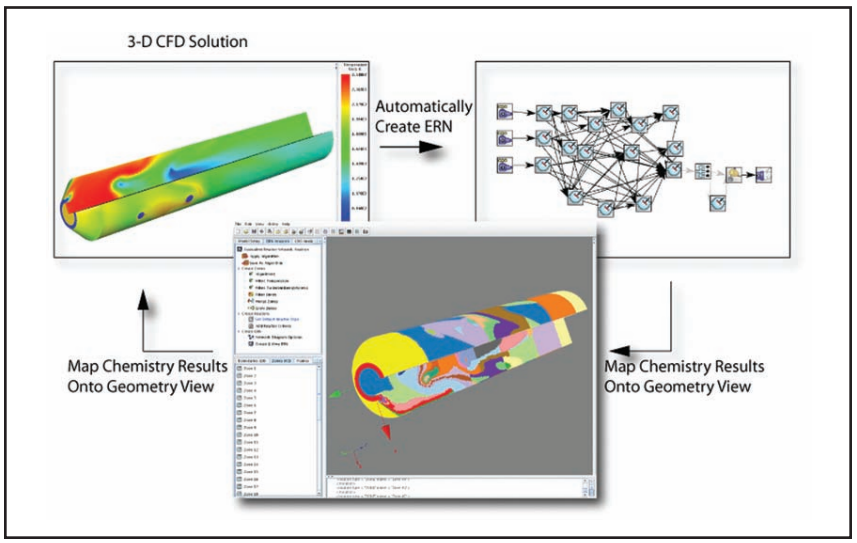
BY MIKE MERCER



The ENERGICO software package from Reaction Design is used to solve complex combustion challenges in gas turbines by virtual simulation. It automatically creates and solves Equivalent Reactor Networks (ERN) from CFD analysis programs. Viewing the ERN results on combustor geometry facilitates the design modifications.

Solving Complex Combustion Challenges

ENERGICO software package chemically simulates combustion in virtual environment for multiple fuels

Reaction Design has introduced its ENERGICO combustion simulation and analysis software for use with gas turbines operating on traditional and nontraditional fuels. With the capability to accurately simulate emissions and combustion stability, ENERGICO is designed to reduce the need for physical engine prototype testing and speed time-to-market for new designs with reduced field failures.

When used in conjunction with Computational Fluid Dynamics (CFD) software, ENERGICO can simulate performance of any continuous-flow combustion device using virtually any type of fuel. User-defined algorithms within the tool can be fully customized for specific applications.

"In field trials using real-world customer design problems, ENERGICO solved critical combustion issues substantially faster than with conventional modeling, test and debugging methods," said Bernie Rosenthal, CEO of Reaction Design. "ENERGICO delivers higher-quality predictions across a much broader operating envelope, including diverse fuel sources and variable environmental conditions and usage scenarios. We believe this technology will be a catalyst in advancing the use of sustainable fuels and reducing environmental impact.

"The software is a stepping stone to help engineers determine cause and effect when it comes to the variables of fuel types and combustor designs," Rosenthal added.

As emissions regulations tighten, and the use of alternative fuels expands, manufacturers continue to develop more complex combustion systems. As new fuels are introduced, combustion uncertainty and mechanisms to capture required effects need to become much more detailed.

"The big challenge for combustion gas turbines, with regard to use of sustainable fuels, is combustion dynamics, emissions compliance and lean-blowout [LBO]," said Rosenthal. "The key benefits of the software are rapid, accurate prediction of emissions for modern combustors, the straightforward determination of LBO tendency, and to evaluate the impacts on combustion performance due to variations in operating conditions, such as fuel composition."

ENERGICO allows engineers to model different types of fuels, and the combustion process. These fuels include: syngas from integrated gasification combined-cycle (IGCC) applications; opportunity fuels such as blast furnace and landfill gases; coal-derived Fischer-Tropsch fuels; biofuels; and oil-sand derived fuels. It also models environmental variables and can simulate combustion under a variety of operating conditions — from tropical jungles to the arctic tundra.

This modeling simulation can help determine key parameters of a design that affects efficiency and emissions. It also allows engineers to simulate conditions that cannot be experimentally tested.

"Most of the time, people take a very simplistic view of the fuel," said Rosenthal. "However, what seems like a fairly innocuous change in a fuel's composition can have drastic effects on emissions output, fuel efficiency, power output and equipment reliability. New fuel types change combustion characteristics, while NO_x and CO emissions vary widely depending on fuel composition and quality."

One way engineers test designs is with the creation of equivalent reactor

networks (ERN) that represent the complex 3-D combustor flow field into a series of idealized 0-D chemical reactors. The benefit of this reduced order ERN model is that fuel reaction mechanisms can be used to track the thousands of reactions and short-lived species that dictate combustion performance and emissions formation.

The ENERGICO software adds chemistry into the design flow and starts by reading in the 3-D CFD solution, and then automatically identifies zones with common characteristics so they can be simulated as a simplified chemical reactor. The combustor flow field is automatically divided into zones through the application of filters on variables such as temperature, velocity, fuel and oxygen concentrations. The zone creation algorithm provides both the flexibility to capture key regions of the flame and to eliminate manual analysis and errors.

The engineer can then adjust and refine the algorithm to capture flow/flame structures. The software tracks all flows to stitch together the zones into an ERN instantly, according to Reaction Design. The ERN can then be solved using accurate detailed fuel chemistry for combustion performance and those results are represented back on the combustor geometry. This allows the engineer to identify where the NO_x emissions are formed, where the CO emissions are quenched, and where soot pre-curser chemicals are present.

Another challenge associated with the low-NO_x combustor designs of gas turbines is LBO. The ENERGICO simulation helps engineers find the cause by conducting a detailed chemistry analysis locally in the flame with the chemical rate from reaction mechanism and mixing rate from CFD. It then determines how close the flame is to LBO and visualizes the flame within geometry to guide design modifications.

ENERGICO has completed a rigorous validation program on actual gas turbine designs. Reaction Design did its own internal benchmarking on the software with turbine designs supplied from the industry prior to release. In addition, three gas turbine manufacturers ran virtual simulations on different, well-understood designs. They included emissions prediction and LBO assessments in order to compare ENERGICO's results with physical prototype experimental data.

"In every case, the ENERGICO-predicted NO_x and CO levels were within 5% of actual emissions for each design using different fuel sources such as natural gas and syngas," said Rosenthal. "The customers reported that this data was far more accurate than estimates delivered by their CFD simulations alone, and that the data was available weeks to months sooner than when using traditional methods."

The software is compatible with many popular commercial CFD codes such as Fluent, Star-CD and CFX. The ENERGICO package only requires a standard CGNS file as input to create a link from virtually any CFD code.

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