Which CHEMKIN is Right for You?

Reaction Design

6440 Lusk Blvd, Suite D205
San Diego, CA 92121

Phone: 858-550-1920
www.reactiondesign.com

Modernization of CHEMKIN

In a world where everyone needs to maximize their resources - the longer it takes to accomplish a job, the more expensive it is. So when you look for tools to help your work, you look for the ones that get the work done in the fastest, most economical manner, with the highest return on your investment.

Time in the lab is expensive time, and some chemical-kinetics questions can only be answered using simulation. When Chemkin was first introduced, it provided a flexible and powerful approach to implementing gas-phase kinetics simulations, allowing home-grown descriptions of the studied systems. However, working with Chemkin II required users to acquire an intimate understanding of programming and scripting languages, code compiling and debugging procedures on different computer operating systems, and to master the intricacies of problem-keyword syntax. It also required time-consuming, manual manipulation of data to allow interpretation of the simulation results. Delving into material at this level of detail took quite a level of devotion, such that the typical researcher spent countless hours in preparing for, maintaining, and processing Chemkin II simulations.

There are now two versions of Modern CHEMKIN available today.

- **CHEMKIN-PRO** is our latest release that is specifically designed for power users who need large mechanisms or models that are computationally intensive. CHEMKIN-PRO also includes several new facilities for Particle Tracking, Multi-Zone Engine simulation, Reaction Path Analysis and Uncertainty Analysis.
- **CHEMKIN 4.1** (*initially released in 2006*) provides an economical alternative for users who do not require the increased speed or feature set of CHEMKIN-PRO.

Modern CHEMKIN provides you with flexible and easy application development and analysis, avoiding the challenges associated with developing, maintaining, transferring and learning homegrown codes. At the same time, Modern CHEMKIN retains the flexibility allowed by Chemkin II, but with continuously improving performance, capabilities, and robustness.

With improved speed and solver performance, numerous new reactor-model applications, a user interface that clarifies and speeds user-software interactions, supported installers for multiple platforms, and professional technical support from a dedicated and expert staff, Modern CHEMKIN gives researchers the ability to focus on the problem and its solution, rather than the implementation of the tool.

There are several myths regarding Chemkin II that this white paper will address.

Myth 1: Chemkin II enables more accurate results

Myth 2: Chemkin II is Free

Myth 3: Chemkin II is more Flexible

Myth 4: Chemkin II is more Respected Technically

Myth 5: It is prohibitive to convert custom codes with integrated Chemkin II to Modern CHEMKIN

Chemkin II Overview

Chemkin originated at Sandia National Laboratories as a software package, whose purpose was to facilitate formation, solution and interpretation of problems involving elementary gas-phase chemical kinetics. At the time of introduction to the combustion field, Chemkin represented an important advance in enabling the testing and interchange of different chemistry mechanisms that were based on elementary kinetics, without the need to restructure code with each change in chemistry. The "Chemkin II" package consisted of several software components: a reaction-mechanism Interpreter, which parsed a symbolic description of an elementary, user-specified chemical reaction mechanism; a gas-phase subroutine library, which contained about 100 FORTRAN subroutines that could be called upon to return information on equations of state, thermodynamic properties and chemical production rates; a thermodynamic data file for many gaseous species; and four application codes that handled simulations of equilibrium, steady-state perfectly stirred reactors, transient adiabatic closed systems with constant pressure or volume, and adiabatic, premixed laminar flames. For the flame calculations, a transport data file for selected species, a transport data-file interpreter, and a transport subroutine library were also included.

To apply Chemkin II to an application, users often had to write their own FORTRAN programs that would include a set of governing equations to describe their particular system of interest, due to the limited number of application codes and options provided in the Sandia distribution. Writing such programs was facilitated by the use of the Chemkin subroutine libraries, which provide easy access to the terms in the governing equations of interest that relate to equations of state, chemical production, transport properties, and thermodynamic properties. (Kee, Rupley et al. 1989). In such cases the user would be responsible for setting up and solving a system of equations using numerical solver modules, compiling and linking code modules, executing pre-processor and application programs via the command line, and extracting results from a separate set of machine-dependent binary solution files.

Improved Performance

As mechanisms have grown in complexity, Modern CHEMKIN has evolved with improved solvers that significantly speed solution times and with advanced reactors and capabilities that assist in modeling real world applications. The solver enhancements in CHEMKIN-PRO provide enhanced solution speed over CHEMKIN 4.1. It is also important to note that CHEMKIN 4.1 is much faster than Chemkin II, when tested using identical reactor models and mechanisms. The performance increase is particularly noticeable for applications with large reaction mechanisms or longer solution times. Results of solution-speed benchmarking tests on CHEMKIN-PRO, CHEMKIN 4.1 and Chemkin II are shown in Table 1. Benchmarks for all cases were run using the same Linux 64-bit platform. Comparing relative solution speed between Modern CHEMKIN and Chemkin II for the most common reactor types shows that CHEMKIN-PRO can be up to 14 times faster than Chemkin II and CHEMKIN 4.1 also provides substantial speed improvement over Chemkin II (see Figure 1).

There are also many reactor model types that are of interest to kinetic modelers that are not available with Chemkin II. Figure 2 illustrates how CHEMKIN-PRO yields much faster solution times than CHEMKIN 4.1 for kinetic models using large mechanisms for reactor types that are not supported in Chemkin II. The solution time improvement can be dramatic for large mechanisms, reducing solution time from days to hours or hours to minutes. For example, the IC Engine Model simulation time was cut from 53 minutes to 3 minutes. More impressive, though, is the improved solution time for the 103-PSR Network from gas turbine combustor, where the solution time was reduced from 5 hours with CHEMKIN 4.1 to 17 minutes with CHEMKIN-PRO.

The improvements made to Modern CHEMKIN have also greatly increased its stability and robustness enabling converged solutions for many applications that did not converge using Chemkin II.

Some of the modeling performance improvements in Modern CHEMKIN include:

- Improved speed of transport-property evaluations
- Increased accuracy in conservation equations for flames
- Improved performance for running problems with and manipulating large mechanisms (100s of species).
- Automation of initial "guess" profiles for steady state reactors, including auto-calculation of equilibrium concentrations when initial guesses are not provided by the user and a simplified specification of initial dependent-variable profiles that can reliably provide convergence.
- Added facilities to easily import and export initial profiles (such as time profiles for transient problems or spatial profiles for initial guesses), which facilitates sharing or generating this information.

Table 1. Speed Performance Benchmarks Between Chemkin II and Modern CHEMKIN

Reactor Model	Chemkin II Application	Chemistry Description	Number of Species	Number of Reactions	Chemkin II Runtime (seconds)	CHEMKIN 4.1 Runtime (seconds)	CHEMKIN-PRO Runtime (seconds)	CHEMKIN 4.1 Speedup	CHEMKIN-PRO Speedup
Flame-speed Calculator	PREMIX	CHEMKIN sample for methane/air flame	17	58	7	6	4	1.2	1.8
Burner-stabilized Flame	PREMIX	Methane flame	53	325	787	241	181	3.3	4.3
Flame-speed Calculator	PREMIX	n-heptane flame	313	1,875	20,393	7,253	2,975	2.8	6.9
Burner-stabilized Flame	PREMIX	fuel-rich benzene flame with soot precursor formation	101	544	1,573	374	197	4.2	8.0
Perfectly Stirred Reactor	PSR	LLNL cyclohexane	1,081	4,269	N/A (Failure)	945	101	infinite	infinite**
Perfectly Stirred Reactor	PSR	LLNL PRF mech	1,034	4,235	798	518	57	1.5	14.0
Transient Closed Homogeneous Batch Reactor	SENKIN	LLNL PRF mech	1,034	4,235	322	447	61	0.7	5.3
Burner-stabilized Flame	PREMIX	CHEMKIN sample for hydrogen/air flames	9	18	< 1	< 1	< 1	N/A	N/A
Perfectly Stirred Reactor	PSR	CHEMKIN sample for h2/air combustion	9	19	<1	<1	<1	N/A	N/A

** 9.3 speed-up factor compared to 4.1

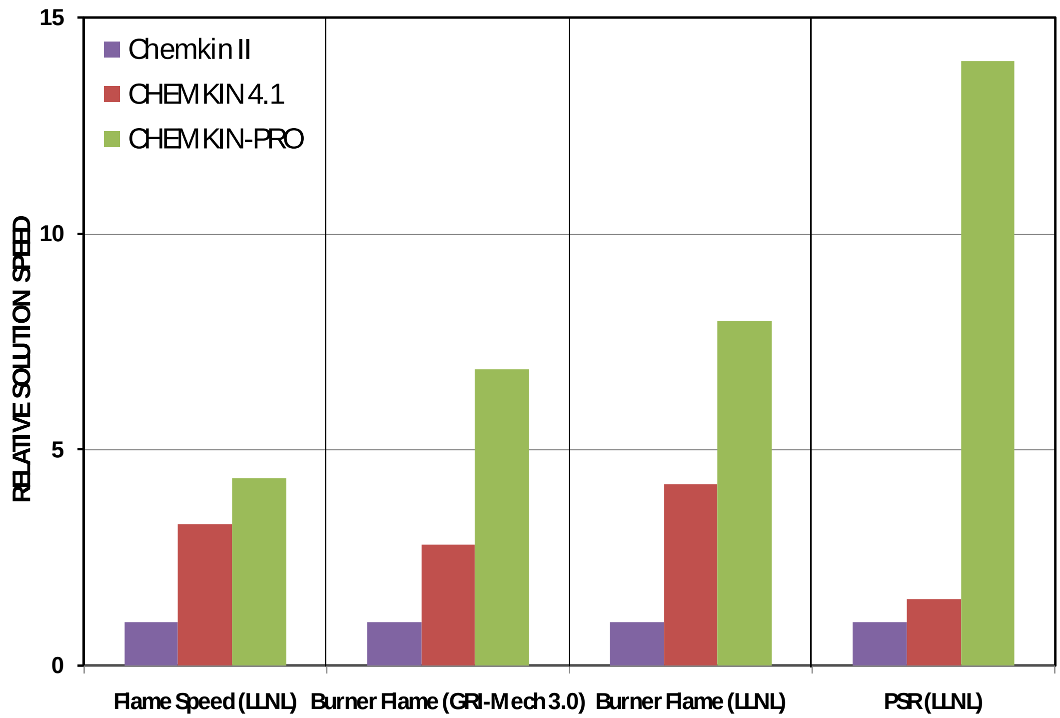


Figure 1. Solution Speed Comparisons between Chemkin II and Modern CHEMKIN (Linux 64-bit Platform)

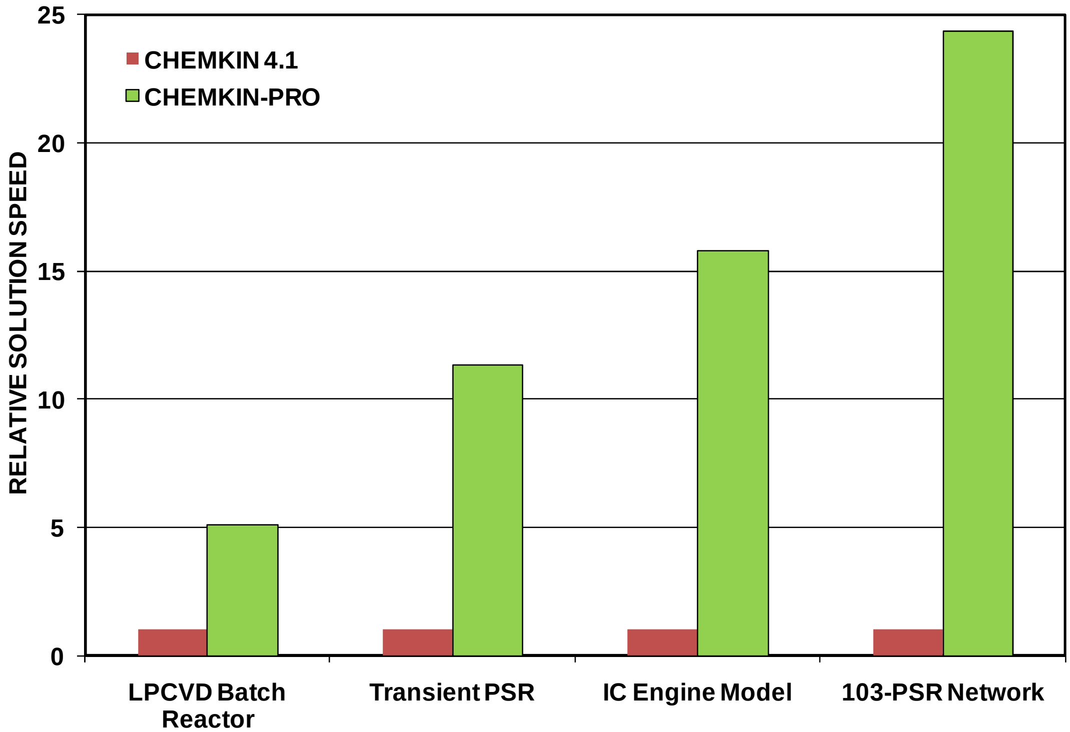


Figure 2. Solution Speed Comparison between CHEMKIN 4.1 and CHEMKIN-PRO on Computationally Intensive Real-World Applications (Linux 64-bit Platform)

Application Programming Interface (API)

One of the innovations of Chemkin II was the ease at which custom programs could be written, in which all chemistry-specific data was encapsulated through pre-processing of an input file. The transfer of that data to the application code was through the use of chemistry-independent calls to the CHEMKIN subroutine library. A key benefit of this functionality was that it facilitated the integration of Chemkin II into custom-developed software as the chemistry solution engine. That provided chemistry solution accuracy and flexibility that was not available through commercial software 20 years ago.

In Modern CHEMKIN, the ability to call any of the routines in the subroutine libraries remains an important feature through the CHEMKIN/API. And, as it turns out, it is relatively easy to switch out, or convert, Chemkin II-based custom applications to interact with the Modern CHEMKIN/API. The documentation for the CHEMKIN/API provides step-by-step instructions for building a user program to link the power of CHEMKIN to your application. In addition, the subroutine libraries are continuously being expanded to return new types of information, including surface chemistry data. The API allows users to write their own custom programs, or to modify or supplement the functionality of Modern CHEMKIN reactor models. The subroutine libraries may be accessed either from user-modified subroutines called by the supported CHEMKIN Reactor Models, or from entirely user-written application programs. User application programs may be written in C, C++, or FORTRAN computer languages. Extensive documentation of the API usage and examples are available as a part of a Modern CHEMKIN installation.

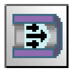
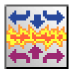
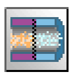
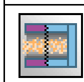
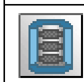
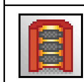
Applications

Reactor Models

While Modern CHEMKIN still allows user access to the CHEMKIN libraries, it also provides a great variety of pre-packaged, customizable Reactor Models, including all of the capability of the Chemkin II application codes with added improvements, as well as various new Reactor Models. Table 2 summarizes the differences between availability of Chemkin II and CHEMKIN-PRO reactor models.

Table 2. Comparison of CHEMKIN-PRO Reactor Models and Chemkin II Application Codes

CHEMKIN-PRO		Chemkin II
	Multi-Zone Engine Model for Reciprocating Engines	none
	Non-reactive Gas Mixer (performs thermodynamic calculations)	none
	Chemical and Phase Equilibrium	Equil - Chemical Equilibrium
	Mechanism Analyzer	none
	Single Zone Closed Internal Combustion Engine Simulator	none
	Closed Homogeneous Batch Reactor with advanced ignition delay calculations and options to constrain the problem using volume vs. time or pressure vs. time profiles	Senkin - Closed Homogeneous Batch Reactor with constant volume or constant pressure
	Closed Partially Stirred Reactor	none
	Closed Plasma Reactor	none
	Perfectly Stirred Reactor (steady state or transient, where transient simulations can use a variety of time-profile constraint options)	PSR - Perfectly Stirred Reactor, steady state only
	Plasma Perfectly Stirred Reactor	none
	Partially Stirred Reactor (PaSR)	none
	Plug Flow Reactor	none
	Honeycomb Plug Flow Reactor	none
	Plasma Plug Flow Reactor	none
	Planar Shear Flow Reactor	none

	Cylindrical Shear Flow Reactor	none
	Premixed Laminar Burner-stabilized Flame with heat loss options	Premix - adiabatic Laminar Burner-stabilized Flame
	Premixed Laminar Flame-speed Calculation, with heat-loss options	Premix - adiabatic Laminar Flame-speed Calculation
	Diffusion or Premixed Opposed-flow Flame	none
	Stagnation Flow CVD Reactor	none
	Rotating Disk CVD Reactor	none
	Normal Incident Shock	Shock
	Normal Reflected Shock	Shock
	Low Pressure CVD (LPCVD) Furnace Model	none
	Low Pressure CVD (LPCVD) Thermal Analyzer	none

Enhancements to the Original Chemkin Reactor Models

In addition to expanding the types of reactor models available, Modern CHEMKIN reactor models include many enhancements compared to their Chemkin II counterparts. Such enhancements include additional capabilities as well as improved convergence and performance. Specific examples include:

- The *Equilibrium Reactor* was expanded to include the ability to perform phase equilibrium as well as chemical equilibrium calculations, with consideration of gas, liquid, and solid phases.
- *Closed Homogeneous Reactors* (including the *IC Engine Model*) have additional capabilities of calculating ignition delay times based on temperature inflection and peak species concentrations.
- All transient 0-D simulations (e.g., all closed reactor models, *PSR*s and *PaSR*s) include the ability to specify input profiles that vary as a function of time for such constraints as temperature, pressure, volume, heat loss and power (plasmas).
- *PSR*s can be run in transient or steady-state mode. The transient capability includes integrated sensitivity analysis for both gas and surface reactions.
- The *Freely Propagating* and *Burner Stabilized Flame Reactors* include improved performance, easier set-up of initial conditions to reach efficient convergence, as well as several heat-loss specification options and a user-programmable radiant-heat-exchange routine.

New Reactors in Modern CHEMKIN

There are many new reactor models in commercially supported CHEMKIN, which are run via user customizable templates. Examples of new reactor models include:

- The *Multi-Zone Engine Model* for HCCI combustion allows the cylinder to be divided up into multiple zones where large, accurate detailed chemistry mechanisms can be applied for more accurate simulation of combustion, yielding better heat release, pressure, and emissions predictions.
- The *Internal Combustion Engine* (ICE) model simulates a combustion cylinder in an internal combustion engine under auto-ignition conditions, which is most relevant to the study of fuel auto-ignition behavior, engine knock, and homogeneous charge compression ignition (HCCI) engines. A variety of heat-transfer correlation options are included.
- *Partially Stirred Reactors* (Open and Closed) allow users to explore turbulent-kinetic interactions by simulating both the mixing process and the detailed kinetics. These reactors use a Monte-Carlo based stochastic model of mixing controlled by a mixing time coupled to detailed kinetics controlled by a specified residence time. Equilibrium conditions can also be assumed.
- The *Plug Flow Reactor* is designed to model the non-dispersive one-dimensional flow of a chemically reacting gas mixture. With full surface chemistry, the PFR allows simulation of fixed bed reactors in which the user can specify area per length for surface chemistry independent of the hydraulic diameter of the flow.
- The *Honeycomb Monolith Reactor* is a special case of the PFR, which allows direct simulation of honeycomb geometry and catalyst loading for automatic calculation of active surface areas for catalyst heterogeneous chemistry.
- The *Opposed Flow Flame* model is designed to model one-dimensional, axisymmetric or planar diffusion flames between two opposing nozzles, using a similarity transformation that reduces the three-dimensional flow field to a one-dimensional problem.
- *Plasma reactors* (PSR, Plug-flow, and Closed systems) are designed to handle non-equilibrium plasma processes where the electrons are not in thermal equilibrium with the background gas. This has particular value in the modeling of plasma chemical-vapor-deposition or etching processes in microelectronics manufacturing and other areas of materials processing.
- The *CHEMKIN LPCVD Furnace Model* and *Thermal Analyzer* provide accurate simulation of multi-wafer LPCVD reactors, allowing users to specify the process chemistry, reactor dimensions, flow rates, pressures, temperatures, wafer quantities and wafer sizes.
- Finally, the *Mechanism Analyzer* presents, in tabular and graphical form, detailed information about the temperature and pressure dependence of chemical reaction rate constants and their reverse rate constants, reaction equilibrium constants, reaction thermochemistry, chemical species thermochemistry and transport properties without requiring the user to do any programming.

Reactor Networks

Not available with Chemkin II, Modern CHEMKIN supports the visual building and execution of reactor networks which allows users to route the flow out of one reactor into an inlet of another reactor, providing representation of more complex reacting flow systems. When the reactors connected in this way are all PSRs, they can form a “cluster” with special capabilities and options. Clusters can include “recycling” flows, where the flow out of one reactor can flow upstream to become an inlet of an upstream reactor. Clusters can also include heat exchange (convection, conduction and/or radiation) between PSRs. The reactors in a cluster are solved simultaneously to provide full coupling of the dependent flows. They can be run in both transient and steady-state modes. A Reactor Network can consist of a mixture of any open reactors, such as PFR, as well as PSR clusters. In CHEMKIN-PRO, such heterogeneous reactor networks can also include upstream or “recycle” flows, which are solved through iteration using a “tear-stream” algorithm. In addition to flow networks, Modern CHEMKIN users can take advantage of the reactor-networking diagramming options to link simulations for purposes of initialization, restart, and information-transfer. These capabilities are facilitated by the use of a unified solution-file structure for all reactor models, based in XML (eXtensible Markup Language).

Surface Chemistry

With Chemkin II, access to surface chemistry capability was restricted, due to export controls and licensing restrictions in place at the time of the initial "Surface Chemkin" release from Sandia. However, in Modern CHEMKIN, all 0-D (closed homogeneous and PSR; steady-state and transient), as well as all plug-flow, shear-flow and CVD reactors provide ready access to the latest surface chemistry capabilities. These capabilities have been greatly expanded since the initial Surface Chemkin report (Kee, Rupley et al. 1989). For example, global reaction mechanisms were enabled, allowing non-elementary kinetics where reactions may be written with non-integer stoichiometric coefficients and arbitrary reaction orders for any species in the system. This facilitates use of semi-empirical reaction mechanisms for catalytic and chemical vapor deposition systems. Another example is the inclusion of a wide range of new reaction formulations to describe plasma-surface interactions, as well as Langmuir-Hinshelwood and Eley-Riedel rate expressions. In addition, several of the reactor models make use of the multiple materials option, which allows Modern CHEMKIN users to specify separate chemistry mechanisms for different materials within the same reactor and to control relative surface areas of those materials. Sensitivity and Rate-of-production analyses are available for all surface species and reactions, in both transient and steady-state reactor models.

Advanced Analysis

Particle Tracking Feature

The most recent capability built on the detailed surface chemistry capability of CHEMKIN-PRO, is the Particle Tracking feature. This feature tracks particle growth and size distributions, including detailed chemical production terms from particle-gas interactions. The module is available for use with all 0-D Closed Homogeneous Reactors, PSRs, PFRs, Shear Flow reactors, and Flame Simulators (for pre-mixed and opposed-flow flames). Particle nucleation reactions are defined and included in the surface chemistry input file, thus allowing multiple nucleation pathways. The user is able to specify surface reactions for growth, reduction, condensation, and deposition on the particle surface. The coagulation of particles is accounted for using built-in coagulation models for various flow regimes. The particle size distributions are determined using the Method of Moments (Appel, Bockhorn et al. 2001).

Reaction Path Analysis

In any detailed chemistry model, understanding of the specific reaction paths that are present, and which are dominant, is critical to filling out your understanding of the kinetic model results. Identifying the dominant reactions that dictate the formation or quenching of pollutant species of NOx, CO and UHC can be extremely valuable in identifying means to reduce their formation through manipulation of reactor geometry and operating conditions. The new Reaction Path Analysis capability in CHEMKIN-PRO allows visual, interactive analysis of dominant reaction paths, and may be used with any of the CHEMKIN Reactor Models for any kind of chemistry set.

Uncertainty Analysis

A new feature in CHEMKIN-PRO provides an assessment of the relative uncertainty in the kinetic model based on the relative accuracy of the various inputs to the model. The Uncertainty Analysis feature in CHEMKIN-PRO tracks how any known variability in the inputs to a kinetic model propagate through the model and results in an assessment of the solution's overall uncertainty. This helps you put "±" or error bars on your model's results. The Uncertainty Analysis feature also can quantify how much of the overall model's uncertainty is related to each input. Adding uncertainty analysis to your kinetic model's result provides a context for improved understanding of the model results and guides better technical and business decisions.

Usability

Application Setup

Chemkin II required that users compile, link, and run FORTRAN files from the command line of a UNIX shell. In order to set up an application, users had to first become familiar with a lexicon of keywords that varied from application to application. In order to make any modifications to application-program behavior, users had to be experts in FORTRAN programming, be able to create their own "make" files and build scripts, and work with code debuggers to diagnose any difficulties encountered. Code modification was required every time the problem size changed to accommodate a larger chemistry set or computational grid.

These limitations are eliminated with Modern CHEMKIN. There is no longer a need to memorize keywords or their usage rules. Memory is allocated dynamically and automatically for each problem, without the need of code recompiling. Problems are defined through panels with mouse-over help for each parameter, including default values and usage guidelines. Although some programming may be required to customize applications and to work with the CHEMKIN/API, the API manual provides step-by-step instructions for both Windows and UNIX/LINUX platforms along with sample code and an integrated build environment. The CHEMKIN User Interface manages the execution of CHEMKIN programs, as well as the organization and specification of input and output files used in the calculations. This point-and-click interface guides users through the pre-processing of chemistry data, reactor-model set-up and results analysis, verifying user input along the way.

The CHEMKIN User Interface (UI) was designed to reduce set-up time for new problems, to speed the learning required for new users, and to enhance retention of knowledge for experienced users. The UI includes visual diagramming options that make it easy to build reactor networks and to perform a series of calculations to represent complex flows. For example, stirred reactors can have multiple inlet flows with mass flow rates that may vary as a function of time. Outlet flow from reactors can be split into two or more parallel streams, where each stream can be fed into different reactors downstream. Multiple flows from different reactors can also be thermodynamically mixed to form a single stream. Within the interactive diagramming facility, inlet streams and reactors can be easily added, deleted or moved.

Reaction Rate Formulations

Many new reaction-rate formulations have been added to those that were originally handled in Chemkin II. The list of differences is shown in Table 3.

Table 3. Comparison of CHEMKIN and Chemkin II Reaction Rate Formulations

CHEMKIN Reactions	Chemkin II
Pressure-dependent reactions with neutral third-body efficiency	equivalent
Reverse Rate Parameters - Supersedes the reverse rates that would normally be computed through the equilibrium constant	equivalent
Troe fall-off for pressure-dependent reactions	equivalent
Chebyshev Polynomial Rate Expressions	none
Ability to supersede Chebyshev polynomial temperature and pressure limits	none
Efficiency of Collision Frequency Expression - If a reaction is bimolecular and the approximate collision diameters are known– the collision frequency efficiency expression can be used to calculate the reaction rate constant.	none

CHEMKIN Reactions	Chemkin II
Duplicate Reactions – When two or more reactions involve the same set of reactants and products, but proceed through distinctly different processes.	equivalent
Ability to specify reactions that depend on a specific species temperature; e.g., the electron temperature for non-equilibrium plasmas.	none
Energy Loss Parameter – Overrides the calculation of energy loss from the change in enthalpy determined by the reaction description and the thermodynamic data of the reactants and products. Useful in describing electron-impact excitation reactions.	none
Ability to use non-integer stoichiometric coefficients to describe non-elementary reactions.	none
Forward Reaction Order Parameter – Supersedes the forward reaction order for any species in the mechanism (with respect to species concentration), regardless of whether the species appears as a reactant or a product in the reaction.	none
Optional Rate Fit Expressions – Supersedes the default reaction rate expression by a Janev-Langer reaction rate (plasma reactions).	none
Landau-Teller Rate expressions.	equivalent
Pressure Dependence Through Logarithmic Interpolation – Provides a general-purpose way of describing pressure-dependent reaction rates.	none
SRI pressure-dependent reaction rate.	equivalent
UNITS option allows specification of different units on a reaction-by-reaction basis.	One unit system must be used for all reaction-rate parameters in the system
Limited to 16 characters for species names.	Limited to 10 characters for species names
Reactions allow up to 6 reactants and 6 products per reaction.	Reactions limited to 3 reactants and 3 products per reaction.
In addition to NASA format, extensions allow inclusion of any number of temperature ranges; species can have more than 5 elements and unlimited number of each element per molecule.	Thermodynamic properties must strictly adhere to NASA 14-coefficient, two-temperature-range format.
Optional User Rate Subroutines – user can define a custom rate-of-progress expression for an individual reaction or net rates of production for all species in user routines designed to be called during any CHEMKIN application run.	none

Parameter Study

In order to perform a parametric study in Chemkin II, users had two choices: Use "continuation" keywords within a keyword input file, or write complex scripts to manage input and output through manipulation of keyword files. Continuation options were limited to certain reactor parameters and were only available for steady-state simulations. To do any kind of parameter variation that involved chemistry parameters, users had to write their own programs or scripts that parsed and modified chemistry-input files, managed file naming and organization, executed programs, and extracted data from binary FORTRAN solution files.

The Parameter Study Facility in CHEMKIN-PRO allows users to perform complex parametric studies without having to write programs or scripts and without running from the command line. Parameter Study can be used with all reactor models and reactor networks, for both steady-state and transient simulations. This capability automates conducting multiple runs to consider the effects of varying one or more input variables. Parameter Studies can be set up with chemistry-set parameters (such as reaction-rate constants or Lennard-Jones potentials) as well as with reactor, inlet, or operating-condition parameters. All or a selection of the Parameter Study cases can be run within a given session, thus allowing the user to return to the project at a later time to continue running additional cases. The Continuation option (which was also available in Chemkin II) can easily be used alongside Parameter Study to provide an added dimension for model refinement.

An important aspect of the parameter-study option is the harvesting of solution data from each of the model runs to provide compound solution sets that may be plotted using line or contour plots, giving quick visualization of parameter-variation effects.

Visualization and Analysis of Results

Graphical Post-Processing

No visualization or post-processing capabilities were built into Chemkin II. Modern CHEMKIN allows users to quickly view CHEMKIN results vs. time, distance, and varied parameters, including ignition times, flame speeds, rates of production, and sensitivity coefficients. Data can be viewed using line plots, or as 2-D or 3-D contour plots. CHEMKIN gives the user interactive control over numerous plot-formatting options as well as allowing for easy exporting of all or selected data in comma-, space- or tab-delimited formats. Figure 3 through Figure 5 demonstrate various capabilities of the CHEMKIN post-processor. In addition to this built-in capability, CHEMKIN-PRO allows direct launch of Excel® as an alternative means for analyzing or plotting the solution data from any CHEMKIN project.

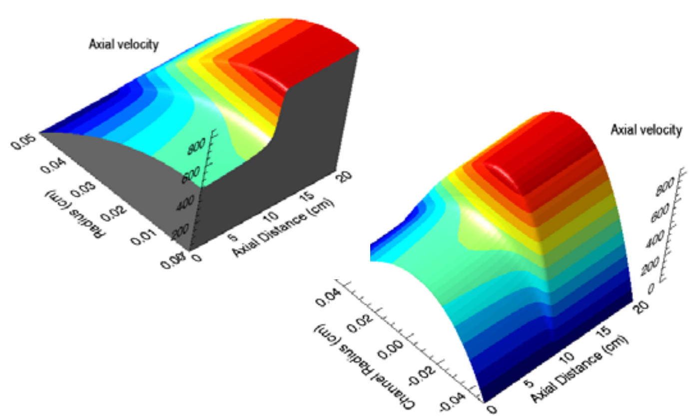


Figure 3. Ability to mirror 3-D contour plots about symmetric axis.

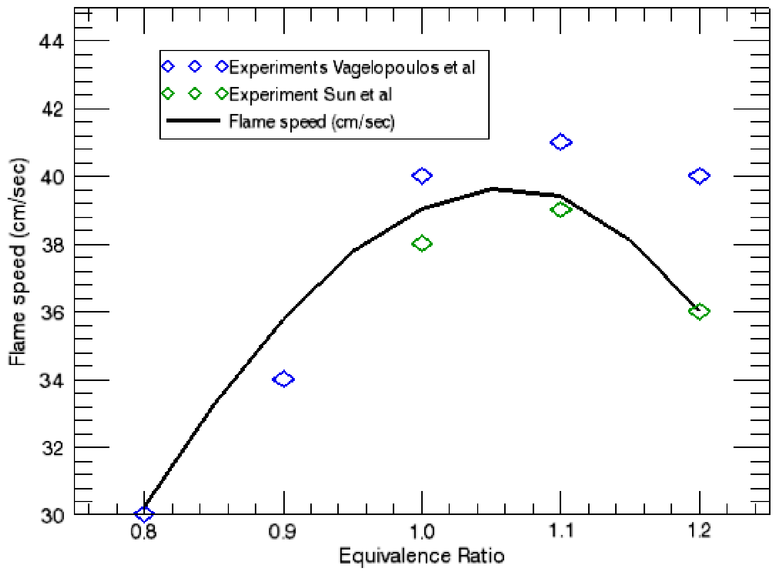


Figure 4. Ability to import experimental data in a variety of delimited formats directly into the same plot as simulations.

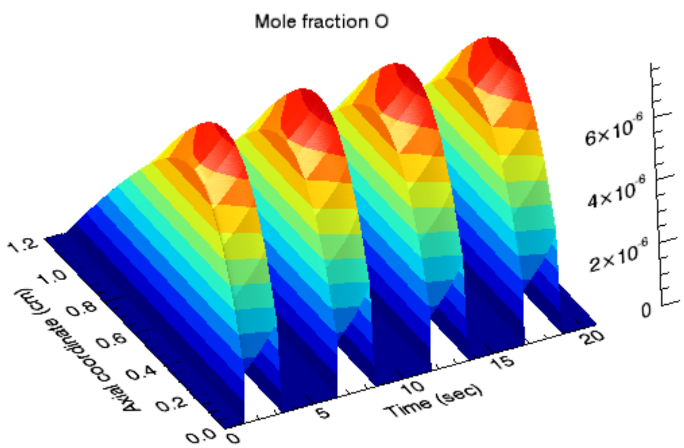


Figure 5. Ability to create plots of variables vs. a parameter varied in the Parameter Study (*Mole Fraction of O species was varied in Parameter Study*).

Support/Maintenance, Documentation

The original Chemkin II functionality is described in static Sandia reports (e.g., Kee, Rupley et al. 1989) that were not maintained as new versions of code were distributed. There was no formal tracking or documentation of changes made to the software, and only limited examples of capabilities were provided.

Commercially supported CHEMKIN is continuously updated and maintained by Reaction Design. Formal documentation is available with every CHEMKIN installation and includes detailed tutorials showing examples of projects related to combustion, materials processing and microelectronics, as well as descriptions of all input parameters and problem set-up procedures. This documentation is updated with every maintenance and major CHEMKIN release, which also includes detailed release notes describing changes made.

Because there was no version control for Sandia distributions of Chemkin, modifications or improvements to the software were often lost during upgrades to later versions, forcing users to continuously re-apply their local modifications. Version control of the commercially supported CHEMKIN allows Reaction Design to track and inform customers of all software updates, new capabilities, enhancements and bug fixes included in each version of CHEMKIN. In addition, Reaction Design maintains a very large suite of regression benchmark tests that are run continuously and expanded for each new capability added to the software. This standardizes results obtained with supported CHEMKIN, assures backwards compatibility, and allows highly-reproducible results among different researchers.

No formal technical support was available for Chemkin II. In contrast, Reaction Design quickly responds to all emailed or phoned-in tech support questions for valid licensed versions of Modern CHEMKIN. Reaction Design also maintains an on-line user group and frequently asked questions (FAQ) forum. Professional support addresses a wide range of problems, ranging from installation issues to problem-specific applications. In addition, frequent training classes and web-based seminars are offered.

History of CHEMKIN

In the early 1980s, Sandia National Laboratories developed Chemkin and Chemkin II. Sandia maintained, all copyright and ownership of the Chemkin programs and the Chemkin name, although it distributed this code widely to collaborators around the world. Until 1997, the only organizations authorized to distribute versions of Chemkin were Sandia and the Department of Energy Office of Scientific and Technical Information (OSTI). In 1995, Sandia initiated a fee-based license program for the then current version of Chemkin II and the initial version of Chemkin III.

In February 1997, Sandia contracted with Reaction Design to become the exclusive worldwide developer and distributor of Chemkin. Reaction Design is the sole legal distributor of CHEMKIN software, although parties that originally obtained their Chemkin II license directly from Sandia National Laboratories maintain the ability and rights to run and modify their original Chemkin codes.

Since 1997, Reaction Design has made available seven major release versions of CHEMKIN.

References

Appel, J., H. Bockhorn, et al. (2001). "A Detailed Numerical Study of the Evolution of Soot Particle Size Distributions in Laminar Premixed Flames." Chemosphere **42**: 635-645.

Kee, R. J., F. M. Rupley, et al. (1989). Chemkin-II: A FORTRAN chemical Kinetics Package for the Analysis of Gas-Phase Chemical Kinetics, SAND89-8009, Sandia National Labs.