

Expert Services for Reaction Mechanisms

Get the results you need with an accurate mechanism tailored to suit your design



- ▶ **Improve the accuracy of your clean-combustion simulation**
- ▶ **Optimize the chemistry employed in CFD models**
- ▶ **Dramatically improve your ability to predict emissions**
- ▶ **Reduce computational time with “smart” mechanism reduction**

Accurate simulation depends on the accuracy of the reaction mechanisms used. When you consider the accuracy your simulations provide, is it good enough to meet your development goals?

Modern designs require the effective use of simulation to improve time-to-market of new products, while reducing the number of costly validation experiments. Today, many system developers use 3-D Computational Fluid Dynamics (CFD) and 0-D and 1-D chemical reactor modeling in their design workflows. These models require the application of a chemical reaction mechanism that is appropriate for the fuels and operating conditions in the system.

Many CFD modelers realize that improved simulation accuracy can only be achieved by replacing commonly used single-step/global reaction mechanisms with multi-step or more detailed mechanisms. Improved temperature and emissions predictions are obtained when using reduced chemistry mechanisms within CFD. Used in conjunction with CHEMKIN® chemical reactor modeling, engineers can take advantage of larger and more accurate reaction mechanisms that provide previously unachievable accuracy for the prediction of system behavior and by-product generation. But, the “smart” development, reduction and assembly of detailed chemistry mechanisms is most successful when performed by chemistry experts.

Reaction Design’s world-renowned, detailed-chemistry experts can work with you to efficiently and effectively optimize reaction mechanisms for use in your simulations. Mechanism development projects can require mechanism assembly from published works, the merging of component mechanisms that are consistent with experimental data, developing and validating new detailed mechanisms for a targeted fuel component, and/or reducing mechanisms for use in CFD.

Expert Mechanism Service — How it works

Typical Reaction-Mechanism Service projects begin with a thorough analysis of your application and specific design goals. Your current use of mechanisms is reviewed against a range of available mechanisms and mechanism services. Next, Reaction Design’s experts recommend the appropriate approach to optimize the use of the mechanism(s) for the most effective and accurate simulation of your application.



Expert Mechanism Service — Step by step:

- ▶ Research appropriate mechanism(s)
- ▶ Create or assemble mechanisms from public and non-public sources
- ▶ Merge mechanism components
- ▶ Assist in validating or refining the mechanism through comparison to available experimental data
- ▶ “Smartly” reduce mechanisms for reactor modeling and for CFD

Reaction-Mechanism Services can be tailored to meet your design and budget constraints

Effective master-mechanism development and validation for modern fuels and additives is a costly process. In fact, it is often prohibitively expensive for individual organizations. However, there are proprietary resources available to Reaction Design that can be used to cost-effectively assemble and reduce reaction mechanisms for CFD or CHEMKIN reactor-modeling applications.

Reaction Design is the world leader in accurate combustion-chemistry mechanism development, enabling effective simulation at all phases of the design process, as well as the analysis of deployed systems. Reaction Design has developed and validated master mechanisms for gasoline, diesel, biodiesel, fuel additives, and Fischer-Tropsch coal-to-liquid fuels. Projects have been performed for the transportation and energy sectors through funding by both commercial and government programs. We also have a broad base of experience in developing gas-phase and gas-surface mechanisms for plasma and chemical vapor deposition systems commonly used in semiconductor and solar-cell manufacturing.

The experts at Reaction Design will quickly assess your application and simulation goals and develop or assemble custom reaction mechanisms that will improve simulation accuracy.

Let's get started

For more information on how Reaction Design can enhance the effectiveness of your combustion chemistry simulation, please contact sales@reactiondesign.com.



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 expert 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. Reaction Design also provides the CHEMKIN-CFD™ software package, extending the capabilities of leading CFD programs. Reaction Design's world-class engineers, chemists and programmers have expertise that spans multi-scale engineering from the molecule to the plant. Today, Reaction Design serves more than 350 customers in the commercial, government and academic markets.

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