Electronic form version 1.4