Dissecting Fire: Model Fully Resolves Ignition Process for the First Time

Research may fuel low-temperature combustion technology to save energy, cut emissions

To flip an old saying, where there's fire, there's smoke. No one knows that better than Jacqueline Chen, a mechanical engineer at Sandia National Laboratories (SNL) who employs some of the world's fastest supercomputers to model combustion.

Jacqueline Chen employs some of the world's fastest supercomputers to gain insight into the flames that ignite and stabilize diesel-engine jets. Photo courtesy Sandia National Laboratories.

With mechanical engineer Chun Sang Yoo at SNL in California and computational scientist Ramanan Sankaran at the National Center for Computational Sciences (NCCS) in Tennessee, Chen used the Cray XT4 Jaguar supercomputer at the NCCS to generate 35 terabytes (trillion bytes) of data about flames similar to those occurring during ignition and stabilization of diesel-engine jets. That's more than three times as much data as contained in the printed contents of the U.S. Library of Congress. In their simulation, the researchers burned the simplest fuel—hydrogen molecules. Hydrocarbon fuels, which contain hydrogen and carbon, are more complex, from the relatively simple methane and ethylene to complex gasoline and diesel fuels.

Engineers are using Chen's data library to develop predictive models to optimize designs for diesel engines and industrial boilers with reduced emissions and increased efficiency. Diesel fuel powers most semitrucks; delivery vehicles; buses; trains; boats; and farm, construction, and military vehicles and equipment in the United States, so development of advanced diesel technology is a leading near-term option by which the country could reduce its fuel consumption and greenhouse gas emissions.

"If low-temperature compression ignition systems employing lean, dilute fuel mixtures make their way into next-generation autos, fuel efficiency could increase by as much as 25 to 50 percent," Chen says. That also means meeting future low-emission vehicle standards with almost undetectable emissions of nitrogen oxide, a major contributor to smog, she adds.

Chen, Yoo, and Sankaran created the first three-dimensional simulation that fully resolves flame features such as chemical composition, temperature profile, and flow characteristics. The model shows feature detail on all size scales—the biggest, the smallest, and everything in between—of a turbulent fuel jet in a hot co-flowing airstream as it ignites.

The researchers modeled in unprecedented detail what happens in the so-called "lifted flames" relevant to industrial boilers and diesel engines. Unlike spark-plug ignition systems in automobiles powered by gasoline in which the fuel and oxidizer (air) are premixed, diesel-injection systems have the diesel fuel entering the engine full of hot air via jet nozzles. Turbulence mixes the fuel and air. Pistons subject the air/fuel mixture to pressure, and the mixture heats further, spurring a chemical pathway that sharply increases the concentration of a highly reactive chemical, hydroperoxyl radical, Chen says. The hydroperoxyl radical produces heat that spurs the production of other radicals. At about 1,520 degrees Fahrenheit, the fuel/air mixture auto-ignites, or bursts into flame, as a result of the rapid, heat-producing oxidation of its own constituents, regardless of heat from external sources. This process creates a lifted flame. The temperature peaks around 3,140 degrees Fahrenheit.
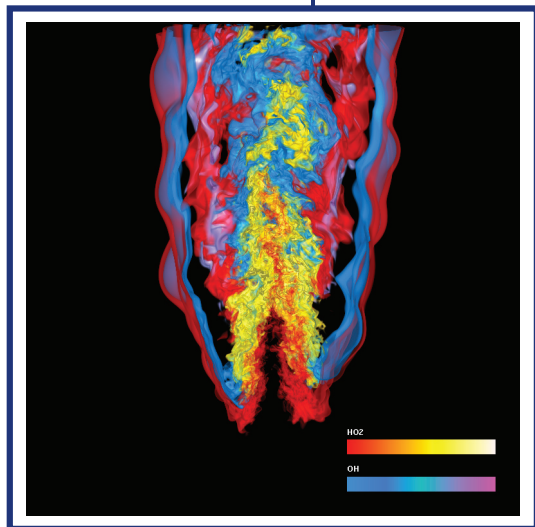
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"Auto-ignition is helpful because it stabilizes the flame," Chen says. "A high-temperature flame base supports its existence."

Before this work by Chen and her colleagues, scientists had modeled only large eddies, or turbulent curlicues, in a burning fuel. They had not simulated the full range of scales down to the smallest eddies, which dictate the viscosity of the system and dissipate heat. Now researchers can resolve the nitty-gritty of the small eddies responsible for flame extinction and reignition.

The Department of Energy (DOE) Office of Basic Energy Sciences and DOE Scientific Discovery through Advanced Computing (SciDAC) program supported the work at SNL. The DOE Office of Science supported the work at the NCCS, located at DOE's Oak Ridge National Laboratory, through its Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program. INCITE grants huge allocations of supercomputing time to a handful of scientists addressing grand challenges in physics, chemistry, biology, and beyond. The program is unique in providing Ph.D.-level computational scientists, such as Sankaran, to optimize tools, help with data analysis, improve algorithms, and aid in other ways so researchers get the most out of high-performance computers.

High-impact code

"In most practical devices, combustion occurs in a very turbulent environment," Sankaran says. The Jaguar supercomputer runs a software code called S3D to understand that turbulence on all length scales. S3D models compressible, reacting flows with detailed chemistry. Chen led the code development by a team that included Sankaran and SNL's Scott Mason, James Sutherland, and Chris Kennedy and Pittsburgh Supercomputing Center's Ravi Subramanya and Raghu Reddy. Written in Fortran, the code continues to evolve. A DOE SciDAC university consortium led by Professors Chris Rutland of the University of Wisconsin, Arnaud Trouve of the University of Maryland, and Hong Im of the University of Michigan contributed recent improvements to better model the physics of sprays, soot particles, and thermal radiation. At SNL, Yoo enhanced the algorithm to better reflect boundary conditions and symmetries, and David Lignell, a doctoral student with the University of Utah who works in Chen's lab at Sandia, advanced soot models.

The strength of the Chen group's code comes from a fluid-dynamics parameter called the Reynolds number, which indicates the range of scales in a system. A fluid system with a lot of turbulence, for example, may have tiny eddy currents with small-scale effects and huge eddies exerting large-scale effects. To understand phenomena at all length scales in a system with a high Reynolds number, researchers need more points in a three-dimensional grid than they do to resolve a system with a low Reynolds number. Chen, Yoo, and Sankaran used nearly a billion grid points spaced 15 microns apart to provide the world's first fully resolved picture of lifted flames surrounded by heated air. The burning mixture they simulated had a Reynolds number of 11,000 and required 2.5 million computing hours at the NCCS to show the complete cascade of different-sized eddy currents and their interaction with the flame. Receiving such a large allocation of time on a supercomputer is rare. It was possible at the NCCS, though, because the center is dedicated to groundbreaking science and committed to helping scientists use the world's most powerful machines for open research.

In their simulation, the researchers burned the simplest fuel—hydrogen molecules. Hydrocarbon fuels, which contain hydrogen and carbon, are more complex, from the relatively simple methane and ethylene to complex gasoline and diesel fuels. Ignition of hydrogen generates eight chemical species and 20 chemical reactions that must be plugged into the model, Chen says, whereas a more complex hydrocarbon fuel such as n heptane, iso-octane, diesel fuel, or the kerosene that powers jet engines may generate hundreds of species and thousands of chemical reactions. Fuel additives, which influence how well and how rapidly the fuel burns and when ignition happens, can further complicate the chemistry, she says.

Chen's group has also simulated combustion of methane, which contains one carbon atom. Later the researchers will study two-carbon fuels such as ethane and ethanol. Lignell is working to model combustion of ethylene, another two-carbon fuel. The researchers are working closely with Professor Chung Law and Associate Research Scholar Tianfeng Lu, both of Princeton University, to eventually simulate diesel surrogate fuels such as n-heptane, a seven-carbon fuel, operating in high-pressure and low-temperature diesel environments. They employ a strategy called mechanism reduction, in which models lessen the number of transported species and keep only the important elementary reactions required to represent the chemical kinetics and thermochemistry with accuracy and computational efficiency. Otherwise, the coupling between detailed chemistry and turbulence would be intractable, even using today's most powerful machines.

"We definitely need petascale [a quadrillion calculations per second] and even exascale [a thousand quadrillion calculations per second] computing for [this]," Chen says. The NCCS is on track to offer such resources in coming years. Its roadmap provides for petascale systems by 2009, and exascale capabilities may be possible within a decade.

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