Simulation

Reaction Design speeds, refines combustion-chemistry simulation

Reaction Design's new software tool, Chemkin-Pro, increases the speed of accurate combustion simulation to meet the needs of engineers designing clean, efficient engines and aftertreatment systems.

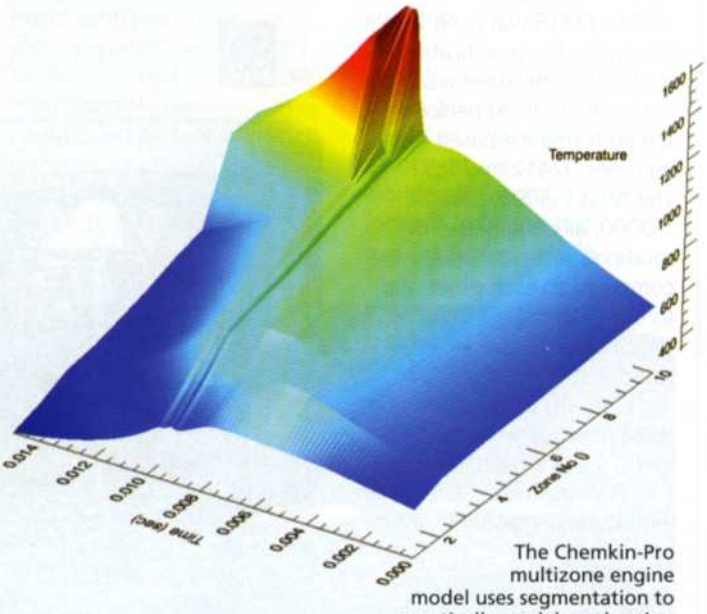
Stringent near-term emissions and fuel-efficiency standards are driving engine designers and fuel providers toward more efficient combustion cycles. Using simulation to help understand design decisions in engines and aftertreatment seems only natural. "What our software does is allow an engineer to understand what is going on inside the engine cylinder," said Bernie Rosenthal, CEO of Reaction Design, Inc.

"Simulation is important in reducing cost," said Rosenthal. "Prototyping even a single-cylinder engine can range from tens of thousands up to millions of dollars before you get one piece of data out of that test cell. We are finding companies are more open to embracing simulation before they commit to bending metal."

He added that people have used combustion and reaction simulations in the past, typically using a single fuel as a model. However, the emissions standards of today require more accurate modeling, he said.

On the other hand, actual fuels are too complex to simulate directly since they are composed of hundreds of components. Computer run time could stretch into weeks with this approach.

The Chemkin software models 'pure' fuel mixtures with surrogate mixtures to simulate real fuels. The model accurately predicts factors such as ignition delay, knocking tendency, flame speeds, pollutant emissions, sooting tendency, density, viscosity, and heating value. Computational fluid dynamics (CFD) does not support the level of detailed chemistry required to simulate accurately these combustion performance criteria. The new multizone engine model in the software compensates by segmenting the cylinder volume into reaction zones. Each zone models detailed chemistry mechanisms while maintaining an accurate representation of the cylinder geometry.



The Chemkin-Pro multizone engine model uses segmentation to practically model combustion processes spatially.

The accomplishments of the Model Fuels Consortium (MFC) inspired the technology, led by Reaction Design to create more accurate combustion simulations. Current members of the MFC include **Chevron**, **Conoco Phillips**, **Cummins**, **Dow Chemical**, **Ford**, **General Motors**, **Honda**, **l'Institut Français du Pétrole**, **Mazda**, **Mitsubishi Motors**, **Nissan**, **PSA Peugeot Citroën**, **Oak Ridge National Laboratory**, **Petrobras**, **Saudi Aramco**, and **Toyota**.

Currently scheduled to end in 2008, the MFC will immediately be followed by a new MFC II consortium. The MFC II will continue work on modeling particulate and soot emissions models, a particular challenge according to Rosenthal. The MFC II will run to 2011.

"As oil hovers near $100 a barrel, alternative sources such as oil from shale becomes economically attractive," said Rosenthal. "We will need to understand how to control emissions from fuels such as these as they become viable."

Membership in the consortium has its benefits. Members have exclusive rights to the data for two years and they help correlate the simulation by providing test facilities and test runs, which is incorporated using a sophisticated design-of-experiments methodology.

"With many different fuel and engine options in development or already available, designers need one simulation tool that quickly and accurately predicts the way various fuel mixtures will interact with different engine designs," said Rosenthal.

The new software makes use of an innovative high-speed solver engine. It is said to cut the time required for solution convergence by five to 10 times over previously available combustion-simulation codes. These results are visible using a new, interactive visual display, called the Reaction Path Analyzer, that also shows which reaction paths are dominant and helps designers determine opportunities for mechanism reduction.

A new particle-tracking module tracks particle growth from inception to oxidation to predict number and size statistics. The new particle-tracking tool also features a user-programmable module called Uncertainty Analysis, which allows designers to evaluate how their inputs propagate through a simulation, helping define tolerances and safety margins and increasing the accuracy of the simulation.

A typical internal combustion engine model that would take 53 min in Chemkin 4.1 now takes 3 min in Chemkin-Pro.

Bruce Morey