GET-035-1
CHEMKIN Collection Release 3.5
July 1999

GETTING STARTED

CHEMKIN RELEASE 3.5

Reaction Design

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Literature Citation for the CHEMKIN Collection:

The *CHEMKIN Collection Release 3.5* should be cited as:

R. J. Kee, F. M. Rupley, J. A. Miller, M. E. Coltrin, J. F. Grcar, E. Meeks, H. K. Moffat, A. E. Lutz, G. Dixon-Lewis, M. D. Smooke, J. Warnatz, G. H. Evans, R. S. Larson, R. E. Mitchell, L. R. Petzold, W. C. Reynolds, M. Caracotsios, W. E. Stewart, and P. Glarborg, *CHEMKIN Collection*, Release 3.5, Reaction Design, Inc., San Diego, CA (1999).

Reaction Design cautions that some of the material in this manual may be out of date. Updates will be available periodically on Reaction Design's web site. In addition, on-line help is available on the program CD. Sample problem files can also be found on the CD and on our web site at www.ReactionDesign.com.

GET-035-1

Overview of Manual

This manual has been designed to get you up and running as quickly as possible with CHEMKIN Release 3.5. The organization of the manual is:

	Chapter	Description
1.	What's New in Release 3.5	A description of the new features in CHEMKIN Release 3.5.
2.	System Requirements	Operating system and computer hardware requirements for installing and running CHEMKIN Release 3.5.
3.	**Installation and Quick Start**	Installation instructions for Windows and UNIX computers. Quick-start instructions for users already familiar with CHEMKIN.
4.	Introduction to the CHEMKIN Collection	A brief overview of the CHEMKIN Collection Utilities and the Applications, as well as background information on Reaction Design.
5.	Problem Solving with the CHEMKIN Collection	Basic strategy for problem formulation and solution using the CHEMKIN Collection. Guidelines for running programs and interpreting results.
6.	The CHEMKIN Application User Interface	An introduction to the *CHEMKIN Application User Interface.*
7.	The CHEMKIN Graphical Post-Processor	An introduction to the *CHEMKIN Graphical Post Processor*.
8.	Using CHEMKIN from the Command Line	Instructions for using CHEMKIN from the command line in an MS-DOS prompt or UNIX shell.
9.	Getting Help and Support	Where to go for more information.

CONTENTS

LIST OF FIGURES

LIST OF TABLES

1. What's New in CHEMKIN Release 3.5

The CHEMKIN Collection is a powerful system for solving complex chemical modeling problems. CHEMKIN is composed of standalone Applications, as well as subroutine libraries and utilities that can be used to create new problem solving environments. CHEMKIN facilitates the formulation, solution, and interpretation of problems involving gas-phase and heterogeneous (gas-surface) chemical kinetics. A wide range of chemical process modeling problems can be addressed including: combustion, catalysis, corrosion, plasma etching and chemical vapor deposition.

Many new features and enhancements have been incorporated by Reaction Design into Release 3.5, including:

- A *CHEMKIN Application User Interface*, which guides users through the set-up and solution of problems using CHEMKIN Applications.
- An integrated *CHEMKIN Graphical Post Processor,* which allows users to display their results and to export their solutions to other applications including spreadsheet programs.
- Dynamic memory allocation, which eliminates the need to recompile the Application and Utility programs for different problem sizes.
- A full suite of sample FORTRAN post-processor routines, which read and process the binary solution files. These routines, distributed as source-code, allow users to tailor post-solution analyses to their own specific needs.
- A planar stagnation-flow option for OPPDIF.
- A new adiabatic boundary-condition option for CRESLAF.
- New flexibility in describing flow conditions in AURORA, using a variable volume.

Getting started with CHEMKIN is easy, the installation takes just a few minutes. This manual guides you through the installation process and helps you navigate through the new graphical user interfaces. Additional details about the CHEMKIN Applications and utilities are provided in a complete set of user manuals. The distribution CD for the CHEMKIN Collection contains all of the program documentation, as well as a set of sample problems for each of the Applications.

2. System Requirements

Before you start, take a minute to verify that you have what you need to install and run CHEMKIN:

1. A suitable computer and operating system. CHEMKIN Release 3.5 will run on the following platforms:

Manufacturer	**Operating System**
Compaq (Digital)	Tru64 (Alpha) UNIX 4.0
Hewlett Packard	HP-UX 10.x
Silicon Graphics	SGI IRIX 6.x
Sun Microsystems	Sun Solaris 2.x
PC-compatible	Win32: Windows NT 4.0 (i386 with Service Pack 3) Windows 95 Windows 98

2. 40 Megabytes of hard disk space.

3. 32 MB of RAM (64 MB recommended). **Note**: You may need more memory if you plan to run very large problems (e.g. problems that involve more than 100 species).

4. A valid License file for the CHEMKIN software

5. Access to the documentation for the applications that you intend to run.

To use CHEMKIN, you should be familiar with the basics of the operating system on your computer. You should know how to use the mouse, how to use menus, manage files and how to enter text. If you are unsure about any of these techniques, consult the documentation that came with your computer.

3. Installation and Quick Start

3.1 Overview of the Installation Process

Installation of CHEMKIN involves three basic steps

1. Install the software from the CD-ROM.
2. Obtain and install a CHEMKIN license file from Reaction design.
3. Run one or more of the samples problems to make sure that the software is installed correctly.

Each of these steps are described in more detail in the following sections. The instructions are divided according to platform. Section 3.2 describes installation procedures for all Windows-based PCs, while Section 3.3 describes installation procedures for all UNIX platforms.

3.2 PC Installation

3.2.1 Running the Setup Program

To install CHEMKIN on your Windows NT, Windows 98, or Windows 95 computer, perform the following steps:

1. Insert the CHEMKIN distribution CD-ROM into your CD-ROM drive. After a short delay, the autoplay program starts. **Note:** If the autoplay program does not start automatically on your computer, double click on your "My Computer" icon and browse to your CD-ROM. Inside the subfolder **`install`**, locate the **`chemkin35_pc_setup.exe`** file and double-click on this.
2. The program will first prompt you to extract the needed files. Click "Setup" to continue.
3. The Welcome dialog introduces you to the Setup program and informs you of several restrictions and cautions. Click "Next" to continue.
4. The next dialog contains some more information about the Release. Click "Next" to continue with the installation.

5. Choose the Destination Location. This is the location on your hard-disk where you would like to install CHEMKIN. The default is "`c:\chemkin`", but you may select any drive or folder name. To choose a different location from the default, click "Browse" and select a location from the Choose Directory dialog. Once you have made your choice (or if you decide to keep the default), click "Next" to continue the installation. Click "Cancel" to leave the installation program and return to Windows.

6. Choose the Setup Type. This allows you to customize what parts of CHEMKIN get installed. We recommend choosing "Typical". If you choose "Compact" you will not install most of the online documentation. Once you have made your selection, click "Next" to continue.

7. Choose the short-cut labels for your Start->Program menu. You modify the settings here to change the way the short-cuts are organized in your Program menu. Click "Next" to continue. At this point the Setup program will begin installing files on your computer's hard disk.

8. After the files have been installed successfully, you will get a Setup Complete dialog. Click "Finish" and you are finished!

3.2.2 Modifying your "Path"

We recommend that you modify your "path" variable to include the "`c:\chemkin\bin`" directory, particularly if you plan to run from the command line, rather than using the new user interface. The following steps will add "`c:\chemkin\bin`" to your path. Note that the instructions are different for Windows NT than for Windows 95 and 98 operating systems.

Windows NT:

1. Right-click on your computer icon on your desktop and choose "Properties" from the system menu.

2. Select the "Environment" tab.

3. Select the "path" variable from the user environment settings.

4. In the "Value" field, scroll to the end of the text box and add a semicolon ";" followed by the full path (e.g., `c:\chemkin\bin`) to your CHEMKIN "`bin`" directory.

Windows 95 and Windows 98:

1. Open your `autoexec.bat` file located in the root of your "C" disk in your favorite text editor (e.g. Notepad).

2. Add the following line at the bottom of the file (substituting the correct path to your CHEMKIN "`bin`" directory if you have not installed in the default location):

   ```
   set PATH=%PATH%;c:\chemkin\bin
   ```

3. Save the file and exit the editor

4. Restart your computer for the change to take effect.

3.2.3 Uninstalling CHEMKIN

After you have installed CHEMKIN with the above steps, you can remove it from your system if you need to. Open the "Add/Remove Programs" folder in the Control Panel (under "Settings" from the "Start" menu). Select "CHEMKIN 3.5" from the "Install/Uninstall" tab and click "Add/Remove". **Note:** If you have added files to or modified files in the CHEMKIN installation, the Uninstall process will not automatically remove these files.

3.3 UNIX INSTALLATION

This section provides detailed instructions for installing CHEMKIN on any one of our supported UNIX platforms.

3.3.1 Mounting the CHEMKIN Distribution CD-ROM

Insert the CHEMKIN distribution CD-ROM into a mounted CD-ROM drive. You must then mount the disk as a file system on your computer. **Note:** on most systems you must be **`root`** to mount a CD-ROM. Specific instructions for mounting the CD on supported platforms are as follows:

Compaq Digital UNIX (Alpha):

Mount the CD using Rock Ridge format by entering:

```
/usr/sbin/mount –t cdfs –r –o rrip <CD-ROM-device> /cdrom
```

replacing *<CD-ROM-device>* with the actual name of the CD-ROM drive on your system. A typical name is `/dev/rz4c`

Hewlett-Packard HP-UX:

Mount the CD by entering:

```
mount –r <CD-ROM-device> /cdrom
```

replacing *<CD-ROM-device>* with the actual name of the CD-ROM drive on your system. A typical name is `/dev/dsk/c1t2d0`

SGI IRIX:

IRIX automatically mounts the CD when you insert it into the CD-ROM drive. It is mounted as:

```
/CDROM
```

Notes: the installation instructions below assume that the CD-ROM is mounted at `/cdrom`. You will therefore need to replace this with the actual path above (all upper case) as you follow the instructions below.

SUN Solaris 2.6:

Solaris includes a "Volume Manager" that automatically mounts the CD when you insert it into the CD-ROM drive. The CD will be mounted as:

```
/cdrom/Chemkin35
```

Notes: the installation instructions below assume that the CD-ROM is mounted at `/cdrom`. You will therefore need to replace this with the actual path above as you follow the instructions below.

3.3.2 Executing the Installation Script

If you are installing CHEMKIN into a public directory, make sure that you have **root** or similar privileges before running the installation script. Once you have the correct permissions, open a UNIX shell and execute the installation script with the following commands (**Note:** for SGI and SUN users, you must substitute the appropriate mount point for `/cdrom` below, as described in Section 3.3.1):

```
cd /cdrom/install
/bin/sh /cdrom/install/chemkin35_unix_setup.sh
```

The installation script will echo information and prompt you for input as it proceeds through the following steps:

1. Verify the current directory and the username. Check that the directory printed is the `install` directory at the CD-ROM mount point. Check that the user login has the correct privileges for installing to your desired destination. If this information is correct, type "y" and <RETURN>.

2. Choose the Destination Location. This is the location on your hard-disk where you would like to install CHEMKIN and is the location where the install script will create a "`chemkin`" subdirectory. The default is the directory identified by the environment variable, `$HOME`, or, if `$HOME` is not set on your computer, the default is `/usr/local`. The prompt asks if you want to change the default. To accept the default, type "n" and <RETURN>. To change the Destination Location, type "y" and <RETURN>, then type in the **full** path of your preferred destination and hit <RETURN> again.

3. Create any needed directories. If the directory you selected for the Destination Location does not already exist, you will be prompted to allow the install script to create the new directory. Type "y" and <RETURN> to continue with the install.

4. Verify the platform for the installation. The install script will determine which platform you are currently running on and will ask you whether this is the correct platform information. If the information is correct, type "y" and <RETURN> to continue. If you want to install onto a different platform than the one specified, type "n" and <RETURN>. You will then be asked to choose from the list of available platforms and enter a corresponding number (e.g. "1" for Compaq (Alpha)). Type the number and <RETURN>.

5. Verify all the information entered thus far before installing the CHEMKIN software. If the information is correct, type "y" and <RETURN>.

6. Install the files. The script will copy compressed tar files from the CD-ROM to your hard disk, uncompress and untar them into the Destination Location, and then delete the tar files. When the installation is complete, information on setting environment variables needed to run CHEMKIN are displayed on your screen, using the UNIX `more` utility. These instructions are also given below and in Section 3.4.

3.3.3 Setting the CHEMKIN_DIR Environment Variable

The UNIX version of the CHEMKIN software requires you to set an environment variable that points to the top-level directory where CHEMKIN was installed. Although you could set the environment variables locally in a UNIX shell every time you run CHEMKIN, we recommend that you instead include the environment settings in your `.cshrc` (for C-shell users) or your `.profile` (for K-shell users) file, which

will result in the variables being set automatically every time you open a new shell. This section gives you detailed instructions for modifying these start-up files.

The following instructions assume that you have installed CHEMKIN in the directory `/usr/local`, such that the top-level CHEMKIN directory is `/usr/local/chemkin`. If you have installed into a different location, you will need to replace "`/usr/local`" in the following instructions with the actual (absolute) path.

1. Modify your .cshrc file (for C-shell users) or your .profile file (for K-shell users) to include the environment variable `CHEMKIN_DIR`. The command(s) that need to be added are shown below for the two shell environments:

   C-shell: `setenv CHEMKIN_DIR /usr/local/chemkin`

   K-shell: `CHEMKIN_DIR=/usr/local/chemkin`

   `export CHEMKIN_DIR`

2. To verify that the CHEMKIN_DIR is set correctly, open a new shell and type:

   `echo $CHEMKIN_DIR`

   This should result in an echo of the directory path to the top-level `chemkin` directory. If not, verify that you have performed step 1 correctly; you may need to log-out and log back in to your computer for the changes to take effect.

3.3.4 Modifying your "Path"

We recommend modifying your "path" variable to include the `/usr/local/chemkin/bin` directory (or the equivalent, if you installed elsewhere from `/usr/local`). This will simplify the commands that you need to type to start the CHEMKIN Application User Interface, the CHEMKIN Graphical Post-processor, or to run programs from the command line. The path variable can be modified in your `.login` or `.cshrc` files for C-shell users, or in your `.profile` for Bourne or Korn shell users with the following added line(s):

C-shell: `set path=( $path /usr/local/chemkin/bin )`

K-shell: `PATH=$PATH:/usr/local/chemkin/bin:`

`export PATH`

Note: if you installed CHEMKIN in a different directory than `/usr/local`, you will need to replace the actual (full) path in the above commands.

3.4 LICENSING

3.4.1 Obtaining a License File

You must obtain and install a set of license keys in order to run the CHEMKIN software. Without the license, you can review the documentation and look at the source code for the sample applications, drivers, and post-processors, but you will not be able to run the software. For purchasing information, contact by email: CHEMKIN@ReactionDesign.com.

Once you have purchased a license, you will be asked to provide the "HOSTID" for the machine on which CHEMKIN will be installed, so that we can generate the needed license file. If you have already installed CHEMKIN, you can get this information by changing directories to the `licenses` subdirectory of the CHEMKIN installation and running the command (at a DOS prompt or in a UNIX window):

```
lmutil lmhostid
```

This returns a unique identifier or HOSTID for your machine. Once you have obtained this identifier, you can send the following information to Reaction Design (email to CHEMKIN@ReactionDesign.com) to receive your license file:

1. The result of the HOSTID command.
2. Your CHEMKIN License Number (located on your "License Specifications Form").
3. The Licensee Contact for your organization (located on your "License Specifications Form").

You should then receive by email a specific license to run CHEMKIN on your system. The file may have either UNIX or PC line-endings, depending on where and how you receive your email; if you need to transfer the license file from one machine to another, be sure to use ftp in *ascii* mode to guarantee the line endings get converted correctly. Save the emailed license keys to a file named `chemkin.lic`.

Once you have installed the CHEMKIN software on your machine and obtained a valid license file from Reaction Design, you will need to activate the license file. This means

1. Copying the license file, `chemkin.lic`, to a known location (for example, in the `licenses` subdirectory of the CHEMKIN install location)
2. Setting the environment variable `LM_LICENSE_FILE` to point to the absolute path of the license file.

Specific instructions for setting the environment variable on UNIX and PC platforms are provided below.

3.4.2 Licensing Instructions for a PC

The following instructions assume that you have installed CHEMKIN in the directory `c:\chemkin`. If you have installed in a different location, you will need to replace "`c:\chemkin`" in the following instructions with the actual (absolute) path.

1. Copy the file `chemkin.lic` to the directory `c:\chemkin\licenses`.
2. In **Windows 95** and **Windows 98**, modify the system `autoexec.bat` file and add the line:

   ```
   set LM_LICENSE_FILE=c:\chemkin\licenses\chemkin.lic
   ```

   You will need to restart before this change takes effect. Not all Windows 95/98 environments have enough environment space to add this variable, so check after the reboot to make sure it is there:

   a. Open a MS-DOS prompt.

   b. Type `set` and press `<RETURN>`

   In the resulting list, make sure that you see the line

   ```
   LM_LICENSE_FILE=c:\chemkin\licenses\chemkin.lic
   ```

   if you do not, you need to expand your environment space. If required, please refer to instructions for your operating system for information concerning increasing the size of your environment space. Also we include detailed instructions in the Frequently Asked Questions section under Customer Support on our website: www.ReactionDesign.com.

3. In **Windows NT** there is no need to modify `autoexec.bat` or to worry about environment space. Simply add the environment variable on the "Environment" tab of the "System Properties" dialog of your computer.

4. To verify that the `LM_LICENSE_FILE` is set correctly, open a new MS-DOS prompt and type `set` and press `<RETURN>`. In the resulting list, make sure that you see the line

   ```
   LM_LICENSE_FILE=c:\chemkin\licenses\chemkin.lic
   ```

   If not, verify that you have performed steps 1 and 2 correctly; you may need to restart your computer for the changes to take effect.

Note for Licensees with Simultaneous Active User Licenses: If you have a network or floating Simultaneous Active User license (rather than a Node-Locked License) you will need to take additional steps to set up your license manager daemon. If you have purchased a Simultaneous Active User License, please have your systems administrator contact Reaction Design Technical Support (email to: Support@ReactionDesign.com) for further assistance.

3.4.3 Licensing Instructions for UNIX

The following instructions assume that you have installed CHEMKIN in the directory `/usr/local`, such that the top-level CHEMKIN directory is `/usr/local/chemkin`. If you have installed in a different location, you will need to replace "`/usr/local`" in the following instructions with the actual (absolute) path.

1. Copy the `chemkin.lic` file to the `licenses` sub-directory in the CHEMKIN installation, `/usr/local/licenses.`
2. Modify your .cshrc file (for C-shell users) or your .profile file (for K-shell users) to include the environment variable `LM_LICENSE_FILE`. The command(s) that need to be added are shown below for the two shell environments:

   C-shell:
   ```
   setenv LM_LICENSE_FILE  /usr/local/chemkin/licenses/chemkin.lic
   ```

   K-shell:
   ```
   LM_LICENSE_FILE=/usr/local/chemkin/licenses/chemkin.lic
   export LM_LICENSE_FILE
   ```

3. To verify that the `LM_LICENSE_FILE` is set correctly, open a new shell and type:

   ```
   cat $LM_LICENSE_FILE
   ```

   This should result in the contents of your license file being echoed to your screen. If not, verify that you have performed steps 1 and 2 correctly; you may need to log-out and log back in to your computer for the changes to take effect.

Note for Licensees with Simultaneous Active User Licenses: If you have a network or floating Simultaneous Active User license (rather than a Node-Locked License) you will need to take additional steps to set up your license manager daemon. If you have purchased a Simultaneous Active User License, please have your systems administrator contact Reaction Design Technical Support (email to: Support@ReactionDesign.com) for further assistance.

3.5 Running the Sample Problems

Once CHEMKIN 3.5 has been installed, you can launch the *CHEMKIN Application User Interface* and run any of the sample problems with just a few mouse clicks.

3.5.1 Launching the CHEMKIN Application User Interface

The way to start the Application User Interface, depends on your platform:

Windows/PC:

In this case, the install program will have placed two icons labeled "`Chemkin`" and "`Chemkin_Post`" on your desktop. Just double-click the "`Chemkin`" icon to launch the Application User Interface.

UNIX:

If you set your "path" variable as instructed in Section 3.3.4 above, then you can open a UNIX shell and simply type:

```
chemkin <RETURN>
```

to launch the Application User Interface. If you did not set the path, you will have to include the full path to the CHEMKIN "`bin`" directory in the above command.

An interface as shown in Figure 1 should appear on your screen. **Note:** this manual includes illustrations from the PC version only; the interface will look slightly different on other platforms. However, the functionality is the same and the instructions provided here are the same for all computer systems.

Figure 1 Startup window for the CHEMKIN Application User Interface.

From here you can choose an Application, as shown in Figure 2.

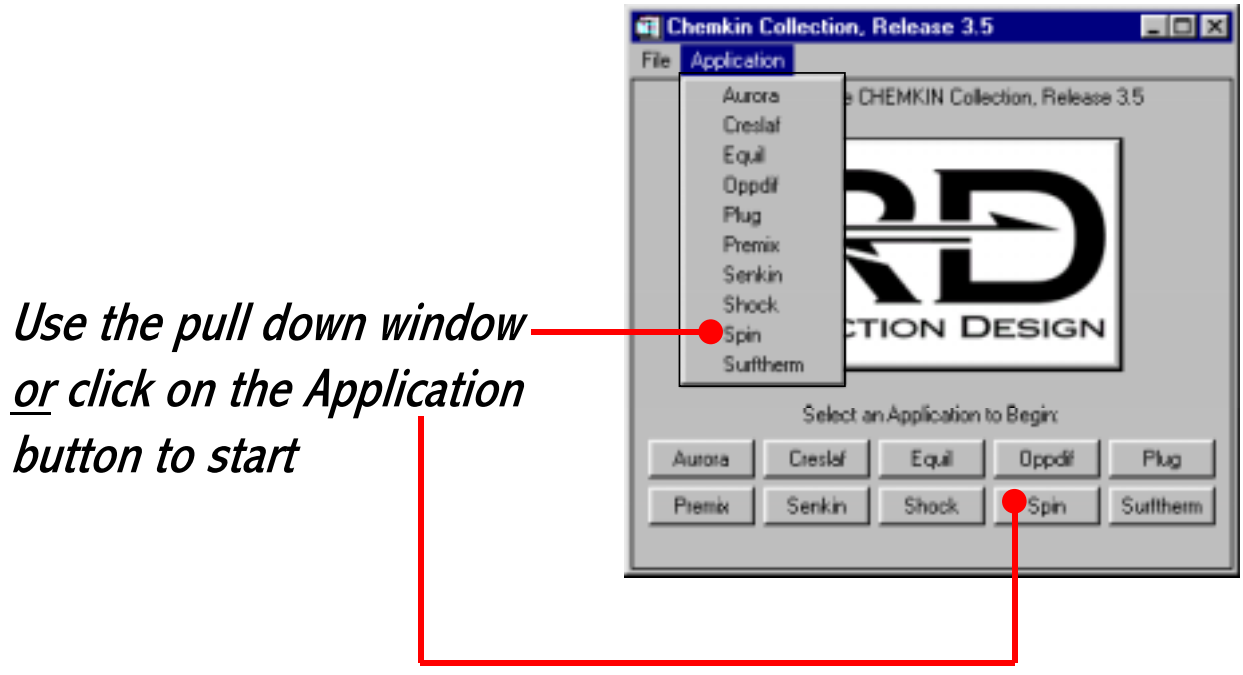

Figure 2 Selecting an Application to run in the Application User Interface.

3.5.2 Running a Sample Problem

For demonstration purposes, select the SPIN Application. The SPIN Application Interface, shown in Figure 3, should appear on your screen.

When CHEMKIN is first installed, the software is pre-set to start the user in a directory containing one of the sample problems for the chosen Application. For SPIN, the "Input" and "Output" directory text boxes should be set to the location of the CHEMKIN sample called "rotating_disk_cvd". The names of the input and output files are also pre-set to the correct files in this sample directory. You can "**Edit**" any of the input files to see their contents. The pre-processors can be run separately by clicking on the individual "**Chem**", "**Surf**" or "**Tran**" buttons, or you can run all of the needed preprocessors and the Application sequentially by clicking on the run "**All**" button.

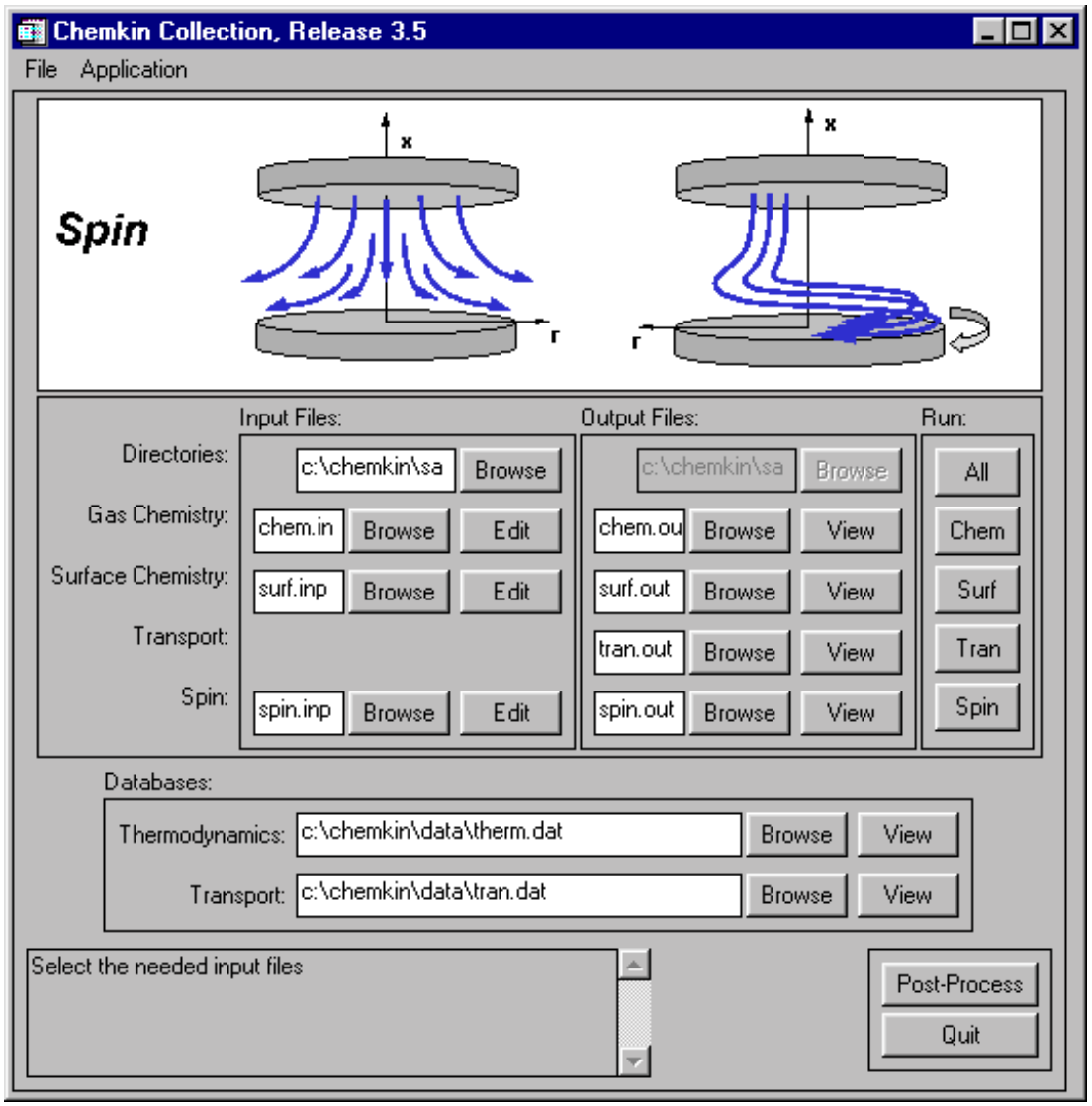

Figure 3 The SPIN Application User Interface

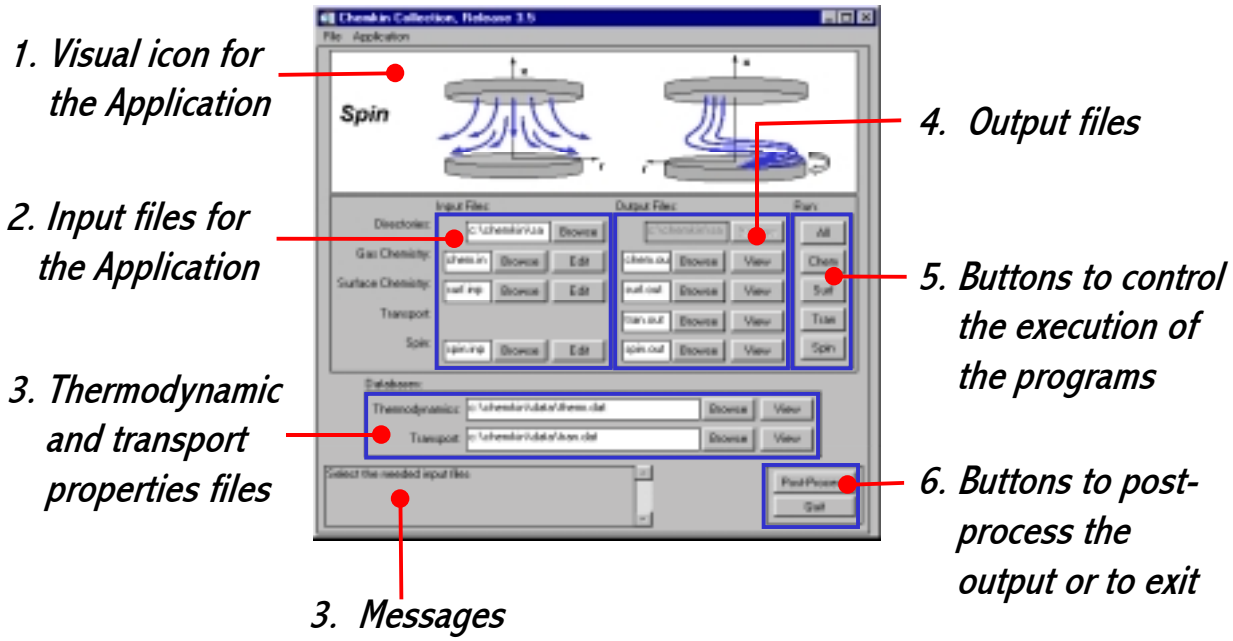

Figure 4 The SPIN Application User Interface with annotations

Click the run "**All**" button now. Messages that describe the progress of the executing programs should appear in the **Message Box** (See No. **3** in Figure 4). If the CHEMKIN installation was successful and the License File has been installed correctly, the messages should report successful completion for the three pre-processors and the SPIN Application.

> **Note for Windows**: On PCs, CHEMKIN 3.5 first creates MS-DOS prompt windows to run each of the CHEMKIN programs. You will see this sequence of windows flash on the screen as programs execute. These events are normal.

To view the results of the SPIN run, you may look at the output files using the "**View**" buttons (See No. **4** in Figure 4). You may also wish to view the results *graphically*. The next section describes the use of the new *CHEMKIN Graphical Post-Processor*.

3.5.3 Launching the CHEMKIN Graphical Post-Processor

From the Application User Interface, you can start the *CHEMKIN Graphical Post-Processor* by simply clicking on the "**Post-Process**" button (See No. **6** in Figure 4). You can also launch the Graphical Post-Processor independently of the Application User Interface, as follows:

Windows/PC:

Just double-click the "`Chemkin_Post`" icon on your desktop to launch the Graphical Post-Processor.

UNIX:

If you set your "path" variable as instructed in Section 3.3.4, then you can open a UNIX shell and simply type:

```
chemkin_post <RETURN>
```

to launch the Graphical Post-Processor. If you did not add the CHEMKIN "`bin`" directory to your path, you will have to include the full path to that directory before "`chemkin_post`" in the above command.

From the Application User Interface, **click "Post-Process"** now. As the post-processor starts up, it will look for a solution file (`save.bin`) in the Output Directory indicated in the Application User Interface or in the user Preferences. (**Note:** If a valid `save.bin` file is not found, a sample plot (sine/cosine) will be displayed.) For the SPIN sample problem, the solution file includes both the solution data itself as well as sensitivity data for the gas-phase reactions, the surface reactions, and the heat-of-formation of species. The Data Selection window, shown in Figure 5 below, allows you to select which solution components will be imported for plotting purposes.

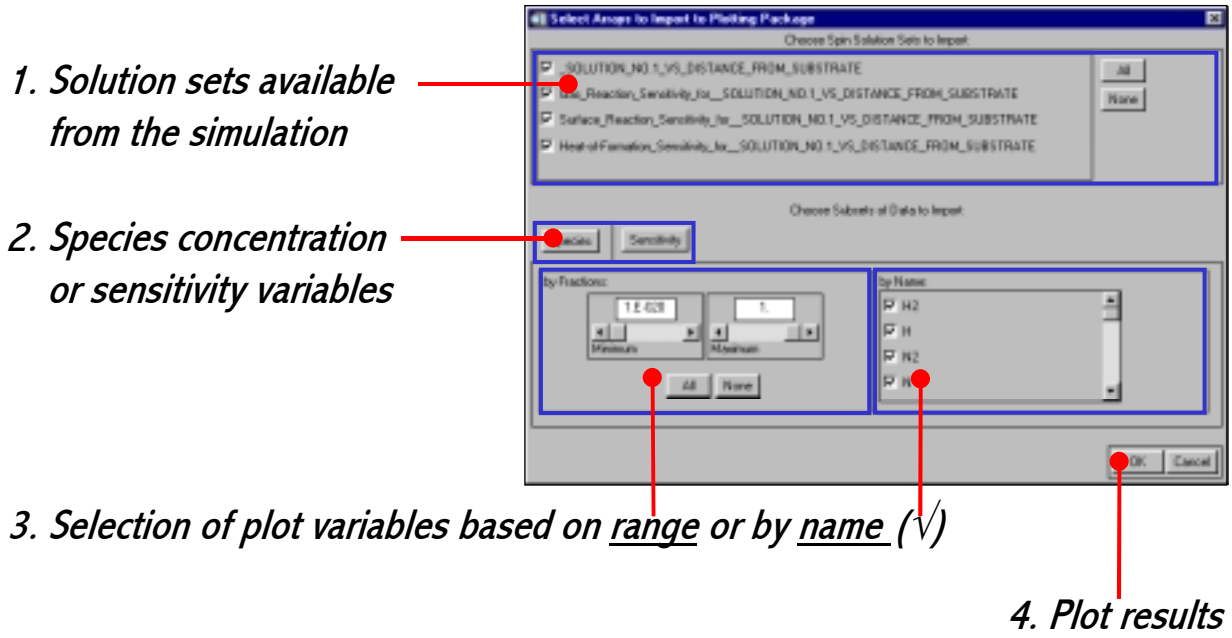

Figure 5 Data Selection window for importing data from the SPIN Sample into the Graphical Post-Processor.

General Note: Any time there is more than one solution "subset", such as sensitivity data or multiple solutions, or when the number of variables in the solution exceeds 20, the program first provides the user with an opportunity to down-select the number of arrays that will be imported into the Graphical Post Processor, with the Data Selection window.

By default, all of the species data for the SPIN solution will be read into the Graphical Post-Processor. **Click "OK"** to read the current selections into the post-processor. Figure 6 shows the default plot that you should now see on your screen.

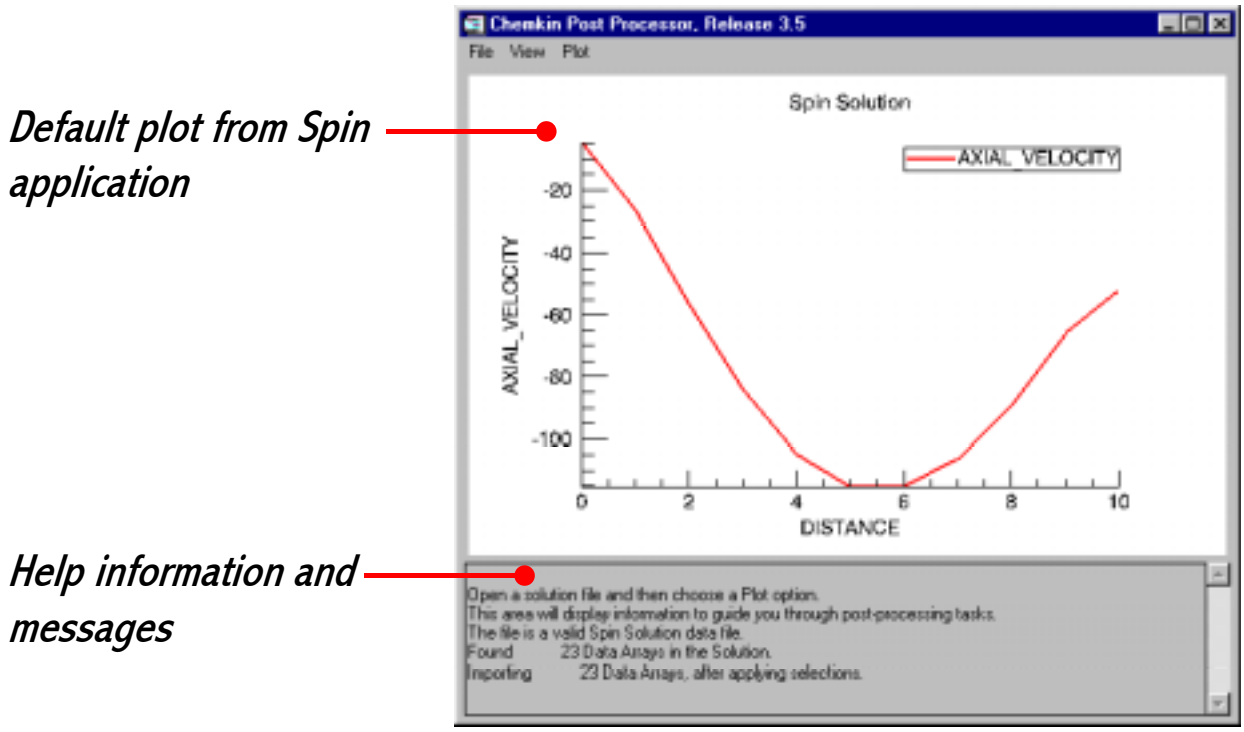

Figure 6 Default plot generated by the Graphical Post-Processor for the SPIN sample.

By default, the Graphical Post-Processor chooses the first two arrays to plot as "X" and "Y" in the initial plot. The dependent variable (in this case "Distance") is typically the first array. To plot a different set of variables, use the "**Plot**" pull-down menu and choose "**XY Plot**". This will give you a menu of the available arrays, as shown in Figure 7. To generate a new plot, leave the "X" variable the same, but select the other two velocity components from the list of available arrays, as shown in Figure 7.

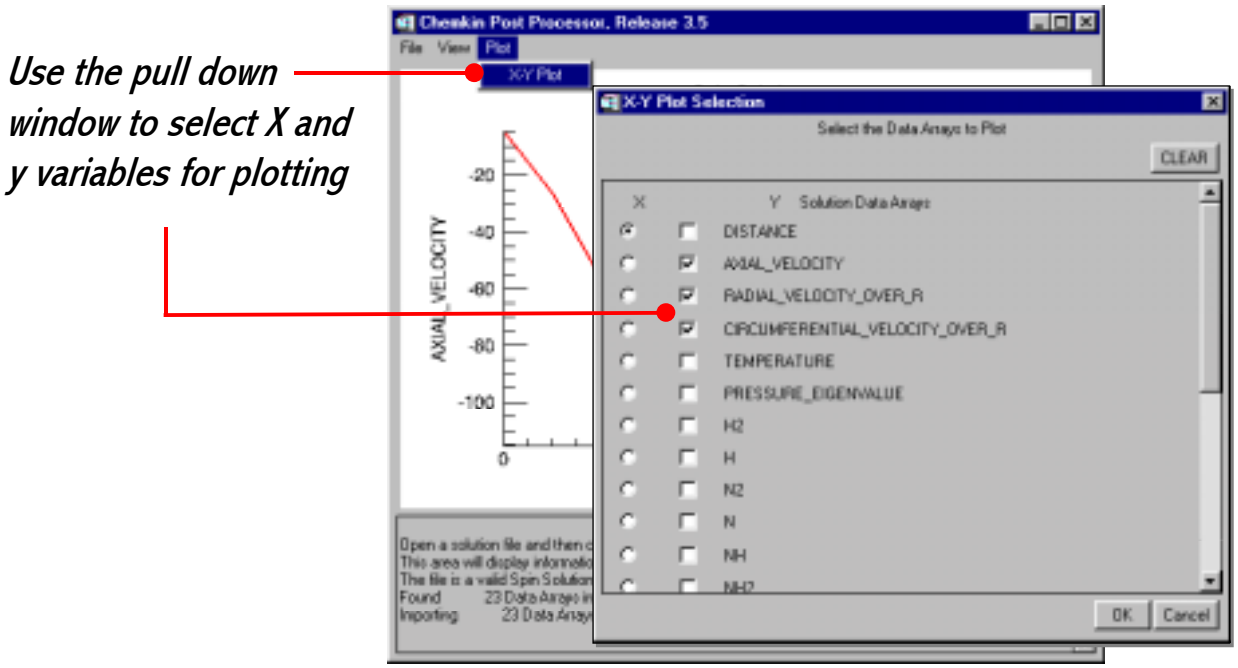

Figure 7 X-Y Plot Selection menu for the SPIN sample in the Graphical Post-Processor

You can now **change the look of the plot by double-clicking on the X-axis, the Y-axis, the Plot Title, or the Legend**, and adjusting the settings in the properties panels. You can also drag-and-drop the Plot Title or the Legend for more optimal placement. Figure 8 shows the results of changing some of the settings for the new velocity plot.

This concludes the "Quick Start" instructions. You can **exit the program by choosing "Quit" from the "File" pull-down menu** or by simply closing the window(s). For more information on the CHEMKIN Collection or about Reaction Design, please see Chapters 4 and 5. For more information on using the CHEMKIN Application User Interface or the CHEMKIN Graphical Post-Processor, see chapters 6 and 7, respectively. If you would like to run CHEMKIN from the command line, rather than through the Application User Interface, you should refer to Chapter 8. Chapter 9 provides information on how to get help if anything has gone wrong in your installation, or if you are having difficulty running any of the programs.

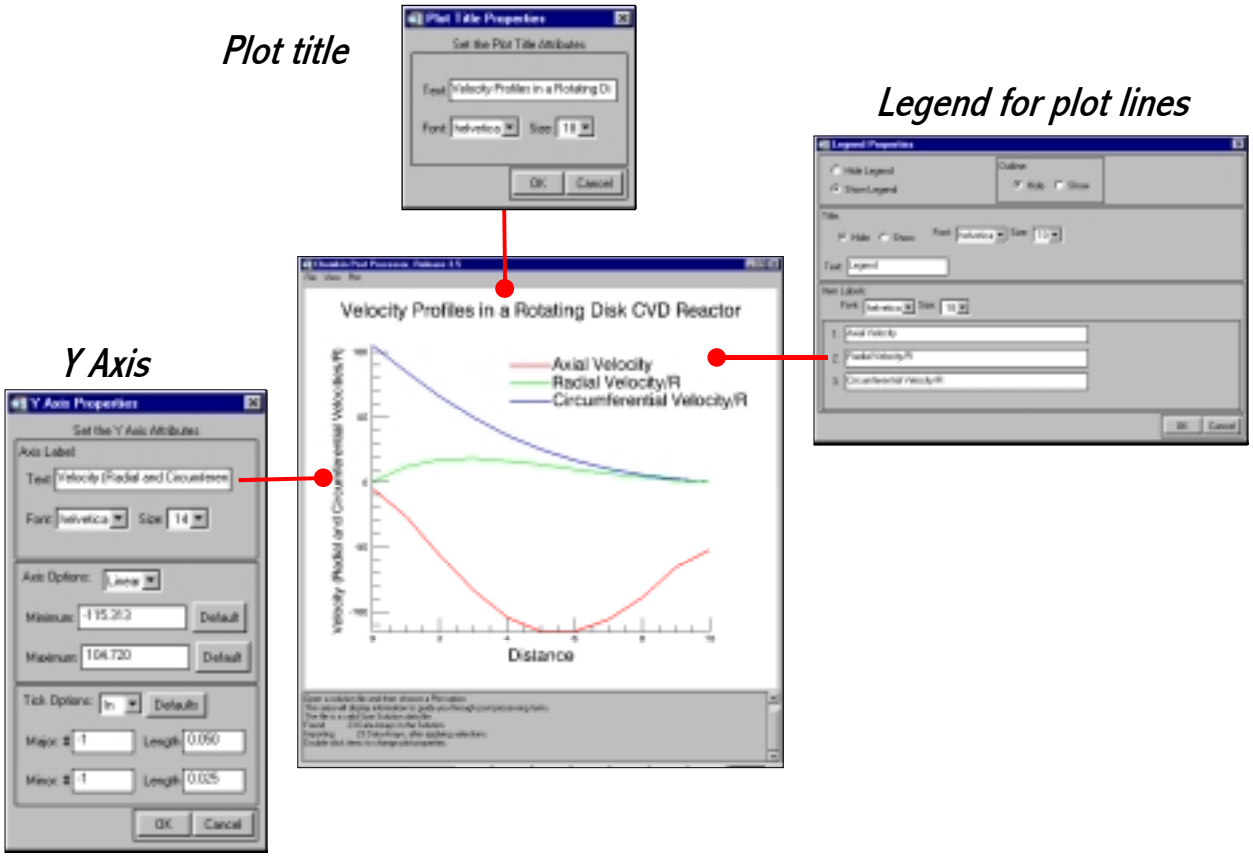

Figure 8 **Example plot generated in the Graphical Post-Processor, where the plot attributes have been modified from the default settings by double-clicking on the plot features (e.g. axis, legend, and title).**

4. Introduction to the CHEMKIN Collection

4.1 About Reaction Design

CHEMKIN Release 3.5 is part of Reaction Design's continuing commitment to expanding the capabilities of the original system developed at Sandia National Laboratories. In 1997, Sandia National Laboratories selected Reaction Design as the exclusive worldwide licensee for its CHEMKIN Collection. Today under this agreement, Reaction Design provides support and new developments for hundreds of industrial and academic users worldwide.

Reaction Design was founded in 1995 to provide software simulation and modeling tools to help process engineers create more efficient and environmentally friendly manufacturing processes. The company is committed to the ongoing development of a comprehensive and easy-to-use set of software simulation tools that incorporate both chemical reaction and transport models. Reaction Design engineers can also provide consulting services and software-based solutions to the customer's specific chemical process problems. These software products and consulting services help industrial customers develop better products faster, with greater yield, higher quality and at a lower cost, with minimized impact on the environment. Reaction Design is focusing its development, consulting and marketing efforts on four chemistry-intensive areas:

Microelectronics:	Integrated circuit manufacturing, semiconductor processing equipment and reactive precursors, protective and optical coatings.
Combustion:	Process heat and power generation, incinerators, jet and automotive engines, gas turbines and fuel design.
Chemical Processing:	Chemical and pharmaceutical, oil refining, paper, high performance materials, corrosion and lubrication, food flavors and fragrances.
Environment Protection:	Pollutant treatment and atmospheric chemistry.

More information about Reaction Design products and services is available through its web site at the address (www.ReactionDesign.com)

4.2 OVERVIEW OF CHEMKIN

The CHEMKIN software architecture represents a modular approach that separates *problem-specific* information from *problem-independent* software. For a reacting flow simulation, Figure 9 illustrates this approach. The Application represents the general model description, independent of what chemical species are included in a specific problem. The general model description typically includes conservation equations for mass, momentum, energy, and species. The upper ovals in Figure 9 contain the input data that make the problem specific, i.e. species identity, species properties, reaction paths, and reaction rates. The CHEMKIN software utilities provide the interface between this problem-specific information and the problem-independent Application. The Application may itself be broken down into modules that perform different functions, such as residual evaluation, matrix manipulation, solution printing, or post-processing. Additional problem-specific information that is non-chemical may also be input directly by the user, such as reactor pressure or inlet flow rate.

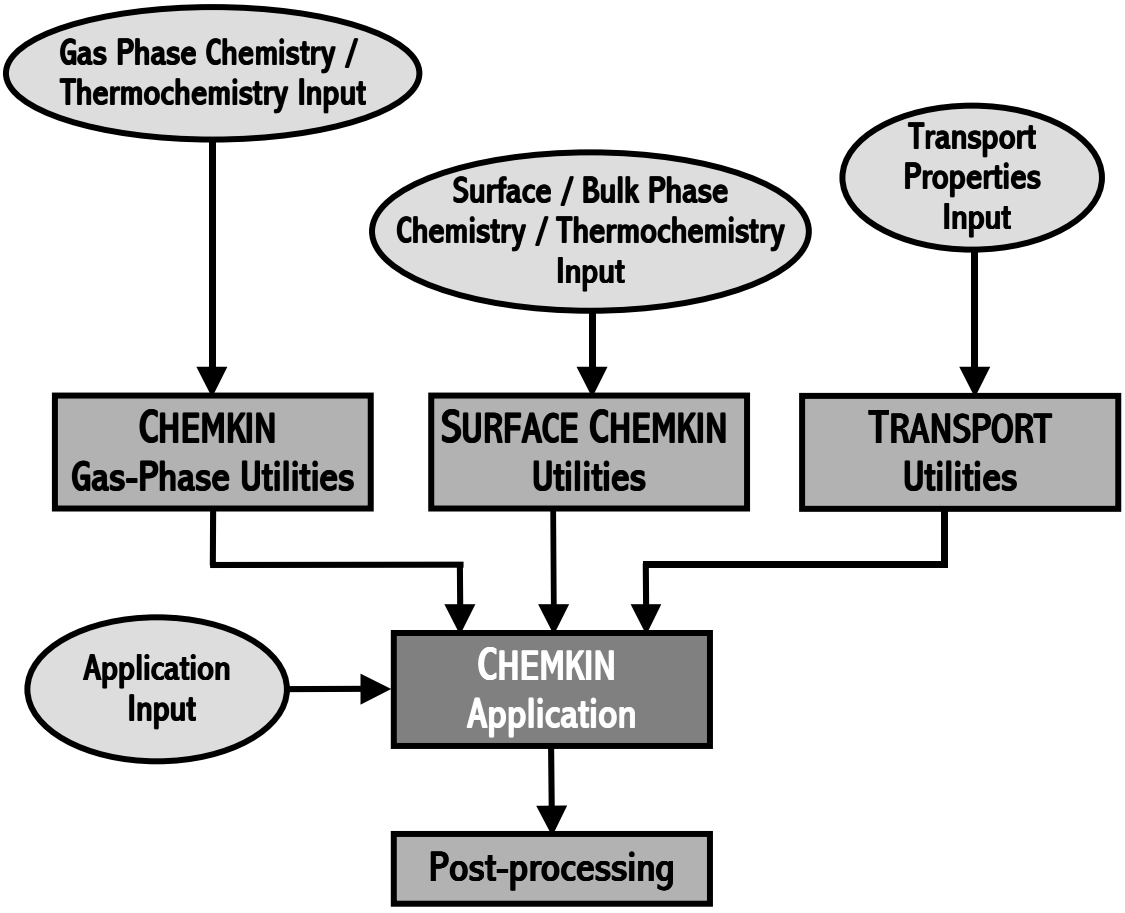

Figure 9 Illustration of the CHEMKIN modular approach to problem solving.

Included in the CHEMKIN distribution are sample problems for each Application, as well as detailed documentation describing each model. In addition to our own Applications and chemistry packages, the CHEMKIN software also includes many utilities that facilitate development of new modular application programs.

4.3 THE CORE UTILITIES OF THE CHEMKIN COLLECTION

The following are brief descriptions of the components of the Core Utilities included in the CHEMKIN Collection:

CHEMKIN III	Pre-Processor (Interpreter) and Subroutine Library for the analysis of gas-phase chemical and plasma kinetics.
SURFACE CHEMKIN III	Pre-Processor (Interpreter) and Subroutine Library for the analysis of heterogeneous chemical kinetics at gas-solid interfaces.
Thermodynamic Database	Compilation of polynomial fits to temperature for species enthalpy, specific heat, and entropy.
TRANSPORT	Pre-processor and Subroutine Library for the evaluation of gas-phase, multi-component transport properties including diffusion coefficients, viscosities, and thermal conductivities of species and their mixtures.
TRANSPORT Database	Compilation of molecular parameters used in the calculation of transport properties.
TWOPNT	A module for solving two-point boundary-value problems using a modified Newton iteration method.
EQUIL	A program for predicting the equilibrium state of systems containing ideal gas mixtures or ideal solutions of gases and liquids.

4.4 CHEMKIN APPLICATIONS

The following are brief descriptions of the Applications available in the CHEMKIN Collection:

AURORA	A program for predicting steady-state or time-averaged properties of a perfectly stirred reactor for plasma or thermal chemical systems. AURORA allows inclusion of surface chemistry on multiple materials in the reactor.
CRESLAF	A program for modeling laminar, chemically reacting, boundary-layer flow in cylindrical or planar channels. Surface chemistry on the inner walls of the channel may be included.
OPPDIF	A program for modeling opposed-flow diffusion flames.
PLUG	A program for the analysis of plug-flow reactors with gas-phase and surface chemistry.
PREMIX	A program for modeling steady, laminar, one-dimensional, pre-mixed flames. PREMIX includes homogenous, gas-phase kinetics with sensitivity analysis.
SENKIN	A program for predicting the time-evolution of homogenous, gas-phase kinetics with sensitivity analysis.
SHOCK	A program for predicting chemical behavior behind incident and reflected shock waves.
SPIN	A program for modeling one-dimensional, rotating-disk or stagnation-flow chemical-vapor-deposition reactors.
SURFTHERM	A program for analyzing thermochemical and kinetic data in gas-surface chemical reaction mechanisms.

There are several advantages of the modular approach to chemically reacting flow simulations. One is that a user may "mix and match" Applications and chemistry descriptions. Users who are interested in the determination of dominant reaction mechanisms, for example, are free from having to repeatedly develop computational tools with large systems of chemical reactions. The CHEMKIN input-file standard also facilitates communication and sharing of reaction sets between researchers. An analyst who must perform calculations for several different chemical mixtures is free from concern over software programming. This also leads to more robust software that is applied to a wide variety of problems.

4.5 CONTENTS OF THE CHEMKIN COLLECTION 3.5 PACKAGES

CHEMKIN can be purchased in several different "packages" tailored to the needs of individual customers. The descriptions in this section provide information on the contents that are currently included in the standard packages.

Full Package

Utility Set CHEMKIN Interpreter and Gas Phase Subroutine Library, SURFACE CHEMKIN Interpreter and Subroutine Library, Thermodynamic Database, TRANSPORT Pre-processor and Database, TWOPNT, and EQUIL

Applications AURORA, CRESLAF, OPPDIF, PLUG, PREMIX, SENKIN, SHOCK, SPIN, and SURFTHERM

Combustion Package

Utility Set (See above)

Applications AURORA, OPPDIF, PLUG, PREMIX, and SENKIN

Microelectronics Package

Utility Set (See above)

Applications AURORA, CRESLAF, SPIN, SENKIN, and SURFTHERM

Customer Designed Packages

Utility Set (See above)

Applications Customer choice

4.6 HOW DOES CHEMKIN WORK?

The CHEMKIN modular approach described in Section 4.4 provides a broad overview of the CHEMKIN philosophy. Here we describe more specifically *how* the CHEMKIN Collection provides the necessary interface between general Applications and chemistry-specific information. The following flow chart illustrates components of the CHEMKIN software for a typical application. The major software components

can be categorized as preprocessors, subroutine libraries, application models, and databases. The flow chart illustrates the communication between these components for a typical application model.

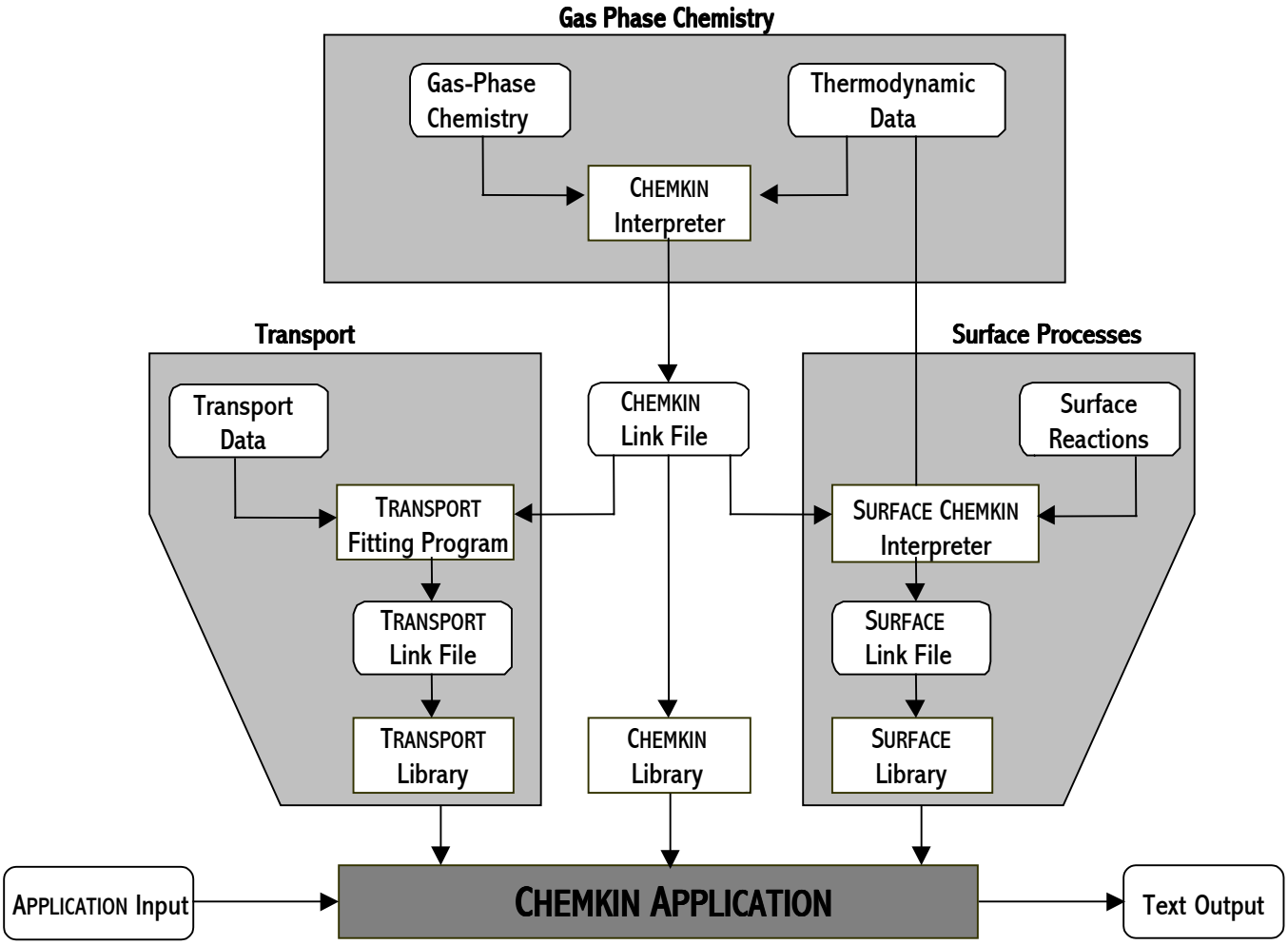

Figure 10 Schematic showing the relationship between the CHEMKIN Utilities and a CHEMKIN Application, including input and output files.

Pre-processors include the CHEMKIN Interpreter, the SURFACE- CHEMKIN Interpreter, and the Transport Fitting Program. The pre-processors read information that is supplied directly by the user, is obtained from one of the CHEMKIN databases, or both. The user-input data tells the pre-processors what species to consider and what reactions can occur between these species. The pre-processors parse and interpret the user information, compile species property information from the databases, and calculate any additional

chemistry-specific information that may be needed by the Application and that are appropriate to determine *a priori*. This information is then stored in "Linking Files" that are later accessed by the CHEMKIN Subroutine Libraries when called by the Application. The CHEMKIN Interpreter must always precede the other pre-processors as it provides information that is used by the others through it's Linking File.

Subroutine libraries include the CHEMKIN Gas-phase Library, the SURFACE CHEMKIN Library, and the TRANSPORT Library. Each of these libraries includes an initialization routine that reads the information in the Linking File, stores the information in arrays and returns these storage arrays to the Application for use in subsequent calls to other library routines. The CHEMKIN Gas-phase Library contains routines that provide information about the size of the chemistry set; information about the elements, species, and reactions; values of physical constants; equation-of-state calculations and units conversions; thermodynamic properties; calculations of chemical production rates; and reaction equilibrium constants. The SURFACE CHEMKIN Library contains routines that perform similar functions for the surface chemistry set. The TRANSPORT Library contains routines that evaluate gas-phase species and gas-mixture transport properties including ordinary diffusion coefficients, thermal diffusion coefficients, thermal conductivities, and viscosities. The transport properties can be evaluated using either mixture-averaged or multicomponent formulations.

Currently, the CHEMKIN collection includes databases of fundamental species data for calculation of transport and thermodynamics properties. Details on the species data available can be found in the Thermodynamic Data and TRANSPORT manuals. Users may also augment or replace database entries by providing their own sets of data.

We have compiled a list of journal articles and other publications that have referenced CHEMKIN Collection software since 1985. These citations may be useful in discovering how other people are using the CHEMKIN Collection in research and industrial applications. The citation bibliography is included on our website (www.ReactionDesign.com) and is updated periodically.

5. Problem Solving with the CHEMKIN Collection

5.1 How to use CHEMKIN 3.5 to Solve Chemical Modeling Problems

The CHEMKIN software can be used in several different ways, depending on your own areas of expertise and your modeling needs. The most straightforward way to use the CHEMKIN software is by direct application of the models included in the CHEMKIN Collection. A brief summary of the Applications is shown in Table 1.

Table 1 CHEMKIN Applications

Application	Brief Description of the CHEMKIN Application
AURORA	Well stirred plasma and thermal reactors with gas and surface reactions
CRESLAF	Laminar, boundary layer flows in cylindrical or planar channels
EQUIL	Chemical equilibrium of and ideal gas or solution mixture
OPPDIF	Diffusion flame between two opposing nozzles
PLUG	Plug flow reactor with gas and surface chemistry
PREMIX	Steady, laminar one-dimensional pre-mixed flames
SENKIN	Sensitivity analysis of homogeneous gas-phase kinetics
SHOCK	Chemical dynamics behind incident and reflected shock waves
SPIN	Rotating-disk/stagnation flow chemical vapor deposition reactors
SURFTHERM	Analysis of thermochemical and kinetic data in gas-surface reaction mechanisms

Additional applications can be built using the sub-components or utilities of the CHEMKIN Collection. This mode requires a much higher level of modeling expertise, but offers more flexibility in describing a specific system of interest to you. Table 2 presents a brief description of the utilities

Table 2 CHEMKIN Utilities and Supporting Databases

CHEMKIN Utility/Database	Brief Description of the CHEMKIN Utility/Database
CHEMKIN III	Library of analysis tools for gas-phase chemical and plasma kinetics
SURFACE CHEMKIN III	Library of analysis tools for chemical kinetics at gas-solid interfaces
Thermodynamic Property Database	Temperature variation of species enthalpy, specific heat, and entropy
TRANSPORT	Library of tools for evaluation of multi-component transport properties
TRANSPORT Property Database	Molecular properties used in calculating transport properties
TWOPNT	Algorithms for solution of two-point boundary value problems

Each of the Application and Utility manuals describe in much more details how to build or extend the capabilities of the existing programs.

5.2 STEPS IN USING CHEMKIN 3.5

There are six basic steps involved in using CHEMKIN to solve a typical chemical process modeling problem. Depending on the particular Application, some of the steps are not required; these are indicated by (.) around the step.

1. **Prepare the chemistry input file(s)**

   Gas-phase chemistry

   (Surface chemistry)

2. **Assemble the thermodynamic and transport databases**

   Gas-phase thermodynamics

   (Surface thermodynamics)

   (Gas-phase species transport data)

3. **Prepare the Application-specific input data**

   (Geometry)

   (Process conditions)

   (Solution method options)

4. **Run the Pre-Processing programs**

   Chem – The CHEMKIN gas-phase reaction mechanism interpreter

   (Tran) – The TRANSPORT property fitting program

   (Surf) – The SURFACE CHEMKIN reaction mechanism interpreter

5. **Run the Application**

6. **Post-process the results**

Table 3 summarizes the input data requirements for each of the CHEMKIN Applications. The specific details of the data formats, and information needs are described in the user manuals for the Applications and the CHEMKIN Utilities.

Table 3 Summary of Input Needed for CHEMKIN Applications

Application	Gas-phase Chemistry	Surface Chemistry	Application-specific Input	Thermodynamic Database	Transport Properties Database
AURORA	✔	✔	✔	✔	
CRESLAF	✔	✔	✔	✔	✔
EQUIL	✔	(✔)	✔	✔	
OPPDIF	✔		✔	✔	✔
PLUG	✔	✔	✔	✔	
PREMIX	✔		✔	✔	✔
SHOCK	✔		✔	✔	
SENKIN	✔		✔	✔	
SPIN	✔	✔	✔	✔	✔
SURFTHERM	✔	✔	✔	✔	(✔)

An illustration of some of the steps is presented in Figure 11

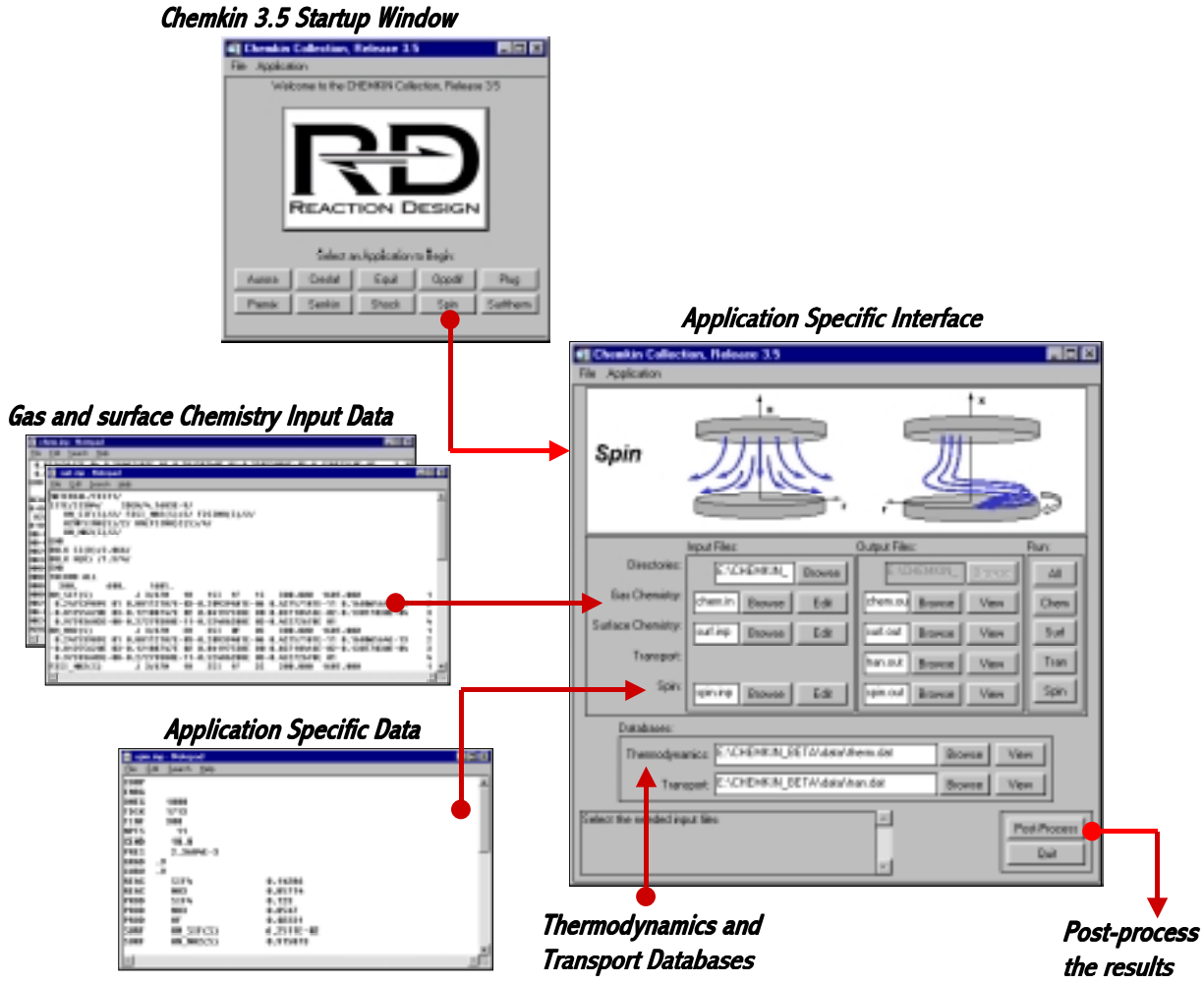

Figure 11 **A Schematic representation of the information flow in running a typical CHEMKIN Application.**

5.3 WHERE TO GET THE NEEDED INPUT DATA?

A typical question is "I can't find data for certain species in the Thermodynamic or Transport database. What should I do?" First, check the complete species list in the Thermodynamic Database and Transport

manuals. These data were originally supplied to Reaction Design by Sandia. While the original data has not been officially updated, Reaction Design continues to assemble information for additional species that will be added to future releases. If you are unable to locate certain species in the Thermodynamic or Transport databases there are several other sources for developing the needed information including:

1. *Original Sources:* These are organizations that generate or critically evaluate data. One of the most important is the National Institute of Standards and Technology (NIST).
2. *Secondary and Tertiary Sources:* These are compilations of data from original sources and are often published in handbooks and journals. For chemical kinetics a good starting point is the *J. Physical and Chemical Reference Data*.
3. *Physical Property Estimation Methods:* These are methods that can be used to evaluate thermo-physical property information. A classical example is the book by Benson (1976) *Thermochemical Kinetics: Methods for the Estimation of Thermochemical Data and Rate Parameters,* Second Edition, John Wiley & Sons, Inc., New York.
4. *Web Sites:* The Reaction Design web site contains links to many different sources of thermochemical and transport property information.

Many other sources of data are described in Maizell (1998), *How to Find Chemical Information: A guide for Practicing Chemists, Educators and Students,* John Wiley & Sons, Inc., New York.

6. The CHEMKIN Application User Interface

This Section provides a more complete description of the elements of the *CHEMKIN Application User Interface*. The information here includes descriptions of menus and buttons as well as quick reference "**Hints**" on program features. We recommend that you first read through Chapter 3, particularly Section 3.5.2 so that you are familiar with starting the Application User Interface and you are sure that your software is installed correctly.

6.1 SELECTING INPUT AND OUTPUT FILES

The Application User Interface is designed to help you organize your input and output files, and to remind you of the steps and input data required to run each Application. For an illustration of the Application User Interface features, see Figure 4, in Chapter 3. These features are described in more detail here.

Directories

You should first set the working directories, where you will store the input and output files. By default, the program assumes that the output directory is the same as the Input Directory.

To select a new directory, you can either type the path to the directory in the text box, or click "**Browse**" to use the mouse to select the desired directory using your computer's file browser.

Hints:

- The directory must already exist.
- You can make the Output Directory independent of the Input Directory by modifying the user Preferences (Choose "**Preferences**" from the "**File**" pull-down menu).
- You can change the default directory that the program assumes at startup in the user Preferences (Choose "**Preferences**" from the "**File**" pull-down menu).

Input File Names

The input files that are used by the pre-processors and the Application must reside in the Input Directory. By default, the program will suggest filenames in the text boxes. To select a different filename, you can either type the new name in the text box or click **"Browse"** to select a new file. You can also click on **"Edit"** to modify the selected file or to create a new file.

Hints:

- Since the text box is small on some platforms, using the "**Browse**" button may be more reliable than typing to ensure that you have the correct input file selected.
- You may change the default editor invoked by the "**Edit**" buttons by modifying the user Preferences (Choose "**Preferences**" from the "**File**" pull-down menu).
- Remember: your input files must exist in the specified Input Directory.

Output File Names

The Pre-processors and the Application program will create output files in the specified Output Directory. By default, this is the same directory as the Input Directory. Also by default, the Application User Interface will suggest filenames in the text boxes. To select a different filename, you can either type the new name in the text box or click "**Browse**" to select a new file. Once you have clicked on "**Browse**" you may still need to type in the filename, since this file typically does not yet exist. **If you choose an existing file, the file will be overwritten when the program is run.** After the programs have been run, you can view the output files by clicking on their **"View"** button.

Hints:

- Since the text box is small on some platforms, using the "**Browse**" button may be more reliable than typing to ensure that you have the correct output filename entered.
- You may change the default editor invoked by the "**View**" buttons by modifying the user Preferences (Choose "**Preferences**" from the "**File**" pull-down menu).
- Remember: the output files will always be created in the specified Output Directory.

Database Files

Unlike the Input and Output Files, the Database Files are specified by providing the full directory path to the required files. These files typically will not reside in the Input Directory or the Output Directory, although it is OK if the directory paths happen to be the same. By default, the database files selected are the standard Thermodynamic Database file and the Transport Database file distributed with CHEMKIN. To change to a different file, click **"Browse"** and navigate to the desired file. You can also click on **"View"** to open the selected file in an editor.

Hints:

If the Transport Database is not required for a specific Application, then the selection features will become inactive.

6.2 RUNNING THE PROGRAMS

As described in Chapter 5, solving a problem using CHEMKIN requires running one or more pre-processors as well as running the Application program itself. The right-hand column of the Application User Interface allows you to run these programs one at a time or, alternatively, to run all needed pre-processors and the Application by clicking the run "**All**" button. In general, the order in which the pre-processors is run is important: all required pre-processors must be run before the Application, and the "**Chem**" pre-processor should always be run first. The two options are described in more detail below.

Run "Chem"

The "**Chem**" button runs the CHEMKIN Interpreter using the specified gas-phase chemistry input file, as well as the Thermodynamic Database File. The CHEMKIN Interpreter creates a Linking File that is required by the other pre-processors and by the Application. For more information about the CHEMKIN Interpreter program and input, refer to the CHEMKIN III user manual.

Run "Surf"

The "**Surf**" button runs the SURFACE CHEMKIN Interpreter using the specified surface chemistry input file, as well as the Thermodynamic Database File. The SURFACE CHEMKIN Interpreter creates a Linking File that is required by the Application. For more information about the SURFACE CHEMKIN Interpret program and input, refer to the SURFACE CHEMKIN III user manual.

Run "Tran"

The "**Tran**" button runs the TRANSPORT Fitting Routine using the specified Transport Database File. The TRANSPORT program creates a Linking File that is required by the Application. For more information about the TRANSPORT program and input, refer to the TRANSPORT user manual.

Run the Application

Each Application User Interface panel has a button labeled with the Application name and aligned with the Application Input and Output File selection features. This Application button runs the Application program using the specified Input File. The Application will create (or overwrite) the Output File. In addition to the text Output File, all of the Applications (except for SURFTHERM) generate a binary solution file named `save.bin`. The `save.bin` file is read by the Graphical Post-Processor to plot the solution results, as described briefly in Chapter 3 and in more detail in Chapter 7.

Running "All"

The "**All**" button automatically runs the required sequence of pre-processors and then runs the Application, as described by the individual buttons above.

Hints:

When running **Chem** and **Surf**, the program will create a local copy of the Thermodynamic Database File in the Output Directory, and rename the file "`therm.dat`". If there is already a `therm.dat` file in that directory, you will be prompted whether or not to overwrite the existing file. Similarly, running **Tran** will try to create a local `tran.dat` file, and will prompt you for a response if an existing file is found. You can allow the program to always overwrite the `therm.dat` and `tran.dat` files found in the Output Directory, by modifying your user Preferences. (Choose "**Preferences**" from the "**File**" pull-down menu).

6.3 INFORMATIONAL MESSAGES AND ERROR REPORTS

The Message Box

The Message Box, located at the bottom of the Application User Interface panel, helps you to follow the progress of your work. The messages tell you what command is being executed, when it has finished executing, and whether or not the process has completed successfully.

Error, Warning and Information Dialogs

In addition to the advisory messages in the Message Box, you may also see pop-up Information, Warning, or Error Dialog boxes. These Dialogs inform you that some operation did not complete properly, that you need to make a choice between one or more options, or that an operation about to occur may result in some unwanted effects (such as overwriting files). The message may also provide some suggested action that you can undertake to correct or avoid the problem. In order to continue working, you must click on a button in the box ("OK", "Yes", "No", etc.).

6.4 THE "FILE" MENU

The "**File**" pull-down menu is located at the left-hand end of the menu bar on the Application User Interface. There are four options available under this menu in Release 3.5: "**Save Session**", "**Recover Session**", "**Preferences**" and "**Quit**". The "**Quit**" option simply exits the *CHEMKIN Application User Interface*. The other three options are discussed further below. Figure 12 demonstrates the selection of "**Preferences**" from the "**File**" menu.

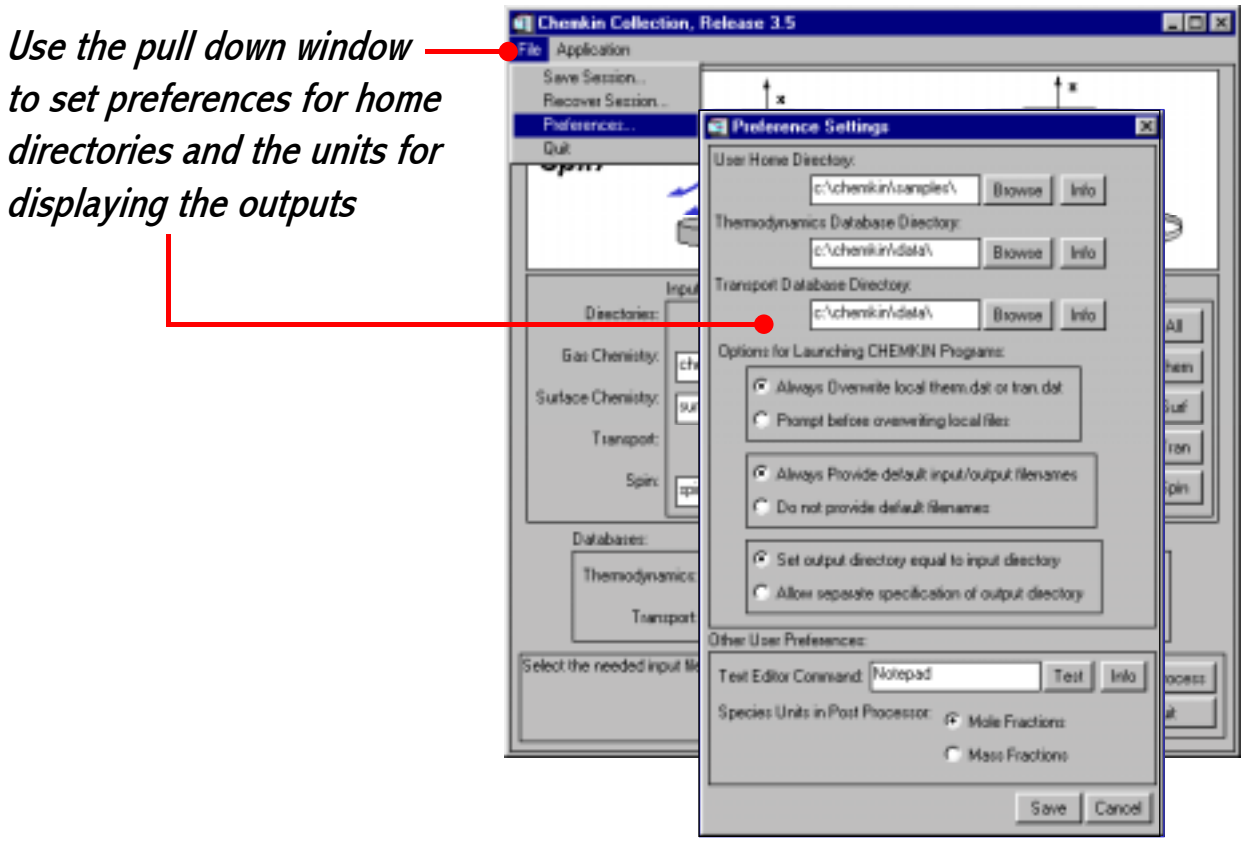

Figure 12 Selection of Preferences from the File pull-down menu.

6.4.1 Preferences

The Preferences option provides you with some control over the settings for the *CHEMKIN Application User Interface*, as well as the settings for the *CHEMKIN Graphical Post-Processor*. The Preferences selection panel is shown in Figure 13.

Note: *If you change the preferences, you will need to restart the CHEMKIN Application User Interface or the CHEMKIN Graphical Post-Processor before the changes take effect.*

> **Hints**:
>
> If the path to the directory containing your Editor program is contained in your environment "path", then only the edit command must be entered in the Preferences Editor box (for example, "`wordpad`" on Windows). If not, then you must include the full directory path to the editor program for the editor command to work properly (for example, "`c:\Program Files\Accessories\wordpad`").

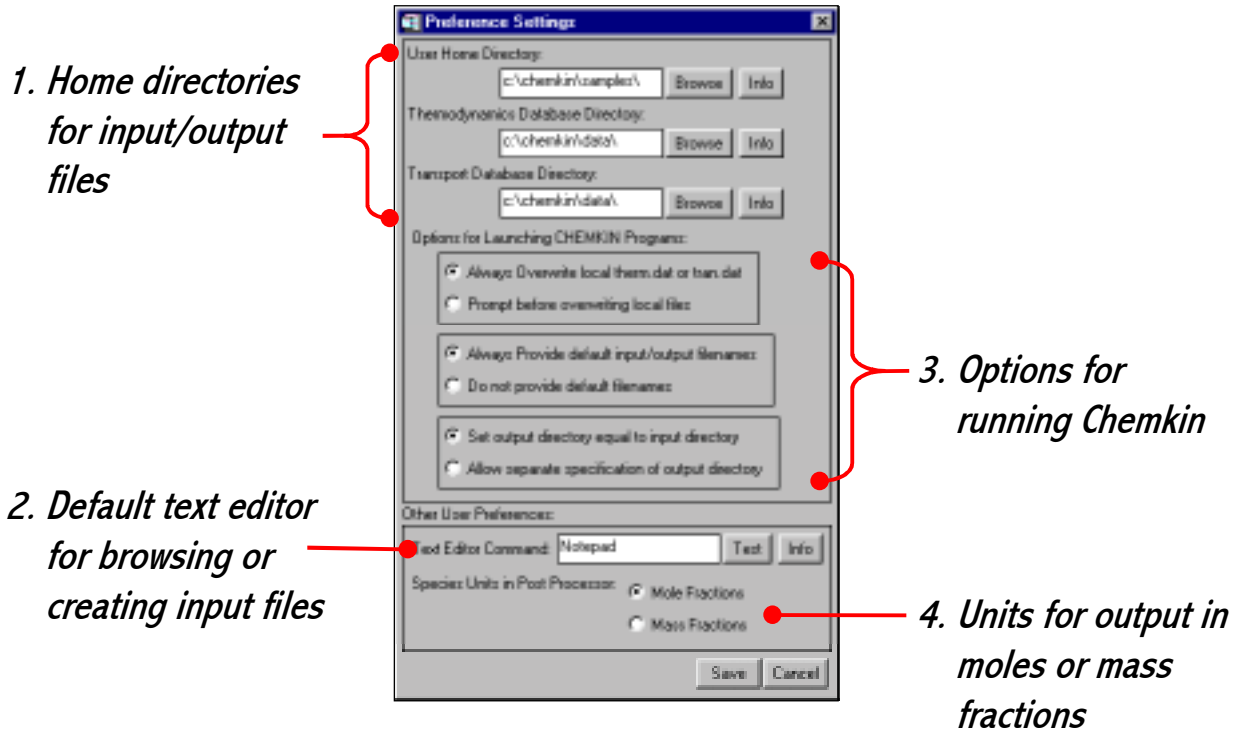

Figure 13 The Preferences selection panel for the Application User Interface and for the Graphical Post-Processor

6.4.2 Saving and Restoring Sessions

Once you have set up a problem in the Applications User Interface panel, you can save your directory, filename, and database settings using the "**Save Session**" option in the "**File**" menu. A dialog will prompt you for a filename and a directory location for the Session File.

A previous session's settings can be recovered by selecting the "**Recover Session**" option in the "**File**" menu. A file browser allows you to select the previously created Session File.

> **Hint**:
>
> When you recover a Session File, you should be in the same Application User Interface panel (e.g. SPIN), as you were when you created the Session File.

7. The CHEMKIN Graphical Post-Processor

This Section provides a more complete description of the elements of the *CHEMKIN Graphical Post-Processor*. The information here includes descriptions of menus and buttons as well as quick reference "**Hints**" on program features. We recommend that you first read through Chapter 3, particularly Section 3.5.3 so that you are familiar with starting the Graphical Post-Processor and you are sure that your software is installed correctly.

7.1 THE "FILE" PULL-DOWN MENU

The "**File**" pull-down menu is located at the left-hand end of the menu bar that runs across the top of the Graphical Post-Processor window. There are six operations available in CHEMKIN Release 3.5: "**Open**", "**Print**", "**Import**", "**Export**", "**Preferences**" and "**Quit**". The "**Quit**" option simply exits the Graphical Post-Processor. The other five options are discussed below.

7.1.1 Open

The "**Open**" option allows you to open a new CHEMKIN binary solution file, which the program expects to have a "`.bin`" suffix. Selecting the "**Open**" option puts you in a file browser on your computer, where you can choose an existing binary solution file. Once the file is selected, the program will attempt to read the data on the file. If there are any difficulties reading the file, a message will appear in the **Message Box** at the bottom of the Graphical Post-Processor window.

As described in Chapter 3, Section 3.5.3, when you open a new binary solution file, the program will either open a Data Selection window, or will directly create a default plot from the data that was read. The Data Selection window is opened whenever there are more than 20 variables in the solution or when there is more than one solution sub-set.

> **Hints**:
>
> Reading in a new `save.bin` file will overwrite any existing data in the Graphical Post-Processor. If you want to examine two or more solutions simultaneously, you can launch multiple Graphical Post-Processor sessions and read in different `save.bin` files. Though you will not be able to compare data in the same window, you will be able to plot results side-by-side on your screen.

7.1.2 Import

You can import x-y data from plain text files into the Graphical Post-Processor using the "**Import**" option in the "**File**" menu. The import utility expects to find columns of data, delimited by tabs, commas, or spaces. Selecting the "**Import**" option opens a dialog box where you can choose the delimiter for the columns in the file, the number of header lines to skip before reading the data, and whether or not to read the first line (after the skipped lines) as character-string labels for the columns. If your selections do not appear to agree with the format of the first couple of lines of data in the file, you will receive an warning message. If you click "**OK**" to read the data in and the import utility encounters errors reading the specified format, you will receive a message in the Message Box, and the data will not be imported. If the format is read correctly, the first two columns found in the file will be used to create a default plot.

7.1.3 Export

To give you more flexibility in analyzing and post-processing your data, you can export all of the data arrays currently stored in the Graphical Post-Processor into a file of text columns. The columns in the exported text files may be delimited by tabs, commas, or spaces. Such formats can be easily imported into spreadsheet programs, as well as other visualization and analysis software. When you select the "**Export**" option from the "**File**" menu, you will be asked to choose the delimiter for the exported data columns, and then the name and location of the data file that will be written. If there are any errors writing the file, a message will appear in the **Message Box** at the bottom of the Graphical Post-Processor window.

7.1.4 Print

Any plot generated on your screen can be printed to a color or black-and-white printer using the "**Print**" utility. This requires that you already have a print driver installed and a default printer set on your computer. You can also print to a Postscript file, by selecting the file option on the printer dialog.

7.1.5 Preferences

As described in Chapter 6, Section 6.3.1, the "**Preferences**" option provides you with some control over the settings for the *CHEMKIN Application User Interface*, as well as the settings for the *CHEMKIN Graphical Post-Processor*. The main setting for the CHEMKIN Graphical Post-Processor is a choice of whether the species composition data are imported from CHEMKIN solution files as mole fractions or mass fractions. The default is to convert the data to mole fractions. **Note:** if you change the settings in the Preferences dialog, you will need to restart the CHEMKIN Graphical Post-Processor before the changes take effect.

7.2 THE "VIEW" PULL-DOWN MENU

Currently, only two options are available from the "**View**" pull-down menu, "**Show/Hide Legend**" and "**Show/Hide Title**". These options allow you show the Plot Title or Legend, if you have previously selected to "**Hide**" them in the Plot Title or Legend Attributes Dialog. Alternatively, if you have previously selected to "**Show**" the Plot Title or Legend (the default), you can use the "**View**" menu to "**Hide**" these items.

7.3 THE "PLOT" PULL-DOWN MENU

Although we plan to have more plot options in future CHEMKIN releases, the current release only allows creation of X-Y plots. Choosing the "**X-Y Plot**" option in the "**Plot**" menu opens a window from which you can select the data arrays to plot as "X" (horizontal axis) or "Y" (vertical axis) variables in the Graphical Post-Processor.

7.4 CHANGING PLOT ATTRIBUTES

By using your mouse to double-click or click-and-drag items in the plot window, you can change the appearance of the plot as displayed in the Graphical Post-Processor. Table 4 summarizes what items can be accessed by the mouse and what attributes can be changed.

Table 4 Plot Attributes That Can Be Changed

Item	Mouse Action	Attributes
X-Axis / Y-Axis	double-click	Axis Label Text Axis Label Font and Font Size Linear/Log Axis Scaling Axis Minimum/Maximum values Tick Direction, Number, and Size
Plot Title	double-click	Title Text Font and Font Size
Plot Title	click-and-drag	Title Position on Plot
Legend	double-click	Hide/Show Legend Hide/Show Outline Hide/Show Legend Title Legend Title Text Legend Title Font and Font Size Legend Item Labels Legend Item Font and Font Size
Legend	click-and-drag	Legend Position on Plot

7.5 UNITS OF SOLUTION VARIABLES

The binary solution files (`save.bin`) produced by the CHEMKIN Applications include values for solution variables, (e.g. velocities, temperatures, pressure, and species fractions), which have physical units (e.g. [cm/s], [K], [dyne/cm^2], and mole fractions). In some cases, the variable names assigned to the arrays indicate the units (e.g. a variable labeled "Pressure_In_Torr" would indicate that the date has the units of Torr instead of the default). In all other cases, you can assume that the units are the standard units for the "cgs" system (centimeters, grams, seconds). Table 5 below indicates the cgs units for some of the common solution variables:

Table 5 CGS Units for Common Solution Variables

Variable	CGS Units
Time	s
Distance	cm
Velocity	cm/s
Area	cm^2
Pressure	$dyne/cm^2$
Density	g/cm^3
Temperature	K
Mass flow rate	g/s
Volume flow rate	cm^3/s
Deposition/Etch Rate	$mole/cm^2$-s
Molecular weight	g/mole
Species Fraction	Determined by user Preferences (see Section 7.1.4)

For variables not listed in Table 5, see the Application manual for information about units of variables specific to that Application.

8. Using CHEMKIN from the Command Line

We recognize that there will always be some users who prefer to run CHEMKIN by typing commands from a command line (in a MS-DOS prompt or a UNIX shell, for example), rather than using the new CHEMKIN Application User Interface. Also, if you are writing your own applications or your own post-processing routines, you will need to be familiar with running CHEMKIN from a command line. This section describes the steps for running a sample problem, the makefiles and build scripts available in the CHEMKIN distribution, as well as the FORTRAN post-processors that are available as templates for writing your own post-processing routines. For most uses of command-line programming, you will need to have a Fortran compiler installed on your platform. For Windows/PC users, the required compiler is Digital Visual Fortran version 5.0D or later.

Note for Windows: To open an MS-DOS prompt in Windows, go to your **Start** menu, select **Programs**, and then select **MS-DOS Prompt** (Windows) or **Command Prompt** (Windows NT)

8.1 RUNNING THE CHEMKIN SAMPLE PROBLEMS

The CHEMKIN distribution includes one or more sample problems for each Application. Generally, each sample consists of a set of input files, a "make" file that builds and runs the sample, and an HTML file that describes what type of problem the sample demonstrates. For the purposes of describing the commands in this section, we will refer to the root of the CHEMKIN installation as `c:\chemkin` for PCs and `~/chemkin` for UNIX. In following the instructions you will need to substitute the actual path where CHEMKIN is installed in place of these references.

8.1.1 Build All Samples

To build and run all the samples in the release, change directories to the `samples` subdirectory of the CHEMKIN installation (`c:\chemkin\samples` for PCs or `~/chemkin/samples` for UNIX) and type:

```
buildsamples
```

Note for UNIX: On UNIX, you may not have the current directory (.) in your "path". If typing `buildsamples` does not work in your UNIX shell, try prefixing the command with your current directory, like this:

```
./buildsamples
```

This command will launch a batch script that will build and run all of the samples by changing into each sample directory in turn and running the make file found there. Under the `samples` directory, there are subdirectories named for each Application. Within these subdirectories, there are different sample problems, such as "`gas_psr`" or "`rotating_disk_cvd`", depending on the Application. Within these sample-problem directories, you can look at the sample input and output files with a standard text editor.

8.1.2 Clean All Samples

You can undo the `buildsamples` command by running `cleansamples` in the same manner as described in Section 8.1.1. This command removes all of the output and intermediate files from the sample sub-directories.

> **General Note:** It is often desirable to run `cleansamples` to reduce the use of disk space.

8.1.3 Using the Make files

As mentioned above, each of the sample sub-directories contains a "make" file that will compile and link programs if necessary, run pre-processors, run the Application, and run a command-line post-processor if required. The make files obtain information about the build dependencies and machine-specific commands from an "include" file located in the "include" directory in the root of the CHEMKIN installation (`c:\chemkin\include` for PCs or `~/chemkin/include` for UNIX). The include file is named `chemkin_make_pc.inc` on the PC and `chemkin_make_unix.inc` on UNIX.

> **General Note:** The make files are designed to be used at the directory level where they are located, since they determine the location of the Include File relative to this directory. If you want to copy a makefile to another directory for your own use, you may need to modify the make file before it will work properly in its new location.

As an example, we will demonstrate here how to run the AURORA sample problem called "gas_psr". First, change directories to the AURORA `gas_psr` sample directory and then run the "make" utility as follows:

Windows/PC:

```
cd c:\chemkin\samples\aurora\gas_psr
nmake –f gas_psr_pc.mak > gas_psr_pc.log
```

UNIX:

```
cd ~/chemkin/samples/aurora/gas_psr
make –f gas_psr_unix.mak > gas_psr_unix.log
```

Note that the results of the make utility are redirected to a log file so that you can review any warnings or error messages that occur during the build process.

Notes for Windows:

- Notice that the "make" utility on the PC is called **`nmake`** instead of `make`
- You must have Digital Visual Fortran installed on your PC for the nmake command to be recognized.

8.1.4 Running Step by Step

If make files give you headaches or you just like to type, you can run each command directly on the command line. Here we will repeat the above example, but show the commands that would need to be typed to the terminal for each step.

1. **Change directories** to the AURORA `gas_psr` sample directory:

   Windows/PC: `cd c:\chemkin\samples\aurora\gas_psr`
   UNIX: `cd ~/chemkin/samples/aurora/gas_psr`

2. **Create a local copy of `therm.dat`.** The `therm.dat` file contains the thermodynamic database used by the CHEMKIN and SURFACE CHEMKIN Interpreters. The utilities assume it is located in the current directory.

   Windows/PC: `copy ..\..\..\data\therm.dat .`
   UNIX: `ln –s ../../../data/therm.dat therm.dat`

   The "`..`" on both UNIX and PC platforms means "one directory up from the current directory". Note that in UNIX you can use a "soft-link" instead of actually copying the data file to the local directory. PC users may want to consider deleting the local `therm.dat` and `tran.dat` files after the pre-processors have been run, to avoid unnecessary use of disk space.

General Note: A similar copy command is required for Applications that require TRANSPORT data (not required by AURORA). In this case you need a local copy of the database file called `tran.dat`.

3. **Run the CHEMKIN Intrepreter:**

   Windows/PC: `..\..\..\bin\chem < chem.inp > chem.out`
   UNIX: `../../../bin/chem < chem.inp > chem.out`

   The "<" and ">" are used to redirect standard input and output, respectively, from and to the specified files. In addition to the `chem.out` file, the CHEMKIN Interpreter creates an output file named `chem.asc`. This is the Linking File required by other CHEMKIN pre-processors and by the Application. You should *always check for errors by reviewing the contents of* `chem.out`, *before proceeding*.

4. **Run the SURFACE CHEMKIN Interpreter:**

   Windows/PC: `..\..\..\bin\surf < surf.inp > surf.out`
   UNIX: `../../../bin/surf < surf.inp > surf.out`

   Note that this particular AURORA sample does not actually deal with surface chemistry, but AURORA still requires you to run the SURFACE CHEMKIN Interpreter. In this case, however, the `surf.inp` file is very simple: it contains nothing but a comment. In addition to the `surf.out` file, the SURFACE CHEMKIN Interpreter creates an output file named `surf.asc`. This is the Linking File required by the Application. You should *always check for errors by reviewing the contents of* `surf.out`, *before proceeding*.

> **General Note:** For Applications that require TRANSPORT data (not required by AURORA), you will also need to run the TRANSPORT pre-processor. This must be run after the CHEMKIN Interpreter and before the Application.

5. **Run the Application**, in this case the AURORA program:

   Windows/PC: `..\..\..\bin\aurora < aurora.inp > aurora.out`
   UNIX: `../../../bin/aurora < aurora.inp > aurora.out`

   In addition to the `aurora.out` file, the AURORA program creates a binary solution file called `save.bin`. This file is required by the CHEMKIN Graphical Post-Processor as well as the FORTRAN post-processor described below. You should *always check for errors by reviewing the contents of* `aurora.out`, *before proceeding*.

6. **Run the FORTRAN Post-Processor** for AURORA, called AURORA_POST:

   Windows/PC: `..\..\..\bin\aurora_post < aurora_post.inp >aurora_post.out`
   UNIX: `../../../bin/aurora_post < aurora_post.inp >aurora_post.out`

   The AURORA_POST program reads the binary solution file, `save.bin`. In addition to the `aurora_post.out` output file, which contains diagnostics information, the post-processor creates one or more files named `psrout_*.txt`, where the "*" is a number from 1 to the number of files created. These files contain columns of data representing the AURORA solution results (such as species mass fractions). The number of rows is determined by the number of continuations (keyword CNTN) included in the AURORA input file. The output file name prefix is determined by the FILE keyword in the `aurora_post.inp` file.

General Note: All of the Applications in the CHEMKIN Release 3.5 have sample FORTRAN post-processors. The release includes full source code for these routines. The source code is located in the "post_processors" directory at the root of the CHEMKIN installation. These post-processors provide examples of how to read the binary solution files for exporting CHEMKIN solution data into custom or third-party applications.

8.2 SETTING UP YOUR OWN PROBLEM

To begin applying CHEMKIN Applications to your own problems, we recommend that you set up a working directory where you will store your input and output files for the application you wish to run. We also recommend that you add the CHEMKIN "`bin`" directory (e.g. `c:\chemkin\bin` on a PC or `~/chemkin/bin` for UNIX) to your local "path" definition, so that you don't have to specify the full path of the executables every time you run them. The procedure for modifying path variables is described in Chapter 3, Sections 3.2.2 (for PCs) and Section 3.3.4 (for UNIX).

You can then follow a similar procedure as when running the sample problems in the step-by-step mode, but this time you will have to create your own input files. For this discussion we will use SENKIN as the target Application. The following are the steps for running SENKIN for your own problem.

1. **Create the input files** that you want to use to describe your reactor and process conditions. Use the text editor you are most comfortable with and save the files to your working directory. (See the Application and Utility user manuals for more guidance in creating the input data.)

2. **Open a MS-DOS Prompt or UNIX shell** and change directories to this working directory.

3. **Make sure that the `LM_LICENSE_FILE` environment variable is correctly set**. (See Chapter 3)

4. **Run the necessary pre-processors**. For the SENKIN Application, you will only need to run the CHEMKIN Gas-phase Interpreter. This requires that you first create a local copy of the thermodynamic database file to your local directory, as described in section 8.1.3 above. You can then run the CHEMKIN Interpreter by typing the following, assuming that you set your path as suggested above and have defined the chemistry in a file named `mychem.inp` :

   ```
   chem < mychem.inp > mychem.out
   ```

   Make sure check the `mychem.out` *file before proceeding.* For other applications, you may also need to run the TRANSPORT pre-processor (which requires the `tran.dat` file to be copied or linked to the local directory) and/or the SURFACE CHEMKIN Pre-processor. To determine which pre-processors and input files are needed, see Table 3 in Chapter 5.

5. **Run the Application** with your input files. For example, to run SENKIN, you would type:

   ```
   senkin < mysenkin.inp > mysenkin.out
   ```

6. Again, you would want to **check the `mysenkin.out` file to see if the program ran successfully**, before attempting to post-process the results.

7. **Run the SENKIN post-processor**:

   ```
   senkin_post < mysenkin_post.inp > mysenkin_post.out
   ```

The SENKIN post-processor (like all of the FORTRAN post-processors) produces a number of text files that contain columns of data according to the options requested in the `mysenkin_post.inp` file. These text files can easily be imported into the *CHEMKIN Graphical Post-Processor*, or into other analysis tools, such as spread-sheet programs.

9. Getting Help and Support

9.1 Online Documentation

CHEMKIN 3.5 provides a complete set of documentation in the form of HTML pages and PDF documents focused precisely on the details of building and running the CHEMKIN software. Included in the CHEMKIN installation are PDF documents for each of the user manuals for the CHEMKIN Utilities and Applications. You can view the PDF documents using Adobe Reader, which is available for your convenience on the CHEMKIN distribution CD-ROM. The HTML pages installed with CHEMKIN describe the installation directory structure and the sample problems available for each Application. You can view the HTML files using any internet browser (such as Internet Explorer or Netscape Navigator).

9.2 Frequently Asked Questions

Reaction Design provides a set of answers to Frequently Asked Questions (FAQs) that we have compiled through our interaction with customers. The up-to-date list of FAQs is maintained in the Customer Support section of our website (www.ReactionDesign.com) . Also, a snapshot of the FAQs compiled at the time of release for CHEMKIN 3.5 have been included as HTML files in the CHEMKIN distribution (see Section 6.1 above).

9.3 Contacting Technical Support

Reaction Design is committed to the highest level of technical support. If the answer to your question is not found in the Frequently Asked Questions (FAQ) section, please email your question to Support@ReactionDesign.com. You may also contact Reaction Design's Technical Support, by Fax: (858) 550-1925, or by Phone: (858) 550-1920.

If you call or send email, you should include the following information in your support request:

1. Your CHEMKIN License Number.
2. The name and email address of the Licensee, if different from yourself.
3. Any input or output files for the problem you are running.
4. Any pertinent error or informational messages you have received from the CHEMKIN software.

Reaction Design

Main Office:
Reaction Design
6440 Lusk Boulevard
Suite D-209
San Diego, CA 92121-2758
(858) 550-1920 (telephone)
(858) 550-1925 (fax)
info@Reaction Design.com (email)
www.ReactionDesign.com

Northern California Office:
Reaction Design
6500 Dublin Boulevard
Suite 214
Dublin, CA 94568
(925) 803-2226 (telephone)
(926) 803-2230 (fax)

CHEMKIN Distributor in Japan:
Best Systems
2-1-6 Sengen
Tsukuba Ibaraki 305-0047 Japan
81-298-60-7080 (telephone)
81-298-60-7081 (fax)