

Advances and Applications of Intrinsic Low Dimensional Manifold Theory

Joseph M. Powers, Samuel Paolucci, and Sandeep Singh
University of Notre Dame

submitted to

Work in Progress Poster Session
28th International Symposium on Combustion
Edinburgh, UK
2000

It is well known that in order to accurately simulate a wide variety of thermochemical phenomena, the effects of detailed finite rate chemistry must be incorporated into models. The development of these detailed models over the past decades has provided a strong link between traditional collision-based gas phase chemistry and fundamental fluid mechanics. However, implementation of fully detailed chemistry models with the obligatory numerical resolution has proved to require a prohibitive amount of computational resources for all but the simplest of flows. While the addition of species and reaction mechanisms induces an increase in computational time required to simulate a given event, a more serious problem is often the severe stiffness associated with the differential equations which model the chemistry. In general, the time scales of reaction, found by eigensystem analysis of locally linearized systems, are often widely disparate; in systems studied here, their ratio is as high as 10^{10} . This leads to computations which routinely take hundreds of hours on supercomputers; such efforts are often impractical.

Consequently, it becomes necessary to implement some strategy to reduce the stiffness introduced by the chemistry. The simplest, full equilibrium, is effectively an intrinsic low dimensional manifold (ILDm) of dimension zero; however, this approach will necessarily miss the coupling of events which occur of time scales of chemical reaction. Simple and often useful strategies which capture some of the kinetic time scales employ explicit one- and two-step models. Also useful are the commonly employed partial equilibrium and steady state modeling assumptions. As shown by Maas and Pope, 1992, such assumptions are often not robust. While they may be useful in the range in which they have been calibrated, it is often easy to find scenarios where such models cannot accurately reproduce the results of full kinetic models. As a consequence, Maas and Pope and simultaneously Goussis and Lam, 1992, have advocated methods which systematically reduce chemical kinetic models in such a way that consistency with full model equations is maintained to a user-specified precision.

We will present recent results of our application of the ILDM method to hydrogen oxygen detonation, to gas phase HMX combustion, and to constant pressure ozone decomposition. In addition, we will demonstrate our general formulation of the ILDM method which is suitable for systems with preferential diffusion and which rationally and consistently accounts for the effects of convection and diffusion.

Joseph M. Powers
Associate Professor
Department of Aerospace and Mechanical Engineering
University of Notre Dame
Notre Dame, Indiana 46556-5637
219-631-5978 (ph)
219-631-8341 (fax)
powers@nd.edu

Samuel Paolucci
Professor
Department of Aerospace and Mechanical Engineering
University of Notre Dame
Notre Dame, Indiana 46556-5637
219-631-8110 (ph)
219-631-8341 (fax)
paolucci@chaos.ame.nd.edu

Sandeep Singh
Ph.D. Candidate
Department of Aerospace and Mechanical Engineering
University of Notre Dame
Notre Dame, Indiana 46556-5637
219-634-3971 (ph)
219-631-8341 (fax)
ssingh@nd.edu