Combustion up close

Direct numerical simulations reveal small-scale structures and processes that experiments cannot measure

Efficient mixing is one of the basic challenges in turbulent combustion, especially in situations where the fuel and air streams are initially separated (so-called *nonpremixed combustion*), as in jet aircraft engines and direct-injection diesel and gasoline engines. The mixing of fuel and air molecules is necessary for the chemical reactions of combustion to take place.

Turbulence increases the mixing rate, so the right amount of turbulence improves the efficiency of combustion. But too much turbulent mixing can interrupt the chemical reaction process and lead to partial extinction of the flame. If extinguished pockets of unburned fuel–air mixture fail to reignite promptly, they may be emitted in the exhaust. Thus extinction may lead to reduced fuel efficiency, increased harmful emissions, and if pervasive enough, destabilization or blowout of the flame—a potentially catastrophic effect for aircraft.

Small-scale turbulence–chemistry effects such as extinction and reignition, flow and flame unsteadiness, and differential diffusion of chemical

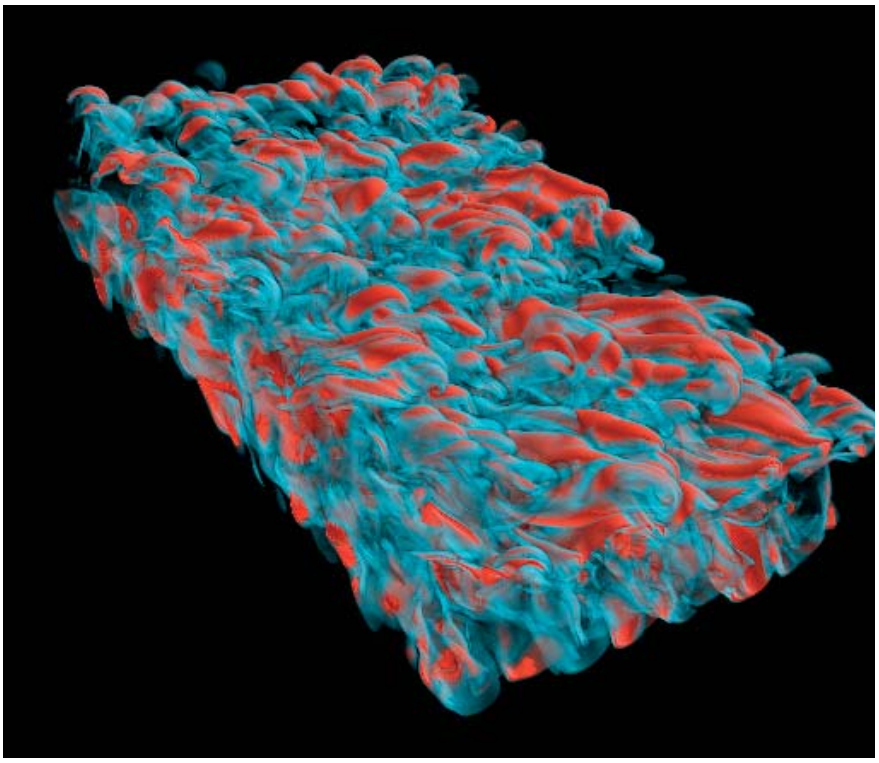

FIGURE 1. A simulated planar jet flame, colored by the rate of molecular mixing (scalar dissipation rate), which is critical for determining the interaction between reaction and diffusion in a flame. The image shows that high scalar dissipation regions exist in thin, highly intermittent structures aligned with principal strain directions. (Visualization created using an application written by Hongfeng Yu and Kwan-Liu Ma, UC Davis.)

species are difficult, if not impossible, to measure experimentally. Engineering-scale combustion simulations, in order to be computationally feasible, must use a spatial grid that is too coarse to capture these small-scale phenomena; to approximate their effects, mathematical models extrapolated from experimental results must be used. But the rapid growth of computational capabilities in recent years has presented new opportunities for high-resolution direct numerical simulations (DNS) of turbulent combustion that address unanswered questions about turbulence–chemistry interactions.

In the 2005 INCITE project "Direct Numerical Simulation of Turbulent Nonpremixed Combustion—Fundamental Insights towards Predictive Modeling," Jacqueline Chen, Evatt Hawkes, and Ramanan Sankaran of Sandia National Laboratories have performed the first 3D DNS simulations of a turbulent nonpremixed H_2/CO–air flame with detailed chemistry (Figure 8). The simulations, including 11 chemical species and 33 reactions, were performed with up to 500 million grid points and 100,000 time steps, and ran for 2.5 million processor hours on Seaborg and 1.5 million hours on Bassi.

An initial analysis of the data shows for the first time how detailed transport and chemistry effects can influence the mixing of chemical molecules.[5] (The mathematical representations of these molecules are called *scalars*.) This is an example of how DNS can be used to assess the validity of assumptions used in combustion models. Mixing models typically assume that the mixing rate is the same for each different scalar and corresponds to the turbulence time scale. In fact, the INCITE simulation reveals that the mixing rates of active (reacting) scalars and passive scalars may vary by a factor of 3. Models may need to incorporate these different mixing rates, because a poor mixing model could incorrectly predict a stable flame when actually extinction occurs. This finding and others yet to come from further analysis may lead to more accurate models for use in lower-resolution simulations.

To ramp up to the large INCITE calculations, Chen's team started by running many test calculations with their highly scalable S3D code, using different numbers of grid points on a variety of large-scale computing systems. After analyzing and optimizing the code's performance with the help of NERSC staff, they improved the code's efficiency by 45%.

The code improvements helped the researchers achieve the highest-ever Reynolds number (ratio of inertial to viscous forces) in a 3D fully resolved DNS of a nonpremixed flame with detailed chemistry. Simulations with different Reynolds numbers shed light on a phenomenon called intermittency—intense, localized fluctuations of any quantity in a turbulent flow—which can result in localized extinction and reignition of the combustion process. The results show a relationship between scalar intermittency and the Reynolds number (Figure 9).

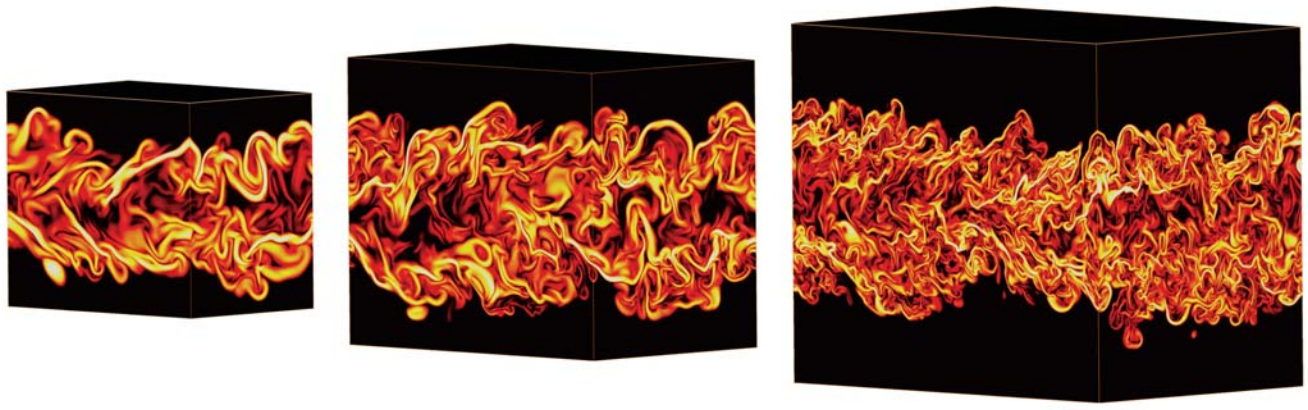

FIGURE 2. Instantaneous isocontours of the total scalar dissipation rate field for successively higher Reynolds numbers at a time when reignition following extinction in the domain is significant. The dissipation fields are organized into thin sheet-like lamellar structures, with lengths far exceeding their thickness, consistent with experimental observations in nonreactive flows. Increasingly fine-scaled structures are observed at higher Reynolds numbers. (From E. R. Hawkes, R. Sankaran, J. C. Sutherland, and J. H. Chen, "Direct Numerical Simulation of Temporally-Evolving Plane Jet Flames with Detailed CO/H_2 Kinetics," submitted to the 31st International Symposium on Combustion, 2006.)

[5] E. R. Hawkes, R. Sankaran, J. C. Sutherland, and J. H. Chen, "Direct numerical simulation of turbulent combustion: Fundamental insights towards predictive models," Journal of Physics Conference Series **16** (SciDAC 2005), 65 (2005).

This project has generated 10 terabytes of raw DNS data, which they intend to share with an ongoing international collaboration of experimentalists and modelers called the Turbulent Nonpremixed Flame Workshops.6 The DNS data will serve as a numerical benchmark, complementary to experimental data, for model validation and the advancement of basic scientific understanding of turbulent combustion.

Extracting and analyzing useful information from this massive dataset is a daunting task. Chen's group is working with Kwan-Liu Ma of the University of California at Davis to develop automated feature extraction tools and multi-variable visualization capabilities that will help researchers understand how turbulent mixing interacts with chemical reactions. Phenomena they are working to visualize include flame edges and cusps, extinction pockets, and ignition kernels.

Research funding: BES, INCITE, SciDAC
Computational resources: NERSC, MSCF, NCCS
This article written by: John Hules