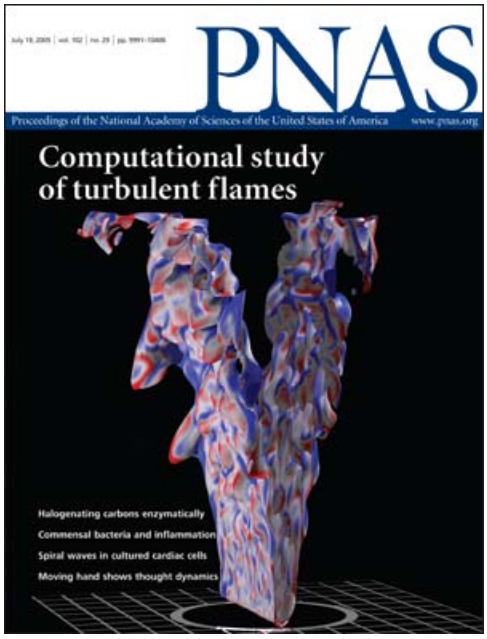
Virtual Combustion Experiments at the Laboratory Scale

Remember when "sticker shock" referred to the price of a new car—not the cost of filling the gas tank? Given rising oil prices, getting the most efficiency out of a gallon of gas has implications ranging from personal finances to national policy. Investing in combustion research at national laboratories and universities is one way the U.S. Department of Energy (DOE) is striving to improve combustion efficiency.

A recent research survey compiled for the DOE noted that 85 percent of the mation's energy needs are fueled by combustion. Interestingly, this process that we take for granted is an extremely complex problem involving chemistry and turbulence in a complicated environment. Recently, researchers at DOE's Lawrence Berkeley National Laboratory's Center for Computational Sciences and Engineering and the Environmental Energy Technologies Division created a three-dimensional combustion simulation of unmatched accuracy, a simulation that closely matches conditions found in laboratory combustion experiments.



This V-flame simulation, which models a full laboratory-scale flame by using detailed chemistry and transport, treats a domain more than three orders of magnitude larger in volume than that of any previous efforts and represents a major increment in simulation complexity.

Although collaborations between computational scientists and experimentalists are increasingly common, the results from this project clearly demonstrate how computing is now an essential component of scientific discovery. The simulation is unprecedented in several aspects—the number of chemical species included, the number of chemical processes modeled and the overall size of the flame. The work was featured on the cover of the July 19, 2005 Proceedings of the National Academy of Sciences.

The article, written by John B. Bell, Marc S. Day, Ian G. Shepherd, Matthew R. Johnson, Robert K. Cheng, Joseph F. Grcar, Vincent E. Beckner and Michael J. Lijewski, described the simulation of "a laboratory-scale turbulent rod-stabilized premixed methane V-flame. This simulation, which models a full laboratory-scale flame by using detailed chemistry and transport, treats a domain more than three orders of magnitude larger in volume than that of any previous efforts and represents a major increment in simulation complexity."

Even a simple fuel like methane burns in a complex sequence of steps. Oxygen atoms gradually replace other atoms in the hydrocarbon molecules, ultimately leaving carbon dioxide and water. Methane oxidation involves on the order of 20 chemical species for releasing energy, and many more minor species that can become pollutants.

The LBNL combustion simulations use a different mathematical approach than has been typically used. Most other combustion simulations are direct numerical simulations, which are very compute-intensive. Because of this, such simulations have been limited to only two dimensions and on a small scale.

The LBNL team has developed an algorithmic approach called an "adaptive low Mach number model," which strips away relatively unimportant components of the simulation and focuses the computing resources on the most important processes. These algorithmic improvements over the past five years have

slashed computational costs for combustion simulations by a factor of 10,000. Even so, the simulation requires substantial computing power—the group ran their application for about 1,000 hours on 256 processors of the IBM SP supercomputer at DOE's National Energy Research Scientific Computing Center.

The code allows the researchers to model a flame about 12 cm in height and consisting of 80 chemical species and more than 300 chemical processes. This has the potential to greatly increase the understanding of how fuels behave in the complicated environments inside turbulent premixed flames, in which fuel and air mix before burning.

Turbulence can distort the distribution of species and the redistribution of thermal energy which are required to keep the flame burning. These turbulence-chemistry interactions. can cause the flame to burn faster or slower or create more or less pollution.

The holy grail of combustion science has been to observe these turbulence-chemistry effects. Over the past few decades amazing progress has been made in observational techniques, including the use of lasers to excite molecules of a given species and produce a picture of the chemical distribution. But laser imaging is limited in the species and concentrations that can be reliably observed and it is difficult to obtain simultaneous images to correlate different chemical species.

As a result, progress in combustion science has to a remarkable degree coincided with advances in scientific computing. For example, while basic concepts for solving 1D flat flames originated in the 1950s, it only became possible to solve the 1D flame equations some 30 years later using 80 MHz Cray-1 supercomputers. Those calculations, which are routine on personal computers today, enabled a renaissance in combustion science by allowing chemists to observe the interrelationships among the many hypothesized reaction processes in the flame.

Simulating 3D turbulent flames took 20 more years of advances in applied mathematics, computer science, and computer hardware, particularly massively parallel systems. The recent simulation results were found to match experiments within a few percent, thereby directly validating both the computational method and the chemical model of hydrocarbon reaction and transport kinetics in a turbulent flame. In effect, a virtual experiment was successfully performed by computer simulation.

Achieving these impressive results underscores the fact that the greater part of the investment in scientific computing is in the years of R&D leading to the complex algorithms and software employed. Once that investment has been made, it continues to pay returns as these supercomputing techniques are put to work on the future's more capable computers, perhaps even one day on the desktop.

More information about LBNL's combustion simulation research can be found at: http://seesar.lbl.gov/ccse/Research/index.html