Enabling **Detailed Chemistry**

Reaction Design provides CHEMKIN-CFD for free to ANSYS FLUENT users who are looking to improve the accuracy of their flow simulations.

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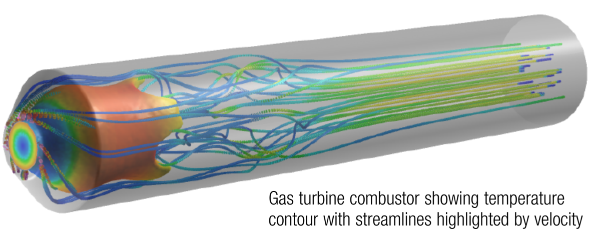
Some of today's automotive and industrial power challenges — increased fuel flexibility, high efficiency and emissions reductions — set the stage for more accurate reactive-flow simulation. Commercial firms are increasingly using more-detailed chemistry in their flow simulations to reduce development costs, achieve low-emissions design and improve operating efficiencies. Innovative companies recognize that these objectives can be met only by improving the accuracy of their reacting-flow simulations.

The benefits of using more-detailed chemistry in simulation are being realized by the transportation, energy and materials processing markets. Employing detailed chemistry can lead to improved predictions of:

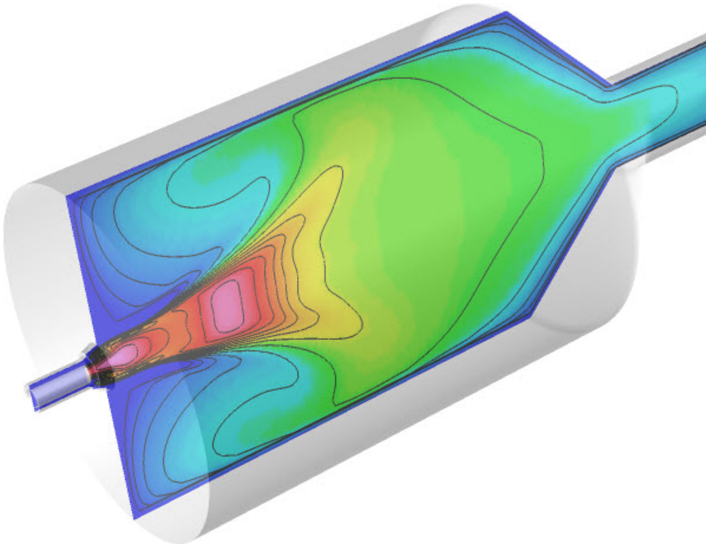
- Ignition and emissions for automotive engine designers
- Emissions, stability and durability for gas-turbine combustor designers
- Increased efficiency, improved yields and reduced manufacturing cost for materials manufacturers that produce everything from glass coatings to semiconductor devices and solar cells

In an ideal world, every reacting-flow simulation would include fully detailed chemistry descriptions: The solution would incorporate a fully detailed master mechanism with potentially thousands of reactions and species to accurately represent chemical reactions. However, it can be difficult to employ such detail given the practicality of simulation run-time requirements and hardware availability.

Significant run time can be experienced when solving detailed-chemistry simulations as a negative consequence of computational stiffness. This characteristic poses a problem for applications that involve sharp chemistry gradients and/or disparate time scales, either between the chemistry and the flow or within the chemistry itself. Reaction Design's CHEMKIN-CFD module specifically addresses the problem by working with ANSYS FLUENT software to provide efficient and accurate solution algorithms, assuring robust coupling of the chemistry and the flow.



Gas turbine combustor showing temperature contour with streamlines highlighted by velocity



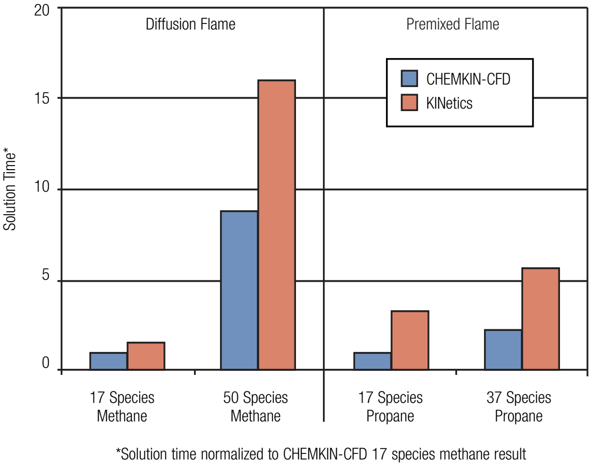
Temperature contour cross section through a natural gas burner
Courtesy Burner Engineering Research Laboratory (BERL).

Further, run time increases as more reactions and species are included in the simulation, necessitating intelligent mechanism reduction of the master mechanism. Mechanism reduction is a process that eliminates "excess baggage" in the master mechanism — reactions and species that are not needed for a specific result and the application conditions of interest. All mechanism reduction techniques employ the same strategy: Remove the reactions and species that are not of interest for the desired results and simplify groups of reactions using similar species into a smaller group of reactions. However, every time you employ a reduced mechanism, you introduce error as you remove information from the fully most accurate form of the mechanism. You must balance the trade-offs between the size of the mechanism and the acceptable error.

ANSYS partner Reaction Design has developed a suite of advanced mechanism-reduction methods, which include both skeletal-reduction and more-severe reduction methods with very good accuracy over a wide range of conditions. Using these tools, an engineer can reduce a master mechanism to a level that can run accurately within the 50-species limit in ANSYS FLUENT software.

Reaction Design's CHEMKIN-PRO, industry-standard chemical kinetic simulation software, can be used to assess which reactions may be removed from the master mechanism without adversely affecting objectives of the simulation. Reduced mechanisms resulting from these methods may be imported directly into ANSYS FLUENT — or into Reaction Design's CHEMKIN-CFD, which can be used in lieu of ANSYS chemistry solvers. CHEMKIN-CFD takes advantage of unique mathematical techniques developed for the CHEMKIN-PRO solvers. The actual calculation speed has been dramatically improved, yielding speed improvements approaching two times the previous version of CHEMKIN-CFD (called KINetics).

Using mechanism reduction is not always required. Integrated circuit, solar cell, industrial glass and HDTV display manufacturers produce their advanced products through processes such as chemical vapor deposition (CVD), plasma etching and atomic layer deposition. They use flow simulation modeling to incorporate system fluid dynamics into the production process for improved product quality and efficiency. CHEMKIN-CFD may be applied with ANSYS FLUENT to simulate these processes using the full chemistry reaction mechanism, given that the full mechanism typically consists of 20 to 30 species for these types of processes. "The combination of ANSYS FLUENT and CHEMKIN-CFD allowed me to accurately model my CVD process using the full chemistry mechanism," said Anthony Dip, process manager of Tokyo Electron America. "Previous attempts to include full chemistry in flow simulation using other chemistry solvers resulted in extremely long computational times, and the simulation runs often failed to converge."



Improvements in solution time with the new CHEMKIN-CFD compared to the previous software version

CHEMKIN is the most widely validated chemical simulation software available on the market today. CHEMKIN CFD is available for free to licensed ANSYS FLUENT users. To learn more, visit www.reactiondesign.com/products/open/chemkin-cfd.html. ■

Auto Manufacturers Take Advantage of Better Fuel Chemistry

The understanding of combustion chemistry has advanced recently with the development of validated fuel reaction mechanisms accurately describing the detailed chemistry involved in various combustion processes. One example of a collaborative effort in this area is the Model Fuels Consortium (MFC, www.reactiondesign.com/support/open/mfc.html), led by Reaction Design, which brings together a total of 17 car and truck engine manufacturers as well as major fuel processors to develop advanced methodology for treating fuel-combustion chemistry for diesel, gasoline and biofuel components.

"Modern, clean-burning, fuel-flexible engine designs are highly dependent upon how effectively we can manipulate the combustion process to our advantage," said Rolf Reitz, professor at the University of Wisconsin. "Effective combustion simulation in flow modeling requires the use of accurate fuel reaction mechanisms to predict key phenomena such as ignition delay, flame speed, and the formation of such undesired emissions as NOx, CO and soot."

The MFC team has developed and continues to improve its set of specialized simulation software to help consortium members take advantage of a comprehensive fuel–chemistry database and to achieve previously unheard-of levels of combustion–simulation accuracy. Benefits to fuel and engine manufacturers include reduction in costly experimental testing, improvement of product quality and reduction in time to market for new products. Computational methods of discerning key combustion characteristics developed under the MFC are now being used by fuel manufacturers to simulate the impact of different fuel compositions on engine performance.

"CHEMKIN-CFD has allowed me to take advantage of the accurate fuel mechanisms developed in the MFC for improved CFD simulation accuracy," said Hidefumi Fujimoto, advanced powertrain development senior specialist for Mazda. "We've seen a five-times speed increase with greater solution stability in the latest version of CHEMKIN-CFD, which has dramatically improved the value of CFD to our design process."

The follow-on program, MFC-II, is now poised to extend this understanding of fuel chemical mechanisms to a wider variety of alternative fuels and to enable use of science-based soot-formation models.