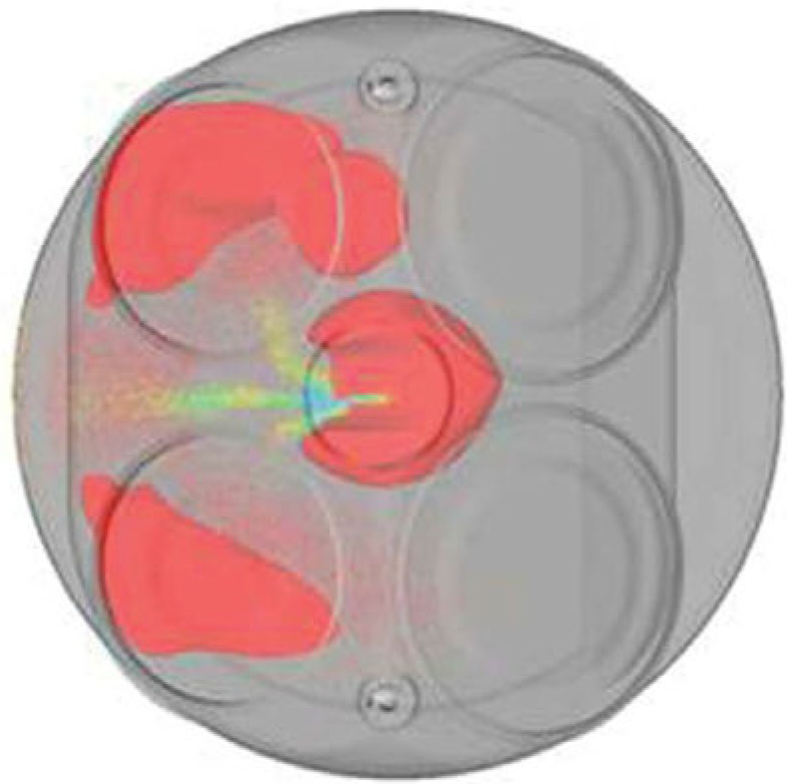
Alternative fuels heat up

"Boosting is an important, practical element of HEDGE, and a single-cylinder engine does not allow you to use a production turbocharger," he said. "You have to mimic the source air from a turbo or supercharger, and that can be misleading."

Some of the research concepts he reports working on include dual fuel combustion, such as pilot injection of diesel igniting gasoline through compression.

"We now have a 13-L, six-cylinder engine running in test cells with 80% gasoline and 20% diesel," he said, achieving over 44% brake thermal efficiency (BTE.) Alger said he would also like to see improvements in engine simulation software: "We need a better kinetic mechanism for 3-D modeling to deal with auto-ignition and flame propagation in high dilute environments."



Auto-ignition locations (red) and liquid spray droplets for dual fuel in a test case using iso-octane and diesel. (Chrysler Group LLC)

Low temperatures and high computation

"One of the biggest advances in ICEs in the last 10 years has been in low-temperature combustion, providing both higher efficiencies and lower NOx," said Rolf Reitz, Mechanical Engineering Professor at the **University of Wisconsin**.

Reitz and his team also developed a new two-fuel combustion scheme he calls Reactivity Controlled Compression Ignition (RCCI.) It too uses direct injection of diesel with gasoline. Unlike other alternative schemes that may only be good for light loads because of high-pressure rise rates at high loads—rates that can damage engines—Reitz has demonstrated RCCI from idle up to full load in diesels.

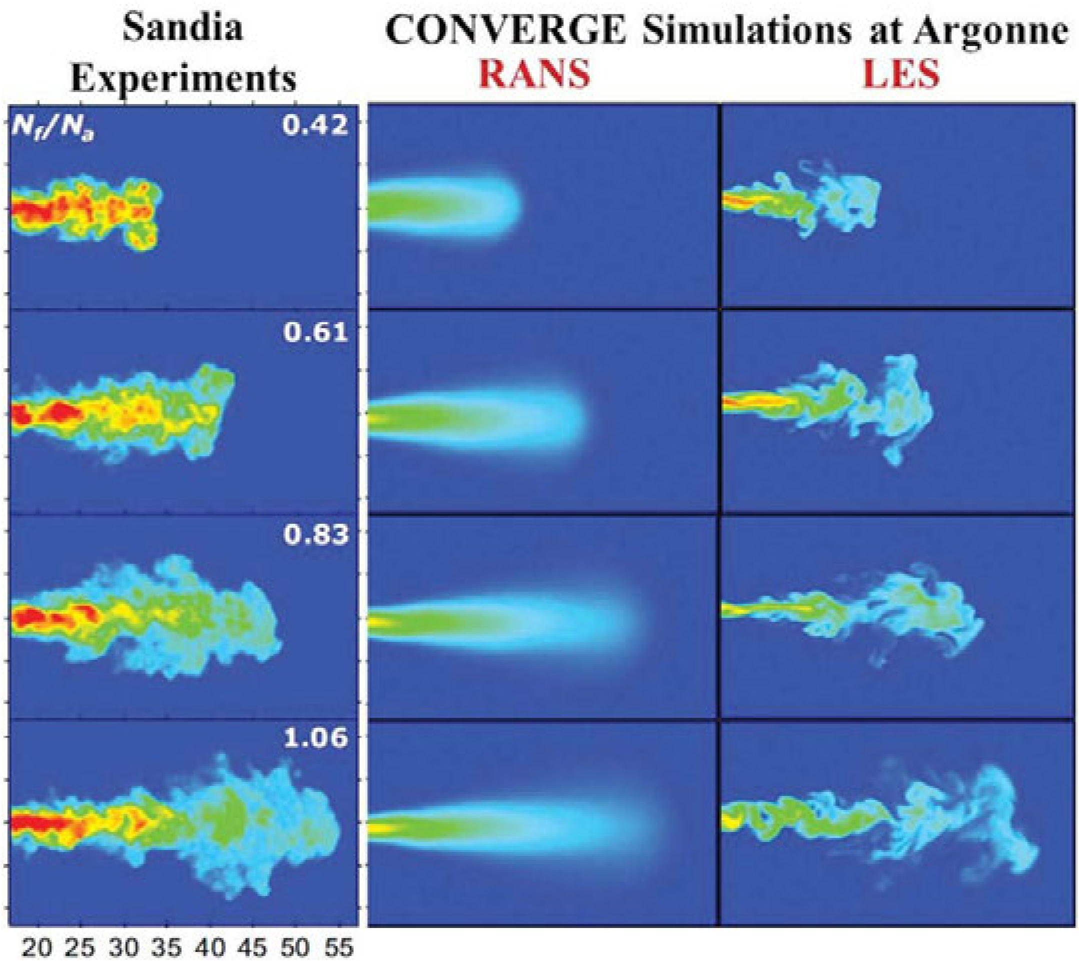
"One of my students ran a [modified] automotive multi-cylinder diesel with two fuels over the whole **EPA** FTP cycle. It produced better fuel efficiency than a standard diesel with no aftertreatment [needed to meet emissions standards.]"

He points to advances in computer modeling as a key enabler in developing such schemes as RCCI.

"We have been working on codes for simulating ICEs for the last 25 years. Computer speeds have improved, and we tackle much bigger problems now," he said, while noting that there is always work needed to keep computational times reasonable.

His team might take a month to simulate a new combustion scheme, running thousands of test cases to find the optimum set of parameters. Simulation gives them complete freedom in number and type of injections, injection pressure, nozzle geometry, and spray geometry, along with combustion chamber geometry.

"It is much better to do this on a computer, and in my opinion, computers are responsible for the rapid rate of progress in new combustion research," he said. Once the codes have predicted the optimum condition—geometry, fuel mix, spray-characteristics—they then build a prototype and test. No surprise,



ANL has developed detailed CFD models of how actual sprays work near the nozzle for advanced combustion computation, clearly showing the advantage of Large Eddy Simulation (LES) models over Reynolds Averaged Navier-Stokes Simulations (RANS).

he reports that the computer predictions are close, but not precise, when compared with actual test data.

Modeling fuels, reducing complexity

For the future, Reitz predicts further development in codes that predict chemical kinetics.

"A typical diesel fuel consists of approximately 1000 individual chemical species—we can only model 30 of them these days," he explained. His team uses the approach from the **Model Fuels Consortium** (MFC), a group led by **Reaction Design**, to whom he also acts as adviser. (For more on MFC, see the article "New software model to help engine makers meet diesel soot standards" on page 18.)

The Model Fuel approach reduces the complexity of a particular fuel by replacing a number of chemical species that have similar chemical properties with a single surrogate, according to Ellen Meeks, Vice President of Product Development at Reaction Design. Meeks is also the Director of the MFC.

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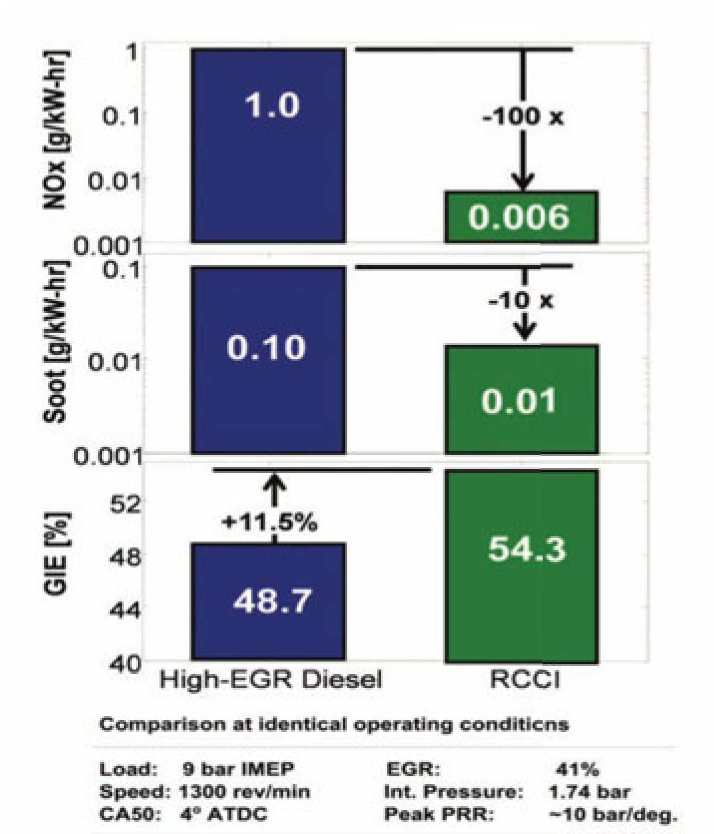

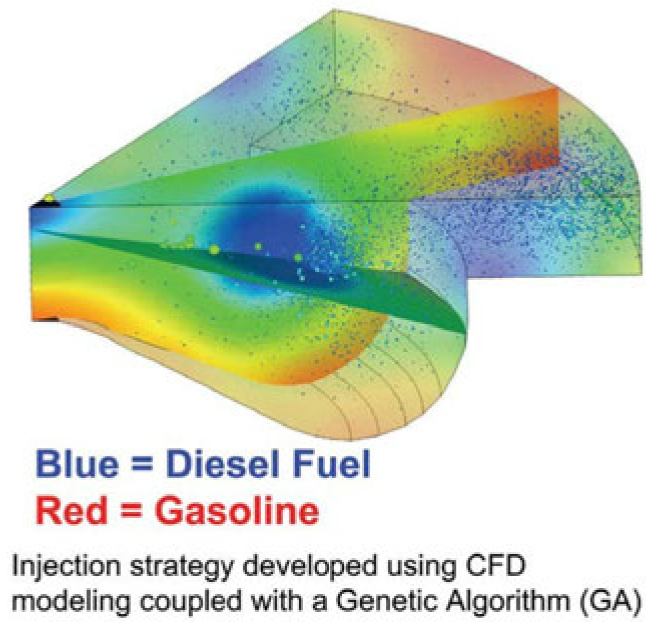

Left: In research conducted by the University of Wisconsin, efficiency and reduced emissions are accomplished with high EGR diesel and dual-fuel Reactivity Controlled Compression Ignition (RCCI). Right: CFD predicted optimal mixture distribution shown in a 60° sector view of the combustion chamber just before the time of compression ignition.

With a Model Fuel, there may be only four or five molecules used to represent the fuel, compared to the 1000 or more in a real fuel. The MFC also works toward both understanding and reducing the complexity of intermediate species and reactions during the burn process. A key function of the MFC (composed of engine manufacturers, universities, and petroleum companies) is validating the surrogate fuel models.

Besides leading the MFC, Reaction Design offers a number of software products for combustion engineering, including CHEMKIN and CHEMKIN-PRO for chemical kinetics; FORTÉ for 3D CFD modeling of fuel effects in ICEs; and CHEMKIN-CFD and ENERGICO for combining chemical kinetics with CFD.

Nozzles, spray models, and 3-D

Convergent Science is another company that offers software for engineering of alternative fuels and combustion methods. It specially designed its CONVERGE CFD code for automatic meshing, including automatic mesh refinement to capture fine detail without excessive computation.

CONVERGE CFD software eliminates the tedious process of making meshes manually by automatically generating a mesh at runtime. It also offers SAGE, a chemistry solver for modeling kinetically limited phenomena such as knocking, auto-ignition, emissions formation, and flame propagation.

According to Dan Lee, Director of Business Development, SAGE incorporates the multi-zone chemistry solver developed