SPECTRAL METHODS FOR UNCERTAINTY QUANTIFICATION IN REACTING-FLOW SYSTEMS

M.T. Reagan[a], H.N. Najm[b], O.M. Knio[c], R.G. Ghanem[d], O.P. Le Maître[e]

[a,b]Combustion Research Facility
Sandia National Laboratories
Livermore, CA 94551
mtreaga@ca.sandia.gov

[c,d]The Johns Hopkins University
Baltimore, MD 21218

[e]Université d'Evry Val d'Essonne
91020 Evry cedex, France

Uncertainty quantification (UQ) in the computational modeling of physical systems is important for scientific investigation, engineering design, and model validation. We have implemented an "intrusive" technique for UQ that allows the construction of simulation codes with embedded uncertainty quantification. Using pseudospectral operators, the deterministic governing equations and field variables are reformulated in terms of stochastic quantities, where the dependence of the process on multiple stochastic dimensions is represented by polynomial chaos expansions in terms of a set of orthogonal Hermite polynomials and Gaussian basis functions. Uncertain parameters, such as reaction-rate coefficients or enthalpies of reaction, are modeled as sets of Gaussian or log-normal random variables. The coefficients of the spectral expansion relate specific modes of uncertainty to their effects on flame structure and composition. In this work, the intrusive reformulation has been applied to a multi-dimensional, low-Mach number, reacting-flow model with detailed chemistry. Using a detailed hydrogen-air mechanism, as well as a global rate expression, the effect of uncertainties in parameters has been quantified for homogeneous ignition and a one-dimensional premixed flame. Comparisons are made with non-intrusive Monte-Carlo-style analysis, with a focus on the efficiency of the computations. This analysis provides new insights into uncertainty propagation in reacting-flow models and the consequences of known uncertainties in model parameters on the predictability of specific model outputs.

References

[1] O.P. Le Maître, M.T. Reagan, H.N. Najm, R.G. Ghanem, and O.M. Knio "A Stochastic Projection Method for Fluid Flow II. Random Process," *J. Comp. Phys.*, v. 181, p. 9-44, 2002.

[2] M.T. Reagan, H.N. Najm, O.M. Knio, and R.G. Ghanem, "Uncertainty Quantification in Reacting Flow Simulations through Non-Intrusive Spectral Projection," *Combustion and Flame*, v. 132, p.545-555, 2003.