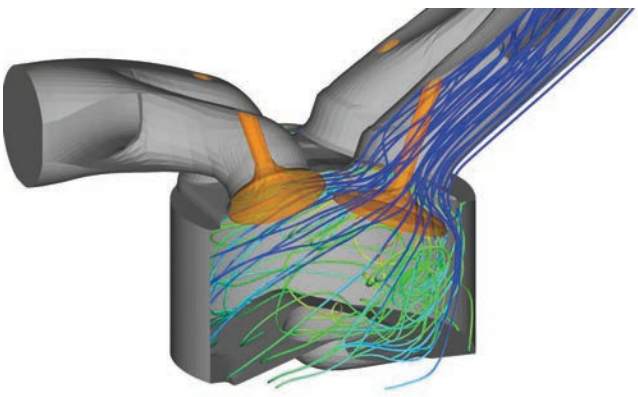
FAST, ACCURATE SIMULATIONS FOR FUEL COMBUSTION APPLICATIONS

The acquisition of Reaction Design broadens the ANSYS simulation offering with industry-leading chemistry solvers to advance clean engine and fuel technologies.

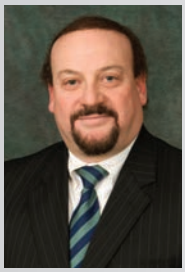
By Bernie Rosenthal, CEO, Reaction Design

Now — more than ever — automobile engine and turbine manufacturers are under intense pressure to develop and deliver higher-performance products with significantly reduced emissions.

In early March 2014, the U.S. Environmental Protection Agency (EPA) announced new, tighter fuel standards for motor vehicles as part of ongoing initiatives to lower greenhouse gas emissions. According to the Union of Concerned Scientists, today's on-road vehicles produce over a third of the carbon monoxide and nitrogen oxides in our atmosphere along with over 20 percent of global-warming pollution [1], while power generation is the single largest source of U.S. global warming emissions [2].



▲ FORTÉ CFD package for advanced, 3-D internal combustion engine design based on detailed fuel chemistry mechanisms



ANSYS is the global leader and innovator of engineering simulation software. Reaction Design creates solutions that automate the analysis of chemical processes through computer simulation and modeling. By joining forces, we provide our customers with the most powerful and effective combustion simulation tools available in the world.

Merging the technical strengths of Reaction Design and ANSYS into a single company creates new opportunities to enable the development of less-polluting, higher-efficiency and more-competitive products in transportation, energy and materials processing sectors.

Effective simulation of underlying detailed chemistry is critical to advancements in engine and fuel technology, and ANSYS customers now have easy access to kinetics tools and fuel libraries from Reaction Design. Understanding and predicting the effects of fuel chemistry in a combustion system with fast, accurate, cost-effective modeling is vital to developing competitive products that translate reliably to real-world functionality.

As the two companies' technologies come together, exciting new integrated capabilities will become available to ANSYS customers, helping to drive increased fuel efficiency around the globe and leading to new advancements in engine and fuel technology.

Bernie Rosenthal, CEO, Reaction Design

Model Fuel Library

Fuel Chemistry Component Class	Number of Components	Relevant for Modeling: Gasoline	Diesel	Jet Fuels or FT Fuels	Natural or Synthetic Gas	Biofuels or Additives
Hydrogen/CO	2				●	
n-Alkanes	9	●	●	●	●	
iso-Alkanes	3	●	●	●	●	
1-Ring Aromatics	5	●	●	●		
2-Ring Aromatics	2	●	●	●		
cyclo-Alkanes	3	●	●	●		
Olefins	6	●	●	●		
Oxygenated Fuels	8				●	●
Soot Precursors and Emissions Pathways	10	●	●	●	●	●

▲ The Model Fuel Library features more than 40 validated fuel component models.

Designing high-performance internal combustion engines and gas turbines that meet regulatory mandates for reduced levels of greenhouse gases and other toxic emissions is perhaps the top challenge that transportation manufacturers and energy producers face today.

Reaction Design products enable designers to achieve their clean technology goals by automating the analysis of chemical processes that take place in a wide range of products and applications. The company serves more than 400 customers from around the globe, including industry-leading internal combustion engine, industrial, and aviation turbine manufacturers, materials processors and energy producers.

Combustion CFD simulation makes it possible for design engineers to create lower-emission combustion systems without spending millions of dollars on physical mockups and costly trial-and-error testing. However, ensuring that simulations accurately predict real-life fuel effects demands using complex algorithms that describe the physics and thermodynamic behavior of combustion. It also requires a detailed understanding of the chemical makeup of the fuels to be burned and types of engine to be deployed.

FAST, HIGHLY ACCURATE SIMULATIONS

Reaction Design products are designed to maximize simulation accuracy and reduce the overall time required to create a fully actionable design. Combustion simulation is a valuable aid to designers in meeting their goals, but only if the results of their modeling gives true insight into the engine's behavior. Obtaining accurate results from combustion simulation requires capturing both the physical and the chemical characteristics that can change radically over a full engine-duty cycle. In an internal combustion engine, for example, spray breakup and evaporation, turbulence, ignition delay and flame propagation are all factors that must be modeled accurately to yield meaningful results.

Thanks to massively parallel computers, engine geometries can be represented with amazing detail using computational meshes in CFD that approach 100 million cells. However, the chemistry solver technology included with most CFD packages is slow relative to the flow calculations. So it is common for engineers to use single-component, severely reduced fuel models in their combustion simulations. These reduced fuel models lack the detail required to accurately predict key engine performance factors, such as ignition delay, flame propagation, NOx, CO and PM (soot) emissions.

In 2005, Reaction Design launched the Model Fuels Consortium, a 20-member group that includes global leaders in energy and engine manufacturing: Chevron, ConocoPhillips, Cummins, Dow Chemical Company, Ford Motor Company, GE Energy, General Motors, Honda, l'Institut Français du Pétrole (IFP), Mazda, Mitsubishi Motors, Nissan, Oak Ridge National Laboratory, Petrobras, PSA Peugeot Citroën, Saudi Aramco, Suzuki, Toyota and Volkswagen. The consortium's goal was to enable more timely and cost-effective design of cleaner-burning, more-efficient engines and fuels through use of chemically accurate fuel component models in software simulation and modeling.

Reaction Design worked with data from the Model Fuels Consortium to develop its Model Fuel Library (MFL), a compendium of detailed chemical kinetics and mechanisms for 56 fully validated, self-consistent fuel components derived from a master reaction mechanism roster of more than 4,000 chemical species. The MFL enables engine designers to accurately simulate fuel effects in virtually all types of automotive, aircraft and power-generation engines; the components can be combined to model a large variety of new or existing fuel blends.

When coupled with Reaction Design's software suite, the fuel model

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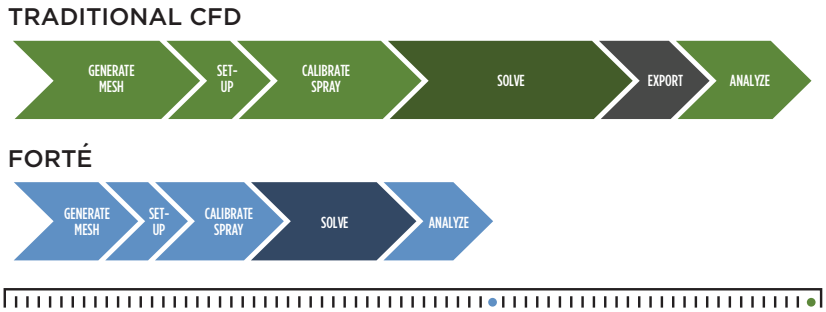
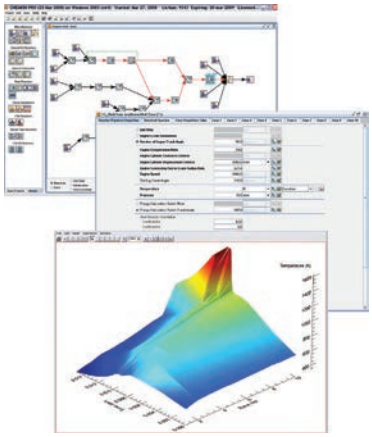
Time to Solution



▲ FORTÉ delivers dramatic reductions in time to solution over conventional CFD approaches.



▲ CHEMKIN is the gold standard simulation software for complex chemical processes.

components greatly increase the accuracy of results across a wide range of operating conditions and fuel types without negatively impacting time to solution, measured as the total wall clock time an engineer experiences from simulation setup through completion of analysis of the visualized results. The Reaction Design products address traditional bottlenecks in the simulation process by offering easy-to-understand, wizard-like graphical user interfaces to ease the setup, solve and analyze steps of the simulation process, and incorporate mathematical solver technologies with the appropriate level of physics and chemistry detail to ensure accuracy.

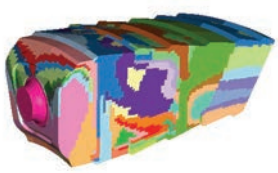
INDUSTRY-LEADING PRODUCTS

CHEMKIN, the gold standard for modeling gas-phase and surface chemistry, was born at the Sandia National Laboratories in the 1980s as a set of command-line–driven codes that describe the complex series of molecular-level chemical reactions that take place during fuel combustion. These led to the development of a suite of detailed-kinetics reactor models that use idealized representations of reacting flows. In time, the 0-D and 1-D flow approximations became the workhorse of fundamental combustion research. CHEMKIN also became an important educational tool in chemical engineering, mechanical engineering and chemistry curricula. The detailed approach to gas-surface reactions led to wide use of CHEMKIN for materials processing studies, such as chemical vapor deposition or plasma etching in microelectronics chip manufacturing.

In 1997, Reaction Design became the exclusive developer and licensor of CHEMKIN technology. CHEMKIN evolved into commercial-quality software that enables engineers and scientists to develop a comprehensive understanding of chemical processes and kinetics and to quickly explore the effects of design variables on performance, by-products production, and engine or process efficiency. Using CHEMKIN, researchers are able to consider thousands of chemical species — and tens of thousands of reactions — for wide ranges of processes and conditions. The advanced solvers developed for CHEMKIN enable fast, accurate simulation of underlying detailed chemical and ignition behaviors, cutting combustion simulation times from days to hours — or hours to minutes — for complex models with large mechanisms. The speed and accuracy of these simulations allow designers to test alternative system configurations and inputs to optimize for performance, efficiency and emissions compliance — virtually, before moving to the prototype stage of their development program.

Reaction Design's ENERGICO simulation package brings the power of detailed kinetic modeling to combustion system design for applications such as gas turbine combustors, burners for boilers and furnaces, and flares and incinerators. ENERGICO uses CFD simulation to help create accurate chemistry models of a system to meet the challenges of emissions reduction and combustion stability for energy production and related industries. Using its strong background and experience in chemistry, Reaction Design created the FORTÉ CFD Package that makes possible realistic 3-D modeling of fuel effects in internal engines. FORTÉ uses proven mathematical techniques and algorithms, coupled with detailed chemical kinetics to simulate the combustion process that takes place inside an engine chamber and predict the effects of operating conditions and fuel variations on the engine's behavior. FORTÉ's superior time-to-solution metrics make it a trusted part of the internal combustion engine design workflow and an invaluable aid in producing cleaner-burning, higher-performance and more-efficient engines.

The Reaction Design team is proud to provide solutions that have helped leading companies to create better products by automating the analysis of chemical processes using computer simulation and modeling. And now, as a part of ANSYS, the team is expanding its vision to provide capabilities to an even broader audience.



▲ The ENERGICO simulation package chemically simulates combustion in a virtual environment for multiple fuels.

REACTION DESIGN SITE
reactiondesign.com

References

[1] Union of Concerned Scientists: Cars, Trucks, and Air Pollution, www.ucsusa.org/clean_vehicles/why-clean-cars/air-pollution-and-health/cars-trucks-air-pollution.html

[2] Union of Concerned Scientists: Clean Energy, www.ucsusa.org/clean_energy/