

### ***Detailed Chemistry in CFD***

Commercial combustion firms and materials manufacturers are recognizing that to achieve low-emissions designs, improve productivity and increase performance, they need to incorporate more detailed chemistry in their simulations. Low-emissions combustion system design depends on the simulation of both chemical and fluid flows. When simulation is used effectively in design workflows, designer ingenuity is enhanced, development costs are reduced, and speed to market for new designs is improved. The dominant simulation tool used in the industry today is Computational Fluid Dynamics (CFD).

In an ideal world, every CFD simulation would include detailed chemistry descriptions as well as accurate geometry representations. However, while CFD has many powerful benefits, it is significantly limited in the amount of chemistry detail that can be included effectively. Typical CFD solutions can only handle global (single-step) reactions or a set of severely reduced chemical reaction steps while still producing a stable solution in a time-frame that suits modern design cycles.

### **Challenge to CFD Implementations of Detailed Chemistry**

The primary challenge to achieving CFD solutions with accurate detailed chemistry is the issue of computational stiffness. Computational stiffness 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. Many CFD tools do not have the necessary sophistication to handle complex chemistry systems that require pressure-dependent gas-phase reaction rates, coverage-dependent surface reactions, or multi-component molecular transport properties.

Modern chemical reaction mechanisms are already providing unparalleled simulation accuracy for commercial combustion and materials processing industries. These mechanisms can be quite large, involving thousands of reactions and hundreds of species. The benefits of using more accurate detailed chemistry in simulation are being realized by the transportation, energy and materials processing markets. Employing detailed chemistry leads to improved predictions:

- Of ignition and emissions for automotive engine designers.
- Of NO<sub>x</sub>, CO and Unburned Hydrocarbons for gas turbine combustor designers.

CFD, unfortunately, is not well equipped to handle these accurate mechanisms— it forces designers to sacrifice chemical accuracy for accuracy in geometry and flow.

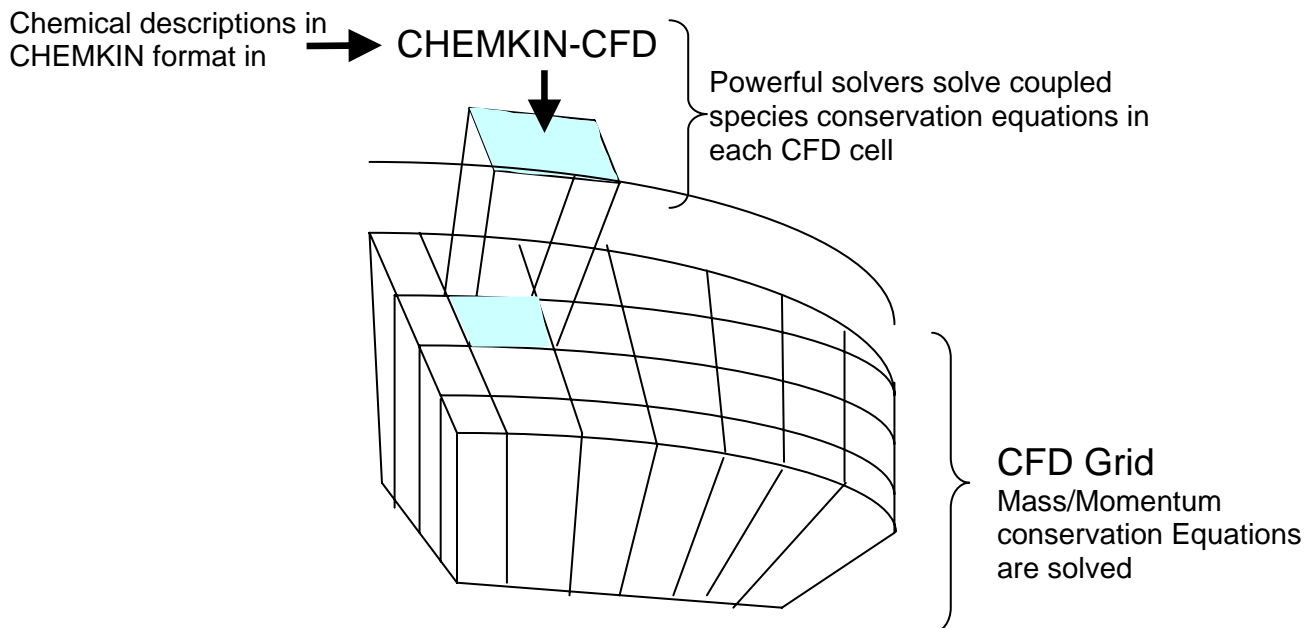
When CFD applies reaction kinetics consisting of more than a few steps, some typical problems are:

- Significantly increased solution times
- Unstable solutions
  - Oscillating solutions
  - Numerical expansion (solution blowing up)

### CHEMKIN-CFD Benefits

CHEMKIN-CFD is a chemistry module that addresses the problem of CFD’s computational stiffness by providing efficient and accurate solution algorithms that assure robust coupling of the chemistry and the flow. CHEMKIN -CFD also includes modern chemistry description options, fully compatible with the latest version of CHEMKIN. Popular commercial CFD codes such as ANSYS FLUENT and STAR-CD can include CHEMKIN-CFD as an integrated feature optionally available from Reaction Design. The CHEMKIN-CFD Application Programming Interface is designed to be easily linked to a CFD code.

If you are satisfied with the simulation results you receive from global or severely reduced reaction kinetics in your CFD solution, then CHEMKIN-CFD might not be right for you . However, if the lack of accurate chemistry in your CFD solution is limiting your results, then CHEMKIN-CFD may be a good option for increased solution speed and stability (robustness).



## CHEMKIN-CFD Q&A

### Q: What is CHEMKIN-CFD?

**A:** Very simply, CHEMKIN-CFD gives your CFD code the power of CHEMKIN to perform its chemistry calculations. CHEMKIN-CFD software is designed to couple detailed chemistry with third-party CFD codes. CHEMKIN-CFD uses CHEMKIN-derived solvers that are able to handle stiff gas-phase and gas-surface chemistry. Just like CHEMKIN, it solves the conservation equations for transient and steady-state problems. As an input, CHEMKIN-CFD needs a chemical-kinetics mechanism and thermodynamic data in CHEMKIN format, as well as optional CHEMKIN-based molecular-transport properties. At every CFD time step, or at every steady-state iteration, and in every CFD cell, it advances the solution of temperature and species profiles by iterating closely with the CFD code of interest. Depending on which CFD code is used, some other information (for example, rate of production of species and/or heat) can also be passed on to be used in the CFD calculations. CHEMKIN-CFD can also provide accurate multi-component molecular transport properties, such as diffusivity, thermal conductivity, and viscosity, for use in the flow simulation by the CFD code.

### Q: What are the benefits of using CHEMKIN-CFD as opposed to treating chemistry directly inside CFD?

**A:** Traditional CFD solution algorithms solve each equation in series and then undergo an iterative process until there is convergence for the entire 3-D problem with momentum, energy, species, and mass conservation equations. If the chemistry is stiff (as it is in most combustion simulations as well as surface-catalytic systems), such an approach leads to instabilities, because each species equation is solved independently of the others. CHEMKIN-CFD solves coupled conservation equations at every cell (or grid point), at every iteration and at every time-step within a CFD simulation. The third-party CFD code then performs transport calculations over all grid points, optionally using the transport properties provided by CHEMKIN-CFD. In this way, CHEMKIN-CFD allows the close coupling required to resolve/converge chemistry terms for complex mechanisms.

### Q: My CFD code advertises detailed chemistry capability. Why use CHEMKIN-CFD instead?

**A:** Many commercial CFD codes offer their own stiff chemistry solvers for large gas-phase reaction flow problems. However, there are still several advantages of using CHEMKIN-CFD.

- 1) Many reaction rate parameter definition options (e.g. surface coverage dependent reaction rate parameters, advanced non-Arrhenius rate expressions, pressure-dependent reactions, etc.) are available in CHEMKIN and CHEMKIN-CFD but are not present or not handled correctly in many CFD codes.
- 2) CHEMKIN-CFD can be more efficient than CFD chemistry solvers in converging to a solution, particularly if a high degree of accuracy is needed. In transient CFD applications, for example, CHEMKIN-CFD finds the optimum time step for solution of the

coupled reaction problem, while CFD codes may keep the time step defined by the user for the flow-segregated problem, often missing key information that occurs at small time scales relative to the flow time scale.

**Q: Will the solution take longer when I use detailed chemistry with CHEMKIN-CFD?**

**A:** Yes. As you add additional chemistry steps into your CFD solution, it will take longer. For example, a single-step global reaction will certainly have a shorter run time without CHEMKIN-CFD than a 25-step reduced mechanism will have running with CHEMKIN-CFD. But remember that the additional chemistry steps included in the CFD simulation will provide you more accurate and valuable results for important results such as emissions and ignition. On the other hand, running a 25-step reduced mechanism with CHEMKIN-CFD will always provide a faster solution than one without CHEMKIN-CFD. Perhaps more importantly, your solution has a better chance of converging and actually reaching a solution with CHEMKIN-CFD than without.

**Q: Is the use of CHEMKIN required in order to run CHEMKIN-CFD?**

**A:** CHEMKIN-CFD does not require the user to run CHEMKIN as well. However there are many benefits of using CHEMKIN along with CHEMKIN-CFD/CFD (see below).

**Q: Why would I want to use CHEMKIN along with CHEMKIN-CFD?**

**A:** CHEMKIN and CHEMKIN-CFD used in conjunction with a CFD code complement each other and represent chemistry simulation best-practices when they are utilized together in a design workflow. CHEMKIN offers the ability to quickly apply very detailed chemistries in a variety of idealized reactors and can even handle more complex problems by combining these simple reactors into networks. Furthermore, individual reactor analyses can be performed very quickly even with large reaction mechanisms. Utilizing this speed of computation and the sensitivity analysis tools of CHEMKIN, users can develop reduced chemistries better suited for application in CFD calculations.

Even with CHEMKIN-CFD, it is not possible to utilize reaction mechanisms of extreme size in CFD owing to the overall computational scale of multidimensional simulations. Of course, CFD can better handle the actual geometry of very complex systems and can add multidimensional and geometry-dependent effects (sprays, turbulence, radiation, etc.) not possible with CHEMKIN. Thus, CHEMKIN can be thought of as a screening tool or a great “what if” tool, that maps out the parameter space of a chemistry-dependent problem, and as an analysis tool for developing and testing reduced reaction mechanisms. These calculations can provide the basis for CHEMKIN-CFD analyses to examine the full multidimensional problem and, by reducing the parameter space and providing the reduced chemistries, reduce the overall simulation time for a given engineering project.

**Q: Is CHEMKIN-CFD limited to the use with only 50 chemical species?**

**A:** Like CHEMKIN, there is no arbitrary limit of 50 species when using CHEMKIN-CFD. This limitation, where it exists, comes from how the particular CFD code in question was originally programmed. For example, ANSYS FLUENT and STAR-CD currently limit the detailed kinetics to only 50 species.

**Q: What are the specific CFD codes (and which versions) can currently be used with CHEMKIN-CFD on various platforms?**

**A:** CHEMKIN-CFD is supported on a variety of modern computer platforms, including 64-bit Windows and Linux systems. For the most up-to-date information on platform availability, please contact [Reaction Design support](#).

## About Reaction Design

Reaction Design helps transportation manufacturers and energy companies rapidly achieve their Clean Technology goals by automating the analysis of chemical processes via simulation and modeling solutions. Reaction Design is the exclusive developer and distributor of CHEMKIN and CHEMKIN-PRO, the *de facto* standards for modeling gas-phase and surface chemistry, providing engineers ultra-fast access to reliable answers that save time and money in the development process. Reaction Design also offers the CHEMKIN-CFD software module, which brings detailed kinetics modeling to other engineering applications, such as Computational Fluid Dynamics (CFD) programs. Reaction Design's world-class engineers, chemists and programmers have expertise that spans multi-scale engineering from the molecule to the plant. Reaction Design serves more than 350 customers in the commercial, government and academic markets.

Reaction Design can be found online at [www.reactiondesign.com](http://www.reactiondesign.com).

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