

# CHEMKIN™ Distribution and Use Guidelines

Dated October 24, 2001

In recent years there has been some confusion over the intellectual property status of CHEMKIN with regard to early versions that Sandia National Laboratories delivered to collaborators in the 1980s and early 1990s. This statement clarifies the intellectual property position and provides guidance to parties utilizing the CHEMKIN capabilities within the IP framework that currently exists.

## **Background**

In the early 1980s, Sandia National Laboratories developed CHEMKIN and CHEMKIN II. Sandia distributed this code widely to collaborators around the world. Sandia has always maintained copyright and ownership of the CHEMKIN programs and the CHEMKIN name. Sandia never placed CHEMKIN in the public domain and has never authorized recipients to re-distribute CHEMKIN either as a software product or as modified and incorporated into subsequently developed software. Until 1997, the only organizations authorized to distribute versions of CHEMKIN were Sandia and Department of Energy Office of Scientific and Technical Information (OSTI).

In 1995, Sandia initiated a fee-based license program for the 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 CHEMKIN distributor. Under this license agreement, Sandia and Reaction Design cooperate on the continuing development of the CHEMKIN software.

## **Redistribution and Use of CHEMKIN software and Use of the CHEMKIN Name**

Parties who received versions of CHEMKIN directly from Sandia in the 1980s and early 1990s or purchased it from OSTI have a right to continue to use and modify that software, and to publish the results. Sandia and OSTI did not grant permission to distribute these early versions of CHEMKIN either in part or in its entirety, or as modified or embedded in third party software.

For parties who may have received CHEMKIN through unauthorized distribution and are currently using CHEMKIN, we request you contact Reaction Design at [chemkin@reactiondesign.com](mailto:chemkin@reactiondesign.com) to obtain the latest information about current CHEMKIN products and extensive CHEMKIN support services.

The CHEMKIN name is a trademark owned by Sandia National Laboratories and needs to be expressed as CHEMKIN™. The trademark name may be used in scientific papers or as a literature citation. All other use of the trademark name "CHEMKIN" requires permission from either Sandia or its exclusive CHEMKIN licensee, Reaction Design.

## **Addressing the Needs of the Scientific Community**

Sandia and Reaction Design encourage and support the widespread use of CHEMKIN in the scientific community. Included in the license agreement with Reaction Design are measures to support this research community, including:

- The right for Sandia to designate active collaborators who are eligible to receive current CHEMKIN versions at no charge.
- Substantially discounted license fees from commercial rates for academic users.
- Establishing a CHEMKIN users' public website to facilitate the free exchange of information and problem solving experience among users.
- Making source code available as needed to researchers who wish to modify the current commercial code and are willing to have their improvements incorporated into future CHEMKIN releases.
- Holding biennial workshops to encourage feedback from users on the future direction of CHEMKIN in conjunction with International Combustion Institute meetings.

## Availability of CHEMKIN Software

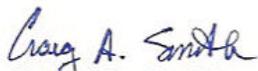
There has been no further development of CHEMKIN II since 1995. Since that date there has been substantial modification and enhancement of the successor version, CHEMKIN III. The current CHEMKIN version, 3.6.1, is the fourth release of CHEMKIN by Reaction Design and provides a number of enhancements that have expanded the scope of its capabilities to improve user productivity. These include:

- A windows interface that facilitates problem set up.
- The ability to utilize global reaction kinetics, derived from empirical methods or experiment.
- Improvements in the robustness, stability and reliability of the software through implementation of standard software configuration management methods.
- Identification and repair of many long-standing bugs and inconsistencies that existed in early versions of CHEMKIN.
- New pressure-dependence formulations.
- Faster computational speed and convergence for many of the applications.
- Ability to model transient chemical processes such as catalyst light-off.
- Integral graphical post-processing capability.
- Direct coupling to several widely used commercial CFD codes.
- Support for versions of CHEMKIN that run on PC, Windows, NT and Linux as well as on Sun, SGI, HP, IBM and Alpha Unix platforms.

Parties still using CHEMKIN II will discover considerable benefit by upgrading to this more advanced version. Those whose special applications require capabilities not yet incorporated in the current version are encouraged to request source code directly from Reaction Design to facilitate such modification under the Reaction Design Collaborative Development agreement.

For more information on these guidelines, the capabilities of CHEMKIN 3.6.1, the comprehensive support for CHEMKIN products and the Reaction Design Collaborative Development Agreement please visit Reaction Design's website at <http://www.reactiondesign.com> or email Reaction Design at [chemkin@reactiondesign.com](mailto:chemkin@reactiondesign.com)

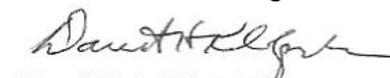
For Sandia,

  
Craig A. Smith

Technology Licensing Manager



For Reaction Design,

  
David H. Klipstein  
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