



CHEMKIN



LEADING SOLUTIONS FOR THE RAPID SIMULATION OF COMPLEX CHEMISTRY

Chemistry Simulation Enables Clean Technology Design

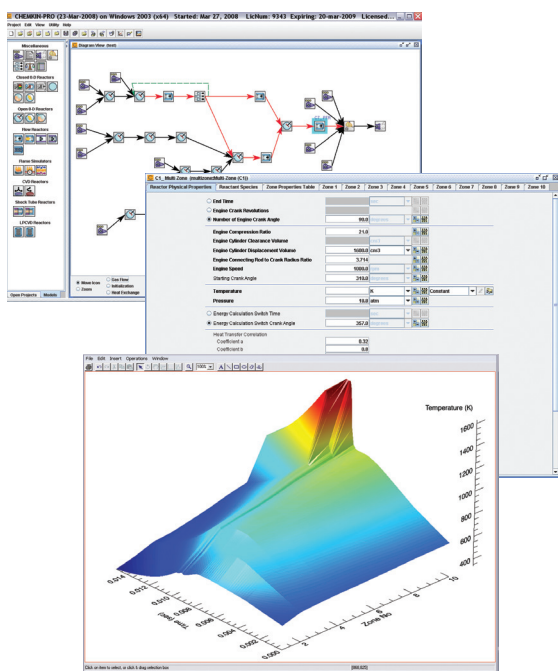
Understanding and predicting chemistry effects is essential in developing Clean Technology solutions in transportation, energy and materials processing applications. As gas turbine, boiler and piston engine designers strive to meet low-emissions regulations with ever widening fuel flexibility, they must also maintain, or even improve, their system's performance. Relying on engine testing for accurate performance validation is prohibitive, given today's fuel diversity, complex engine designs and shortening design cycles. Effective simulation of the underlying detailed combustion chemistry is required for cost-effective design of systems with reduced pollutant emissions.

CHEMKIN® — the de facto standard simulation tool for solving complex chemical design problems

At its most fundamental level, CHEMKIN software enables the simulation of complex chemical reactions. With the advanced capabilities now available, sophisticated Design-of-Experiments (DoE) can be created to parametrically explore potential design solutions well before costly hardware is built.

CHEMKIN evolved from its origin as a Sandia National Laboratory combustion code (Chemkin II) into today's commercial-quality software suite with a user-friendly interface, best-in-class simulation speed, and unparalleled accuracy. No other chemistry simulation product is more widely validated or cited in technical peer-reviewed journals.

Reaction Design offers multiple CHEMKIN products to satisfy unique requirements. CHEMKIN-PRO™ is specifically designed for large chemical simulation applications requiring complex mechanisms. CHEMKIN-PRO's advanced solvers and full feature set support the quick and accurate development of models for specific applications. CHEMKIN provides industry-leading simulation technology for the simulation of less complex systems at an affordable price. CHEMKIN-CFD™ extends the power of CHEMKIN into Computational Fluid Dynamics (CFD) and enables the introduction of more accurate chemistry into reacting, fluid-flow simulations.



FEATURE COMPARISON	CHEMKIN-PRO	CHEMKIN
Combustion Reactors	•	•
Surface Chemistry	•	•
Parameter Study	•	•
Reactor Networks	Enhanced	Basic
Solver Speed	Enhanced	Basic
64-bit Support	•	•
Reaction Path Analyzer	•	
Extinction Model	•	
Multi-Zone Engine Model	•	
Particle Tracking	•	
CFD Flamelet Table Generation	•	
Uncertainty Analysis	•	

CHEMKIN-PRO — fast, accurate chemistry for power users

Incorporating advanced functionality and the latest analytical algorithms and methods, CHEMKIN-PRO delivers the ultimate in speed, accuracy and solution robustness.

Accurate solutions, in a fraction of the time

For complex models with large mechanisms, core solver enhancements incorporated into CHEMKIN-PRO cut simulation times from days to hours, or hours to minutes. CHEMKIN-PRO can be over 50 times faster than previous versions of CHEMKIN in demanding applications.

A whole new view

To help you gain key insights into kinetics dependencies, CHEMKIN-PRO includes the Reaction Path Analyzer. Employing an interactive, visual display, the Reaction Path Analyzer provides a clear view of dominant reaction paths that facilitate mechanism development and reduction.

Use complex flow-field representations to enable more accuracy

Enabling the most efficient prediction of emissions with detailed chemistry, Equivalent Reactor Networks allow you to link mixed-type reactors representing real world designs.

Gain better understanding of low emissions combustion stability

The Extinction Model provides fast and accurate calculations of the extinction strain rate that is used to determine the combustion stability of a system. This is especially important in low NO_x premixed combustion systems.

Easily create CFD flamelet tables with speed and accuracy

Many modern combustion system developers are using flamelet table combustion models in their CFD simulations. CHEMKIN-PRO provides a robust and fast method to create these flamelet tables for input into CFD models.

Understand and predict soot and particle formation

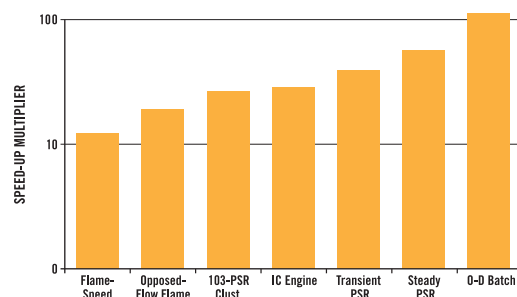
The innovative Particle Tracking feature of CHEMKIN-PRO follows particle inception, growth and oxidation. You can apply number and size statistics to predict soot emissions or optimize particle production.

Explore how input uncertainties affect simulation results

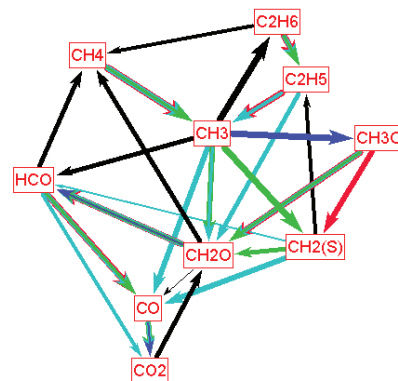
Enhance the robustness of simulation results with the ability to calculate error bars based on user-defined input accuracy ranges.

Multi-Zone Engine Model for piston engines

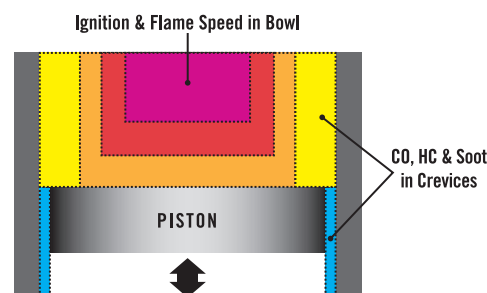
CHEMKIN-PRO's Multi-Zone Engine Model simplifies and optimizes the analysis of key combustion effects including ignition, flame speed, plus CO, HC and Soot emissions.



Simulation Speed-Up of CHEMKIN-PRO vs. CHEMKIN



Visualize reactions with the Reaction Path Analyzer



Multi-Zone Engine Model

CHEMKIN — Industry-leading technology in an affordable, flexible and easy to use solution

For designers who do not require the speed or advanced features offered in CHEMKIN-PRO, Reaction Design offers CHEMKIN as an economical alternative. Up to 6x faster than freeware and academic codes, CHEMKIN is a robust and mature chemistry simulation tool that has been widely used for an impressive range of applications. CHEMKIN is a cost effective solution for simulation projects employing small or reduced mechanisms and/or comprise less complex reactions.

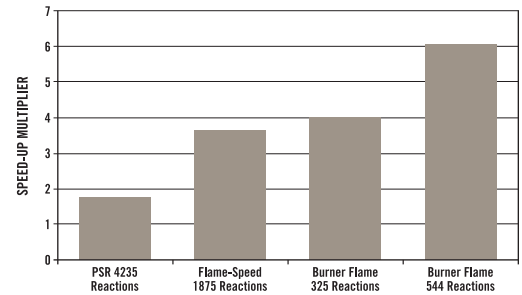
CHEMKIN-CFD — Detailed kinetics modeling meets CFD

CFD software has become a standard design tool for combustor and engine designers. Most CFD cases are run with simplified, or global mechanisms, because computation time prohibits use of more detailed chemistry. However, emission predictions, ignition and stability issues require a much more detailed accounting of chemistry effects to ensure useful analysis. To solve complex chemical kinetics problems faster and more accurately, Reaction Design enables detailed kinetics modeling through its CHEMKIN-CFD software package. CHEMKIN-CFD couples with, and extends the capabilities of, leading CFD software and engine modeling software from CD-Adapco Group, Fluent (ANSYS, Inc), Gamma Technologies, Ricardo plc, and Los Alamos National Laboratory (KIVA).

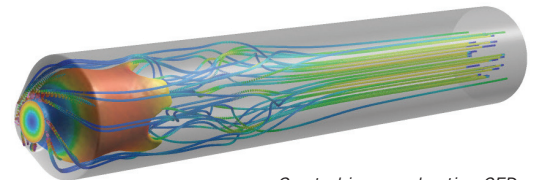
About Reaction Design

Reaction Design empowers transportation manufacturers and energy companies to achieve their Clean Technology goals with comprehensive, easy-to-use software simulation tools, chemical models and consulting services. Reaction Design is the exclusive developer and distributor of CHEMKIN and CHEMKIN-PRO software — the de facto standards for modeling and simulating gas-phase and surface chemistry. For the automatic generation of reactor networks from CFD solutions for emissions and combustion stability simulations, Reaction Design provides the ENERGICO Simulation Package. Reaction Design also offers the CHEMKIN-CFD software package to extend the capabilities of leading CFD programs. Reaction Design's world-class engineers, chemists and programmers have expertise spanning multi-scale engineering from the molecule to the plant.

To learn how Reaction Design can help you solve your most complex chemical design problems, send an email to info@reactiondesign.com or visit www.reactiondesign.com



Simulation Speed-Up of CHEMKIN vs. Chemkin II



Gas turbine combustion CFD using FLUENT® and CHEMKIN-CFD

Reaction Design

6440 Lusk Boulevard, Suite D-205
San Diego, CA 92121

web:

www.reactiondesign.com

telephone:

(+1) 858-550-1920

fax:

(+1) 858-550-1925

sales information:

sales@reactiondesign.com

technical support:

support@reactiondesign.com

