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Studies in Nonlinear Problems of Energy

Progress Report

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We concentrate on modeling, analysis and large scale scientific computation of combustion and flame propagation phenomena, with emphasis on the transition from laminar to turbulent combustion. More than 165 papers citing the grant have been published, and our efforts have twice been recognized for top accomplishment by DOE's Basic Energy Sciences Division.

Determining the transition from laminar to turbulent fluid flow is one of the most fundamental problems in science. While some progress has been made on this problem, far less is known about the transition from laminar to turbulent combustion. In the transition process a flame passes through stages exhibiting increasingly complex spatial and temporal patterns which serve as signatures identifying each stage. Often the transitions arise via bifurcation. We investigate nonlinear dynamics, bifurcation and pattern formation in the successive stages of transition. We describe the stability of combustion waves, and transitions to combustion waves exhibiting progressively higher degrees of spatio-temporal complexity.

Combustion involves compressible fluids in which exothermic chemical reactions occur. Strong coupling exists among chemical reactions, transport processes and fluid dynamics, so that the resulting system is extremely difficult to analyze. Scientists therefore resort to approximate descriptions. One aspect of our research program is the systematic derivation of appropriate, approximate models from the original models governing combustion. The approximate models are then analyzed. We are particularly interested in understanding the basic mechanisms affecting combustion, which is a prerequisite to effective control of the process. We are interested in determining the effects of varying various control parameters, such as Nusselt number, Lewis number, heat release, activation energy, Damkohler number, Reynolds number, Prandtl number, Peclet number, etc.

Combustion waves are characterized by large activation energies, so that chemical reactions are significant only in thin layers, termed reaction zones, in which the solutions of the very highly nonlinear partial differential equations vary rapidly. In the limit of infinite activation energy, the zones shrink to moving surfaces, termed fronts, which must be found during the course of the analysis, so that the problems are moving free boundary problems. The analytical studies are carried out for the limiting case with fronts, while the numerical studies are carried out for the case of finite, though large, activation energy, thus corresponding to reaction zones. Accurate resolution of the solution in the reaction zones is essential, so that false predictions are avoided. The fact that the reaction zones move, and their location is not known a-priori, poses a challenge to numerical computations. To meet this challenge we have developed adaptive pseudo-spectral methods, which have proven to be very useful for the accurate, efficient computation of solutions of combustion, and other, problems.

Our approach is based on a synergism of analytical and numerical methods so that the results obtained are greater than the mere sum of results obtained by each method separately. Our numerical computations build on and extend information obtained analytically. In addition, solutions obtained analytically serve as benchmarks for testing the accuracy of computations. Moreover, ideas from analysis are also used to suggest new and better computational methods. Finally, the computational results suggest new analysis to be considered. Among the results recently obtained were descriptions of a variety of transitions to flames exhibiting increasingly complex spatio-temporal behavior.

We have also considered a number of problems in self-propagating high-temperature synthesis (SHS), in which combustion waves are employed to synthesize advanced materials. Our efforts are directed toward understanding fundamental mechanisms. A finely ground powder mixture in the form of a cylinder, say, is ignited at one end, initiating a combustion wave which propagates through the porous solid mixture, converting unreacted powder into the desired product. Among the results recently obtained were descriptions of methods of enhancing the propagation of the synthesis wave by pumping gas through the porous solid, a description of deformation of the porous solid during the synthesis process, and a description of melting of one or more of the solid components of the mixture followed by flow of the liquid melt through the pores.

During the past year invited talks were presented on our work at: (i) Bilateral US/Russia Workshop on Fundamental Aspects of SHS, Honolulu, Hawaii, (ii) Second International Symposium on SHS, Honolulu, Hawaii, (iii) Dynamics Days - Europe, Budapest, Hungary, (iv) International Conference on Pattern Formation in the Natural Environment, Noordwijkerhout, Netherlands, (v) Joint US/Japan Workshop on Mathematical Modeling in Combustion and its interaction with Numerical Computation, Kauai, Hawaii, (vi) Gordon Conference on Oscillations and Dynamical Instabilities in Chemical Systems, Newport, RI, and (vii) Annual meeting of Amer. Inst. Chem. Engineers, St. Louis, MO, as well as a number of colloquia at various universities and institutes.

A cumulative list of publications citing the grant is appended.

CUMULATIVE LIST OF PUBLICATIONS

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"On inhibiting runaway in catalytic reactors," SIAM J. Appl. Math. 35(2) (1978), pp. 307-314 (with D. S. Cohen).

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