CS&E—Tackling Computational Modeling of Turbulent Combustion

Combustion accounts for 85 percent of the energy used in the U.S., and it is likely that such a high percentage will remain for some time to come. Vast amounts of fossil fuel are consumed, and significant amounts of pollutants are emitted in transportation, power generation, and process industries. More advanced combustion technologies are required to address the vital issues of energy conservation and environmental protection. Computational modeling of turbulent combustion plays an increasingly crucial role in the design and development of advanced combustion equipment.

In addition to its practical importance, turbulent combustion poses a great intellectual and computational challenge. The fundamental process of fluid flow is well understood, and the complexities of the chemistry of combustion are yielding to continued research. However, the combination of turbulence and combustion chemistry creates great difficulties. The turbulence causes large fluctuations of velocity, temperature, and other properties over a large range of time and length scales. The combustion chemistry is exquisitely sensitive to temperature, and hence to the turbulent temperature fluctuations.

Stephen B. Pope, Mechanical and Aerospace Engineering, tackles several aspects of the turbulent combustion problem. Computationally, combustion chemistry is expensive to treat, because of the large number of chemical species involved (for example, 50) and because the chemical timescales vary over at least six orders of magnitude. To alleviate these problems, Pope has developed a two-pronged strategy to dramatically reduce the computational cost of implementing combustion chemistry. First, the researchers use ideas from dynamical systems and thermodynamics to perform a dimension reduction (for example, from 50 to 20 degrees of freedom). Then, having developed a method of *in situ* adaptive tabulation, chemical information can be stored and retrieved to avoid expensive, repetitive calculations. Overall, the researchers can achieve a computational speed-up of a factor of a thousand.

Pope's research group has developed computational approaches to turbulent combustion called PDF (probability density function) methods in which a conservation equation is solved for the joint probability density function of the flow and thermochemical variables. In this way, full account is taken of all of the turbulent fluctuations and their impact on the chemical reactions. The PDF equations are solved by a particle-mesh Monte Carlo method.

As an example of the application of the PDF approach, the figure (below) shows a scatter plot comparison of experiments and computations for a non–premixed flame close to extinction. The distribution of the scattered points represents the distribution of the properties in the turbulent flame. As may be seen, the PDF method accurately captures the distribution observed in the experiments.

Through the power of modern computers, and the development of appropriate algorithms and models, the researchers are now able to use their basic knowledge of fluid mechanics and combustion chemistry to tackle the important task of developing better combustion technologies for increased efficiency and decreased environmental impact.

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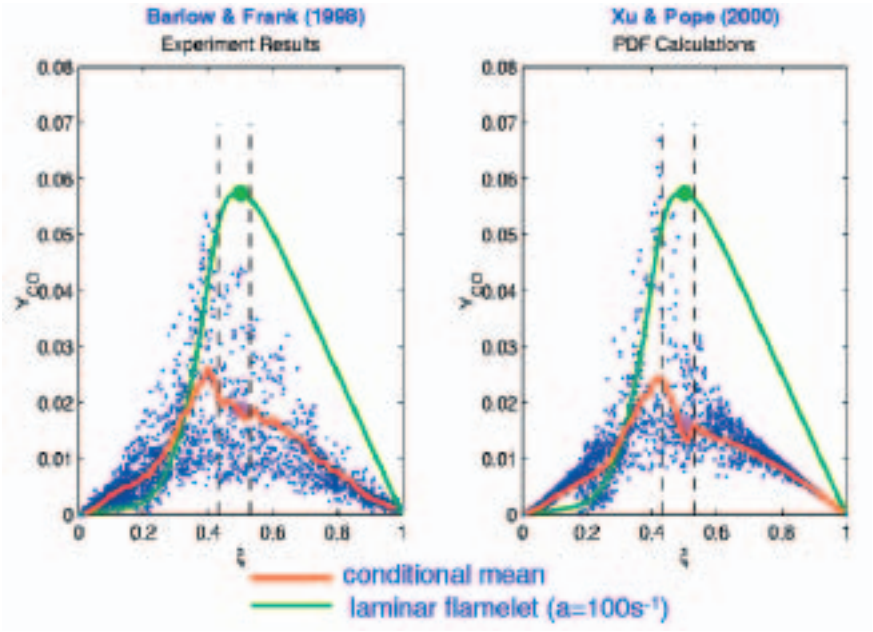

The flame being studied is a challenging test case, because the flame is close to extinction, i.e., it is almost "going out." If, on the contrary, the flame were far from extinction, then all of the points would lie close to the green line, which corresponds to a laminar flame far from extinction. The fact that the experimental data (left plot) is scattered off the green line shows the local extinction that occurs in this flame. And, as may be seen, the PDF calculations (right plot) match well the experimental observations.