ANSYS Chemkin-Pro Input Manual

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Table of Contents

Note: PDF user guides
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List of Figures

Note: PDF user guides
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after release 19.0

List of Tables

Note: PDF user guides
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after release 19.0

Chapter 1: Introduction

The Chemkin-Pro Input Manual (p. 1) is designed to serve as a reference to ANSYS Chemkin-Pro users who require more information about the input parameters needed in defining a chemically reacting flow simulation. In particular, information about syntax and format of chemical reaction mechanism input files, thermodynamic data, and transport-property data are described in detail. In addition, detailed information about all of the input parameters associated with reactor models, including default values and usage guidelines, are included in the Keywords section.

The ANSYS Chemkin-Pro Interface guides users through problem setup and execution, as well as quick analysis with the Chemkin-Pro Visualizer. The operation of the Chemkin-Pro Interface and Post-Processing are described in detail in Chemkin-Pro Getting Started Guide. In some cases, however, users may wish to work from the command line instead of the User Interface and manually assemble Reactor Model input files. For this purpose, the Chemkin-Pro Input Manual (p. 1) describes the necessary syntax and usage of the reactor-input Keywords, as well as a quick reference of what keywords are available for each Reactor Model.

For background information on the equations and theory behind the input parameters, the Chemkin-Pro Theory Manual provides further reading. In many cases, equations in the Chemkin-Pro Theory Manual are references in the discussions of reactor parameter input Keywords.

In Thermodynamic Data (p. 3) through Transport Database (p. 87), we describe the syntax and format required for thermodynamic, gas-phase kinetics, surface kinetics, and transport-property input data. Description and Properties of Particles (p. 95) has the description of fundamental particle properties for Particle Tracking. CHEMKIN Project Input: Keyword Syntax and Rules (p. 113) provides an overview of the syntax and rules for Keyword input, which make up the Reactor Model input files. Reactor Model input files are ordinarily created by the User Interface but can also be manually assembled for command-line usage. Reference Guide to Project Input Keywords (p. 115) provides a Quick Reference of the Keywords, organized by Reactor Model and other concepts, while Alphabetical Listing of Project Input Keywords (p. 123) contains alphabetical listings of keywords.

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Chapter 2: Thermodynamic Data

Any chemical species that appears in a problem must have thermodynamic data associated with it. The format required for these data is described in this chapter. Also Standard State Enthalpies and Entropies at 298 K (p. 10) includes a discussion and listing of the standard-state enthalpies and entropies for the data contained in the therm.dat database file, which is included with every ANSYS Chemkin-Pro installation.

Thermodynamic data may be extracted from a database file (for example, *therm.dat*) and/or read from the *Gas-phase Kinetics* or *Surface Kinetics* input file. If all of the thermodynamic data are to be extracted from a database file, then no thermodynamic data input in the *Gas-phase Kinetics* or *Surface Kinetics* input file is required. However, if the user wishes to override information in the database or to provide data on species not in the database, then thermodynamic data are needed in the *Gas-phase Kinetics* or *Surface Kinetics* input file. In any case, the format for the information is the same.

2.1. Thermodynamic Data Format

ANSYS Chemkin-Pro expects the thermodynamic data to be provided in a specific format. In addition to the fourteen polynomial fitting coefficients (described in Standard-state Thermodynamic Properties in the *Chemkin-Pro Theory Manual*), the database also contains the species' name, its elemental composition, its electronic charge, and an indication of its phase (gas, liquid or solid). The data for each species requires four formatted lines of length 80 characters. Figure 2.1: Excerpts from the *therm.dat* Thermodynamic Database File (p. 4) is a sample of the lines required for a species and Table 2.1: Summary of the Rules for Thermodynamic Data (p. 4) provides a detailed specification of the format required for entry of thermodynamics data. The first two lines in Figure 2.1: Excerpts from the *therm.dat* Thermodynamic Database File (p. 4) are required at the top of a thermodynamic database file; the first line specifies that the following is a set of thermodynamic data, while the second line provides the three temperatures used in the fitting process (a low temperature, break temperature, and high temperature). The user must also adhere to these specifications when placing thermodynamic data within the *Gas-phase Kinetics* or *Surface Kinetics* input file.

The default format (see Table 2.1: Summary of the Rules for Thermodynamic Data (p. 4) and Table 2.2: Fortran Format Descriptions from Table 2.1: Summary of the Rules for Thermodynamic Data (p. 5)) is a minor modification of that used by Gordon and McBride[1] (p. 331) for the Thermodynamic Database in the NASA Chemical Equilibrium code. However, ANSYS Chemkin-Pro allows a different midpoint temperature for the fits to the properties of each chemical species. We also allow a species to be composed of a maximum of nine elements, not four, on Line 3. Additional extensions allowed by Chemkin-Pro for multiple temperature ranges and for very large molecular clusters are described in Using More than Two Temperature Ranges (p. 7) and Creating Very Large Molecules with Unlimited Number of Elements (p. 8) , respectively. Despite these extensions, however, Chemkin-Pro can use the NASA database directly without any modification. The format conventions are summarized in Table 2.2: Fortran Format Descriptions from Table 2.1: Summary of the Rules for Thermodynamic Data (p. 5) .

As indicated in Table 2.1: Summary of the Rules for Thermodynamic Data (p. 4) , the pertinent information includes the species name, the elemental composition of the species, and the temperature ranges over which the polynomial fits to thermodynamic data are valid. The fits to C_p^o/R, H^o/RT, and S^o/R

consist of seven coefficients for each of two temperature ranges, see Equation 2.18 , Equation 2.22 and Equation 2.28 of the Chemkin-Pro Theory Manual . Further information about the fitting procedure can be found in the Chemkin-Pro Theory Manual as well as Using the FITDAT Utility (p. 99) .

Figure 2.1: Excerpts from the *therm.dat* Thermodynamic Database File

```
THERMO
   300.000  1000.000  5000.000
(CH2O)3            70590C   3H   6O   3     G  0300.00   4000.00  1500.00      1
 0.01913678E+03 0.08578044E-01-0.08882060E-05-0.03574819E-08 0.06605142E-12    2
-0.06560876E+06-0.08432507E+03-0.04662286E+02 0.06091547E+00-0.04710536E-03    3
 0.01968843E-06-0.03563271E-10-0.05665403E+06 0.04525264E+03                   4
AL                 62987AL  1               G  0300.00   5000.00  0600.00      1
 0.02559589E+02-0.10632239E-03 0.07202828E-06-0.02121105E-09 0.02289429E-13    2
 0.03890214E+06 0.05234522E+02 0.02736825E+02-0.05912374E-02-0.04033937E-05    3
 0.02322343E-07-0.01705599E-10 0.03886794E+06 0.04363879E+02                   4
END
```

Table 2.1: Summary of the Rules for Thermodynamic Data

Line #	Contents	Format[a]	Note in following table [b]	Column
1	THERMO (or THERMO ALL)[c]	Free	c	Any
2	Temperature ranges for 2 sets of coefficients: lowest T, common T, and highest T [d]	3F10.0	d	1 to 30
3	Species name (must start in Column 1)	16A1	e	1 to 16
	Date (not used)	6A1	f	19 to 24
	Atomic symbols and formula	4(2A1, I3)	g	25 to 44
	Phase of species (S, L, or G for solid, liquid, or gas)	A1	h	45
	Low temperature	E10.0	i	46 to 55
	High temperature	E10.0	i	56 to 65
	Common temperature (if needed, else blank)	E8.0	j	66 to 73
	Atomic symbols and formula (if needed, else blank)	2A1, I3	k	74 to 78

Line #	Contents	Format[a]	Note in following table [b]	Column
	The integer 1. This is a **mandatory** element and **must** appear in column 80.	I1	I	80
	Atomic symbols and formula (if needed, else blank), or & to indicate continuation to next line (See Creating Very Large Molecules with Unlimited Number of Elements (p. 8) for further information)	4(2A1, I3)	g	81 to 100
4	Coefficients a_1 through a_5 in Equation 2.18 , Equation 2.22 and Equation 2.28 of the Chemkin-Pro Theory Manual , for upper temperature interval	5(E15.8)	m	1 to 75
	The integer 2	I1	I	80
5	Coefficients a_6, a_7 for upper temperature interval, and a_1, a_2, and a_3 for lower temperature interval	5(E15.8)	m	1 to 75
	The integer 3	I	I	80
6	Coefficients a_4, a_5, a_6, a_7 for lower temperature interval	4(E15.8)	n	1 to 60
	The integer 4	I1	I	80
..	Repeat lines 3 - 6 for each species			
last	End (Optional, end of thermodynamic data.)	Free	c	Any

[a]The format string in this column follows the convention of FORTRAN documentation, as detailed in the notes provided in Table 2.2: Fortran Format Descriptions from Table 2.1: Summary of the Rules for Thermodynamic Data (p. 5) .

[b]See Table 2.2: Fortran Format Descriptions from Table 2.1: Summary of the Rules for Thermodynamic Data (p. 5)

[c]Use only when all thermodynamic data are to be taken from Pre-processor input.

[d] When inserting thermodynamic data directly in the *Gas-phase Kinetics* and *Surface Kinetics* input files, Line 2 should only be included with `THERMO ALL` option (See *Gas-phase Kinetics* and *Surface Kinetics* for more information).

Table 2.2: Fortran Format Descriptions from Table 2.1: Summary of the Rules for Thermodynamic Data (p. 4)

Note	Format	Format Description
c	FREE	The particular input described can be in any column of the input line.
d	3F10.0	3 Floating-point (real) values are allowed; each is allocated 10 columns.
e	16A1	16 Alpha-numeric characters are allowed in these columns (some may be blank).
f	6A1	6 Alpha-numeric characters are allowed in these columns (some may be blank).

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Note	Format	Format Description
g	4(2A1,I3)	There can be 4 sets of data; each set is allowed 2 Alpha-numeric columns (an element symbol) followed by 3 columns containing an Integer value (element count).
h	A1	1 Alpha-numeric character is allowed.
i	E10.0	10 columns are allocated for a real value, and scientific notation (E format) is allowed.
j	E8.0	8 columns are allocated for a real value, and scientific notation (E format) is allowed.
k	2A1,I3	2 Alpha-numeric columns (an element symbol) followed by 3 columns for an integer value (element count).
l	I1	One column is allowed for an integer value.
m	5(E15.8)	5 real values are allowed, with 15 columns allocated for each value, and scientific notation is allowed to have up to 8 values after the decimal point.
n	4(E15.8)	4 real values are allowed, with 15 columns allocated for each value, and scientific notation is allowed to have up to 8 values after the decimal point.

The first thermodynamic data line must start with the word THERMO (or THER). If the data appears inside of a *Gas-phase Kinetics* or *Surface Kinetics* input file, then the addition entry ALL (i.e., the first line reads THERMO ALL) tells the pre-processor that all thermodynamic data for the species associated with that chemistry input are included in the chemistry input file. This will cause the pre-processor not to try to open or read a Thermodynamic database file.

If the data are in a thermodynamics database file, or if THERMO ALL precedes within a *Gas-phase Kinetics* or *Surface Kinetics* input file, then the next line must be Line 2 of Table 2.1: Summary of the Rules for Thermodynamic Data (p. 4) . Otherwise Line 2 is skipped. In any case, the subsequent thermodynamic data lines must be in the format of Lines 3 - 6 of Table 2.1: Summary of the Rules for Thermodynamic Data (p. 4) . (For the THERMO option within a kinetics input file, the midpoint temperature is taken from Line 2 information already in the Thermodynamic Database associated with the chemistry set.)

Figure 2.2: Examples of Thermodynamic Data (p. 7) shows some examples of thermodynamic property input, as they might occur within a *Gas-phase Kinetics* input file. In these examples for OH, OH+, and OH-, it is seen from columns 25 - 34 that the elemental composition of each molecule is one O atom and one H atom. In addition, columns 35 - 39 indicate that two of the species, OH+, and OH-, are ionic since they contain -1 and +1 electrons (E), respectively. The G in column 45 indicates that all three species are gaseous. (This phase information is ignored by *Gas-phase Kinetics*.) The 1000.00 in columns 66 - 73 for OH indicates that the common temperature between the high- and low-temperature fits is 1000.00 K. If columns 66 - 73 are left blank, as they are for OH+ and OH-, then the common temperature is that given in columns 11 - 20 in Table 2.1: Summary of the Rules for Thermodynamic Data (p. 4) , which in this example is in the Thermodynamic Database. An alternative format is shown for OH if more than two temperature ranges are required. In this case we've given the molecule a different name, "MyOH ", but the elemental composition is the same as for OH. The line after the elemental composition contains the TEMP description of minimum, common, and maximum temperatures, and a set of coefficients for each temperature range, ordered from highest to lowest.

Figure 2.2: Examples of Thermodynamic Data

```
THERMO
OH                121286O   1H   1          G  0300.00   5000.00  1000.00      1
 0.02882730E+02 0.10139743E-02-0.02276877E-05 0.02174683E-09-0.05126305E-14    2
 0.03886888E+05 0.05595712E+02 0.03637266E+02 0.01850910E-02-0.16761646E-05    3
 0.02387202E-07-0.08431442E-11 0.03606781E+05 0.13588605E+01                   4
OH+               121286O   1H   1E  -1     G  0300.00   5000.00              1
 0.02719058E+02 0.15085714E-02-0.05029369E-05 0.08261951E-09-0.04947452E-13    2
 0.15763414E+06 0.06234536E+02 0.03326978E+02 0.13457859E-02-0.03777167E-04    3
 0.04687749E-07-0.01780982E-10 0.15740294E+06 0.02744042E+02                   4
OH-               121286O   1H   1E   1     G  0300.00   5000.00              1
 0.02846204E+02 0.10418347E-02-0.02416850E-05 0.02483215E-09-0.07775605E-14    2
-0.01807280E+06 0.04422712E+02 0.03390037E+02 0.07922381E-02-0.01943429E-04    3
 0.02001769E-07-0.05702087E-11-0.01830493E+06 0.12498923E+01                   4
MyOH                   0O   1H   1    0    0G   300.000  5000.000            0 1
TEMP   300.000  1000.000  2500.000  5000.000
 0.30563941E+01 0.89059362E-03-0.20849917E-06 0.24115927E-10-0.10516720E-14
 0.37260112E+04 0.44780081E+01
 0.34298433E+01-0.25250392E-03 0.80470663E-06-0.33336490E-09 0.43425671E-13
 0.37097800E+04 0.26751302E+01
 0.37695923E+01-0.59256858E-03-0.21359336E-06 0.13644331E-08-0.63575666E-12
 0.35908836E+04 0.78130486E+00
END
```

The following is a summary of the possibilities for specifying thermodynamic data:

- **Case 1**: All thermodynamic data from database file

  1. A database file is opened during pre-processing (e.g. *therm.dat*).
  2. No THERMO data required in the *Gas-phase* or *Surface Kinetics* input file.

- **Case 2**: Thermodynamic data from database and input files

  1. A database file is opened during pre-processing (e.g. *therm.dat*).
  2. Include the following lines in the *Gas-phase* or *Surface Kinetics* input file, after the species data:

     ```
     THERMO
     Data in Table 2.1: Summary of the Rules for Thermodynamic Data (p. 4)
      format (lines 3 - 6 repeated) for each species not in the database or to override species in database
     END
     ```

- **Case 3**: All thermodynamic data from input file

  1. No Thermodynamic database file is required.
  2. Include the following lines in the *Gas-phase* or *Surface Kinetics* input file, after the species data:

     ```
     THERMO ALL
     Data in Table 2.1: Summary of the Rules for Thermodynamic Data (p. 4)

     format (lines 3 - 6 repeated) for at least all species named in the species data
     END
     ```

2.1.1. Using More than Two Temperature Ranges

An alternative input data format allows specification of more than two temperature ranges. Use of this format provides more flexibility in describing the thermodynamic data for complex functions of temperature. This alternative approach is summarized in Table 2.3: Alternative Format for Specifying More than Two Temperature Ranges (p. 8) . The alternative lines used in place of lines 4 - 6 of Table 2.1: Summary

of the Rules for Thermodynamic Data (p. 4) . Line 1 specifies all of the temperature values that define the temperature intervals. Lines 2 and Line 3 are then repeated for each specified temperature interval, in descending order of temperature ranges.

Table 2.3: Alternative Format for Specifying More than Two Temperature Ranges

Alternative lines for more than 2 temperature intervals (in place of Lines 4 - 6 in Table 2.1: Summary of the Rules for Thermodynamic Data (p. 4)):			
Line #	**Contents**	**Format**	**Column**
1	TEMP followed by space-delimited minimum fit temperature, common temperatures in increasing order, and maximum fit temperature.	A4, Free	1 to 80
2	Coefficients a_1 - a_5 for a temperature interval	5(E15.8)	1 to 75
3	Coefficients a_6, a_7 for a temperature interval	2(E15.8)	1 to 30

2.1.2. Creating Very Large Molecules with Unlimited Number of Elements

There are some cases where users may want to define very large molecules that contain many elements or that may be composed of a very large number of atoms for a particular element. For this purpose, we have extended the thermodynamic data format to allow users to provide un-limited number of elements and un-constrained composition. Figure 2.3: Examples of Very Large Molecules (p. 8) shows an example (for illustration purposes only) of using this extended format to describe a molecule called CLUSTER1 that consists of 2326 carbon atoms, 895 hydrogen atoms, 18 nitrogen atoms, 53 oxygen atoms, and 32 sulfur atoms. The extended format is enabled by putting a & character at the end of Line 3 (Table 2.1: Summary of the Rules for Thermodynamic Data (p. 4)), in column 81. Any number of continuation lines may subsequently be included by adding an ampersand (&) at the end of a preceding line. The composition information used on these continuation lines is in free format, which consists of an element symbol, followed by the number of those atoms in the molecule, followed by another element symbol, and so forth.

Figure 2.3: Examples of Very Large Molecules

```
CLUSTER1          121086                    G   300.000  5000.000 1000.00      1&
C 2326  H 895 N 18  O 53  S 32

 2.60208700e+00-1.78708100e-04 9.08704100e-08-1.14993300e-11 3.31084400e-16    2

 8.54215400e+04 4.19517700e+00 2.49858500e+00 8.08577700e-05-2.69769700e-07    3

 3.04072900e-10-1.10665200e-13 8.54587800e+04 4.75345900e+00                   4
```

2.1.3. Surface-Coverage Dependent Enthalpy of Surface Species

The enthalpy of surface species can be specified to be dependent on surface coverage by entering a block of data starting with HFCOV within a block of thermodynamics data that is being specified for surface species. Coverage-dependent coefficients are a subset of the thermodynamic data, and are specified at the end of the surface thermodynamic data input. The linear coverage-dependent coefficients are explicitly specified under the HFCOV block, as shown below. The required input for each line consists of the species (*species_namej*) whose enthalpy is dependent on the second mentioned species coverage

(*species_namem*), and the coverage-dependent coefficient. The coverage-dependent coefficients must be specified in units of Kelvin.

Species_name $_j$ *Species_name* $_m$ $c_{j,m}$

Figure 2.4: HFCOV Thermodynamic Auxiliary Keyword Example

```
THERMO
O(S)                    C   0H   0O   1AG  1S  0300.00   5000.00  1000.00      1
 0.02542059E+02-0.02755061E-03-0.03102803E-07 0.04551067E-10-0.04368051E-14    2
 0.02923080E+06 0.04920308E+02 0.02946428E+02-0.16381665E+02 0.02421031E-04    3
-0.16028431E-08 0.03890696E-11 0.02914764E+06 0.02963995E+02                   4
C2H4(S)                 C   2H   4O   0AG  1S  0298.00   5998.00  1298.00      1
 0.68302018E+01 0.10144574E-01-0.34419787E-05 0.52897660E-09-0.30353490E-13    2
-0.98191467E+04-0.14816284E+02-0.40212793E+00 0.23298220E-01-0.80872187E-05    3
-0.25065598E-08 0.15984527E-11-0.71721868E+04 0.24925868E+02                   4
Cl(S)                   C   0H   0Cl  1AG  1S  0298.00   5998.00  1298.00      1
 0.68302018E+01 0.10144574E-01-0.34419787E-05 0.52897660E-09-0.30353490E-13    2
-0.98191467E+04-0.14816284E+02-0.40212793E+00 0.23298220E-01-0.80872187E-05    3
-0.25065598E-08 0.15984527E-11-0.71721868E+04 0.24925868E+02                   4

HFCOV ! UNITS ARE KELVIN (ENTHALPY UNITS/GAS CONSTANT)

 O(S)  O(S)     17966.784

 O(S) C2H4(S)   -1811.777

 O(S) Cl(S)    1409.160

 C2H4(S) Cl(S)  -4932.058

END

END
```

2.1.4. Gas Species Radiation Absorption Coefficients

For a gas species to absorb or emit infrared energy, its molecular structure must allow rotational and vibrational transitions and change in dipole moment. Accordingly, all monatomic species, such as O and H, and homonuclear diatomic species, such as O_2, H_2, and N_2, are "transparent" with respect to thermal radiation transfer. Most species that are actively absorbing and emitting infrared energy in flames can be neglected in the radiation calculation because they either have very low concentrations (e.g., NO and NO_2) or exist in cooler regions of the flow domain (e.g., hydrocarbon fuel species and CH_3 OH). The most important radiating species in hydrocarbon flames are CO_2 and H_2 O. The next important gas species are CO and CH_4, which emit about 1/10 as much infrared energy as the two dominant species.

The Planck mean absorption coefficients *a* for CO_2, H_2 O, CO, and CH_4 can be calculated by a narrow-band absorption coefficient model such as RADCAL.[2] (p. 331) Since narrow-band calculations require integrating absorption-line intensities over all wavelengths, direct integration of a narrow-band model into the radiation model would greatly decrease the computational performance.In order to incorporate good absorption coefficient data without sacrificing performance, we instead use polynomials to fit to temperature to represent the absorption coefficient data for individual gas species.[3] (p. 331)

Two types of temperature polynomials are accepted by the radiation model for gas species:

- **Polynomial 1:**

$$a_i(T) = \sum_j c_j T^j \quad \text{with } j = 0, \ldots, 6. \quad \left(\text{m}^{-1}\text{atm}^{-1}\right) \tag{2.1}$$

- **Polynomial 2:**

$$a_i(T) = \sum_j c_j / T^j \quad \text{with } j=0,\ldots,6. \quad \left(\text{m}^{-1}\text{atm}^{-1}\right) \tag{2.2}$$

The curve-fitting parameters c_j are entered as optional-data lines in the thermodynamic data file or in the thermodynamic data section of the mechanism input file. The absorption coefficient data line is formatted as

```
![_ AbsorptionCoefficient=" polynomial_form Tmin Tmax c0 c1 c2 c3 c4 c5 c6 " _]
```

`AbsorptionCoefficient` is the tag indicating the data are for species absorption coefficient calculation.`polynomial_form` indicates the form of polynomial used to fit the absorption coefficient. This must have a value of 1.0 or 2.0, corresponding to Equation 2.1 (p. 9) or Equation 2.2 (p. 10) , respectively.`Tmin` is the lower temperature bound in [K] for the fitted curve to be valid.`Tmax` is the upper temperature bound in [K] for the fitted curve to be valid. `cj` are the seven parameters of the polynomial.

This data line must appear before the thermodynamic data of the associated gas species. Different gas species can use a different form of polynomial. Each gas species can have as many as two absorption-coefficient data lines, which allows two sets of parameters of different temperature ranges. If there are two tag lines for a given gas species, they must be of the same type of polynomial and the low-temperature line should appear before the high-temperature line. The gas radiation model will not be activated if no absorption-coefficient data are included in the thermodynamic data file.

For example, the absorption coefficient data of CO are fitted to two type-1 polynomials over temperature ranges of 300—750 K and 750—2500 K, with the coefficients included in the optional-data lines as follows:

```
! [_ AbsorptionCoefficients=" 1 300 750 4.8E0 -6.95E-2 2.96E-4 -4.26E-7  2.03E-10 0 0 " _]
! [_ AbsorptionCoefficients=" 1 750 2500 10. -1.2E-2 4.78E-6 -5.87E-10 -2.53E-14 0 0 " _]
CO                TPIS79C   1O   1   00   00G   200.000  3500.000  1000.000    1
 2.71518561E+00 2.06252743E-03-9.98825771E-07 2.30053008E-10-2.03647716E-14    2
-1.41518724E+04 7.81868772E+00 3.57953347E+00-6.10353680E-04 1.01681433E-06    3
 9.07005884E-10-9.04424499E-13-1.43440860E+04 3.50840928E+00 8.67100000E+03    4
```

2.2. Standard State Enthalpies and Entropies at 298 K

Table 2.4: Standard State Enthalpies and Entropies at 298 K (p. 11) contains the standard state enthalpies and entropies for 778 species that are in the thermodynamic database file, *therm.dat* (see Figure 2.1: Excerpts from the *therm.dat* Thermodynamic Database File (p. 4) and Table 2.1: Summary of the Rules for Thermodynamic Data (p. 4) for the data and formats), which is included with all ANSYS Chemkin-Pro installs. The values in the table were determined by evaluating the polynomial expressions (Equation 2.3 (p. 10) and Equation 2.4 (p. 10) of the Chemkin-Pro Theory Manual) at the standard temperature of 298 K. Note the measured or derived data for $H^o(298)$ and $S^o(298)$ that were used in generating the coefficients in *therm.dat* are also included in Table 2.4: Standard State Enthalpies and Entropies at 298 K (p. 11) for comparison.

$$H^o(298) = RT\left[a_1 + \frac{a_2}{2}T + \frac{a_3}{3}T^2 + \frac{a_4}{4}T^3 + \frac{a_5}{5}T^4 + \frac{a_6}{T}\right] \tag{2.3}$$

$$S^o(298) = R\left[a_1 \ln T + a_2 T + \frac{a_3}{2}T^2 + \frac{a_4}{3}T^3 + \frac{a_5}{4}T^4 + a_7\right] \tag{2.4}$$

The units for enthalpies are (kcal)/mole and for entropies cal/(mole · K). The entries in Table 2.4: Standard State Enthalpies and Entropies at 298 K (p. 11) correspond to the *therm.dat* distributed with ANSYS Chemkin-Pro.

Table 2.4: Standard State Enthalpies and Entropies at 298 K

Species	$H^o(298)\text{kcal/mole}$		$S^o(298)\text{cal/(mole·K)}$	
	Data	**Fit**	**Data**	**Fit**
(CH2O)3	-110.70	-110.71	69.42	69.38
(CH3)2SICH2	12.30	12.37	80.37	82.41
AL	78.80	78.80	39.30	39.30
AL2H6	21.35	21.35	62.75	62.75
AL2ME6	-61.20	-61.20	131.05	131.06
ALAS	107.33	107.32	60.65	60.65
ALH	62.00	62.00	44.88	44.87
ALH2	41.95	41.95	54.40	54.40
ALH3	18.83	18.83	52.30	52.30
ALME	19.75	19.75	60.68	60.68
ALME2	12.75	12.75	77.40	77.40
ALME3	-20.30	-20.30	83.68	83.68
AR	0.00	0.00	36.98	36.98
AR+	364.91	364.91	39.75	39.74
AS	75.48	75.48	43.53	43.52
AS2	47.08	47.08	59.83	59.83
AS3	65.35	65.35	77.53	77.53
AS4	37.13	37.13	78.45	78.45
ASALME	70.00	70.00	81.60	81.60
ASALME2	63.25	63.25	91.00	91.00
ASGAET	82.75	82.75	95.20	95.20
ASGAET2	69.55	69.55	109.83	109.83
ASGAME	83.50	83.50	85.75	85.75
ASGAME2	81.25	81.25	91.00	91.00
ASGAMEH	93.75	93.75	84.73	84.73
ASH	61.75	61.75	50.20	50.20
ASH2	42.25	42.25	46.45	46.45
ASH3	16.63	16.63	55.65	55.65
ASME	59.20	59.20	63.80	63.80
ASME2	34.20	34.20	79.50	79.50
ASME3	2.93	2.93	85.78	85.78
B	133.80	133.80	36.65	36.64
B(S)	0.00	0.00	1.41	1.41

Species	$H^o(298)$ kcal/mole		$S^o(298)$ cal/(mole·K)	
	Data	**Fit**	**Data**	**Fit**
BCL	33.80	33.80	50.94	50.94
BCL2	-19.00	-19.00	65.14	65.15
BCL3	-96.31	-96.31	69.33	69.33
BE	78.25	78.25	32.54	32.54
BE(S)	0.00	0.00	2.28	2.28
BE2SIO4(S)	-506.03	-506.03	15.34	15.33
BE3B2O6(S)	-741.96	-741.96	24.00	23.97
BE3N2(A)	-140.60	-140.60	8.16	8.15
BE3N2(L)	-116.40	-116.41	9.43	9.41
BEAL2O4(S)	-549.90	-549.90	15.84	15.84
BEB2O4	-323.00	-323.00	78.08	78.08
BEBO2	-115.20	-115.20	63.40	63.41
BEBR	28.71	28.71	54.59	54.59
BEBR2	-54.80	-54.80	65.44	65.44
BEBR2(S)	-85.00	-85.00	24.00	23.99
BECL	14.50	14.50	51.98	51.98
BECL2	-86.10	-86.10	60.26	60.26
BECL2(A)	-117.34	-117.34	19.76	19.75
BECL2(B)	-118.60	-118.60	18.12	18.11
BECLF	-137.00	-137.00	58.89	58.89
BEF	-40.60	-40.60	49.15	49.14
BEF2	-190.25	-190.25	54.36	54.36
BEF2(L)	-244.27	-244.28	14.32	14.32
BEH	76.77	76.77	42.24	42.23
BEH+	276.40	276.40	40.76	40.75
BEH2	30.00	30.00	41.35	41.33
BEH2O2	-161.70	-161.70	55.89	55.91
BEH2O2(A)	-215.80	-215.81	12.80	12.78
BEH2O2(B)	-216.50	-216.51	12.00	11.98
BEI	40.63	40.63	56.69	56.69
BEI2	-15.30	-15.30	69.65	69.65
BEI2(S)	-45.10	-45.11	28.80	28.78
BEN	101.98	101.98	49.87	49.87
BEO(A)	-145.40	-145.39	3.29	3.31
BEO(B)	-143.80	-143.79	3.97	3.99
BEOH	-27.40	-27.40	50.07	50.07
BES(S)	-56.00	-56.00	8.85	8.84

Species	$H^o(298)$ kcal/mole		$S^o(298)$ cal/(mole·K)	
	Data	**Fit**	**Data**	**Fit**
BESO4(A)	-287.00	-287.01	18.64	18.60
BESO4(B)	-286.73	-286.75	18.94	18.91
BESO4(GAM)	-282.06	-282.07	24.09	24.06
BN	-59.97	-59.97	3.54	3.53
C	171.29	171.29	37.76	37.76
C(S)	0.00	0.00	1.37	1.37
C+	432.47	432.02	36.94	36.93
C-	140.61	140.61	36.16	36.16
C2	200.22	200.23	47.63	47.63
C2-	106.00	106.00	46.96	46.96
C2CL3	54.37	54.36	79.93	79.89
C2CL5	7.38	7.39	94.52	94.75
C2CL6	-32.43	-32.44	93.15	93.04
C2F6	-321.20	-321.20	79.37	79.38
C2H	135.00	135.00	51.10	49.55
C2H2	54.19	54.19	48.00	48.01
C2H3	0.00	68.41	0.00	55.32
C2H4	12.54	12.54	52.40	52.37
C2H5	0.00	28.01	0.00	60.13
C2H6	0.00	-20.04	0.00	54.72
C2HCL	51.10	51.10	57.81	57.82
C2HCL5	-35.19	-35.19	91.61	91.51
C2N	133.00	133.00	55.16	55.16
C2N2	73.87	73.87	57.71	57.72
C2O	68.50	68.50	55.68	55.67
C3	196.00	196.00	56.68	56.66
C3H2	129.39	129.60	62.01	64.81
C3H2(S)	141.43	141.43	59.74	59.75
C3H4	47.67	47.63	57.99	57.94
C3H4C	67.99	68.00	57.94	57.95
C3H4P	45.77	45.77	58.89	58.89
C3H6	0.00	4.89	0.00	61.51
C3H8	0.00	-24.82	0.00	64.56
C3O2	-22.38	-22.38	65.96	65.96
C4	232.00	232.00	54.54	54.55
C4H	0.00	155.08	0.00	60.89
C4H10	-32.02	-31.84	70.94	71.79

Species	$H^o(298)$ kcal/mole		$S^o(298)$ cal/(mole·K)	
	Data	**Fit**	**Data**	**Fit**
C4H2	0.00	111.70	0.00	59.77
C4H6	0.00	34.96	0.00	68.16
C4H8	0.00	-0.13	0.00	73.55
C5	234.00	234.01	57.81	57.82
C5H	0.00	185.99	0.00	62.20
C5H12	0.00	-34.98	0.00	83.48
C5H2	0.00	165.23	0.00	63.69
C5H5	63.83	63.84	68.10	68.13
C5H6	0.00	31.99	0.00	64.45
C6H	0.00	213.15	0.00	74.10
C6H10	0.00	-1.00	0.00	74.75
C6H14	0.00	-39.91	0.00	92.87
C6H2	0.00	169.66	0.00	70.92
C6H3	0.00	158.45	0.00	76.30
C6H4	99.66	99.67	68.25	68.26
C6H5	79.42	79.43	69.81	69.82
C6H5(L)	140.58	140.58	83.39	84.26
C6H5O	10.34	10.35	74.86	74.87
C6H5OH	-25.13	-25.01	76.96	76.93
C6H6	0.00	19.81	0.00	64.35
C6H7	47.94	47.96	73.07	73.07
C8H	0.00	288.86	0.00	78.39
C8H2	0.00	226.15	0.00	75.94
CA	42.85	42.85	36.99	36.98
CA(A)	0.00	0.00	9.93	9.93
CA(B)	0.12	0.12	10.15	10.15
CA(L)	2.61	2.60	12.11	12.10
CA+	185.30	185.30	38.37	38.37
CA2	82.66	82.66	61.29	61.29
CABR	-11.81	-11.81	60.42	60.41
CABR2	-92.00	-92.00	75.20	75.20
CABR2(S)	-163.30	-163.30	31.00	30.99
CACL	-25.00	-25.00	57.71	57.71
CACL2	-112.70	-112.70	69.35	69.35
CACL2(S)	-190.20	-190.20	25.00	24.99
CAF	-65.00	-65.00	54.86	54.86
CAF2	-187.50	-187.50	65.41	65.42

Species	$H^o(298)$kcal/mole		$S^o(298)$cal/(mole·K)	
	Data	**Fit**	**Data**	**Fit**
CAH2O2	-145.98	-145.97	68.23	68.25
CAH2O2(S)	-235.68	-235.68	19.93	19.93
CAI	-1.21	-1.21	62.43	62.42
CAI2	-61.70	-61.70	78.26	78.26
CAO	10.50	10.50	52.49	52.52
CAO(S)	-151.79	-151.79	9.13	9.15
CAOH	-46.34	-46.34	56.25	56.26
CAOH+	88.21	88.21	54.92	54.93
CAS	29.54	29.52	55.56	55.55
CCL	106.10	106.10	52.46	52.45
CCL2	53.02	53.02	63.29	63.28
CCL2CCLO	-24.27	-24.27	85.06	84.97
CCL2CCLOH	-44.66	-44.69	83.09	82.88
CCL2CH	62.30	62.29	71.95	71.93
CCL2HOO	-1.37	-1.33	78.30	79.17
CCL2OHCH2	-22.77	-22.60	79.91	80.63
CCL2OHCHCL	-31.69	-31.54	87.57	89.10
CCL3	16.58	16.58	72.20	72.20
CCL3CCLH2	-35.29	-35.28	85.57	85.59
CCL3CCLO	-56.49	-56.47	89.99	90.43
CCL3CH2	18.79	18.89	81.61	82.80
CCL3CHCL	11.06	11.09	88.40	89.03
CCL3CHO	-45.51	-45.47	83.71	85.04
CCL3OO	-0.74	-0.71	83.14	83.46
CCL4	-20.22	-20.22	78.91	78.91
CCLH2OO	1.22	1.27	71.06	71.68
CH	142.00	142.00	43.72	43.71
CH+	388.80	388.80	41.00	41.00
CH2	92.48	92.48	46.72	46.71
CH2(S)	101.50	101.50	45.10	45.10
CH2CCL	61.43	61.39	64.24	64.15
CH2CCL2	0.75	0.71	68.84	68.76
CH2CCLOH	-37.01	-36.94	69.00	69.35
CH2CHCCH	69.14	69.14	66.49	67.33
CH2CHCCH2	74.11	74.14	74.70	75.31
CH2CHCH2	38.70	38.64	64.39	64.73
CH2CHCHCH	86.13	86.09	72.75	73.06

Species	$H^o(298)$ kcal/mole		$S^o(298)$ cal/(mole·K)	
	Data	**Fit**	**Data**	**Fit**
CH2CHCHCH2	28.33	28.29	69.74	70.44
CH2CHCL	4.69	4.67	63.03	62.98
CH2CL	27.08	27.07	59.28	59.28
CH2CL2	-22.83	-22.83	64.57	64.57
CH2CLCCL2	6.02	6.05	82.70	83.32
CH2CLCCLO	-58.33	-58.30	77.51	78.10
CH2CLCH2	23.00	23.10	68.36	69.46
CH2CLCH2CL	-32.35	-32.33	72.20	72.45
CH2CLCHCL	13.10	13.14	75.92	76.80
CH2CLCHCL2	-35.23	-35.22	80.05	80.12
CH2CLCHO	-41.67	-41.66	72.11	74.04
CH2CO	0.00	-12.40	0.00	57.78
CH2F2	-107.71	-107.71	58.94	58.91
CH2HCO	0.00	6.00	0.00	63.99
CH2O	-27.70	-27.70	52.26	52.24
CH2OH	-4.21	-4.10	58.93	58.87
CH2OHCCL2	-23.26	-23.21	82.18	82.65
CH2OHCHCL	-16.90	-16.79	74.35	74.94
CH2SICL	45.68	45.67	69.39	69.33
CH2SICL3	-87.71	-87.71	90.16	91.94
CH2SIH2CL	-0.90	-0.87	74.23	75.92
CH2SIHCL2	-44.67	-44.67	83.30	85.08
CH3	34.82	34.82	46.38	46.37
CH3C(O)CL	-56.93	-56.86	70.60	71.87
CH3CC	123.81	123.82	60.28	60.27
CH3CCCH2	74.33	74.34	78.57	80.35
CH3CCCH3	40.92	40.94	71.58	73.36
CH3CCH2	61.04	61.09	69.12	69.24
CH3CCL	61.68	61.73	66.18	67.81
CH3CCL2	10.33	10.42	75.42	76.27
CH3CCL3	-33.55	-33.51	76.48	76.61
CH3CCLO	-56.93	-56.86	70.60	71.87
CH3CH2CCH	44.66	44.75	71.46	71.43
CH3CH2CH2CH3	-30.64	-30.50	72.68	73.31
CH3CH2CL	-27.17	-27.10	66.00	66.33
CH3CH2O	-0.51	-0.44	65.48	65.81
CH3CHCH	64.70	64.75	68.49	68.74

Species	$H^o(298)$ kcal/mole		$S^o(298)$ cal/(mole·K)	
	Data	**Fit**	**Data**	**Fit**
CH3CHCL	18.22	18.30	68.46	69.48
CH3CHCL2	-32.08	-32.02	72.79	73.04
CH3CHOH	-14.34	-14.17	66.73	67.77
CH3CL	-20.00	-20.00	55.99	55.97
CH3CO	0.00	-5.40	0.00	63.73
CH3F	-56.00	-56.00	53.25	53.22
CH3HCO	0.00	-39.51	0.00	63.04
CH3NO	18.88	18.95	62.33	63.46
CH3NO2	-16.83	-16.84	70.26	72.03
CH3O	0.00	3.89	0.00	54.60
CH3OCH3	-43.80	-43.72	63.74	64.35
CH3OCL	-14.06	-13.98	64.97	65.42
CH3OH	0.00	-48.06	0.00	57.27
CH3ONO	-15.30	-15.25	66.63	66.87
CH3ONO2	-26.12	-26.06	71.34	71.63
CH3SICL	-2.47	-2.44	70.99	72.63
CH3SIH2SIH	-10.12	-9.96	88.03	91.66
CH3SIH2SIH2CH3	-10.92	-10.79	88.03	90.60
CH3SIHCL2	-93.81	-93.74	79.61	80.53
CH4	-17.90	-17.90	44.49	44.46
CHCL	80.00	80.00	56.12	56.11
CHCL2	19.51	19.51	65.08	65.08
CHCL2CCL2	8.53	8.53	90.99	92.74
CHCL2CCLO	-57.87	-57.85	84.59	85.22
CHCL2CH2	20.23	20.24	78.03	79.99
CHCL2CHCL	10.32	10.35	82.79	83.54
CHCL2CHCL2	-36.03	-36.02	85.18	85.39
CHCL3	-23.25	-23.25	70.64	70.64
CHCLCCL	55.99	55.98	72.48	72.40
CHCLCCLOH	-43.59	-43.51	76.26	76.42
CHCLCH	64.77	64.81	64.47	64.48
CHCLCHCL	-1.15	-1.15	69.24	69.19
CHCLCHOH	-38.64	-38.56	68.93	69.13
CHCLOH	-16.71	-16.65	65.30	65.41
CHCLOHCH2	-15.20	-15.08	74.53	76.30
CHCLOHCHCL	-24.95	-24.85	82.31	83.81
CHF	30.00	30.00	53.36	53.35

Species	$H^o(298)$ kcal/mole		$S^o(298)$ cal/(mole·K)	
	Data	**Fit**	**Data**	**Fit**
CHF3	-166.60	-166.60	62.03	62.02
CHOHCLCCL2	-31.95	-31.84	88.72	90.27
CHSICL	89.13	89.13	70.30	70.30
CHSICL2	29.60	29.61	81.07	82.86
CHSICL3	-35.28	-35.27	88.41	90.19
CHSIH2CL	50.52	50.55	73.11	74.85
CHSIHCL	67.86	67.93	70.62	72.26
CHSIHCL2	7.19	7.22	80.87	82.62
CL	28.99	28.99	39.45	39.45
CL(CH3)SICH2	-13.11	-13.08	78.44	79.58
CL2	0.00	0.00	53.29	53.29
CL2CCCL2	-5.66	-5.67	81.51	81.41
CL2CCHCL	-3.95	-3.96	77.64	77.54
CL2CCHO	-12.45	-12.46	77.67	77.57
CL2CHOH	-66.56	-66.41	71.53	72.50
CL2CO	-52.70	-52.70	67.64	67.64
CL2COH	-22.80	-22.68	73.07	73.68
CL2HCO	-4.12	-4.12	71.65	71.64
CL2SI(CH3)2	-113.74	-113.59	88.72	90.45
CL2SI(CH3)CH2	-64.26	-64.18	92.21	94.86
CL2SICH2	-34.22	-34.25	75.18	75.10
CL2SICH3	-52.78	-52.71	80.76	81.74
CL2SISI	32.71	32.71	79.88	79.88
CL2SISICL	-24.42	-24.41	92.40	92.46
CL2SISICL2	-95.69	-95.69	102.08	102.02
CL3CCO	1500.00	1500.02	-5.27	87.34
CL3CO	-4.37	-4.37	78.35	78.35
CL3COH	-66.33	-66.23	77.64	79.21
CL3SICH3	-137.81	-137.74	84.47	85.28
CL3SISI	-26.17	-26.17	89.43	89.43
CL3SISICL	-99.56	-99.55	101.49	103.27
CLCCCL	56.20	56.20	64.28	64.28
CLCCO	42.24	42.25	68.92	68.87
CLCH2OH	-55.49	-55.49	69.49	71.45
CLCO	-6.48	-6.48	64.39	64.39
CLCOH	1.17	1.13	62.43	62.37
CLH2CO	-2.35	-2.35	64.42	64.41

Species	$H^o(298)\mathrm{kcal/mole}$		$S^o(298)\mathrm{cal/(mole{\cdot}K)}$	
	Data	**Fit**	**Data**	**Fit**
CLHCO	-44.30	-44.30	61.80	61.79
CLO	29.20	29.19	53.00	52.99
CLOCL	19.71	19.71	63.65	63.65
CLOO	33.60	33.60	63.54	63.53
CLSI(CH3)2	-26.19	-26.06	82.72	84.80
CLSI(CH3)2CH2	-37.20	-37.04	92.86	96.44
CLSI(CH3)3	-86.29	-86.08	90.84	93.65
CLSICH3	-2.86	-2.82	70.99	72.64
CLSISI	99.11	99.11	71.44	71.44
CLSISICL	33.48	33.48	81.76	81.88
CN	104.00	104.00	48.41	48.40
CN+	430.87	430.87	50.99	50.98
CN-	14.50	14.50	46.81	46.81
CN2	113.00	113.00	54.04	54.03
CNN	139.70	139.70	55.35	55.35
CNO	97.64	97.64	55.57	55.57
CO	-26.42	-26.42	47.21	47.21
CO2	-94.05	-94.05	51.07	51.07
CO2-	-105.50	-105.50	57.49	57.48
COS	-33.08	-33.08	55.32	55.33
CS	67.00	67.00	50.30	50.29
CS2	27.95	27.95	56.85	56.85
CSICL	146.05	146.06	68.07	68.07
CSICL2	89.11	89.11	76.71	76.71
CSICL3	9.05	9.05	86.79	86.79
CSIH2CL	105.85	105.85	69.88	69.88
CSIHCL	119.47	119.47	67.68	67.68
CSIHCL2	63.16	63.16	77.47	77.47
D	52.99	52.99	29.46	29.45
D2	0.00	0.00	34.62	34.62
DH	0.08	0.08	34.34	34.34
DIOXANE	-75.11	-75.12	71.76	71.72
E	0.00	0.00	0.00	4.98
F	18.90	18.90	36.15	36.14
F-	-61.08	-61.08	34.77	34.76
F2	-0.09	-0.09	48.14	48.14
F2N2(C)	16.40	16.40	62.07	62.08

Species	$H^o(298)$kcal/mole		$S^o(298)$cal/(mole·K)	
	Data	**Fit**	**Data**	**Fit**
F2O2	14.00	13.99	64.42	64.33
F2SINH	-146.95	-146.93	70.92	70.92
F3SIN	-200.02	-200.02	73.86	73.87
FNNF	17.88	17.88	63.07	63.47
FNO3	2.50	2.50	69.99	69.99
FO	26.00	26.00	51.77	51.76
FO2	3.00	3.00	61.90	61.90
FONO(C)	10.18	10.16	64.43	64.34
FONO(T)	14.13	14.12	64.88	64.79
FSIN	54.37	54.37	63.67	63.67
GA	68.53	68.52	43.83	43.82
GA2H6	31.50	31.50	69.05	69.05
GAAS	88.40	88.40	63.23	63.23
GAAS(3,C)	245.75	245.75	100.00	100.00
GAAS(3,L)	256.25	256.25	127.75	127.75
GAAS(5,C)	357.75	357.75	130.50	130.50
GAAS(5,L)	420.00	420.00	193.50	193.50
GAET	17.75	17.75	81.60	81.60
GAET2	4.50	4.50	100.43	100.43
GAET3	-17.05	-17.05	112.98	112.98
GAH	54.80	54.80	49.18	49.17
GAH2	41.00	41.00	56.00	56.00
GAH3	27.00	27.00	54.50	54.50
GAME	18.53	18.53	63.80	63.80
GAME2	16.42	16.43	80.55	80.55
GAME3	-10.88	-10.87	87.88	87.88
H	52.10	52.09	27.39	27.39
H(CH3)SICH2	26.36	26.39	70.27	71.37
H+	367.17	367.15	26.01	26.01
H-	33.23	33.19	26.02	26.01
H2	0.00	0.00	31.21	31.21
H2ALME	6.00	6.00	61.73	61.73
H2ASME	24.05	24.05	64.85	64.85
H2C4O	54.58	54.59	66.42	66.43
H2CCC	160.67	160.67	61.07	61.07
H2CCC(S)	133.42	133.42	58.50	58.49
H2CCCCCH	128.19	128.19	75.36	75.37

Species	$H^o(298)$ kcal/mole		$S^o(298)$ cal/(mole·K)	
	Data	**Fit**	**Data**	**Fit**
H2CCCCH	111.34	111.32	72.83	72.94
H2CCCCH2	75.53	75.49	64.77	65.12
H2CCCH	83.03	83.04	61.48	61.48
H2CCCLO	-11.53	-11.54	69.74	69.67
H2CCH(SICL2H)	-66.26	-66.22	84.68	85.71
H2CCH2OH	-4.57	-4.46	69.01	71.17
H2CCHO	3.55	3.51	61.95	61.87
H2CCHSI	97.77	97.77	66.01	65.94
H2CCHSIH	73.54	73.58	66.68	66.79
H2CCHSIH2	58.21	58.21	69.03	68.94
H2CCHSIH3	20.65	20.70	68.95	69.47
H2CLSICH3	-50.13	-50.06	72.04	73.01
H2CLSISICL3	-146.58	-146.56	100.61	101.70
H2CN	59.10	59.11	53.59	53.59
H2CNCH2	56.61	56.53	61.18	61.01
H2CNCH2O	45.02	44.98	68.50	68.38
H2CNCHO	-0.52	-0.56	66.78	66.64
H2CNH	21.89	21.85	54.81	55.45
H2CNNHO	49.78	49.72	67.28	67.10
H2CNNO	58.35	58.36	66.42	66.98
H2CNNO2	33.62	33.64	72.48	73.06
H2CNO	41.46	41.42	61.08	61.01
H2CNO2	36.44	36.47	65.53	65.58
H2CONO	33.07	33.10	68.31	68.54
H2GAET	-2.30	-2.30	83.68	83.68
H2GAME	15.00	15.00	64.85	64.85
H2NF	-6.49	-6.49	54.73	54.72
H2NNO	18.25	18.21	60.27	60.18
H2NO	15.82	15.82	55.69	55.68
H2NOH	-12.23	-12.16	56.04	56.17
H2O	-57.80	-57.80	45.11	45.10
H2O(L)	0.00	-68.31	0.00	16.71
H2O(S)	0.00	-69.96	0.00	10.71
H2O2	0.00	-32.53	0.00	55.65
H2S	-4.90	-4.90	49.15	49.14
H2SI(CH3)2	-23.20	-23.08	72.44	73.83
H2SI(CH3)CH2	25.55	25.61	77.77	79.83

Species	$H^o(298)$ kcal/mole		$S^o(298)$ cal/(mole·K)	
	Data	**Fit**	**Data**	**Fit**
H2SI(NH2)2	-37.30	-37.15	71.62	72.38
H2SIC	167.19	167.19	60.31	60.21
H2SICCH	90.95	90.95	66.92	66.80
H2SICH	105.35	105.42	62.48	63.58
H2SICH2	40.75	40.72	59.94	59.85
H2SICH3	33.05	33.11	64.52	65.41
H2SIN	149.19	149.19	59.51	59.51
H2SINH	40.99	40.95	59.90	60.09
H2SINH2	28.03	28.09	65.77	65.79
H2SINH3	23.78	23.85	66.78	66.78
H2SISIH2	62.90	62.87	66.69	66.89
H3ASGAET3	-11.00	-11.00	124.48	124.48
H3ASGAME3	-4.70	-4.70	102.50	102.50
H3CONHO	6.46	6.56	71.67	72.65
H3SIC	147.61	147.61	61.79	61.71
H3SICCH	53.02	53.02	64.11	64.02
H3SICH	92.67	92.67	65.63	66.94
H3SICH2	41.54	41.54	67.62	68.97
H3SICH3	-7.32	-7.25	61.75	62.43
H3SIN	234.59	234.60	56.93	56.93
H3SINH	51.32	51.34	65.52	66.21
H3SISIH	74.91	74.96	67.99	69.32
H3SISIH3	19.11	19.16	68.06	68.06
HALME	27.25	27.25	62.78	62.78
HALME2	-6.73	-6.72	75.32	75.33
HASALME	56.50	56.50	83.68	83.68
HASGAET	69.15	69.15	97.28	97.28
HASGAME	70.00	70.00	87.88	87.88
HASME	42.58	42.58	65.90	65.90
HASME2	18.10	18.10	78.45	78.45
HCCCHCCH	134.95	134.95	73.15	73.17
HCCCL	54.95	54.95	57.29	57.29
HCCHCCH	129.91	129.88	68.80	69.06
HCCO	42.44	42.44	60.74	60.73
HCCOH	20.42	20.43	58.69	58.70
HCCSICL2H	-31.76	-31.76	82.04	82.04
HCL	-22.06	-22.06	44.65	44.64

Species	$H^o(298)$ kcal/mole		$S^o(298)$ cal/(mole·K)	
	Data	**Fit**	**Data**	**Fit**
HCL2SICH3	-94.23	-94.16	79.61	80.53
HCL2SISICL2H	-145.25	-145.24	99.80	101.08
HCLCCCLO	-19.42	-19.43	77.51	77.40
HCLCCHO	-6.02	-6.03	70.20	70.09
HCLSI(CH3)2	-68.24	-68.09	81.59	83.53
HCLSI(CH3)CH2	-19.15	-19.06	83.79	86.52
HCLSICH2	2.62	2.59	68.45	68.37
HCLSICH3	-9.10	-9.03	72.91	74.00
HCLSISI	67.05	67.05	71.34	71.34
HCN	31.89	31.89	48.21	48.21
HCNH	66.15	66.10	55.58	55.90
HCNO	38.42	38.43	53.75	53.79
HCO	10.40	10.40	53.67	53.65
HCO+	199.10	199.10	48.59	48.59
HCOOH	-92.57	-92.61	59.32	59.26
HE	0.00	0.00	0.00	30.12
HE+	0.00	568.46	0.00	31.50
HF	-65.14	-65.14	41.51	41.50
HG2BR2(S)	-48.80	-48.80	52.28	52.27
HG2CL2(S)	-63.32	-63.32	46.02	46.00
HG2F2(S)	-116.00	-116.00	38.40	38.39
HG2I2(S)	-28.46	-28.47	57.67	57.66
HGAET	22.90	22.90	83.68	83.68
HGAET2	-2.30	-2.30	100.50	100.50
HGAME	29.00	29.00	65.90	65.90
HGAME2	2.50	2.50	79.50	79.50
HGBR	24.90	24.90	64.88	64.87
HGCL2	-34.97	-34.96	70.43	70.43
HGCL2(S)	-55.00	-55.00	34.54	34.53
HGF2	-70.19	-70.18	63.55	63.55
HGF2(S)	-101.00	-101.00	27.80	27.79
HGH	57.00	57.00	52.49	52.48
HGI	31.90	31.90	67.07	67.06
HGO	10.00	10.00	57.13	57.13
HGO(S)	-21.70	-21.70	16.80	16.79
HMEGAET	4.00	4.00	88.90	88.90
HN(OH)2	-24.72	-24.64	61.98	62.09

Species	$H^o(298)\text{kcal}/\text{mole}$		$S^o(298)\text{cal}/(\text{mole}\cdot\text{K})$	
	Data	**Fit**	**Data**	**Fit**
HN3	71.87	71.87	239.08	57.14
HNC	43.85	43.85	48.93	48.93
HNCN	76.43	76.43	59.36	59.36
HNCNH	35.61	35.71	57.31	57.42
HNCO	-28.22	-28.22	57.05	57.05
HNF	32.00	32.00	54.98	54.97
HNF2	-13.79	-13.79	60.06	60.06
HNNHO	21.91	21.86	58.70	58.63
HNNO	55.25	55.20	60.59	60.53
HNNONO	59.02	58.99	70.98	70.97
HNO	23.80	23.80	52.73	52.72
HNO2	-14.15	-14.15	56.75	56.73
HNO3	-32.10	-32.10	63.66	63.66
HNOH	21.05	21.06	55.78	55.78
HO2	2.50	2.50	54.73	54.72
HOCH2OH	-96.64	-96.53	61.14	61.31
HOCL	-18.64	-18.64	56.34	56.33
HOCN	-3.55	-3.53	57.66	59.25
HOCO	-46.31	-46.29	60.12	60.11
HONO	-18.34	-18.34	59.59	59.58
HONO2	-30.18	-30.18	63.20	63.16
HSI(CH3)2	18.27	18.38	74.81	76.56
HSI(CH3)2CH2	9.32	9.44	86.18	88.89
HSI(CH3)3	-39.40	-39.24	83.61	85.87
HSI(NH2)2	5.62	5.77	72.56	73.38
HSI(NH2)3	-64.86	-64.68	78.65	79.52
HSIC	184.85	184.85	58.24	58.13
HSICCH	104.97	104.97	64.44	64.32
HSICH2	85.83	85.81	60.64	60.53
HSICH3	48.84	48.90	62.04	63.21
HSICL	17.00	17.00	59.80	59.80
HSIN	92.99	92.99	54.76	54.75
HSINH	84.80	84.79	60.63	60.68
HSINH2	26.33	26.29	59.77	60.05
HSISICL	79.13	79.11	73.04	72.96
I*C3H7	0.00	18.20	0.00	60.09
K	21.31	21.31	38.30	38.30

Species	$H^o(298)$ kcal/mole		$S^o(298)$ cal/(mole·K)	
	Data	**Fit**	**Data**	**Fit**
K(L)	0.55	0.55	17.08	17.07
K+	122.90	122.90	36.92	36.92
K2	30.37	30.37	59.67	59.66
K2B4O7(S)	-796.90	-796.89	49.80	49.82
K2B6O10(S)	-1107.44	-1107.50	60.00	59.87
K2B8O13(S)	-1420.92	-1420.93	70.20	70.18
K2CO3(S)	-274.90	-274.91	37.17	37.15
K2H2O2	-156.50	-156.50	78.37	78.35
K2O(S)	-86.80	-86.79	22.50	22.51
K2O2(S)	-118.50	-118.47	27.00	27.05
K2SO4	-261.50	-261.50	87.49	87.50
K2SO4(A)	-343.62	-343.62	41.96	41.94
K2SO4(B)	-340.40	-340.41	45.96	45.94
K3CL6AL(S)	-500.00	-499.97	90.00	90.08
K3CL9AL2(S)	-683.60	-683.61	112.00	111.96
K3F6AL(S)	-795.00	-794.96	68.00	68.11
KBF4	-371.00	-371.00	75.35	75.36
KBO2	-161.10	-161.10	71.06	71.06
KBO2(S)	-237.80	-237.81	19.12	19.10
KBR	-43.04	-43.04	59.85	59.85
KBR(L)	-89.98	-89.99	25.23	25.22
KBR(S)	-94.12	-94.12	22.93	22.92
KCL	-51.31	-51.31	57.12	57.11
KCL(L)	-100.81	-100.81	20.71	20.71
KCL(S)	-104.37	-104.37	19.73	19.73
KCL4AL(S)	-286.00	-286.01	47.00	46.98
KCLO4(S)	-102.80	-100.21	36.10	40.62
KCN	19.00	19.00	60.48	60.47
KCN(L)	-24.89	-24.89	32.10	32.09
KCN(S)	-27.12	-27.12	30.54	30.53
KF	-78.10	-78.10	54.14	54.13
KF(L)	-132.52	-132.52	16.17	16.16
KF(S)	-135.90	-135.90	15.91	15.91
KH	29.40	29.40	47.30	47.30
KH(S)	-13.82	-13.81	12.00	12.02
KI	-30.00	-30.00	61.70	61.70
KI(L)	-74.77	-74.77	27.27	27.26

Species	$H^o(298)$kcal/mole		$S^o(298)$cal/(mole·K)	
	Data	**Fit**	**Data**	**Fit**
KI(S)	-78.37	-78.37	25.43	25.42
KO	17.00	17.00	56.86	56.86
KO-	-33.00	-33.00	54.06	54.06
KO2(S)	-68.00	-68.00	29.28	29.27
KOH	-98.64	-98.65	23.09	23.07
KOH+	119.00	119.00	59.80	59.81
ME2GAET	-5.25	-5.25	97.28	97.28
MEGAET	14.25	14.25	89.95	89.95
MEGAET2	-7.33	-7.32	106.70	106.71
MG	35.28	35.28	35.50	35.50
MG(L)	2.16	2.16	10.16	10.16
MG(S)	0.00	0.00	7.81	7.81
MG+	213.09	213.09	36.88	36.88
MG2	68.91	68.91	58.28	58.27
MG2BR4	-183.50	-183.50	110.24	110.23
MG2C3(S)	19.00	19.00	24.00	24.01
MG2F4	-410.70	-410.69	80.52	80.55
MGAL2O4(S)	-549.50	-549.49	21.20	21.22
MGB2(S)	-21.98	-21.99	8.60	8.59
MGBR	-8.45	-8.45	58.52	58.52
MGBR2	-72.40	-72.40	71.92	71.92
MGBR2+	174.80	174.80	76.87	76.87
MGC2(S)	21.00	21.00	13.00	13.01
MGCL	-10.40	-10.40	55.76	55.76
MGCL2	-93.80	-93.80	66.18	66.18
MGCL2(S)	-153.35	-153.35	21.42	21.42
MGCO3(S)	-265.70	-265.70	15.74	15.73
MGF	-56.60	-56.60	52.81	52.81
MGF2	-173.70	-173.70	61.28	61.28
MGF2(S)	-268.70	-268.70	13.68	13.67
MGF2+	141.49	141.49	61.67	61.68
MGH	40.40	40.40	46.15	46.14
MGH2(S)	-18.20	-18.20	7.43	7.42
MGH2O2	-136.80	-136.80	63.85	63.87
MGH2O2(S)	-221.00	-221.00	15.12	15.10
MGN	69.00	69.00	53.71	53.71
MGO(S)	-143.70	-143.70	6.44	6.45

Species	$H^o(298)$ kcal/mole		$S^o(298)$ cal/(mole·K)	
	Data	**Fit**	**Data**	**Fit**
MGOH	-39.38	-39.38	54.10	54.11
MGOH+	139.68	139.68	52.75	52.76
MGS	34.71	34.71	53.87	53.84
MGS(S)	-82.63	-82.63	12.03	12.02
MGSO4(S)	-301.57	-301.58	21.84	21.83
N	112.98	112.95	36.61	36.61
N*C3H7	0.00	22.60	0.00	64.13
N2	0.00	0.00	45.77	45.76
N2F2(C)	17.88	17.88	62.26	62.24
N2F2(T)	20.08	20.07	62.14	62.06
N2F4	-2.00	-2.00	71.96	71.98
N2H2	50.90	50.90	52.22	52.20
N2H3	0.00	36.78	0.00	54.61
N2H4	22.79	22.79	57.03	57.02
N2H4(L)	12.10	12.09	29.05	29.03
N2O	19.61	19.61	52.55	52.55
N2O+	318.69	318.69	55.87	55.86
N2O4	2.17	2.17	72.72	72.72
N3	99.00	99.00	54.10	54.10
NA	25.76	25.75	36.71	36.71
NA(L)	0.58	0.57	13.83	13.82
NA+	145.76	145.75	35.34	35.33
NA2	32.87	32.87	54.99	54.99
NA2B4O7(S)	-783.16	-783.17	45.29	45.27
NA2B6O10(S)	-1094.76	-1094.79	55.50	55.43
NA2C2N2	-2.10	-2.10	82.93	82.93
NA2F2	-202.30	-202.30	68.66	68.67
NA2H2O2	-145.20	-145.20	73.44	73.43
NA2O(L)	-89.11	-89.12	21.90	21.88
NA2O(S)	-99.90	-98.48	17.94	19.10
NA2O2	-122.66	-121.57	22.66	24.05
NA2SO4	-247.04	-247.04	82.87	82.89
NA2SO4(D)	-329.66	-329.66	39.01	38.99
NA2SO4(i)	-330.04	-330.04	38.30	38.28
NA2SO4(iii)	-330.99	-330.99	37.02	37.01
NA2SO4(iv)	-331.63	-331.64	35.89	35.87
NA2SO4(v)	-331.70	-331.70	35.75	35.74

Species	$H^o(298)$ kcal/mole		$S^o(298)$ cal/(mole·K)	
	Data	**Fit**	**Data**	**Fit**
NA3CL6AL(S)	-473.00	-472.97	83.00	83.08
NA3F6AL(S)	-792.76	-792.77	57.00	56.97
NABH4(S)	-45.85	-45.85	24.23	24.23
NABO2	-155.00	-155.00	68.63	68.63
NABO2(S)	-233.20	-233.21	17.58	17.56
NABR	-34.40	-34.40	57.63	57.63
NABR(L)	-81.11	-81.11	24.94	24.93
NABR(S)	-86.38	-86.38	20.75	20.74
NACH	22.53	22.53	58.14	58.14
NACL	-43.36	-43.36	54.90	54.90
NACL(S)	-98.26	-98.26	17.24	17.23
NACL4AL(S)	-273.00	-273.01	45.00	44.97
NACN	22.53	22.53	58.14	58.14
NACN(S)	-21.68	-21.68	28.32	28.31
NAF	-69.42	-69.42	51.98	51.98
NAF2-	-160.00	-160.00	59.89	59.89
NAF4AL	-440.00	-440.00	82.41	82.43
NAH	29.70	29.70	45.00	44.99
NAI(S)	-68.80	-68.80	23.54	23.54
NAO	20.00	20.00	54.74	54.74
NAO-	-29.00	-29.00	51.95	51.95
NAO2(S)	-62.30	-62.30	27.70	27.69
NAO2AL(S)	-270.84	-270.59	16.83	17.17
NAOH	-47.27	-47.26	54.57	54.58
NAOH(L)	-99.64	-99.64	18.13	18.12
NAOH+	162.00	162.00	57.96	57.96
NCN	107.59	107.59	54.77	54.76
NCO	31.51	31.51	54.14	54.14
NF	53.93	53.93	50.82	50.82
NF2	7.87	7.87	59.40	59.39
NF3	-27.97	-27.97	61.79	61.79
NFO	-15.70	-15.70	59.27	59.27
NFO2	-26.00	-26.00	62.18	62.18
NH	85.20	85.20	43.29	43.29
NH2	45.50	45.50	46.51	46.50
NH3	-10.97	-10.97	46.05	46.03
NNH	58.57	58.57	53.63	53.62

Species	$H^o(298)\text{kcal}/\text{mole}$		$S^o(298)\text{cal}/(\text{mole}\cdot\text{K})$	
	Data	**Fit**	**Data**	**Fit**
NO	21.58	21.58	50.35	50.34
NO+	236.66	236.66	47.35	47.34
NO2	7.91	7.91	57.34	57.33
NO2-	-48.45	-48.45	56.52	56.51
NO2F	-23.10	-23.09	61.26	61.26
NO3	17.00	17.00	60.35	60.35
NO3F	3.34	3.34	68.94	68.85
NOF	-16.91	-16.90	58.63	58.63
NOF3	-39.00	-39.00	66.54	66.55
O	59.55	59.55	38.47	38.46
O+	374.95	374.95	37.01	37.01
O-	24.32	24.32	37.69	37.68
O2	0.00	0.00	49.01	49.00
O2-	-11.61	-11.62	50.06	50.06
O2F	22.56	22.56	60.57	60.56
O3	34.10	34.10	57.08	57.08
OC(OH)2	-147.04	-147.04	64.46	64.40
OCHCHO	-49.55	-49.53	64.82	64.98
OCHNNHO	-2.05	-2.09	69.36	69.15
OF	23.73	23.73	50.43	50.43
OF2	4.60	4.60	58.54	58.54
OH	9.32	9.32	43.88	43.87
OH+	314.80	314.80	43.66	43.65
OH-	-34.32	-34.32	41.19	41.19
ONHNHO	23.55	23.52	62.66	62.55
ONHNOH	-1.77	-1.77	65.04	64.93
P	79.80	79.80	38.98	38.98
P2	42.68	42.68	52.11	52.11
P4	30.77	30.78	66.89	66.92
S	66.20	66.20	40.09	40.09
S(L)	0.00	0.44	0.00	8.77
S(S)	0.00	0.00	0.00	7.62
S+	306.48	306.47	39.08	39.08
S-TRIAZINE	56.36	56.37	64.49	64.49
S2	30.71	30.71	54.51	54.50
SH	33.30	33.30	46.73	46.73
SI	107.70	107.70	40.12	40.12

Species	$H^o(298)$kcal/mole		$S^o(298)$cal/(mole·K)	
	Data	Fit	Data	Fit
SI(CH3)2	32.16	32.19	74.55	77.23
SI(CH3)3	3.12	3.28	84.75	87.23
SI(CH3)3CH2	-6.88	-6.71	96.57	99.89
SI(CH3)4	-55.74	-55.51	93.08	96.05
SI(L)	11.59	11.58	10.63	10.62
SI(NH2)3	-18.77	-18.63	84.34	84.27
SI(NH2)4	-92.88	-92.67	84.54	85.38
SI(S)	0.00	0.00	4.50	4.50
SI2	145.79	145.79	54.83	54.83
SI2C	128.00	128.00	57.88	57.88
SI2CL5	-151.65	-151.64	109.12	110.10
SI2CL5H	-188.98	-188.97	108.00	108.98
SI2CL6	-232.75	-232.73	111.13	111.85
SI2F6	-569.62	-569.61	97.16	97.16
SI2H2	95.63	95.62	58.84	58.83
SI2H3	105.70	105.70	65.51	65.51
SI2H5	55.70	55.70	68.85	68.85
SI2H6	19.10	19.10	64.54	64.53
SI3	152.00	152.00	64.00	64.01
SI3H8	28.90	28.90	81.57	81.56
SI3N4(A)	-178.00	-178.00	27.00	26.99
SIC	172.00	172.01	50.89	50.93
SIC(B)	-17.50	-17.50	3.97	3.98
SIC2	147.00	147.00	56.55	56.55
SICCH	125.77	125.77	60.40	60.26
SICH	124.39	124.39	54.94	54.83
SICH2	74.15	74.15	55.99	55.92
SICH3	74.53	74.53	60.16	60.13
SICL	37.90	37.90	56.80	56.80
SICL2	-40.30	-40.30	67.20	67.20
SICL2H2	-74.50	-74.50	68.40	68.40
SICL3	-76.50	-76.50	75.50	75.50
SICL3CH2CH	-140.60	-140.59	93.99	95.65
SICL3H	-118.60	-118.60	74.90	74.89
SICL4	-158.40	-158.40	79.10	79.09
SICLH3	-32.20	-32.20	59.80	59.79
SIF	-12.42	-12.42	52.71	52.71

Species	$H^o(298)$ kcal/mole		$S^o(298)$ cal/(mole·K)	
	Data	**Fit**	**Data**	**Fit**
SIF(NH2)2	-95.48	-95.33	76.93	77.70
SIF(NH2)3	-170.70	-170.55	87.97	87.91
SIF2	-149.86	-149.86	61.38	61.38
SIF2(NH2)2	-247.30	-247.19	82.82	82.77
SIF2N	-63.11	-63.11	70.51	70.51
SIF2NH2	-167.24	-167.21	77.17	77.48
SIF3	-237.42	-237.42	67.76	67.76
SIF3NH	-249.65	-249.65	82.15	83.70
SIF3NH2	-317.89	-317.89	79.98	81.03
SIF3NHSIH3	-320.19	-320.16	95.97	96.88
SIF3NSIH3	-252.84	-252.83	97.65	99.34
SIF4	-385.98	-385.98	67.55	67.54
SIFH3	-85.50	-85.50	57.00	57.00
SIFNH	-13.57	-13.49	68.88	68.95
SIFNH2	-80.01	-80.04	64.68	64.62
SIH	91.70	91.70	44.20	44.20
SIH2	64.80	64.80	49.50	49.49
SIH2CL	7.80	7.80	62.30	62.30
SIH2F	-42.16	-42.16	59.70	59.70
SIH2F2	-186.38	-186.38	62.81	62.81
SIH3	47.43	47.43	51.81	51.80
SIH3NH2	-11.45	-11.40	65.66	65.66
SIH3NHSIH3	-14.32	-14.32	83.54	85.95
SIH3NSIH3	48.90	48.90	83.75	86.69
SIH3SIH2CH3	4.03	4.14	79.43	81.90
SIH4	8.09	8.10	48.90	48.90
SIHCL2	-34.30	-34.30	70.30	70.30
SIHF	-35.70	-35.70	57.07	57.07
SIHF2	-139.57	-139.57	65.05	65.05
SIHF3	-288.63	-288.63	66.65	66.65
SIN	115.55	115.55	51.95	51.95
SINH	38.39	38.39	51.66	51.66
SINH2	48.67	48.67	58.56	58.56
SN	63.00	63.00	53.06	53.05
SO	1.20	1.20	53.02	53.01
SO2	-70.95	-70.95	59.30	59.29
SO3	-94.59	-94.59	61.34	61.34

Species	$H^o(298)\mathrm{kcal/mole}$		$S^o(298)\mathrm{cal/(mole{\cdot}K)}$	
	Data	**Fit**	**Data**	**Fit**
TI	113.20	113.20	43.07	43.06
TICL	36.90	36.90	59.54	59.54
TICL2	-56.70	-56.70	66.50	66.50
TICL3	-128.90	-128.90	75.70	75.71
TICL4	-182.40	-182.40	84.79	84.80

Chapter 3: Gas-phase Kinetics Input

The *Gas-phase Kinetics* input file provides a symbolic description of an elementary chemical reaction mechanism. This file is used during Pre-processing to create a *Gas-phase Kinetics* linking file (*chem.asc*) that stores pertinent information about that mechanism for access during the reactor-model simulation. The information in the Linking File is subsequently accessed by an initialization routine that copies the needed information into memory during a reacting-flow simulation. The stored information is used in calculations related to the equation of state, thermodynamic properties, and chemical production rates.

The *Gas-phase Kinetics* input file includes information on elements, species, thermodynamic data, and the reaction mechanism. Element data are read first, species data are second, followed by optional thermodynamic data, with reactions specified last. The thermodynamic data for the species may come be included in the *Gas-phase Kinetics* input file and/or from a Thermodynamic Database (e.g., *therm.dat*). With the exception of the thermodynamic data, all input is free format. The required syntax for the four types of input is described in Element Data (p. 33) through Reaction Mechanism Description (p. 39) . The auxiliary keywords for gas-phase reactions are described in Table 3.7: Alphabetical Listing of Gas-phase Reaction Auxiliary Keywords (p. 43) and the options for specifying units on the REACTIONS line are described in Table 3.4: Alphabetical Listing of REACTIONS-line Options for Gas-phase Kinetics Data (p. 39). Alphabetical Listing of Project Input Keywords (p. 123) describes the meaning and usage of each keyword entry that may be included as part of a Reactor Model input file.

Note

Input information in the *Gas-phase Kinetics* input file must be contained within the first **100 columns, or it will be ignored**.

3.1. Element Data

All chemical species in the reaction mechanism must be composed of chemical elements or isotopes of chemical elements. Each element and isotope must be declared as a one- or two-character symbol. The purpose of the element data is to associate atomic weights of the elements with their character symbol representations and to identify the order in which arrays of element information in the *Gas-phase Kinetics* Subroutine Library are referenced. For example, an array of atomic weights for the elements is in exactly the same order in which the elements were declared in the element data. In other words, if the atomic weights are stored in an array AWT, then AWT(3) is the atomic weight of the third element declared in the element data.

Element data must start with the word ELEMENTS (or ELEM), followed by any number of element symbols on any number of lines. Element symbols may appear anywhere on a line, but those on the same line must be separated by blanks. Any line or portion of a line starting with an exclamation mark (!) is considered a comment and will be ignored. Blank lines are ignored.

If an element is on the periodic chart, then only the symbol identifying the element need appear in the element data.

Note

The elements that ANSYS Chemkin-Pro recognizes are as follows: H, HE, LI, BE, B, C, N, O, F, NE, NA, MG, AL, SI, P, S, CL, AR, K, CA, SC, TI, V, CR, MN, FE, CO, NI, CU, ZN, GA, GE, AS, SE, BR, KR, RB, SR, Y, ZR, NB, MO, TC, RU, RH, PD, AG, CD, IN, SN, SB, TE, I, XE, CS, BA, LA, CE, PR, ND, PM, SM, EU, GD, TB, DY, HO, ER, TM, YB, LU, HF, TA, W, RE, OS, IR, PT, AU, HG, TL, PB, BI, PO, AT, RN, FR, RA, AC, TH, PA, U, NP, PU, AM, CM, BK, CF, ES, FM, D, E

For the elements appearing on the periodic chart, the ANSYS Chemkin-Pro pre-processors have the atomic weight (in grams per mole) stored internally. For isotopes, a one- or two- character symbol must be input by the user to identify each isotope, and a symbol and an atomic weight (in grams per mole) for each must be defined. The same symbol must be used in the thermodynamic data to identify the elemental composition of species involving the isotope. Once an isotope has been so defined, it is treated exactly as a new element. If an ionic species is used in the reaction mechanism (i.e., `OH+`), an electron must be declared as the element `E`.

For an isotope, the atomic weight must follow the identifying symbol and be delimited by slashes (`/`). The atomic weight may be in integer, floating-point, or E format (e.g., `2`, `2.0`, `0.2E1`), but internally it will be converted to a floating point number. For example, the isotope deuterium may be defined as `D/2.014/`. If desired, the atomic weight of an element in the periodic chart may be altered by including the atomic weight as input just as though the element were an isotope.

Figure 3.1: Examples of Species Data (p. 34) shows several equivalent ways to describe element information. In this example the elements are hydrogen, oxygen, nitrogen, and the isotope deuterium.

Figure 3.1: Examples of Species Data

```
ELEMENTS   H   D /2.014/  O   N   END

ELEM                                ! ELEM is equivalent to ELEMENTS
   H
   D / 2.014 /
   O
   N
END                                 ! an END line is optional

ELEM H
ELEM D/2.014/
ELEM O
ELEM N
```

Table 3.1: Summary of the Rules for Element Data (p. 34) summarizes the rules for element data.

Table 3.1: Summary of the Rules for Element Data

Rule	Description
1	The first element line must start with the word `ELEMENTS` (or `ELEM`).
2	Element or isotope names are either one- or two-character symbols.
3	An isotope name (i.e., a name not on the periodic chart) must be followed by its atomic weight (in grams per mole) delimited by slashes.
4	Each element or isotope should be declared only once; however, duplicated element symbols will be ignored.

Rule	Description
5	An element or isotope name may appear anywhere on the line.
6	Any number of element or isotope names may appear on a line, and more than one line may be used.
7	Element or isotope names that appear on the same line must be separated by at least one blank space.
8	An element or isotope name that begins on one line may not continue to the next line.
9	Any blank spaces between an element or isotope name and the first slash are ignored and any blank spaces between slashes and an atomic weight are also ignored. However, no blank spaces are allowed within an element name or an atomic weight.
10	There may be more than one ELEMENT statement.
11	All characters following an exclamation mark are comments.
12	It is recommended that an END statement follow a group of elements.
13	Elements required by *Surface Kinetics* surface species must be declared in the *Gas-phase Kinetics* input file.

3.2. Species Data

Each chemical species in a problem must be identified on one or more species line(s). Any set of up to 16 upper or lower case characters can be used as a species name. In addition each species must be composed of elements that have been identified in the element data. As for the element data, one of the primary purposes of the species data is to identify the order in which arrays of species information are referenced in the *Gas-phase Kinetics* Subroutine Library.

Species data must start with the word SPECIES (or SPEC), followed by any number of species symbols on any number of lines. Species symbols may appear anywhere on a line, but those on the same line must be separated by blank spaces. Any line or portion of a line starting with an exclamation mark (!) is considered to be a comment and will be ignored. Blank lines are ignored. Figure 3.2: Examples of Species Data (p. 35) shows several equivalent ways to describe species information.

Figure 3.2: Examples of Species Data

```
SPECIES    H2  O2  H  O  OH  HO2  N2  N  NO  END

SPEC                                    ! SPEC is equivalent to SPECIES
  H2  O2
  H  O  OH  HO2  N2  N  NO
END

SPEC H2
spec O2
```

The rules for species data are summarized in Table 3.2: Summary of the Rules for Species Data (p. 35) .

Table 3.2: Summary of the Rules for Species Data

Rule	Description
1	Species data must start with the word SPECIES (or SPEC).

Rule	Description
2	Species names are composed of up to 16-character upper- or lower- case symbols. The names cannot begin with the characters +, =, or a number; an ionic species name may end with one or more + 's or - 's.
3	Each species should be declared only once; however, duplicated species symbols will be ignored.
4	Each species that subsequently appears in a reaction must be declared.
5	A species name may appear anywhere on the line.
6	Any number of species names may appear on a line, and more than one line may be used.
7	Species named on the same line must be separated by at least one blank space.
8	A species name that begins on one line may not continue to the next line.
9	There may be more than one SPECIES statement.
10	All characters following an exclamation mark are comments.
11	For best results, an END statement should follow a species group.

3.3. Thermodynamic Data

All gas-phase species that appears in the reactions contained in the *Gas-phase Kinetics* input or in the *Surface Kinetics* input, must have associated thermodynamic data. The data may be extracted from a database file (e.g. *therm.dat*) and/or read directly from the *Gas-phase Kinetics* input file. Details on the thermodynamic data format, whether including in the *Gas-phase Kinetics* input file or in a thermodynamic database file, are provided in Thermodynamic Data Format (p. 3) .

Note

When thermodynamic data input is included in the *Gas-phase Kinetics* input file, it must immediately follow species data.

Note

The *therm.dat* file distributed with ANSYS Chemkin-Pro represents a historical (not necessarily best) collection of data accumulated by Sandia National Laboratories over the period from 1980 to 1995. The data fits in this collection are based on a variety of sources, including JANAF Tables, NASA, and computational chemistry calculations performed at Sandia and elsewhere. This data set has been fixed and not updated in order to assure backwards compatibility and consistency with published Chemkin-Pro results.

3.4. Real Gas Data

ANSYS Chemkin-Pro employs the cubic equation of state (EOS) to capture the P-T-V relationship of a real gas mixture at high pressures. For each gas species in the real gas mixture, the cubic equation of state models require additional properties that are not part of the regular thermodynamic data. These properties include the critical point, P_c, T_c, and V_c, and the acentric factor ω, and would be provided in the real gas data block of the gas-phase mechanism. The real gas data block starts with the keyword EOS_. Immediately following this keyword (no space), a phrase indicating the choice of the cubic

equation of state model to be used with this gas mechanism is appended. There are five cubic EOS models available in ANSYS Chemkin-Pro. (For more details, see Real Gas Model in the *Chemkin-Pro Theory Manual*) These cubic equation of state models, along with their key phrases, are listed in Table 3.3: Cubic equation of state models available in Chemkin-Pro (p. 37). For example, the keyword EOS_PR will cause the Peng-Robinson equation of state to be applied whenever this gas mechanism is used in a ANSYS Chemkin-Pro simulation.

Table 3.3: Cubic equation of state models available in Chemkin-Pro

Cubic EOS Model	Key Phrase
van der Waals	**VAND** or **VDW**
Redlich-Kwong	**REDL** or **RK**
Soave-Redlich-Kwong	**SOAV** or **SRK**
Aungier-Redlich-Kwong	**AUNG** or **ARK**
Peng-Robinson	**PENG** or **PR**

The required properties of all gas species in the mechanism are given below the EOS_ keyword. Each gas species will have its properties listed in one single line. The line must start with the species name and be followed by, in the exact same order, the values of P_c, T_c, V_c, and ωω for this gas species. The critical pressure P_c is in bar, the critical temperature T_c in Kelvin, and the critical molar volume V_c in cm^3/mole. All four parameters are required. If V_c or ω are not available for a species, set the value to zero.

The parameters are format-free and separated by blank space(s). If the binary interaction coefficients between this gas species and other species are known, the coefficients can be given as auxiliary keywords in the line(s) below the property data line. The interacting species name and the corresponding binary interaction coefficient should be provided in the format illustrated here with the coefficient value delimited by slashes (/):

```
<interacting species name>/<interaction coefficient>/
```

For example, the binary interaction coefficient between O2 and N2 can be given in a line below the properties data line of O2 (or N2) as `N2/-0.0078/` (or `O2/-0.0078/`).

If you have multiple binary interaction coefficients to specify, they should be separated by blank space(s) and can be written in a single line or in several lines. The binary interaction coefficient is only required once for each pair of species.

All species in the mechanism must have their real gas data given in the real gas data block, and the species data lines can appear in any order. The real gas data block should be closed by the keyword `END`.

Figure 3.3: Example of Real Gas data input (p. 38) shows some examples of the real gas data input.

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Figure 3.3: Example of Real Gas data input

```
! Real Gas Information
! R.C. Reid, J.M. Prausnitz, and B.E. Poling, The Properties of Gases & Liquids, 4th ED.
EOS_SRK
!Soave-Redlich-Kwong EOS
!Species symbol, TC[K],    PC[bar], VC[cm3/mol], Best-fitted Acentric Factor
H                33.2      13.64     0.0          0.0
H2               33.15     13.0      65.1        -0.2324
! Binary Inteaction Coefficients
O                44.5      26.9      0.0          0.0
O2              154.6      50.4      73.4         0.0298
! Binary Inteaction Coefficients
OH              400.0     149.0      0.0          0.1
HO2             400.0      82.0      0.0          0.2
H2O             647.37    221.2     57.1          0.3443
H2O2            730.10     21.68     0.0          0.5
CH4             190.56     46.0      99.2         0.01142
! Binary Inteaction Coefficients
CO2/0.093/  N2/0.028/ CO/0.032/
CO              132.9      35.0      93.2         0.0295
! Binary Inteaction Coefficients
CH4/0.032/
CO2             304.1      73.8      93.9         0.2373
! Binary Inteaction Coefficients
N2/-0.032/
CH4/0.093/
N2              126.2      33.9      89.8         0.0358
! Binary Inteaction Coefficients
CO2/-0.032/ CH4/0.028/
END
```

3.5. Transport Data

Gas-phase species transport data is required for a collision-frequency reaction formulation, and for reactor models or other programs that require a transport linkfile. The data can be read from a database file (e.g., *tran.dat*) and/or read directly from the *Gas-phase Kinetics* input file. To include transport data in the input file, the first line of the data should be the word TRANSPORT (or TRAN), and the last line should be the word END. If TRANSPORT ALL is used, it is expected that all required transport data is given in this section, or else a database file is used to supplement data not provided here.

The TRANSPORT . . . END data block's format should resemble this:

```
TRANSPORT
C2H4 2 280.800 3.971 0.000 0.000 1.500
END
```

For the collision frequency reaction, the required collision diameter of species will be obtained from the transport data and stored in the gas-phase linkfile. For reactor models or other programs that require a supplemental transport linkfile, the User Interface provides a check-box option on the Pre-Processing panel, Process Transport Properties; if this is checked, transport-data coefficient fitting is performed, and a transport linkfile written.

Details on the transport data format, whether included in the *Gas-Phase Kinetics* input file or in a transport properties database file, are provided in Transport Data Format (p. 87) .

Note

If the *Gas-Phase Kinetics* input file includes transport properties data input, this data must follow species data and precede reaction data.

3.6. Reaction Mechanism Description

The reaction mechanism may consist of any number of chemical reactions involving the species named in the species data. A reaction may be reversible or irreversible; it may be a three-body reaction with an arbitrary third body and/or enhanced third-body efficiencies; it may have a Lindemann [4] (p. 331), Troe [5] (p. 331) or SRI [6] (p. 331) pressure fall-off formulation; it may have an arbitrary pressure-dependence defined by special fits or interpolation; it may involve a photon; and it may depend on a species temperature other than that of the bulk gas. Pressure-dependent Reactions of the Chemkin-Pro Theory Manual provides more detailed discussion of these different formulations. In this section, we describe the rules and syntax needed to enter different types of reactions in the *Gas-phase Kinetics* input file. The keywords for controlling these reaction parameters are described in Alphabetical Listing of Project Input Keywords (p. 123) .

Reaction data must start with a line that contains the word REACTIONS (or REAC). The lines following the REACTIONS line contain reaction descriptions, together with their Arrhenius rate coefficients. The reaction description is composed of a reaction path, reaction rate coefficients, and (optionally) some auxiliary information or keywords.

3.6.1. REACTIONS Line Options

On the same line as the REACTIONS word, you may specify units of the Arrhenius rate coefficients (Equation 3.5 of the Chemkin-Pro Theory Manual) followed by the word CAL/MOLE, KCAL/MOLE, JOULES/MOLE, KJOULES/MOLE, KELVINS, or EVOLTS for E_i, and/or MOLES or MOLECULES for A_i. If MOLECULES is specified, then the units for A_i are cm, molecules, sec, and K.

Note

If units are not specified, A_i and E_i must be in cm, mole, sec, K, and cal/mole, respectively. Note that T is always in Kelvin. ANSYS Chemkin-Pro uses the thermal calorie, 4.184 Joules.

Table 3.4: Alphabetical Listing of REACTIONS-line Options for Gas-phase Kinetics Data

Keyword	Definition
CAL/[MOLE]	Reiterates the default units for all gas-phase reactions that follow the REACTIONS header line for parameters with energy units such as E_i. **Notes** - Default units for E_i are cal/mole.
EVOL[TS]	Supersedes the default units for all gas-phase reactions which follow the REACTIONS header line for parameters with energy units such as E_i. **Notes** - Default units for E_i are cal/mole.
JOUL[ES/MOLE]	Supersedes the default units for all gas-phase reactions which follow the REACTIONS header line for parameters with energy units such as E_i. **Notes** - Default units for E_i are cal/mole.

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Keyword	Definition
KCAL[/MOLE]	Supersedes the default units for all gas-phase reactions which follow the REACTIONS header line for parameters with energy units such as E_i. **Notes** - Default units for E_i are cal/mole.
KELV[INS]	Supersedes the default units for all gas-phase reactions which follow the REACTIONS header line for parameters with energy units such as E_i. **Notes** - Default units for E_i are cal/mole.
KJOU[LES/MOLE]	Supersedes the default units for all gas-phase reactions which follow the REACTIONS header line for parameters with energy units such as E_i. **Notes** - Default units for E_i are cal/mole.
MOLEC[ULES]	Supersedes the default units for all gas-phase reactions which follow the REACTIONS header line for pre-exponential factors A_i. **Notes** - Default units for A_i are cgs (cm, sec, K, mole), the exact units depending on the order of the reaction.
MAXSP	Increases the maximum number of reactants or products allowed in a reaction. The number given by this keyword must be greater than the default limit of 6. For example, `REACTIONS MAXSP=11`. **Notes** -This keyword is available to both the gas-phase and surface reaction mechanism.
MOLE[S]	Supersedes the default units for all gas-phase reactions which follow the REACTIONS header line for pre-exponential factors A_i. **Notes** - Default units for A_i are cgs (cm, sec, K, mole), the exact units depending on the order of the reaction.
USRPROD	Indicates that the user will provide a user-written rate routine that will supply all of the species net rates of production, overriding any other reaction input in the *Gas-phase Kinetics* input file. The net rate-of-production for all species will be obtained by calling the user-supplied subroutine, CKUPROD. An optional slash(/)-delimited integer parameter allows the user to select from more than one type of rate formulation. Wherever the species production rates are required, they will be obtained by calling the user-written subroutine called CKUPROD. A template of CKUPROD is provided in the ANSYS Chemkin-Pro installation, in the file *cklib_user_routines.f* located in the directory *user_subroutines*. Information about how to compile and link user routines into Chemkin-Pro is included in Chemkin-Pro Application Programming Interface Manual.

Keyword	Definition
	Notes - USRPROD cannot be used in conjunction with USRPROG (entered after a particular reaction).

Note

This API does not support user-written programming, so you are cautioned to use the CKUPROD user-routine feature at your own risk. Also, there are some features in ANSYS Chemkin-Pro that will be incompatible with the global replacement of species rates of production, such as sensitivity analysis and rate-of-production analysis. Such features will return zero values when user-rate programming is encountered.

3.6.2. Reaction Data

Reaction Data follows the REACTIONS line and precedes an END statement that concludes the Reactions Data section. Each reaction entry line is divided into two fields. The first contains the symbolic description of the reaction path for that reaction while the second contains the Arrhenius rate coefficients. Both fields are format-free and blank spaces are ignored. Any line or portion of a line starting with an exclamation mark (!) is considered a comment and is ignored. Blank lines are also ignored.

The reaction description, given in the first field, must be composed of the species symbols, coefficients, delimiters, and any special symbols defined in Table 3.5: Reaction Data Criteria (p. 41) .

Table 3.5: Reaction Data Criteria

Species Symbols	
	Each species in a reaction is described with the unique sequence of characters as they appear in the species data and the thermodynamic data (e.g., H2).
Coefficients	
	A species symbol may be preceded by an integer or real coefficient. The coefficient has the meaning that there are that number of moles of the particular species present as either reactants or products; e.g. 2OH, is equivalent to OH + OH. Non-integer coefficients are allowed in *Gas-phase Kinetics input*, but the element balance in the reaction must still be maintained.
Delimiters	
+	A plus sign is the delimiter between each reactant species and each product species.
=	An equality sign is the delimiter between the last reactant and the first product in a reversible reaction.
<=>	An equality sign enclosed by angle brackets can also be used as the delimiter between the last reactant and the first product in a reversible reaction.
=>	An equality sign with an angle bracket on the right is the delimiter between the last reactant and the first product in an irreversible reaction.
Special Symbols	
+M	An M as a reactant and product stands for an arbitrary third body. An M in the reaction description indicates that a third body is participating in the reaction. In a reaction containing an M, species can be specified to have enhanced third body efficiencies, in which case auxiliary information (described below) must

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Species Symbols	
	follow the reaction line. If no enhanced third body efficiencies are specified, then all species act equally as third bodies and the effective concentration of the third body is the total concentration of the mixture.
(+M)	An `M` as a reactant and product surrounded by parentheses indicates that the reaction is a pressure-dependent reaction, in which case auxiliary information line(s) (described below) must follow the reaction to identify the fall-off formulation and parameters. A species may also be enclosed in parenthesis. Here, for example, (+`H2O`) indicates that water is acting as the third body in the fall-off region, not the total concentration `M`.
E	The symbol E as a reactant and/or product is used to represent an electron. An electron is treated just like any other species, and is composed of the element E, which must be declared as element data. If an E appears in any reaction, then it must also be declared as a species in the species data.
!	An exclamation mark means that all following characters are comments on the reaction. For example, the comment may be used to give a reference to the source of the reaction and rate data.

The second field of the `REACTIONS` line is used to define the Arrhenius rate coefficients A_i, β_i, and E_i, in that order, as given by Equation 3.5 of the Chemkin-Pro Theory Manual . At least one blank space must separate the first number and the last symbol in the reaction. The three numbers must be separated by at least one blank space, be stated in either integer, floating point, or "E" format (e.g., `123`, `123.0` or `123E1`), and have units associated with them.

Note

Unless modified by options specified on the `REACTIONS` line or in Auxiliary Reaction Keywords, the default units for A_i are in cgs (cm, sec, K, mole), the exact units depending on the reaction. The factor β_i is dimensionless. The default units for the activation energies are cal/mole.

Examples of reaction data are shown in Figure 3.4: Examples of Reaction Data (p. 42) .

Figure 3.4: Examples of Reaction Data

```
REACTIONS                          CAL/MOLE   ! these are the default units for the reaction rates
H2 + O2 = 2OH                                        1.7E13  0  47780.  !  Ref. 21
! H2 + O2 = OH + H                    1.7E13  0  47780.  !  same as previous reaction,
                                         ! commented to prevent a duplication error
H  + O2 + M = HO2 + M                                2.0E15  0.000  -870.
!  H + O2 + M = HO2                                  2.0E15  0.000  -870.
!  H + O2 = HO2 + M                                  2.0E15  0.000  -870.
OH+ + H + E = H2O                                           1.E19  0  0.0
O = O(*)                                                    1.3E5  0  0

0.5H2 + 0.5O2 = OH                                   ! photoactive reaction, represented without HV
END                                                             ! example of real coefficients
                                   ! END statement is optional;  ! <eof> condition is equivalent
```

Table 3.6: Summary of the Rules for Reaction Data (p. 43) is a summary of the reaction data rules.

Table 3.6: Summary of the Rules for Reaction Data

Rule	Description
1	The first reaction line must start with the word REACTIONS (or REAC), and may include units definition(s).
2	The reaction description can begin anywhere on the line. All blank spaces, except those between Arrhenius coefficients, are ignored.
3	Each reaction description must have =, <=> or => between the last reactant and the first product.
4	Each reaction description must be contained on one line.
5	Three Arrhenius coefficients must appear in order (A_i, β_i, and E_i) on each Reaction line, separated from each other and from the reaction description by at least one blank space; no blanks are allowed within the numbers themselves.
6	There cannot be more than six reactants or six products in a reaction.
7	Comments are any and all characters following an exclamation mark.
8	For best results an END statement should follow the reaction input.

3.6.3. Auxiliary Reaction Data

Auxiliary Reaction Data is entered in lines immediately following the Reaction Data for a specific reaction path. The format of an auxiliary information line is a character-string keyword followed by a slash-delimited (/) field, which begins and ends with a slash (/), and which contains an appropriate number of parameters (either integer, floating point, or "E" format).

These data or keywords are used to indicate different reaction-rate expressions, units, pressure-dependency, and other ways in which the reaction behavior may be modified. Table 3.8: Summary of the Rules for Auxiliary Reaction Data (p. 57) provides detailed information about the meaning and usage of each auxiliary keyword entry option for gas-phase reactions. Also, Figure 3.5: Examples of Auxiliary Reaction Data (p. 56) provides some additional examples of reaction data.

Table 3.7: Alphabetical Listing of Gas-phase Reaction Auxiliary Keywords

<table>
<tr><th>Keyword</th><th>Definition</th></tr>
<tr><td><SpeciesName></td><td>Neutral Third Body Efficiency - If a reaction contains M as a reactant and/or product, auxiliary information lines may follow the reaction line to specify enhanced third-body efficiencies of certain species (i.e., a_{ki}, Equation 3.19 of the Chemkin-Pro Theory Manual). To define an enhanced third body efficiency, the keyword is the species name of the third body, and its one parameter is its enhanced efficiency factor. A species that acts as an enhanced third body must be declared as a species. Examples of third body efficiencies are shown in the first three reactions in Figure 3.5: Examples of Auxiliary Reaction Data (p. 56) .
<table>
<tr><th>Parameters</th><th>Optional/Reqd.</th><th>Units</th><th>Examples</th></tr>
<tr><td>Species name</td><td>Required</td><td>--</td><td>CO/1.87/</td></tr>
<tr><td>Stoichiometric coefficient υ'_{ki}</td><td>Required</td><td>--</td><td>CO/1.87/</td></tr>
</table>
</td></tr>
</table>

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<table>
<tr><th>Keyword</th><th colspan="4">Definition</th></tr>
<tr><td></td><td>Reaction Example</td><td colspan="3">REACTIONS CAL/MOLE

HCO+M=H+CO+M 0.250E+15
0.000 16802.000
! Warnatz

CO/1.87/ H2/1.87 CH4/2.81/
CO2/3./ H2O/5./</td></tr>
<tr><td>CHEB</td><td colspan="4">Chebyshev Polynomial Rate Expressions - Supersedes the default reaction rate expression by a Chebyshev polynomial evaluation (see Equation 3.43 of the Chemkin-Pro Theory Manual). CHEB must be followed by (slash delimited) parameters; for the first CHEB, the first value is N, the number of basis functions along the temperature axis; the second is M, the number of basis functions along the pressure axis; and the remainder are the N x M coefficients anm from Equation 3.41 in the order of a_{11}, a_{12}, …, a_{1M}, a_{21}, a nm, in this or additional CHEB declarations.</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td></td><td>Number of temperature functions N</td><td>Required</td><td>--</td><td>CHEB / 7 3 -4.1624 .9394 -.18563 12.438/</td></tr>
<tr><td></td><td>Number of pressure functions M</td><td>Required</td><td>--</td><td>CHEB / 7 3 -4.1624 .9394 -.18563 12.438/</td></tr>
<tr><td></td><td>Chebyshev coefficients a</td><td>Required</td><td>--</td><td>CHEB / 7 3 -4.1624 .9394 -.18563 12.438/</td></tr>
<tr><td></td><td>Reaction Example</td><td colspan="3">C2H5 + O2 (+M) <=> C2H4E + HO2 (+M) 1.00E+00 .000
0. ! mecon 7/97

CHEB/ 7 3 1.0216E+01 -
1.1083E+00 -1.9807E-01 7.8325E-01/

CHEB/ 1.1609E+00 1.1762E-01 -
9.5707E-02 1.0928E-01 1.1551E-01/

CHEB/ -8.0290E-02 -1.0978E-01
3.7074E-04 -1.4830E-02 -6.0589E-02/

CHEB/ -2.8056E-02 6.9203E-03 -
9.7259E-03 -1.3556E-02 7.6648E-03/

CHEB/ 6.6865E-03 -8.8244E-04/</td></tr>
<tr><td></td><td>Notes</td><td colspan="3">• More than one set of CHEB data can appear for a given reaction, as many as required to input exactly N x M + 2 values.

• Pressure limits of the Chebyshev polynomial for this reaction may be provided by keyword PCHEB .</td></tr>
</table>

Keyword	Definition	
		• Temperature limits of the Chebyshev polynomial for this reaction may be provided by keyword TCHEB .

COLLEFF	**Efficiency of Collision Frequency Expression** - If a reaction is bimolecular and the approximate collision diameters are known, then the collision frequency efficiency expression can be used to calculate the reaction rate constant.
	
	The Arrhenius parameters for the correction factor are specified on the reaction line. On the line following, the keyword COLLEFF is required to tell the interpreter the type of reaction.
	
	`A+B<=>Products a b c`
	
	`COLLEFF`
	
	In addition to the parameters for the correction factor *a*, *b* , and *c*, the diameters for each reacting species must be specified. ANSYS Chemkin-Pro uses the Lennard-Jones diameter as an approximation for the spherical diameter of a species. The Lennard-Jones diameter is one of the inputs read by the *Transport* Pre-Processor that are specified as outlined in Transport Data Format (p. 87) .	

	Reaction Example	`C6H6 + C6H6 => C12H10 + H2 0.02 0 0`
		
		`COLLEFF`

DUP	**Duplicate Reactions** - Two or more reactions can involve the same set of reactants and products, but proceed through distinctly different processes. In these cases, it may be appropriate to state a reaction mechanism that has two or more reactions that are the same, but have different rate parameters. However, duplicate reactions are normally considered errors by the *Gas-phase Kinetics* Pre-Processor. If the user requires duplication (e.g., the same reactants and products with different Arrhenius parameters), the keyword DUP must follow the reaction line of each duplicate reaction, including the first occurrence of the reaction that is duplicated. For example, if the user wishes to specify different rate expressions for each of two identical reactions, there must be two occurrences of the DUP keyword, one following each of the reactions. No auxiliary parameters are required. Examples are shown in Figure 3.5: Examples of Auxiliary Reaction Data (p. 56) .	

	Reaction Example	`HO2+HO2=H2O2+O2`
		`4.20E14 0.0 11982`
		
		`DUP`
		
		`HO2+HO2=H2O2+O2`
		`1.3E11 0.0 -1629`
		
		`DUP`

<table>
<tr><th>Keyword</th><th>Definition</th></tr>
<tr><td>EXCI</td><td>Energy Loss Parameter - Auxiliary data may be used to specify the energy loss per reaction event by specifying the keyword EXCI, followed by the value of the energy loss per event, in units of electron volts. This option 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. The option is useful in describing electron-impact excitation reactions, for example, where the user does not wish to keep track of the excited-species density, but wants to include the energy loss to the electrons due to the excitation process. An example of the use of EXCI is given in Figure 3.5: Examples of Auxiliary Reaction Data (p. 56) . The EXCI keyword represents the ΔH_r parameter that is used to describe inelastic collisions in Equation 8.88 of the Chemkin-Pro Theory Manual for the electron balance in plasma simulations.
<table>
<tr><th>Parameters</th><th>Optional/Reqd.</th><th>Units</th><th>Examples</th></tr>
<tr><td>Energy loss per event</td><td>Required</td><td>electron-volts</td><td>TDEP/E/ EXCI/11.60/</td></tr>
<tr><td>Reaction Example</td><td colspan="3">E + AR => AR + E 2.235E16 0.0 3.47E5

TDEP/E/ EXCI/11.60/

DUP</td></tr>
</table></td></tr>
<tr><td>FIT1</td><td>Supersedes the default reaction rate expression by the reaction rate described by Equation 3.50 of the Chemkin-Pro Theory Manual . FIT1 must be followed by the four slash-delimited FIT1 parameters, bni.
<table>
<tr><th>Parameters</th><th>Optional/Reqd.</th><th>Units</th><th>Examples</th></tr>
<tr><td>FIT1 parameters b_1 - b_4</td><td>Required</td><td>--</td><td>FIT1/33756 -1.695E8 1.08E13 0.0/</td></tr>
<tr><td>Reaction Example</td><td colspan="3">E + O2 => O + O-
4.60E-11 0.0 0.

TDEP/E/

FIT1/33756 -1.695E8 1.08E13 0.0/</td></tr>
</table></td></tr>
<tr><td>FORD</td><td>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. FORD is followed, in slash-delimited format, by the species name and the new reaction order. This option overrides the values of υ'_{ki} in Equation 3.4 of the Chemkin-Pro Theory Manual pertaining to the particular species named on the line. The reaction order for all other species maintain their default values.
<table>
<tr><th>Parameters</th><th>Optional/Reqd.</th><th>Units</th><th>Examples</th></tr>
<tr><td>Species name</td><td>Required</td><td>--</td><td>FORD /Pt(S) 1.0/</td></tr>
<tr><td>Stoichiometric coefficient υ'_{ki}</td><td>Required</td><td>--</td><td>FORD /Pt(S) 1.0/</td></tr>
</table></td></tr>
</table>

<table>
<tr><th>Keyword</th><th colspan="4">Definition</th></tr>
<tr><td></td><td>Reaction Example</td><td colspan="3">JP10+14O2 => 10CO2 + 8H2O
6.454323E+13 0.0
29188.8

FORD / JP10 1.153923 /

FORD / O2 0.738210 /</td></tr>
<tr><td></td><td>Notes</td><td colspan="3">Multiple occurrences of the FORD construct may appear on the auxiliary line.</td></tr>
<tr><td>HIGH</td><td colspan="4">Defines the high-pressure limit for pressure-dependent chemically activated bimolecular reactions (see Equation 3.26 of the Chemkin-Pro Theory Manual). HIGH must be followed by the three slash-delimited high-pressure limit Arrhenius parameters A_∞, β_∞, and E_∞, and the Arrhenius coefficients on the reaction line represent the low-pressure limit Arrhenius parameters A_o, β_o, and E_o.</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td></td><td>Pre-exponential factor A_∞</td><td>Required</td><td>Depends on reaction</td><td>HIGH /6.85E-12 6.53 -834./</td></tr>
<tr><td></td><td>Temperature exponent β_∞</td><td>Required</td><td>--</td><td>HIGH /6.85E-12 6.53 -834./</td></tr>
<tr><td></td><td>Activation energy E_∞</td><td>Required</td><td>cal/mole</td><td>HIGH /6.85E-12 6.53 -834./</td></tr>
<tr><td></td><td>Reaction Example</td><td colspan="3">C2H5+O2(+M)= C2H4+HO2(+M) 1.41E7 1.09 -1975.

HIGH/6.85E-12 6.53 -834./

TROE/0.45 1.E-10 1.E10/

H2/2/ CO/2/ CO2/3/ H2O/5/</td></tr>
<tr><td></td><td>Notes</td><td colspan="3">• Required when SRI or TROE is present
• Additional pressure-dependency parameters may be provided by keywords SRI or TROE.
• If no additional parameters, the Lindemann formulation is applied.</td></tr>
<tr><td>JAN</td><td colspan="4">Optional Rate Fit Expressions - Supersedes the default reaction rate expression by a Janev-Langer reaction rate (see Equation 3.49 of the Chemkin-Pro Theory Manual). JAN must be followed by the nine slash-delimited Janev-Langer rate parameters, b_{ni}.</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
</table>

Keyword	Definition			
	Janev-Langer parameters b1 - b9	Required	eV	JAN / -19.73476 3.992702 -1.773436 0.5331949 -0.1 0.02 -0.002 8.E-5 -2.E-6/

	Reaction Example	`H* + E = H+ + 2E 1.0 0.0 0.0`
		
		`JAN / -19.73476 3.992702 -1.773436 0.5331949 -0.1 0.02 -0.002 8.E-5 -2.E-6/`		

	Notes	• If fewer than 9 parameters are required for the fit, the user must provide zeros for the remainder of the parameters. • The Janev rate expression was originally designed for usage with plasmas, and the temperature unit is eV (i.e., electron-volt). When the rate is calculated, the system temperature is first converted to eV. For temperatures in kelvin, it will be T/11595 in eV. Therefore the temperature needs to be in eV when fitting the JAN rate coefficients, while other reactions in the mechanism still use temperature in K.		
LOW	Defines the low-pressure limit for pressure-dependent unimolecular fall-off reactions (see Equation 3.25 of the Chemkin-Pro Theory Manual). LOW must be followed by the slash-delimited low-pressure limit Arrhenius parameters A_o, β_o, and E_o, and the Arrhenius coefficients on the reaction line represent the three high-pressure limit Arrhenius parameters A_∞, β_∞, and E_∞.			
	Parameters	Optional/Reqd.	Units	Examples
	Pre-exponential factor A_o	Required	depends on reaction	LOW /1.73E69 -15.07 60491./
	Temperature exponent β_o	Required	--	LOW /1.73E69 -15.07 60491./
	Activation energy E_o	Required	cal/mole	LOW /1.73E69 -15.07 60491./

	Reaction Example	`O+CO(+M)<=>CO2(+M) 1.800E+10 .000 2385.00`
		
		`LOW/ 6.020E+14 .000 3000.00/`		

	Notes	• Required when SRI or TROE is present • Supplemental pressure-dependency parameters may be provided by keywords SRI or TROE. • If no additional parameters, the Lindemann formulation is applied.		

<table>
<tr><th>Keyword</th><th>Definition</th></tr>
<tr><td>LT</td><td>Landau-Teller Reactions - Supersedes the default reaction rate expression by the Landau-Teller reaction rate (see Equation 3.47 of the Chemkin-Pro Theory Manual). LT must be followed by the two slash-delimited Landau-Teller reaction rate parameters Bi and Ci.
<table>
<tr><th>Parameters</th><th>Optional/Reqd.</th><th>Units</th><th>Examples</th></tr>
<tr><td>Landau-Teller parameter B _i</td><td>Required</td><td>--</td><td>LT /-67 62.1/</td></tr>
<tr><td>Landau-Teller parameter C _i</td><td>Required</td><td>--</td><td>LT /-67 62.1/</td></tr>
<tr><td>Reaction Example</td><td colspan="3">H2(1)+H2O(000)=H2(0)+H2O(001)
2.89E15 0 0

LT / -67 62.1/</td></tr>
<tr><td>Notes</td><td colspan="3">If explicit REV parameters are given for the reaction, then explicit reverse Landau-Teller parameters must also be given by keyword RLT.</td></tr>
</table></td></tr>
<tr><td>MOME</td><td>Plasma Momentum-Transfer Collision Frequency Options - Indicates that the reaction parameters describe the momentum-transfer collision frequency for electrons. This keyword requires no supplemental data, but changes the treatment of the reaction-rate coefficients. The option causes the reaction to be flagged as an electron momentum-transfer reaction, and assumes that the reaction rate constant is in units of cm^3 /mole-s or cm^3 /molecule-s, depending on the units specified in the REACTIONS statement. These reactions are treated as special cases when Gas-phase Kinetics subroutines evaluate reaction rates-of-progress, as described in Rates of Creation and Destruction of Species of the Chemkin-Pro Theory Manual .
<table>
<tr><td>Reaction Example</td><td>E + AR* => E + AR* 1.0502E-08
2.5929E-01 1.7464E+04

TDEP/E/

MOME</td></tr>
<tr><td>Notes</td><td>These options would generally not be used (or would be ignored) with any of the standard ANSYS Chemkin-Pro reactor models; they are there for users who may be incorporating Chemkin-Pro into a multi-dimensional plasma simulation user program.</td></tr>
</table></td></tr>
<tr><td>PCHEB</td><td>Supersedes the default pressure limits for a Chebyshev polynomial rate expression (see Equation 3.42 of the Chemkin-Pro Theory Manual). PCHEB must be followed by the two slash-delimited values Pmin and Pmax.
<table>
<tr><th>Parameters</th><th>Optional/Reqd.</th><th>Units</th><th>Examples</th></tr>
<tr><td>Minimum pressure Pmin</td><td>Required</td><td>atm</td><td>PCHEB / 1.0 100.0/</td></tr>
<tr><td>Maximum pressure Pmax</td><td>Required</td><td>atm</td><td>PCHEB / 1.0 100.0/</td></tr>
</table></td></tr>
</table>

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<table>
<tr><th>Keyword</th><th colspan="4">Definition</th></tr>
<tr><td></td><td>Reaction Example</td><td colspan="3">C2H5+O2(+M)=C2H4E+HO2 (+M) 1.0 0.0 0.0

LOW / 1.0 0.0 0.0 /

PCHEB / 1.0 100.0/

CHEB/ 7 3 10.216 -1.1083 -0.19807 0.78325/

CHEB/ 1.1609 0.1.1762 -0.095707 0.10928 0.11551/

CHEB/ -0.08029 -0.10978 3.7074E-04 -0.01483 -0.060589/

CHEB/ -0.028056 6.9203E-03 -9.7259E-03 -0.013556 7.6648E-03/

CHEB/ 6.6865E-03 -8.8244E-04/</td></tr>
<tr><td></td><td>Notes</td><td colspan="3">• The default Chebyshev polynomial pressure limits are P_{min}=0.001, P_{max}=100.

• Chebyshev polynomial parameters must be provided by use of keyword CHEB.

• Default Chebyshev polynomial temperature limits may be superseded by keyword TCHEB.</td></tr>
<tr><td>PLOG</td><td colspan="4">Pressure Dependence Through Logarithmic Interpolation - Provides a general-purpose way of describing pressure-dependent reaction rates. Using the PLOG keywords, you can enter any number of sets of Arrhenius reaction-rate coefficients at different reactor pressures. The PLOG data will override the Arrhenius coefficients provided on the reaction line. The PLOG keyword must be followed by the slash-delimited values for the pressure at which the reaction rates are given and the three Arrhenius parameters, A_i, β_i, and E_i, for that pressure. Multiple PLOG entries can be provided, but they must be included in ascending order of pressure. See the ANSYS Chemkin-Pro Theory Manual, General Pressure Dependence Using Logarithmic Interpolation , General Pressure Dependence Using Logarithmic Interpolation .</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td></td><td>Pressure</td><td></td><td>atm</td><td>PLOG /0.03947 2.9512E+09 1.28 13474./</td></tr>
<tr><td></td><td>Pre-exponential factor A_i</td><td></td><td>Depends on reaction</td><td>PLOG /0.03947 2.9512E+09 1.28 13474./</td></tr>
</table>

Keyword	Definition			
	Temperature exponent β_i		--	PLOG /0.03947 2.9512E+09 1.28 13474./
	Activation energy E_i		cal/mole	PLOG /0.03947 2.9512E+09 1.28 13474./

	Reaction Example	`H2CCCH+H=C3H2(S)+H2 2.9512E+09 1.28 13474.`
		
		`PLOG /0.03947 2.9512E+09 1.28 13474./`
		
		`PLOG /1. 1.0965E+10 1.13 13929./`
		
		`PLOG /10. 3.3113E+13 0.195 17579./`
		
		`PLOG /100. 3.3113E+13 0.195 17579./`		

	Notes	There should not be more than one `PLOG` entry for the same pressure for a reaction. However, you can use the `DUPLICATE` option to have two reactions that are the same and that both use `PLOG` entries; in this case the resulting reaction-rates will be summed as is the usual case for `DUPLICATE` reactions.		
REV	**Reverse Rate Parameters** - Supersedes the reverse rates that would normally be computed through the equilibrium constant, Equation 3.6 of the Chemkin-Pro Theory Manual . REV must be followed by the three slash-delimited Arrhenius coefficients (A_i, β_i, and E_i) to specify the reverse rate.			
	Parameters	Optional/Reqd.	Units	Examples
	Pre-exponential factor A_i		depends on reaction	REV / 6.61E-14 0.0 9561./
	Temperature exponent β_i		--	REV / 6.61E-14 0.0 9561./
	Activation energy E_i		cal/mole	REV / 6.61E-14 0.0 9561./

	Reaction Example	`C2F4 + M = CF2 + CF2 + M 1.126E-07 0. 27528.0`
		
		`REV / 9.381E-14 0. 31404.1 /`		

RLT	Supersedes the default reverse reaction rate expression by the Landau-Teller reaction rate (see Equation 3.47 of the Chemkin-Pro Theory Manual). `RLT`			

<table>
<tr><th>Keyword</th><th>Definition</th></tr>
<tr><td></td><td>must be followed by the two slash-delimited Landau-Teller reaction rate parameters Bi and Ci.
<table>
<tr><th>Parameters</th><th>Optional/Reqd.</th><th>Units</th><th>Examples</th></tr>
<tr><td>Landau-Teller parameter B _i</td><td>Required</td><td>--</td><td>RLT /-67 62.1/</td></tr>
<tr><td>Landau-Teller parameter C _i</td><td>Required</td><td>--</td><td>RLT /-67 62.1/</td></tr>
<tr><td>Reaction Example</td><td colspan="3">H2(1)+H2O(000)=H2(0)+H2O(001)
2.89E15 0 0

RLT / -67 62.1/</td></tr>
<tr><td>Notes</td><td colspan="3">• Required when the combination of LT and REV keywords is present.

• If explicit REV parameters are given for the reaction, then explicit reverse Landau-Teller parameters must also be given by keyword RLT.</td></tr>
</table></td></tr>
<tr><td>RORD</td><td>Reverse Reaction Order Parameter - Supersedes the reverse 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. RORD must be followed by the slash-delimited species name and the new reaction order, and supersedes the values of υ''_{ki} in Equation 3.4 of the Chemkin-Pro Theory Manual pertaining to the particular species named on the line; the reaction order for all other species maintain their default values. Multiple occurrences of the RORD construct may appear on the auxiliary line.
<table>
<tr><th>Parameters</th><th>Optional/Reqd.</th><th>Units</th><th>Examples</th></tr>
<tr><td>Species name</td><td>Required</td><td>--</td><td>RORD /OH 2.0/</td></tr>
<tr><td>Stoichiometric coefficient υ''_{ki}</td><td>Required</td><td>--</td><td>RORD /OH 2.0/</td></tr>
<tr><td>Reaction Example</td><td colspan="3">H2+O2=2OH
0.170E+14 0.00 47780

RORD /OH 2.0/</td></tr>
<tr><td>Notes</td><td colspan="3">See also FORD.</td></tr>
</table></td></tr>
<tr><td>SRI</td><td>Defines the SRI pressure-dependent reaction rate (see Equation 3.34 of the Chemkin-Pro Theory Manual). SRI must be followed by either three, or five, slash-delimited parameters a, b, c, d, and e. The fourth and fifth parameters are optional and if omitted, they are by default d =1 and e =0.
<table>
<tr><th>Parameters</th><th>Optional/Reqd.</th><th>Units</th><th>Examples</th></tr>
<tr><td>SRI reaction rate parameters a - e</td><td>Required</td><td>--</td><td>SRI /0.45 797. 979. 1.0 0.0/</td></tr>
</table></td></tr>
</table>

<table>
<tr><th>Keyword</th><th colspan="4">Definition</th></tr>
<tr><td></td><td>Reaction Example</td><td colspan="3">CH3+H(+M) = CH4(+M) 6.0E16
-1.0 0

LOW/8.0E26 -3.0 0/

SRI/0.45 797.0 979.0/

H2/2/ CO/2/ CO2/3/ H2O/5/</td></tr>
<tr><td></td><td>Notes</td><td colspan="3">• Additional SRI parameters are required, by use of keywords LOW or HIGH.</td></tr>
<tr><td>TCHEB</td><td colspan="4">Supersedes the default temperature limits for a Chebyshev polynomial rate expression (see Equation 3.41 of the Chemkin-Pro Theory Manual). TCHEB must be followed by the slash-delimited values, Tmin and Tmax.</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td></td><td>Minimum temperature Tmin</td><td>Required</td><td>K</td><td>TCHEB / 300.0 2500./</td></tr>
<tr><td></td><td>Maximum temperature Tmax</td><td>Required</td><td>K</td><td>TCHEB / 300.0 2500./</td></tr>
<tr><td></td><td>Reaction Example</td><td colspan="3">C2H5+O2(+M)=C2H4E+HO2 (+M) 1.0
0.0 0.0

LOW / 1.0 0.0 0.0 /

TCHEB / 300. 2500./

CHEB/ 7 3 10.216 -1.1083
-0.19807 0.78325/

CHEB/ 1.1609 0.1.1762 -0.095707
0.10928 0.11551/

CHEB/ -0.08029 -0.10978 3.7074E-
04 -0.01483 -0.060589/

CHEB/ -0.028056 6.9203E-03 -
9.7259E-03 -0.013556 7.6648E-03/

CHEB/ 6.6865E-03 -8.8244E-04/</td></tr>
<tr><td></td><td>Notes</td><td colspan="3">• The default Chebyshev polynomial temperature limits are Tmin=300, Tmax=2500.

• Required Chebyshev polynomial parameters must be provided by use of keyword CHEB.

• Supplemental Chebyshev polynomial pressure limits may be provided by use of keyword PCHEB.</td></tr>
</table>

<table>
<tr><th>Keyword</th><th>Definition</th></tr>
<tr><td>TDEP</td><td>Species Temperature Dependence - Causes the reaction rate constant to be evaluated using the specified species temperature and the rate parameters given in the reaction data. In the case when there is more than one temperature defined in the system, the Application must call the Gas-phase Kinetics subroutine CKKTFL to indicate which temperature in the temperature array corresponds to each species. Examples of the TDEP input are shown in Figure 3.5: Examples of Auxiliary Reaction Data (p. 56).
<table>
<tr><th>Parameters</th><th>Optional/Reqd.</th><th>Units</th><th>Examples</th></tr>
<tr><td>Species name</td><td>Required</td><td>--</td><td>TDEP/E/</td></tr>
<tr><td>Keyword Usage</td><td colspan="3">E + CL2 => CL- + CL 5.8901E-09 - 2.5619E-01 1.5834E+04

TDEP/E/</td></tr>
</table></td></tr>
<tr><td>TROE</td><td>Defines the Troe pressure-dependent reaction rate (see Equation 3.33 of the Chemkin-Pro Theory Manual). TROE must be followed by the slash-delimited 3 or 4 parameters α, T^{***}, T^{*}, and T^{**}; the fourth parameter is optional and if omitted, the last term in Equation 3.33 is not used.
<table>
<tr><th>Parameters</th><th>Optional/Reqd.</th><th>Units</th><th>Examples</th></tr>
<tr><td>α</td><td>Required</td><td>Depends on reaction</td><td>TROE /0.5336 629.2 2190. 626.5/</td></tr>
<tr><td>T***</td><td>Required</td><td>K</td><td>TROE /0.5336 629.2 2190. 626.5/</td></tr>
<tr><td>T*</td><td>Required</td><td>K</td><td>TROE /0.5336 629.2 2190. 626.5/</td></tr>
<tr><td>T**</td><td>Optional</td><td>K</td><td>TROE /0.5336 629.2 2190. 626.5/</td></tr>
<tr><td>Reaction Example</td><td colspan="3">C2H5+O2(+M)= C2H4+HO2(+M) 1.41E7 1.09 -1975.

HIGH/6.85E-12 6.53 -834./

TROE/0.45 1.E-10 1.E10/

H2/2/ CO/2/ CO2/3/ H2O/5/</td></tr>
<tr><td>Notes</td><td colspan="3">Other required TROE parameters must be provided by use of keywords LOW or HIGH.</td></tr>
</table></td></tr>
<tr><td>UNITS</td><td>Reaction Units - Supersedes the current units for a particular reaction rate fit that may differ from the default units specified for other reaction expressions in the chemistry mechanism. UNITS must be followed by the slash-delimited character-string string, where string is one of the following: EVOL[TS], KELV[INS], CAL/[MOLE], KCAL[/MOLE], JOUL[ES/MOLE], or KJOU[LES/MOLE] for parameters with energy units such as E_i, or MOLES or MOLEC[ULES] for pre-exponential factors A_i, where the letters in brackets are optional. The inclusion of MOLEC[ULES] would indicate</td></tr>
</table>

<table>
<tr><th>Keyword</th><th>Definition</th></tr>
<tr><td></td><td>
that the reaction rate expression is in units of molecules/cm^3 rather than mole/cm^3. The UNITS auxiliary keyword allows only one string parameter, but the user can repeat the UNITS as many times as needed for a given reaction.
<table>
<tr><th>Parameters</th><th>Optional/Reqd.</th><th>Units</th><th>Examples</th></tr>
<tr><td>Reaction units character string</td><td>Required</td><td>--</td><td>UNITS /MOLECULES/</td></tr>
<tr><td>Reaction Example</td><td colspan="3">CF3+ + E + #WSIO2(B) => #SIO2 + CF3 0.33 0.0 0.0

BOHM !

YIELD /0.01 20. 0.5 1.0/
UNITS/EVOLTS/</td></tr>
<tr><td>Notes</td><td colspan="3">• Default units for A_i are cgs (cm, sec, K, mole), the exact units depending on the order of the reaction.

• Default units for E_i are (cal/mole).

• If any of the units strings are given on the REACTIONS header line, it applies to all reactions, but may be superseded for a particular reaction by the auxiliary UNITS keyword

• Even if the default energy units are changed by giving the UNITS keyword, the temperature appearing in the Arrhenius expression of Equation 3.5 of the Chemkin-Pro Theory Manual is still in Kelvins.</td></tr>
</table>
</td></tr>
<tr><td>USRPROG</td><td>
Optional User Rate Subroutine CKUPROG - The net rate-of-progress for the reaction will be obtained by calling a user-supplied subroutine, CKUPROG. An optional slash(/)-delimited integer parameter allows the user to select from more than one type of rate formulation. Wherever the net reaction rate is required, it will be obtained by calling the user-written subroutine. A template of CKUPROG is provided in the ANSYS Chemkin-Pro installation, in the file cklib_user_routines.f located in the directory user_routines. Information about how to compile and link user routines into Chemkin-Pro is included in Chemkin-Pro Application Programming Interface Manual.
<table>
<tr><th>Parameters</th><th>Optional/Reqd.</th><th>Units</th><th>Examples</th></tr>
<tr><td>Rate formulation type</td><td>Optional</td><td>--</td><td>USRPROG /1/</td></tr>
<tr><td>Reaction Example</td><td colspan="3">H2+O2=>2OH 1.7E13 0.0 47780.

USRPROG/1/</td></tr>
</table>
</td></tr>
</table>

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Keyword	Definition	
	Notes	• USRPROG applies only to irreversible reactions, and cannot be used in conjunction with USRPROD (entered on the REACTIONS header line).
XSMI	Flags a reaction as representing collision cross-section information for the determination of ion momentum-transfer collision frequencies in a plasma simulation. No auxiliary parameters are required. The evaluated rate-constant is assumed to be in cm^2, and is left as such when *Gas-phase Kinetics* subroutines evaluate rates of progress for other reactions. For more detail, see Rates of Creation and Destruction of Species of the Chemkin-Pro Theory Manual . Examples are given in Figure 3.5: Examples of Auxiliary Reaction Data (p. 56) .	

	Reaction Example	`CL+ + CL => CL+ + CL`
		`1.03E-13 -0.5  0.0`
		
		`  TDEP/CL+/`
		
		`XSMI     !momentum-transfer x-sec`

	Notes	• These options would generally not be used (or would be ignored) with any of the standard ANSYS Chemkin-Pro reactor models; they are there for users who may be incorporating Chemkin-Pro into a multi-dimensional plasma simulation user program.

Figure 3.5: Examples of Auxiliary Reaction Data

```
REACTIONS            CAL/MOLE   ! these are the default units for the reaction rates
HCO+M=H+CO+M             0.250E+15  0.000  16802.000                     !  Warnatz
CO/1.87/  H2/1.87  CH4/2.81/ CO2/3./  H2O/5./

H+C2H4(+M)=C2H5(+M)      0.221E+14  0.000  2066.000                       ! Michael
   LOW / 6.369E27  -2.76  -54.0 /                      !Lindemann fall-off reaction
   H2/2/  CO/2/  CO2/3/  H2O/5/                  ! enhanced third-body efficiencies

CH3+CH3(+M)=C2H6(+M)   9.03E16  -1.18  654.
   LOW / 3.18E41  -7.03  2762 /
   TROE / 0.6041  6927.  132. /          ! TROE fall-off reaction, with 3 parameters
   H2/2/  CO/2/  CO2/3/  H2O/5/                  ! enhanced third-body efficiencies

CH3+H(+M)=CH4(+M)   6.0E16  -1.0  0.0
   LOW / 8.0E26  -3.0  0.0/
   SRI  / 0.45  797.  979. /                                ! SRI fall-off reaction
   H2/2/  CO/2/  CO2/3/  H2O/5/                  ! enhanced third-body efficiencies

CH3+CH3(+M)=H + C2H5(+M)   4.989E12 0.099   10600.0 ! Stewart
   HIGH/ 3.80E-7  4.838   7710. /                   ! Chemically activated reaction
   SRI  / 1.641  4334  2725 /                             ! SRI pressure dependence

CH4+H=CH3+H2               1.25E14  0  1.190E4                          ! Westbrook
   REV / 4.80E12  0  1.143E4 /

! The following two reactions are acceptable duplicates:

H2+O2 = 2OH                    1.7E13   0   47780
   DUPLICATE
H2+O2 = 2OH                    1.0E13   0   47000.
   DUPLICATE

H2(1)+H2O(000)=H2(0)+H2O(001)  2.89E15  0  0
```

```
   LT / -67  62.1/                                          ! Landau-Teller reaction

! The following is a Chebyshev polynomial rate description

C2H5 + O2 (+M)       <=> C2H4E + HO2 (+M)  1.00E+00     .000       0.     ! Bozzelli
   TCHEB/ 300 2500/          PCHEB/1 100/
   CHEB/  7   3       1.0216E+01 -1.1083E+00 -1.9807E-01  7.8325E-01/
   CHEB/  1.1609E+00  1.1762E-01 -9.5707E-02  1.0928E-01  1.1551E-01/
   CHEB/ -8.0290E-02 -1.0978E-01  3.7074E-04 -1.4830E-02 -6.0589E-02/
   CHEB/ -2.8056E-02  6.9203E-03 -9.7259E-03 -1.3556E-02  7.6648E-03/
   CHEB/  6.6865E-03 -8.8244E-04/

! The following reactions allow plasma kinetics descriptions
E + E + AR+ <=> AR  +  E  1.414E+39   -4.500  0.00                ! Mansbach & Keck
   TDEP/E/   REV/6.807E+31  -3.0 364218./           !electron temperature dependence

E + AR => AR + E          4.9E-7   0.162  8.7634E3
   TDEP/E/  MOME                              !Momentum-transfer collision frequency
   UNITS/KELVIN/

AR+ + AR => AR+ + AR      1.E-16   0.0   0.0                          !units of cm^2
   XSMI                              !Ion momentum-transfer collision cross-section

E + AR => AR + E          2.235E16  0.0  3.47E5
   TDEP/E/   EXCI/11.60/  ! metastable excitation reaction
   DUP
H2O+H = OH+H2             0.117E+10  1.30   3626
   FORD /H2O 1.1/

END                                                        !END line is optional
```

3.6.3.1. Problems Having No Reactions

In some problems only information about the elements and species is needed (e.g., chemical equilibrium computations). For these it is not necessary to include reaction data. The *Gas-phase Kinetics* Pre-processor will create the Linking File (e.g., *chem.asc*), but it will not contain any reaction information. Therefore, no subroutines in the *Gas-phase Kinetics* Subroutine Library that deal with chemical reactions (e.g., chemical production rates) may be used.

Table 3.8: Summary of the Rules for Auxiliary Reaction Data (p. 57) summarizes the rules for auxiliary reaction data.

Table 3.8: Summary of the Rules for Auxiliary Reaction Data

Rule	Description
1	Auxiliary information lines may follow reaction lines that contain an `M` to specify enhanced third-body efficiencies, a reversible reaction to specify the reverse rate parameters explicitly, or any reaction that specifies Landau-Teller parameters. Auxiliary information must follow any duplicate reactions as well as all reactions that indicate pressure-dependent behavior by (`+M`) (i.e., provide fall-off parameters).
2	A species may have only one enhanced third body efficiency associated with it in any one reaction.
3	Only one radiation wavelength may be declared in a reaction.
4	The order in which the enhanced third body declarations are given is the order in which arrays of enhanced third body information are referenced in the subroutine package.
5	There cannot be more than ten enhanced third bodies in a reaction.
6	Keyword declarations may appear anywhere on the line, in any order.

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Rule	Description
7	Any number of keywords may appear on a line and more than one line may be used; however, a keyword and its parameter(s) must appear on the same line.
8	Keyword declarations that appear on the same line must be separated by at least one blank space.
9	Any blank spaces between a keyword and the first slash are ignored and any blanks between the slashes and parameter(s) are also ignored. However, no blank spaces are allowed within a keyword or a parameter.
10	All characters following an exclamation mark are comments.
11	In ion momentum-transfer collision cross-section reactions there must be exactly two reactant species, one of which must be an ion.
12	In electron momentum-transfer collision frequency reactions, there must be exactly two reactant species, one of which must be the electron.

3.6.4. Error Checks

The *Gas-phase Kinetics* Pre-processor checks each input line for proper syntax and writes diagnostic messages on logical file `LOUT` if errors are encountered. If an error condition occurs, the Pre-processor continues to read and diagnose the input, but an error flag is written to the Linking File and the *Gas-phase Kinetics* subroutine `CKINIT` will not initialize the work arrays. Therefore, the input must be error free before any of the *Gas-phase Kinetics* subroutines can be called. The possibilities for an error condition are listed Table 3.9: Error Checks (p. 58) .

Table 3.9: Error Checks

Data Type	Possible Errors
Element Data	Atomic weight for an element or isotope is not declared, and the element is not found in the Pre-processor's database.
	Atomic weight has been declared, but not enclosed by two slashes (/).
	If an element is declared twice, a diagnostic message is printed, but the duplicate is simply eliminated from consideration and is not considered a fatal error.
Species Data	If a species is declared twice, a diagnostic message is printed, but the duplicate is eliminated from consideration and is not considered a fatal error.
	No thermodynamic data have been found for a declared species.
Thermodynamic Data	Thermodynamic data are format sensitive and therefore provide possibilities for error if not formatted exactly as described by Table 2.1: Summary of the Rules for Thermodynamic Data (p. 4) .
	An element in the thermodynamic data for a declared species has not been included in the element data.
	With the `THERMO ALL` option, line 2 (Table 2.1: Summary of the Rules for Thermodynamic Data (p. 4)) is not found.

Data Type	Possible Errors
Reaction Data	A delimiter =>, <=>, or = between the reactants and the products is not found.
	Three Arrhenius parameters are not found.
	Reactants and/or products have not been properly delineated by a plus sign (+).
	A species as a reactant or product has not been declared in the species data.
	The reaction does not balance in elements.
	The reaction does not balance in electronic charge.
	A reaction is a duplicate not declared by the auxiliary data keyword DUP.
	A third-body species enclosed in parentheses in a fall-off reaction appears as reactant or product, but not both.
	A species is a third-body in a fall-off reaction, and +M also appears in the reaction.
	More than one +M or third body appear as reactants and/or products.
	There are more than six reactants or six products.
Auxiliary Reaction Data	There is an unknown or misspelled keyword or enhanced third-body species name.
	Parameters for a keyword are not enclosed in slashes.
	The wrong number of parameters appear for a keyword.
	There are duplicate keywords for a reaction.
	LOW, HIGH, TROE, SRI, PCHEB, TCHEB, or CHEB are found after a reaction that did not have a species or M in parentheses.
	LOW, HIGH, or CHEB is not found after a pressure-dependent reaction.
	A combination of TROE, SRI, CHEB and/or PLOG is found.
	LT and REV are found for a Landau-Teller reaction, but RLT is not found.
	LT is given for a fall-off reaction.
	There are more than ten enhanced third bodies.
	There are more than or less than two reactants specified with XSMI or MOME keywords.
	An ionic species is not specified as a reactant with the XSMI keyword.
	The electron is not a reactant when using the MOME keyword.
	USRPROG given for a USRPROD mechanism.
	USRPROG given for a reversible reaction.

Chapter 4: Surface Kinetics Input

The *Surface Kinetics* input file provides symbolic description of a surface reaction mechanism. Pre-processing this file requires obtaining information stored in the *Gas-phase Kinetics* linking file (e.g., *chem.asc*) that was created from the gas-phase mechanism associated with the chemistry set. Pre-processing the *Surface Kinetics* input file results in the creation of an additional linking file (e.g., *surf.asc*) that contains information about the surface mechanism and the species it involves. The information in the *Surface Kinetics* Linking File is subsequently accessed by the initialization routine in the *Surface Kinetics* Subroutine Library to store information in memory during a reacting-flow simulation. This stored information is then used to call other routines in the *Surface Kinetics* Subroutine Library to provide information on thermodynamic properties and chemical production rates.

The *Surface Kinetics* input includes information on surface sites (phases), surface species, bulk phases, bulk species, thermodynamic data, and the reaction mechanism. The order of data entry in the *Surface Kinetics* input file is: material name, site data, bulk data, thermodynamic data, reaction data, and a material-end statement. All input data is optional, but species included in reaction strings must be declared as site or surface species (or as gas species in the Gas Kinetics input file) and must have associated thermodynamic data included either directly in the *Surface Kinetics* input file or in a thermodynamic database file (e.g., *therm.dat*). Such sets of information can be repeated for any number of different materials within the same *Surface Kinetics* input file. With the exception of the thermodynamic data, all input is format free. The syntax and rules for all of the data input is described in this chapter. The auxiliary keywords for surface reactions are described in Table 4.6: Alphabetical Listing of Surface Reaction Auxiliary Keywords (p. 72) and the options for specifying units on the REACTIONS line are described in Table 4.3: Alphabetical Listing of REACTIONS-line Options for Surface Reaction Data (p. 66). Alphabetical Listing of Project Input Keywords (p. 123) describes the meaning and usage of each keyword entry that may be included as part of a Reactor Model input file.

Note

The *Surface Kinetics* Input File allows **259** columns for the presentation of the input data.

4.1. Material Declaration

Entirely different surface reaction mechanisms (i.e., with different surface and bulk phases and species, and different surface reactions) can be specified in the same *Surface Kinetics* input file through the use of multiple materials. At the beginning of each separate portion of the input file corresponding to a given material, the user gives an input line with the keyword MATERIAL followed by an optional slash-delimited material name. If no name for the material is supplied, a default name MATERIAL **n** is provided, where **n** is the number of the material (e.g., MATERIAL2 for the second material given in an input file). An example of the usage of multiple materials is given in Figure 4.1: Examples of Material Declarations (p. 61) .

Figure 4.1: Examples of Material Declarations

```
!--------------------GAS-PHASE KINETICS PRE-PROCESSOR INPUT-----------------
ELEMENTS  SI CL E AL
SPECIES   E CL2+ CL+ SICL4 SICL2 CL
```

```
NOTE THAT ABOVE IS A CHEM.INP FILE, WHILE BELOW IS A SURF.INP FILE.

!---------------------------SURFACE KINETICS PRE-PROCESSOR INPUT--------------
MATERIAL WAFER
SITE/POLY/ SDEN/2.25e-9/
 SI(S)  SICL(S) SICL2(S) SICL3(S)
END
BULK SI(B)/2.33/
REACTIONS  MWOFF
    CL + SI(S)    => SICL(S)                          1.0   0.0  0.0
       STICK
    E + CL2+ + 2SI(S) => 2SICL(S)                     0.4   0.0  0.0
       BOHM
    E + CL+ + SICL3(S) + SI(B) => SICL4 + SI(S)       0.50  0.0  0.0
       BOHM
       ENRGDEP/1. 0.5 1.0/  UNITS/EVOLT/
    E + CL+ + #SICL3(S) + #SI(B) + SICL(S) &
          => SICL2(S) + #SICL2 + #SICL(S)             0.50  0.0  0.0
       BOHM
       YIELD/0.0712 1.21 0.5 1.0/  UNITS/EVOLT/
!           /A   Eth[eV] a b /   for #=A(Ei^a-Eth^a)^b
END
MATERIAL WALL
SITE/METAL/ SDEN/2.25E-9/
 AL(S) ALCL(S)
END
REACTIONS  MWOFF
    CL+ + E       => CL                   0.6   0.0  0.0
       BOHM
    CL + AL(S)    => ALCL(S)              1.0   0.0  0.0
       STICK
END
```

4.2. Site Data

Surface-phase species exist on sites, and a site and its species must be identified on one or more lines of site data. The first line in a set of site data must start with the word SITE ; an optional name may be associated with a site if it immediately follows SITE and is delimited by slashes(/). If no name for the site is supplied, a default name SITE **n** is provided, where **n** is the number of a site (e.g., SITE2 for the second site type listed). Following SITE and/or the site name, the word SDEN and a slash-delimited density (the standard state site density for this site, in mole/cm^2) for the site is required. The species that can reside on the site type are declared by a list of species symbols (names) on the same line or on additional lines.

Note

The name of a site species must not duplicate the name of a gas-phase species or a bulk species, and must be unique among the site species for all materials.

An optional slash-delimited site occupancy number may follow a species name, i.e., the number of individual sites that this species occupies. (For example, a large chemical species might cover two or more sites.) The default site occupancy for a surface species is 1. The sets of SITE data input can continue for as many site types as are needed.

Any set of up to sixteen upper- or lower-case characters can be used as a site name or species symbol. In addition, each species must be composed of elements that have been identified in the *Gas-phase Kinetics* Pre-processor and thus contained in the *Gas-phase Kinetics* Linking File. One of the purposes

of the site data is to define the order in which arrays of site species information are referenced in the *Surface Kinetics* Subroutine Library.

Note

Species symbols may not begin with a number, a plus sign (+), a pound sign (#), or an equality sign (=), have imbedded blanks, or include a slash (/). An ionic species may end with any number of plus or minus signs; an imbedded plus sign must be enclosed in parentheses.

Any line starting with or any portion of a line following an exclamation mark (!) is considered a comment and will be ignored. Blank lines are also ignored. Figure 4.2: Examples of Site Data (p. 63) shows sample site data. The rules for site data are summarized in Table 4.1: Summary of the Rules for Site Data (p. 63)
.

Figure 4.2: Examples of Site Data

```
SITE / PLANE /               SDEN/1.04E-9/   ! PLANAR SITE
  ASH(V)                                      ! FIRST SPECIES ON PLANE SITE
 ASH2(V) ASH3(V) H(S) CH3(V) AS(V) AS2(V)/2/
 V                                           ! EMPTY PLANAR SITE
END                                          ! AN END STATEMENT IS OPTIONAL
SITE / LEDGE /   SDEN/1.66E-10/              ! LEDGE SITE
  GACH(L)                                    ! FIRST SPECIES ON LEDGE
  DMG(L)/2/                                  ! THIS SPECIES OCCUPIES 2 SITES
  L                                          ! EMPTY LEDGE SITE
SITE SDEN/1.0E-10/ GA(S)                      ! SITE WITH ONLY ONE SPECIES
                                               ! SITE NAME NOT INCLUDED
```

Table 4.1: Summary of the Rules for Site Data

Rule	Description
1	Site data must start with a line containing the word SITE, followed by an optional slash-delimited name (i.e., SITE/ name /).
2	The standard state site density is required as a slash-delimited number (in mole/cm^2) following the word SITE and/or the site name, and preceded by the word SDEN.
3	The site density is followed by one or more site species name declarations. Declaring a site with no site species is an error.
4	Site and species names are composed of up to sixteen upper- or lower-case character symbols. The names cannot begin with the characters +, =, #, or a number; an ionic species name may end with one or more + or - signs; an embedded plus sign must be enclosed in parentheses (+). Names cannot include a slash (/).
5	All species names should be unique; duplicate species names will be ignored and a warning issued. A species name may not duplicate a name of a gas-phase species, another surface species, or a bulk species.
6	A site name must not duplicate the name of any other phase (gas, surface site, or bulk phase).
7	Each surface species that subsequently appears in a surface reaction must have been declared in this section.
8	A site species name may appear anywhere on the line.

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Rule	Description
9	A site species may have a slash-delimited site occupancy (the number of sites that this species occupies on the surface) following the species name.
10	A species name declaration that begins on one line may not continue to the next line (i.e., do not break a species name into two lines).
11	There may be more than one set of SITE data.
12	All characters on a line following an exclamation mark are considered comments.
13	SITE data are not required.

4.3. Bulk Data

A set of bulk data may consist of one or more condensed-phase species. The first line in a set of bulk data must start with the word BULK and may be followed by an optional slash-delimited name for the bulk phase. If a name is not supplied for bulk phase *n*, then the name BULKn is supplied. Bulk species are declared by a list of unique species symbols (names) on the same line or on additional lines. An optional slash-delimited density (in g/cm^3) may follow a species name. If no density is supplied, the unphysical value of -1.0 is stored as a flag. The rules for bulk species symbols (names) are essentially the same as those for site species. Figure 4.3: Examples of Bulk Data (p. 65) shows sample bulk data. The rules for bulk data are summarized in Table 4.2: Summary of the Rules for Bulk Data (p. 64) .

Table 4.2: Summary of the Rules for Bulk Data

Rule	Description
1	Bulk data must start with a line containing the word BULK, and may be followed by a slash-delimited name for the bulk phase (i.e., BULK/ name /).
2	The BULK declaration and/or bulk name must be followed by one or more bulk species declarations. Declaring a bulk phase with no bulk species is an error.
3	Bulk and bulk species names are composed of up to sixteen upper- or lower-case character symbols. The names cannot begin with the +, =, #, or a number; an ionic species name may end with one or more + or - signs; an embedded plus sign must be enclosed in parentheses (+). Names cannot include a slash (/).
4	All species names should be unique; duplicate species names will be ignored and a warning issued. A species name may not duplicate a name of a gas-phase species, a surface species, or another bulk species.
5	All phase names must be unique. For example, a bulk phase name may not duplicate the name of any other phase (gas, surface site, or bulk phase).
6	Each bulk species that subsequently appears in a surface reaction must have been declared in this section.
7	A bulk species declaration may start anywhere on the line.
8	A bulk species name may be followed by an optional slash-delimited mass density (in g/cm^3).
9	A bulk species declaration that begins on one line may not continue to the next line (i.e., do not break species names into two lines).
10	There may be more than one set of BULK data.

Rule	Description
11	All characters on a line following an exclamation mark are considered comments and are ignored.
12	BULK data are not required.

Figure 4.3: Examples of Bulk Data

```
BULK / GA_RICH /  GA2AS(1)/3.0/  GA3AS(1)/3.0/     END
                                                !an END statement is optional
BULK / GA_RICH /
GA2AS(1)/3.0/
GA3AS(1)/3.0/
GA2AS(1)/2.0/               !THIS NAME IS A DUPLICATE AND WILL BE IGNORED
BULK AS(B)                                !BULK PHASE WITH NO NAME SUPPLIED
                           !ONLY ONE BULK SPECIES AND NO DENSITY SUPPLIED
END
```

4.4. Thermodynamic Data

Any chemical species that appears in a problem must have thermodynamic data associated with it. This data is used in evaluation of thermodynamic properties (entropy, enthalpy, heat capacity) and reverse reaction rate constants through the equilibrium constant. Often thermodynamic data for a species, for instance a surface species, is unknown. Such data can sometimes be calculated via theoretical techniques. However, the user can work around the need for actual thermodynamic data for all species by making the reactions irreversible. In this case, the user can supply " dummy" thermodynamic data for the surface species to satisfy the requirement.

Note

If every reaction in the mechanism is either irreversible, or if Arrhenius rate parameters are given explicitly for the reverse reaction, then the thermodynamic data for species are not actually used for anything related to the kinetics. They may, however, be used in surface heat balances if such are enabled for a particular reacting-flow problem.

The data may be extracted from a database file (e.g. *therm.dat*) and/or read directly from the *Surface Kinetics* input file. Details on the thermodynamic data format, whether including in the *Surface Kinetics* input file or in a thermodynamic database file, are provided in Thermodynamic Data Format (p. 3) .

Note

When thermodynamic data is included in the *Surface Kinetics* Input file, it must immediately follow phase (SITE and BULK) data.

4.5. Reaction Mechanism Description

The surface reaction mechanism may consist of any number of chemical reactions involving the solid species named in the site and bulk data, as well as the gas-phase species declared in the *Gas-phase Kinetics* input file. A reaction may be reversible or irreversible. Reaction data must start with a line containing the word REACTIONS (or REAC). The lines following the REACTIONS line contain reaction descriptions together with their Arrhenius rate coefficients. The reaction description is composed of reaction data and perhaps optional auxiliary reaction data.

4.5.1. REACTIONS Line Options

On the same line as the REACTIONS word, you may define certain options that will apply globally to all surface reactions. In some cases, Auxiliary Reaction Keywords given for a specific reaction may override these global settings. A summary of the REACTIONS -line options are provided in Table 4.3: Alphabetical Listing of REACTIONS-line Options for Surface Reaction Data (p. 66).

Note

Even if the default energy units are changed by giving one of these keywords, the temperature appearing in the Arrhenius expression of Equation 3.5 , i.e., in T raised to the β power and in the denominator of the activation energy term, is still in Kelvins.

Note

If units are not specified, A_i and E_i are assumed to be in (cm, mole, sec, K) and cal/mole, respectively.

Table 4.3: Alphabetical Listing of REACTIONS-line Options for Surface Reaction Data

Keyword	Definition
ATM	Supersedes the default units for all surface reactions that follow the REACTIONS header line for pre-exponential factors A_i ; the units of gas species are partial pressures in atm.
	Notes Default units for A_i are cgs (cm, sec, K, mole), the exact units depending on the order of the reaction.
BAR	Supersedes the default units for all surface reactions that follow the REACTIONS header line for pre-exponential factors A_i; the units of gas species are partial pressures in bar.
	Notes Default units for A_i are cgs (cm, sec, K, mole), the exact units depending on the order of the reaction.
CAL/[MOLE]	Re-iterates the default units for all surface reactions that follow the REACTIONS header line for parameters with energy units such as E_i.
	Notes Default units for E_i are cal/mole.

Keyword	Definition
DYN[ES]	Supersedes the default units for all surface reactions which follow the REACTIONS header line for pre-exponential factors A_i; the units of gas species are partial pressures in dyne/cm^2.
	Notes Default units for A_i are cgs (cm, sec, K, mole), the exact units depending on the order of the reaction.
EVOL[TS]	Supersedes the default units for all surface reactions which follow the REACTIONS header line for parameters with energy units such as E_i.
	Notes Default units for E_i are cal/mole.
JOUL[ES/MOLE]	Supersedes the default units for all surface reactions which follow the REACTIONS header line for parameters with energy units such as E_i.
	Notes Default units for E_i are cal/mole.
KCAL[/MOLE]	Supersedes the default units for all surface reactions which follow the REACTIONS header line for parameters with energy units such as E_i.
	Notes Default units for E_i are cal/mole.
KELV[INS]KCAL/MOLE	Supersedes the default units for all surface reactions which follow the REACTIONS header line for parameters with energy units such as E_i.
	Notes Default units for E_i are cal/mole.
KJOU[LES/MOLE]	Supersedes the default units for all surface reactions which follow the REACTIONS header line for parameters with energy units such as E_i.
	Notes

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Keyword	Definition
	Default units for E_i are cal/mole.
MAXSP	Increases the maximum number of reactants or products allowed in a reaction. The number given by this keyword must be greater than the default limit of 6. For example, `REACTIONS MAXSP=11`.
	Notes This keyword is available to both the gas-phase and surface reaction mechanism.
MOLEC[ULES]	Supersedes the default units for all surface reactions which follow the `REACTIONS` header line for pre-exponential factors A_i.
	Notes Default units for A_i are cgs (cm, sec, K, mole), the exact units depending on the order of the reaction.
MOLE[S]	Re-iterates the default units for all surface reactions which follow the `REACTIONS` header line for pre-exponential factors A_i.
	Notes Default units for A_i are cgs (cm, sec, K, mole), the exact units depending on the order of the reaction.
MWOFF	Turns off the Motz-Wise correction of Equation 4.15 of the Chemkin-Pro Theory Manual for all sticking-coefficient reactions which follow the `REACTIONS` header line.
	Notes By default, the Motz-Wise correction is off for all sticking coefficient reactions; the default may be superseded for a particular sticking-coefficient reaction by use of the auxiliary reaction keyword MWOFF or MWON.
MWON	Turns on the Motz-Wise correction of Equation 4.15 of the Chemkin-Pro Theory Manual for all sticking-coefficient reactions which follow the `REACTIONS` header line.
	Notes By default, the Motz-Wise correction is off for all sticking coefficient reactions; the default may be superseded for a particular sticking-coefficient reaction by use of the auxiliary reaction keyword MWOFF or MWON .

Keyword	Definition
NONCON	Allows non-conservation of sites in any surface reaction which follows the REACTIONS header line. Normally, any reaction that does not conserve the number of surface sites in each surface phase is considered to be in error; the inclusion of NONCON on the REACTIONS line supersedes that rule.
PAS[CALS]	Supersedes the default units for all surface reactions that follow the REACTIONS header line for pre-exponential factors A_i; the units of gas species are partial pressures in pascals.
	Notes Default units for A_i are cgs (cm, sec, K, mole), the exact units depending on the order of the reaction.
SITE[FR]	Supersedes the default units for all surface reactions which follow the REACTIONS header line for pre-exponential factors A_i; the units of surface species are site fraction and the reaction rate unit is 1/sec.
	Notes Default units for A_i are cgs (cm, sec, K, mole), the exact units depending on the order of the reaction.
TOR[R]	Supersedes the default units for all surface reactions which follow the REACTIONS header line for pre-exponential factors A_i; the units of gas species are partial pressures in torr.
	Notes Default units for A_i are cgs (cm, sec, K, mole), the exact units depending on the order of the reaction.
USRPROD	The net rate-of-production for all species will be obtained by calling a user-supplied subroutine, SKUPROD. An optional slash(/)-delimited integer parameter allows the user to select from more than one type of rate formulation. Wherever the net rates of production of species are required, they will be obtained by calling the user-written subroutine. A template of SKUPROD is provided in the ANSYS Chemkin-Pro installation, in the file *sklib_user_routines.f* located in the directory *user_subroutines*. Information about how to compile and link user routines into Chemkin-Pro is included in Chemkin-Pro Application Programming Interface Manual.
	Notes

Keyword	Definition
	USRPROD cannot be used in conjunction with USRPROG (entered after a particular reaction).

Note

Chemkin-Pro does not support user-written programs, so you are cautioned to use the SKUPROD user routine feature at your own risk. Also, there are some features in the program executables that will be incompatible with the global replacement of species rates of production, such as sensitivity analysis and rate-of-production analysis. Such features will return zero values when user-rate programming is encountered.

4.5.2. Reaction Data

Each reaction entry is divided into two fields, (an entry may use multiple lines if it is more than 80 characters long). A reaction data entry is continued on the next line using the special character "& " at the end of the line; any information following the & symbol on the same line is ignored. The first field in the reaction entry contains the symbolic description of the reaction, while the second contains the Arrhenius rate coefficients. Both fields are format free, and blank spaces are ignored. All characters on a line following an exclamation mark (!) are considered comments and are ignored. Blank lines are also ignored.

The reaction description, given in the first field, must be composed of the species symbols, coefficients, and delimiters as summarized below.

Table 4.4: Surface Reaction Data Criteria

Species Symbols	
	Each species in a reaction is described with the unique sequence of characters as they appear in the species data and the thermodynamic data.
Coefficients	
	A species symbol may be preceded by an integer or real coefficient. The coefficient has the meaning that there are that many moles of the particular species present as either reactants or products; e.g., 2OH is equivalent to OH +OH. The "# " symbol is used to mark stoichiometric coefficients that are additionally multiplied by a YIELD coefficient. This is explained in Auxiliary Reaction Data (p. 72) .
Delimiters	
+	A plus sign is the delimiter between each reactant species and each product species.
=	An equality sign is the delimiter between the last reactant and the first product in a reversible reaction.
<=>	An equality sign enclosed by angle brackets can also be used as the delimiter between the last reactant and the first product in a reversible reaction.
=>	An equality sign with an angle bracket on the right is the delimiter between the last reactant and the first product in an irreversible reaction.

The second field of the reaction line is used to define the Arrhenius rate coefficients A_i, β_i, and E_i in that order, as given by Equation 3.5 of theChemkin-Pro Theory Manual . At least one blank space must

separate the last species name in the reaction and first number. The three numbers must be separated by at least one blank space, be stated in either integer, floating point, or "E" format (e.g., `123` or `123.0` or `12.3E1`), and have units associated with them (although the units do not appear on the input line). Unless modified by the `REACTIONS` line or by the `UNITS` auxiliary keyword, the default units for A_i are cgs (cm, sec, K, mole), the exact units depending on the order of the reaction. The factor β_i is dimensionless. The default units for the activation energies are cal/mole.

The second field of the reaction line may optionally be used to specify the coefficients a_i, b_i, and c_i of Equation 4.10 of theChemkin-Pro Theory Manual for a sticking coefficient. In order for the second field to apply to sticking coefficient parameters, the next line of input must contain the auxiliary keyword `STICK`.

Examples of some reaction data are shown in Figure 4.4: Examples of Reaction Data (p. 71) . Table 4.5: Summary of the Rules for Reaction Data (p. 71) summarizes the reaction data rules.

Figure 4.4: Examples of Reaction Data

```
REACTIONS  KCAL/MOLE NONCON
ASH3 + AS(P) <=> ASH3(P) + AS(D)      4.0E11   0 25   ! Ref. 21
! ASH3 + AS(P) <=> ASH3(P) + AS(D)    4.0E11   0  0   ! same as previous
ASH <=> AS(D) + H(S)    1.0   0  0
      STICK
GA(CH3)3(L) + GA2AS(A) <=> AS + GA(CH3)(L) + 2 GAME & ! continued on next line
                                      1.0E13   0  4000.
```

Table 4.5: Summary of the Rules for Reaction Data

Rule	Description
1	The first reaction line must start with the word `REACTIONS` (or REAC), and may be followed by units definition(s), the word `MWON`, `MWOFF`, `NONCON`, or the word USRPROD.
2	The word `MWOFF` can be used to turn off the Motz-Wise correction of Equation 4.15 of the Chemkin-Pro Theory Manual , for all sticking-coefficient reactions, or the word `MWON` can be used to specify that the Motz-Wise correction is to be used for all sticking-coefficient reactions (the default). Including `MWOFF` or `MWON` as an auxiliary keyword for an individual reaction (discussed later) will override the setting given on the `REACTIONS` line.
3	Valid unit declarations are `EVOLTS`, `KELVINS`, `CAL/MOLE`, `KCAL/MOLE`, `JOULES/MOLE`, `KJOULES/MOLE`, `MOLES`, `MOLECULES`, `SITEFR`, `ATM`, `BAR`, `DYN`, `TOR`, and PASCAL.
4	The word `NONCON` is required on the first reaction line if any of the reactions do not conserve the number of surface sites of a given type.
5	The reaction description can begin anywhere on this line. All blank spaces, except those separating the Arrhenius coefficients, are ignored.
6	Each reaction description must have =, <=>, or => between the last reactant and the first product.
7	Each species in a reaction is described with a unique sequence of characters (name) as they appear in the species data and the thermodynamic data. However, if a species name is not unique (because it is duplicated in another phase), the name must be modified by appending its slash-delimited phase name, i.e. as `name / phase /`.

Rule	Description
8	Stoichiometric coefficients are represented by an integer or real number preceding a species name. The default is to assume a stoichiometric coefficient of `1`. The "`#` " symbol preceding the stoichiometric coefficient denotes a coefficient which is additionally multiplied by a "`yield` " multiplier.
9	A reaction description may be contained on more than one line. If a line contains the symbol &, all information following the & symbol will be ignored and the next line will be considered a continuation of the first.
10	Three Arrhenius coefficients must appear in order (A_i, β_i, and E_i) on each Reaction line, separated from each other and from the reaction description by at least one blank space; no blanks are allowed within a number.
11	There cannot be more than six reactants or six products in a reaction.
12	To specify a sticking coefficient rather than a rate constant the three numbers after the reaction description have the meaning a_i, b_i, and c_i (see Equation 4.10 of the Chemkin-Pro Theory Manual) and the auxiliary reaction data word `STICK` must appear on the next line of input. To use this option the reaction must have only one gas-phase species as a reactant and its stoichiometric coefficient must be `1`.
13	All characters on a line following an exclamation mark are comments.
14	For best results, an `END` statement should follow reaction input.

4.5.3. Auxiliary Reaction Data

Auxiliary information appears on one or more separate lines after the reaction data line is read, and serves to modify or give additional parameters needed to evaluate that reaction's rate expression. The format in an auxiliary information line is a character string keyword followed by a slash-delimited (/) field containing an appropriate number of parameters (either integer, floating point, E format, or character). Examples of many of the auxiliary options described in this section are shown in Figure 4.5: Examples of Auxiliary Reaction Data (p. 81) . Table 4.6: Alphabetical Listing of Surface Reaction Auxiliary Keywords (p. 72) provides detailed information on the meaning and usage of each auxiliary keyword entry that may be included as part of the Surface Reaction Data.

Table 4.6: Alphabetical Listing of Surface Reaction Auxiliary Keywords

Keyword	Definition	
BOHM	**Bohm Velocity Limit for Ions** - Applies the Bohm velocity correction for a reaction involving a positive ionic species (see Equation 4.29 of the Chemkin-Pro Theory Manual). No auxiliary parameters are required.	

	Reaction Example	`CL+ + E => CL 0.4 0.0 0.0`
		
		`BOHM`

	Notes	• The three coefficients given in the second field of the reaction line are interpreted as the parameters a_i, b_i, c_i, in Equation 4.29 of the Chemkin-Pro Theory Manual). • The reaction can have only one gas-phase reactant species, which must be a positive ion, and its stoichiometric coefficient must be 1.

<table>
<tr><th>Keyword</th><th>Definition</th></tr>
<tr><td>COV</td><td>Coverage Dependent Reactions - Modifies the expression for the forward rate constant by coverage parameters (see Equation 4.7 of the Chemkin-Pro Theory Manual). Must be followed by (slash delimited) surface species name and the three parameters η_{ki}, μ_{ki} and ε_{ki}.
<table>
<tr><th>Parameters</th><th>Optional/Reqd.</th><th>Units</th><th>Examples</th></tr>
<tr><td>Species name</td><td>Required</td><td>--</td><td>COV /Pt(S) 0.0 0.0 0.9/</td></tr>
<tr><td>Coverage parameter η_{ki}</td><td>Required</td><td>--</td><td>COV /Pt(S) 0.0 0.0 0.9/</td></tr>
<tr><td>Coverage parameter μ_{ki}</td><td>Required</td><td>--</td><td>COV /Pt(S) 0.0 0.0 0.9/</td></tr>
<tr><td>Coverage parameter ε_{ki}</td><td>Required</td><td>cal/mole</td><td>COV /Pt(S) 0.0 0.0 0.9 /</td></tr>
<tr><td>Reaction Example</td><td colspan="3">O(S) +O(S) =>Pt(S) +Pt(S) +O2
3.700E+23 0.0 213.0

COV/O(S) 0.0 0.0 -93.3/</td></tr>
<tr><td>Notes</td><td colspan="3">• More than one set of COV data can appear for a given reaction, and these would be applied multiplicatively as in Equation 4.7 of the Chemkin-Pro Theory Manual .</td></tr>
</table></td></tr>
<tr><td>DCOL</td><td>The reaction rate is proportional to the collision frequency between a gas molecule and a particle surface (see Equation 18.79 of the Chemkin-Pro Theory Manual). Must be followed by the (slash delimited) collision-diameter of the gas-phase reactant.
<table>
<tr><th>Parameters</th><th>Optional/Reqd.</th><th>Units</th><th>Examples</th></tr>
<tr><td>Collision diameter</td><td>Required</td><td>cm</td><td>DCOL /2.45E-8/</td></tr>
<tr><td>Reaction Example</td><td colspan="3">A1 + 8H(se) => 5H(se) + 6C(B) +
3open(se) + 4H2 + H 0.1 0.0 0.0

FORD/H(se) 2.0/

DCOL/2.46E-8/

STICK</td></tr>
<tr><td>Notes</td><td colspan="3">• The reaction must be irreversible.

• The reaction may have only one gas-phase.</td></tr>
</table></td></tr>
<tr><td>DUP</td><td>Duplicate Reactions - Two or more reactions can involve the same set of reactants and products, but proceed through distinctly different processes. In these cases, it may be appropriate to state a reaction mechanism that has two or more reactions that are the same, but have different rate parameters. However, duplicate reactions are normally considered errors by the Surface Kinetics Pre-Processor. If the user requires duplication (e.g., the same reactants and products with different Arrhenius parameters), keyword DUP must follow the reaction line of each duplicate reaction (including the first occurrence of the reaction that is duplicated). For example, if the user wishes to specify different rate expressions for each of</td></tr>
</table>

<table>
<tr><th>Keyword</th><th>Definition</th></tr>
<tr><td></td><td>two identical reactions, there must be two occurrences of the DUP keyword, one following each of the reactions. No auxiliary parameters are required.
<table>
<tr><td>Reaction Example</td><td><pre>O2 + 2PT(S) => 2O(S)
        1.80E+21   -0.5   0.0

DUP

O2 + 2PT(S) => 2O(S)
        0.023   0.00   0.00

DUP</pre></td></tr>
<tr><td>Notes</td><td>DUP is required for each of any duplicated reaction in the mechanism.</td></tr>
</table></td></tr>
<tr><td>ENRGDEP</td><td>Ion-energy Dependent Rates - Allows the rate constant to depend on ion energy according to Equation 4.30 of the Chemkin-Pro Theory Manual . ENRGDEP must be followed by the three (slash delimited) $E_{ion,0}$, f_i, and g_i.
<table>
<tr><th>Parameters</th><th>Optional/Reqd.</th><th>Units</th><th>Examples</th></tr>
<tr><td>Threshold energy E ion, 0</td><td>Required</td><td>cal/mole</td><td>ENRGDEP /1.0 0.5 1.0/</td></tr>
<tr><td>Exponential constant f i</td><td>Required</td><td>--</td><td>ENRGDEP /1.0 0.5 1.0/</td></tr>
<tr><td>Exponential constant g i</td><td>Required</td><td>--</td><td>ENRGDEP /1.0 0.5 1.0/</td></tr>
<tr><td>Reaction Example</td><td colspan="3"><pre>E + CL+ + SICL3(S) + SI(B) => SICL4 + SI(S)   0.50   0.0   0.

BOHM

ENRGDEP/1. 0.5 1.0/ UNITS/EVOLT/</pre></td></tr>
<tr><td>Notes</td><td colspan="3">• There must be exactly one positive ionic reactant species in the reaction.
• Only irreversible reactions are allowed with this option.</td></tr>
</table></td></tr>
<tr><td>FORD</td><td>Arbitrary Reaction Orders - 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. FORD is followed, in slash-delimited format, by the species name and the new reaction order. This option overrides the values of υ'_{ki} in Equation 3.4 of the Chemkin-Pro Theory Manual pertaining to the particular species named on the line; the reaction order for all other species is maintained at the default values.
<table>
<tr><th>Parameters</th><th>Optional/Reqd.</th><th>Units</th><th>Examples</th></tr>
<tr><td>Species name</td><td>Required</td><td>--</td><td>FORD /Pt(S) 1.0/</td></tr>
<tr><td>Stoichiometric coefficient</td><td>Required</td><td>--</td><td>FORD /Pt(S) 1.0/</td></tr>
</table></td></tr>
</table>

<table>
<tr><th>Keyword</th><th colspan="4">Definition</th></tr>
<tr><td></td><td>Reaction Example</td><td colspan="3">A1 + 8H(se) => 5H(se) + 6C(B) +
3open(se) + 4H2 + H 0.1 0.0 0.0

FORD/H(se) 2.0/

DCOL/2.46E-8/

STICK</td></tr>
<tr><td></td><td>Notes</td><td colspan="3">• Multiple occurrences of the FORD construct may appear on the auxiliary line.</td></tr>
<tr><td>LANG</td><td colspan="4">Langmuir-Hinshelwood Reaction Parameters - Indicates the use of the Langmuir-Hinshelwood rate expression. One auxiliary line should be supplied for each species appearing in the denominator of Equation 4.21 of the Chemkin-Pro Theory Manual . The keyword is followed, in slash delimited format, by the species name, the pre-exponential multiplier, the temperature factor, the enthalpy for the equilibrium constant, and the reaction order for that species (usually equal to one). The equilibrium constant is defined as $K=AT^{\beta}\exp\left(-H/RT\right)$, similar to the standard expression for rate constants.
<table>
<tr><th>Parameters</th><th>Optional/Reqd.</th><th>Units</th><th>Examples</th></tr>
<tr><td>Species name</td><td>Required</td><td>--</td><td>LANG /C6H6 1.26 0.0 0.0 1.0/</td></tr>
<tr><td>Pre-exponential factor A</td><td>Required</td><td>Depends on reaction</td><td>LANG /C6H6 1.26 0.0 0.0 1.0/</td></tr>
<tr><td>Temperature exponent β</td><td>Required</td><td>--</td><td>LANG /C6H6 1.26 0.0 0.0 1.0/</td></tr>
<tr><td>Equilibrium enthalpy H</td><td>Required</td><td>cal/mole</td><td>LANG /C6H6 1.26 0.0 0.0 1.0/</td></tr>
<tr><td>Reaction order</td><td>Required</td><td>--</td><td>LANG /C6H6 1.26 0.0 0.0 1.0/</td></tr>
<tr><td>Reaction Example</td><td colspan="3">C6H5CH3 + H2 => C6H6 + CH4

2.507E-8 0.0 0.0 ! rate at 600C

LANG /C6H6 1.26 0.0 0.0 1.0/

LANG /C6H5CH3 1.01 0.0 0.0 1.0/

LHDE /1/

LHNU /C6H5CH3/

LHPR /atm/</td></tr>
<tr><td>Notes</td><td colspan="3">• Only irreversible reactions are allowed with this option.</td></tr>
</table></td></tr>
</table>

Note: PDF user guides no longer in Chemkin-Pro install after release 19.0

<table>
<tr><th>Keyword</th><th colspan="4">Definition</th></tr>
<tr><td></td><td colspan="4">Each species listed in a LHNU statement must have a LANG statement.
Additional keywords LHDE , LHNU , and LHPR provide more flexibility in the form of the Langmuir-Hinshelwood or Eley-Rideal rate expressions.</td></tr>
<tr><td>LHDE</td><td colspan="4">Langmuir-Hinshelwood Denominator Exponent Parameter - Allows the default value of 2 for the overall exponent for the denominator (m) to be overridden when LANG is used to specify a Langmuir-Hinshelwood rate expression. To specify an Eley-Rideal reaction, this keyword would be used and m set to 1. The use of any positive number is permitted, including real or fractional numbers.</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td></td><td>Denominator exponent m</td><td>Required</td><td>--</td><td>LHDE /1/</td></tr>
<tr><td></td><td>Reaction Example</td><td colspan="3">C6H5CH3 + H2 => C6H6 + CH4

2.507E-8 0.0 0.0 ! rate at 600C

LANG /C6H6 1.26 0.0 0.0 1.0/

LANG /C6H5CH3 1.01 0.0 0.0 1.0/

LHDE /1/

LHNU /C6H5CH3/

LHPR /atm/</td></tr>
<tr><td>LHNU</td><td colspan="4">Allows the explicit inclusion of equilibrium constants in the numerator of the LANG rate expression (the use of k rather than k', see Langmuir-Hinshelwood and Eley-Rideal Reactions of the Chemkin-Pro Theory Manual) when LANG is used to specify a Langmuir-Hinshelwood rate expression. This keyword is followed by a slash delimited list of species names. For each species in the list, a multiplier of K will be applied to the rate constant.</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td></td><td>Species name</td><td>Required</td><td>--</td><td>LHNU /C6H5CH3/</td></tr>
<tr><td></td><td>Reaction Example</td><td colspan="3">C6H5CH3 + H2 => C6H6 + CH4

2.507E-8 0.0 0.0 ! rate at 600C

LANG /C6H6 1.26 0.0 0.0 1.0/

LANG /C6H5CH3 1.01 0.0 0.0 1.0/

LHDE /1/

LHNU /C6H5CH3/</td></tr>
</table>

<table>
<tr><th>Keyword</th><th colspan="4">Definition</th></tr>
<tr><td></td><td></td><td colspan="3">LHPR /atm/</td></tr>
<tr><td></td><td>Notes</td><td colspan="3">• Each species listed in a LHNU statement must have a LANG statement.</td></tr>
<tr><td>LHPR</td><td colspan="4">Indicates that the equilibrium constants are given in pressure units when LANG is used to specify a Langmuir-Hinshelwood rate expression. The LHPR keyword will affect the equilibrium constants for the specified reaction only; the reaction rate will still be assumed to be in the units specified on the REACTIONS line, or in the default moles, cm, and sec. The keyword is followed by the slash-delimited name of the pressure unit being used: ATM, BAR, TORR, PASC (for Pascals), or DYNE (for dynes per square cm), where the names are not case sensitive.</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td></td><td>Pressure units character string</td><td>Required</td><td>--</td><td>LHPR /atm/</td></tr>
<tr><td></td><td>Reaction Example</td><td colspan="3">C6H5CH3 + H2 => C6H6 + CH4

2.507E-8 0.0 0.0 ! rate at 600C

LANG /C6H6 1.26 0.0 0.0 1.0/

LANG /C6H5CH3 1.01 0.0 0.0 1.0/

LHDE /1/

LHNU /C6H5CH3/

LHPR /atm/</td></tr>
<tr><td>MWOFF</td><td colspan="4">Motz-Wise Correction - Turns off the Motz-Wise correction of Equation 4.15 of the Chemkin-Pro Theory Manual for a sticking-coefficient reaction.</td></tr>
<tr><td></td><td>Reaction Example</td><td colspan="3">AR* => AR 1.0 0.0 0.0

STICK

MWOFF</td></tr>
<tr><td></td><td>Notes</td><td colspan="3">• By default, the Motz-Wise correction will be off for all sticking coefficient reactions; the default may be changed by including the keyword MWON on the REACTIONS line.</td></tr>
<tr><td>MWON</td><td colspan="4">Motz-Wise Correction - Turns on the Motz-Wise correction of Equation 4.15 of the Chemkin-Pro Theory Manual for a sticking-coefficient reaction, superseding the default. By default the Motz-Wise will be off for all reactions using sticking coefficients unless the MWON keyword is given on the REACTIONS line, in which the new default will be to include the correction term.</td></tr>
<tr><td></td><td>Reaction Example</td><td colspan="3">ALMe3 + O(S) => ALMe2(S) + 0.5C2H6
0.1 0.0 0.0

STICK</td></tr>
</table>

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Keyword	Definition			
		MWON		
	Notes	• By default, the Motz-Wise correction will be off for all sticking coefficient reactions; the default may be changed by including the keyword MWON on the REACTIONS line.		
NATIVE	Indicates the native species of a particle; see Native Surface Sites of the Chemkin-Pro Theory Manual .			
	Reaction Example	OPEN(S) /NATIVE/		
NUCL	Supersedes the default rate calculation with the nucleation reaction rate expression; see Nucleation Reaction Data of the Chemkin-Pro Theory Manual .			
	Reaction Example	2A4 => 32C(B) + 20 H(se) + 28.72 open(se) 1.0E10 0.5 0.0 NUCL		
REV	**Reverse Reaction Parameters** - Supersedes the reverse rates that would normally be computed through the equilibrium constant, Equation 3.6 of the Chemkin-Pro Theory Manual . REV must be followed by the three slash-delimited Arrhenius coefficients (A_i, β_i, and E_i) to specify the reverse rate.			
	Parameters	Optional/Reqd.	Units	Examples
	Pre-exponential factor A_i		Depends on reaction	REV /**1.0E13** 0.0 15000./
	Temperature exponent β_i		--	REV /1.0E13 **0.0** 15000./
	Activation energy E_i		cal/mole	REV /1.0E13 0.0 **15000**./
	Reaction Example	C(S,R) + CH3 <=> D + CH3(S) 4.0E12 0.0 1200.0 REV /1.0E13 0.0 15000./		
RORD	**Arbitrary Reaction Orders** - Supersedes the reverse 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. RORD must be followed by the slash-delimited species name and the new reaction order, and supersedes the values of υ''_{ki} in Equation 3.4 of the Chemkin-Pro Theory Manual pertaining to the particular species named on the line; the reaction order for all other species maintain their default values. Multiple occurrences of the RORD construct may appear on the auxiliary line.			
	Parameters	Optional/Reqd.	Units	Examples
	Species name	Required	--	RORD /OH 2.0/
	Stoichiometric coefficient υ''_{ki}	Required	--	RORD /OH 2.0/
	Reaction Example	H2+O2=2OH 0.170E+14 0.00 47780		

Keyword	Definition	
		RORD /OH 2.0/
	Notes	• See also FORD .
STICK	**Sticking Coefficients** - The three coefficients given in the second field of the reaction line are to be interpreted as the parameters a_i, b_i, and c_i in Equation 4.10 of the Chemkin-Pro Theory Manual for a sticking coefficient (rather than as a rate constant). There can be only one gas-phase reactant species in a sticking-coefficient reaction; moreover, its stoichiometric coefficient must be 1.	
	Reaction Example	A1 + 8H(se) => 5H(se) + 6C(B) + 3open(se) + 4H2 + H 0.1 0.0 0.0 FORD/H(se) 2.0/ DCOL/2.46E-8/ STICK
UNITS	**Unit Specifications for Reactions** - Supersedes the current units for a particular reaction rate fit that may differ from the default units specified for other reaction expressions in the chemistry mechanism. UNITS must be followed by the slash-delimited character-string **string**, where **string** is one of the following (letters in brackets are optional): Parameters with energy units such as E_i : EVOL[TS], KELV[INS], CAL/[MOLE], KCAL[/MOLE], JOUL[ES/ MOLE], or KJOU[LES/MOLE]. Pre-exponential factors A_i : MOLE[S] or MOLEC[ULES], where the inclusion of MOLEC would indicate that the reaction rate expression is in units of molecules/cm^3 rather than mole/cm^3. ATM, BAR, PAS[CALS], DYN[ES], TOR[R] for pre-exponential factors A_i, where the units of gas species are partial pressures. SITE[FR], where the units of surface species are site fractions and the rate units are 1/sec.	

Parameters	Optional/Reqd.	Units	Examples
Reaction units character string	Required	--	UNITS /MOLECUES/

Reaction Example	CF3+ + E + #WSIO2(B) => #SIO2 + CF3 0.33 0.0 0.0 BOHM ! YIELD /0.01 20. 0.5 1.0/ UNITS/EVOLTS/
Notes	• Default units for A_i are cgs (cm, sec, K, mole), the exact units depending on the order of the reaction. • Default units for E_i are cal/mole. • Even if the default energy units are changed by giving the UNITS keyword, the temperature appearing in the Arrhenius expression of Equation 3.5 of the Chemkin-Pro Theory Manual , i.e., in T raised to the β power and in the denominator of the activation energy term, is still in Kelvins.

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<table>
<tr><th>Keyword</th><th colspan="4">Definition</th></tr>
<tr><td></td><td colspan="4">If any of the units strings are given on the REACTIONS header line, it applies to all reactions, but may be superseded for a particular reaction by the auxiliary UNITS keyword.
UNITS allows only one string parameter, but the user can repeat UNITS as many times as needed for a given reaction.</td></tr>
<tr><td>USRPROG</td><td colspan="4">Optional User Rate Subroutine SKUPROG - The net rate-of-progress for the reaction will be obtained by calling a user-supplied subroutine, SKUPROG. An optional slash(/)-delimited integer parameter allows the user to select from more than one type of rate formulation. Wherever the net reaction rate is required, it will be obtained by calling the user-written subroutine. A template of SKUPROG is provided in the ANSYS Chemkin-Pro installation, in the file sklib_user_routines.f located in the directory user_subroutines. Information about how to compile and link user routines into Chemkin-Pro is included in Chemkin-Pro Application Programming Interface Manual.
<table>
<tr><th>Parameters</th><th>Optional/Reqd.</th><th>Units</th><th>Examples</th></tr>
<tr><td>Rate formulation type</td><td>Optional</td><td>--</td><td>USRPROG /1/</td></tr>
<tr><td>Reaction Example</td><td colspan="3">CH3OH +H2O => CO2 + 3H2 1.0 0.00 0.0

USRPROG/3/</td></tr>
<tr><td>Notes</td><td colspan="3">USRPROG applies only to irreversible reactions, and cannot be used in conjunction with USRPROD (entered on the REACTIONS header line).</td></tr>
</table></td></tr>
<tr><td>YIELD</td><td colspan="4">Ion-energy-dependent Yield - Ion-enhanced reaction yield can be applied to a reaction using the following two steps. First, place a pound sign (#) in front of the species symbol (or stoichiometric coefficient if given) for each species that is subject to the ion-energy yield enhancement. The “sub-reaction” of species and coefficients demarcated with the # sign must satisfy mass, elemental, charge and site balance. Second, the auxiliary keyword YIELD must appear after the reaction, followed by the four parameters, h_{yield}, $E_{yield,0}$, t_i, and u_i (as described in Equation 4.33 of the Chemkin-Pro Theory Manual). These parameters are included as a slash-delimited set following the YIELD auxiliary keyword. An example of a YIELD reaction is shown in Figure 4.5: Examples of Auxiliary Reaction Data (p. 81) .
<table>
<tr><th>Parameters</th><th>Optional/Reqd.</th><th>Units</th><th>Examples</th></tr>
<tr><td>Multiplicative factor h_{yield}</td><td>Required</td><td>Depends on reaction</td><td>YIELD /0.053 4.0 0.5 1.0/</td></tr>
<tr><td>Energy threshold E $_{yield,0}$</td><td>Required</td><td>cal/mole</td><td>YIELD /0.053 4.0 0.5 1.0/</td></tr>
</table></td></tr>
</table>

Keyword	Definition			
	Exponential constant t_i	Required	--	YIELD /0.053 4.0 **0.5** 1.0/
	Exponential constant u_i	Required	--	YIELD /0.053 4.0 0.5 **1.0**/

	Reaction Example	`CF3+ + E + #WSIO2(B) => #SIO2 + CF3`
		`0.33 0.0 0.0`
		
		`BOHM !`
		
		`YIELD /0.01 20. 0.5 1.0/ UNITS/EVOLTS/`		

	Notes	• A reaction declared with ion-enhanced yield must contain one (and only one) positive ionic reactant species.		

Note

Even if the default energy units are changed by giving one of the UNITS keyword, the temperature appearing in the Arrhenius expression of Equation 3.5 of the Chemkin-Pro Theory Manual , i.e., in T raised to the β power and in the denominator of the activation energy term, is still in Kelvins.

4.5.3.1. Summary of Auxiliary Reaction Data

Any number of auxiliary information lines may follow a reaction line, in any order, and any number of keywords may appear on an auxiliary information line; however, an auxiliary keyword and its parameter(s) must appear on the same line.

Examples of auxiliary information are shown in Figure 4.5: Examples of Auxiliary Reaction Data (p. 81) . The above rules are summarized in Table 4.7: Summary of the Rules for Auxiliary Reaction Data (p. 82) .

Figure 4.5: Examples of Auxiliary Reaction Data

```
REACTIONS   KCAL/MOLE
! THE FOLLOWING ARE *CONTRIVED* EXAMPLES OF AUXILIARY KEYWORD USAGE
    SICL(S)  <=>  CL + SI(S)                                  1.0E-3  0.0    2.
                                                              REV/1.0E13  0.0   37./
    CL + SICL(S) <=>  CL2 + SI(S)                             0.1     1.1   20.
          DUPLICATE   STICK
          RORD /SI(S)  0/
    CL + SICL(S) <=>  CL2 + SI(S)                             1.4E11  0.0   15.
          DUPLICATE   COV/SICL(S)  -1.2  0.5  32./  FORD/CL+  1.0/
    CL*       =>  CL                                          1.0     0.0    0.
          STICK       MWOFF
    E + CL+ + SICL3(S) + SI(B) => SICL4 + SI(S)               0.50    0.0    0.
       BOHM
       ENRGDEP/1. 0.5 1.0/  UNITS/EVOLT/
    AR+ + E + #SIO2(D) => #SIO2  + AR                  1.0   0.0  0.0
       BOHM
       YIELD /0.023052 35. 0.5 1.0/ UNITS/EVOLTS/
    E + CL2+ + SICL3(S) + SI(B) => SICL4 + SICL(S)     0.50  0.0  0.0       FORD/ CL2+  2.43/
    C6H5CH3  +  H2 => C6H6 + CH4             1.4E-8   0.0     0.0   ! rate at 600C
       LANG /C6H6  1.26  0.0  0.0  1.0/
       LANG /C6H5CH3  1.01  0.0  0.0  1.0/
       LHDE /1/
```

```
LHNU /C6H5CH3/
LHPR /atm/
```

Table 4.7: Summary of the Rules for Auxiliary Reaction Data

Rule	Description
1	Auxiliary information lines may follow a reversible reaction to specify the reverse rate parameters explicitly; auxiliary information must follow any reactions that are duplicated.
2	Auxiliary keyword declarations may appear anywhere on the line, in any order.
3	Any number of auxiliary keywords may appear on a line, and more than one line may be used, but a keyword and its parameter(s) must appear on the same line.
4	Multiple keywords appearing on the same line must be separated by at least one blank space.
5	Any blank spaces between a keyword and the first slash are ignored and any blanks between the slashes and parameter(s) are also ignored. However, no blank spaces are allowed within a keyword or parameter.
6	The keyword REV followed by three slash-delimited Arrhenius coefficients may be used to specify the reverse rate parameters.
7	The keyword DUPLICATE (or DUP) must follow every occurrence of a duplicated reaction.
8	The keyword STICK indicates that the three coefficients on the reaction line are to be interpreted as the parameters a_i, b_i, and c_i in Equation 4.10 of the Chemkin-Pro Theory Manual . There must be exactly one gas-phase reactant species; its stoichiometric coefficient must be 1.
9	The keyword COV is used to modify the forward rate constant by the expression in Equation 4.7 of the Chemkin-Pro Theory Manual . The word COV is followed by a surface species name and the three coverage parameters $\eta_{ki'}$ μ_{ki} and ε_{ki}. The four entries after the word COV are slash-delimited.
10	The keyword BOHM indicates that the three coefficients on the reaction line are to be interpreted as the parameters a_i, b_i, and c_i in Equation 4.29 of the Chemkin-Pro Theory Manual ; the Bohm velocity correction is applied. There must be exactly one gas-phase reactant species and that species must be a positive ionic species; its stoichiometric coefficients must be 1. Only irreversible reactions are allowed with this option. The electron must be declared in the list of species names in the *Gas-phase Kinetics* Pre-processor input.
11	The keyword ENRGDEP allows the rate constant to depend on ion energy according to Equation 4.30 of the Chemkin-Pro Theory Manual . The keyword is followed by the three parameters $E_{ion,0}$, f_i, and g_i which are slash-delimited. There must be exactly one positive ionic reactant species in the reaction. Only irreversible reactions are allowed with this option.
12	The keywords FORD and RORD can be used to change the reaction order (with respect to species concentration) of the forward or reverse reaction, respectively, for any species in the mechanism, regardless of whether the species appears as a reactant or a product in the reaction. The species name and the new reaction order (slash-delimited) follow the keyword.

Rule	Description
13	The YIELD keyword allows modification of the stoichiometric coefficients in a sub-reaction using the ion-yield option. The usage requires preceding each species in the sub-reaction (or its stoichiometric coefficient) with the pound sign (#). Following the reaction line, declare the YIELD keyword, then the four parameters h_{yield}, $E_{yield,0}$, t_i, and u_i of Equation 4.33 of the Chemkin-Pro Theory Manual , between slashes. There must be exactly one positive ionic reactant species in the reaction. Only irreversible reactions are allowed with this option. The sub-reaction demarcated with the # symbols must satisfy mass, elemental, charge and site balance. An example of the YIELD keyword appears in Figure 4.5: Examples of Auxiliary Reaction Data (p. 81) .
14	The UNITS keyword can be used to override the current default units for parameters with energy units or the pre-exponential factor for a given reaction. The usage is UNITS/ **string** /, where **string** is one of the following: EVOLTS, KELVINS, CAL/MOLE, KCAL/MOLE, JOULES/MOLE, or KJOULES/MOLE (for parameters with energy units), or MOLES or MOLECULES (for pre-exponential factors).
15	The string MWON can be used to turn on the Motz-Wise correction of Equation 4.15 of the Chemkin-Pro Theory Manual or the string MWOFF can be used to turn off this correction for a sticking coefficient reaction. Using the MWOFF or MWON keyword overrides the default option set up on the REAC TIONS line or the default supplied by *Surface Kinetics* (which is MWOFF).
16	The LANG keyword can be used to input a Langmuir-Hinshelwood rate expression. The keyword is followed by a species name, three parameters giving the equilibrium constant, and a fourth parameter giving the order of that species in the reaction. Additional keywords LHDE, LHNU, and LHPR provide more flexibility in the form of the Langmuir-Hinshelwood or Eley-Rideal rate expressions.
17	The keyword LHDE allows the default value of 2 for the overall exponent for the denominator (m) to be overridden when LANG is used to specify a Langmuir-Hinshelwood rate expression. To specify an Eley-Rideal reaction, this keyword would be used to set m to 1. The use of any positive number is permitted, including real or fractional numbers.
18	The keyword LHNU allows the explicit inclusion of equilibrium constants in the numerator of the LH rate expression (the use of k rather than k', see Langmuir-Hinshelwood and Eley-Rideal Reactions of the Chemkin-Pro Theory Manual) when LANG is used to specify a Langmuir-Hinshelwood rate expression. This keyword is followed by a slash delimited list of species names. For each species in the list, a multiplier of K will be applied to the rate constant. Each species listed in a LHNU statement must have a LANG statement.
19	The keyword LHPR indicates that the equilibrium constants are given in pressure units when LANG is used to specify a Langmuir-Hinshelwood rate expression. The LHPR keyword will affect the equilibrium constants for the specified reaction only; the reaction rate will still be assumed to be in the units specified on the REACTIONS line, or in the default moles, cm, and sec. The keyword is followed by the name of the pressure unit being used: atm, bar, torr, Pasc (for Pascals), or dyne (for dynes per square cm), where the names are not case sensitive.

4.5.4. Problems Having No Reactions

In some problems only information about the surface and bulk species is needed (e.g., chemical equilibrium computations). For these cases it is not necessary to include reaction data. The Pre-processor will create the linking file *surf.asc*, but it will not contain any reaction information. Therefore, no subroutines in the *Surface Kinetics* Subroutine Library that deal with chemical reactions (e.g., chemical production rates) will be used (although doing so would not generate an error; the production rates of all species would be returned as zero).

4.5.5. Error Checks

Each input line is checked for proper syntax and diagnostic messages are written to the pre-processor output file if errors are encountered. If an error occurs, the pre-processor continues to read and diagnose the input, but an error flag is written to the Linking file and *Surface Kinetics* subroutine `SKINIT` will not initialize the work arrays. Therefore, the input must be error free before a Reactor Model can be run or before any of the *Surface Kinetics* subroutines can be called in a Reactor Model.

Possibilities for an error condition are as follows:

Table 4.8: Error Checks

Data Type	Possible Errors
Site and Bulk Species Data	A duplicated species symbol (name) is not considered a fatal error, but is eliminated from consideration and a warning diagnostic message is printed.
	No site density is found for a declared site, or the site density is negative.
	No thermodynamic data are found for a declared species.
	A site or bulk phase name duplicates another phase name (gas surface site, or bulk phase name).
	A phase or species name contains an illegal character.
	Site occupancy number is negative.
	Bulk density for a bulk species is negative.
Thermodynamic Data	Thermodynamic data are format sensitive and therefore provide possibilities for error if not formatted exactly as described by Table 2.1: Summary of the Rules for Thermodynamic Data (p. 4) .
	An element in the thermodynamic data for a declared species is not included in the *Gas-phase Kinetics* Pre-processor input element data.
	With the `THERMO ALL` option, line 2 (of Table 2.1: Summary of the Rules for Thermodynamic Data (p. 4)) is not found.
Reaction Data	A delimiter =>, <=>, or = between the reactants and the products is not found.
	Three Arrhenius parameters are not found.
	Reactants and/or products species names are not properly delineated by a plus sign (+).

Data Type	Possible Errors
	A species listed as a reactant or product is not declared in the species data.
	A reaction does not satisfy elemental balance.
	The number of sites in a reaction does not balance and the word NONCON was not included on the first REACTIONS line.
	The charge of the reaction does not balance.
	A reaction is a duplicate not declared by the auxiliary data keyword DUP.
	There are more than six reactants or six products in a reaction.
Auxiliary Reaction Data	An unknown or misspelled keyword occurs.
	Parameters for a keyword are not enclosed in slashes.
	There are the wrong number of parameters for a keyword.
	REV is declared for an irreversible reaction.
	Pre-exponential factor for a sticking coefficient is negative.
	For a sticking-coefficient reaction, there is more than one gas-phase species, or the stoichiometric coefficient for the gas-phase species is not 1.
	More than one BOHM declaration appeared for a given reaction.
	BOHM keyword is given for a reversible reaction.
	A positive ionic species did not appear as a reactant or its stoichiometric coefficient was not 1 in a Bohm reaction.
	More than 1 positive ionic species was a reactant in a Bohm reaction.
	The electron species was not declared in the list of species in the *Gas-phase Kinetics* Pre-processor input.
	Invalid string given with the UNITS auxiliary keyword.
	More than one ENRGDEP declaration appeared for a given reaction.
	A positive ionic species did not appear as a reactant or its stoichiometric coefficient was not 1 in a ENRGDEP reaction.
	Wrong number of ENRGDEP parameters given.
	Invalid species name given for FORD or RORD auxiliary keywords.
	A reaction order value was not found with the FORD or RORD keyword.
	RORD given for an irreversible reaction.
	No species coefficients were demarcated with a # symbol for a YIELD reaction.
	YIELD keyword given for a reversible reaction.
	A positive ionic species did not appear as a reactant or its stoichiometric coefficient was not 1 in a YIELD reaction.
	Wrong number of YIELD parameters given.

Data Type	Possible Errors
	More than 1 positive ionic species was a reactant in a YIELD reaction.
	LANG is declared for a reversible reaction, or for the same reaction as STICK, COV, BOHM, YIELD, or ENRGDEP.
	USRPROG given for a USRPROD mechanism.
	USRPROG given for a reversible reaction.

Chapter 5: Transport Database

In this section we list the database file that is currently included with the *Transport* software. While this database file is more of a historical record, we expect that users will want to add their own collection of data to suit their own needs.

The database file included with ANSYS Chemkin-Pro should not be viewed as the last word in transport properties. Instead, it is a good starting point from which a user will provide the best available data for his particular application. Some of the numbers in the database have been determined by computing "best fits" to experimental measurements of a macroscopic transport property (for example, viscosity). In other cases the Lennard-Jones parameters have been estimated following the methods outlined in Svehla.[7] (p. 331) In still other cases they have been determined by computational chemistry techniques.

5.1. Transport Data Format

The first 16 columns in each line of the database are reserved for the species name. Presently ANSYS Chemkin-Pro is programmed to allow no larger than 16-character names. Columns 17 through 80 are free-format, and they contain the molecular parameters for each species. They are, in order:

1. An index indicating whether the molecule has a monatomic, linear or nonlinear geometrical configuration. If the index is 0, the molecule is a single atom. If the index is 1 the molecule is linear, and if it is 2, the molecule is nonlinear.

2. The Lennard-Jones potential well depth ε / k_B in Kelvins.

3. The Lennard-Jones collision diameter σ in angstroms.

4. The dipole moment μ in Debye.

5. The polarizability α in cubic angstroms.

6. The rotational relaxation collision number Z_{rot} at 298 K.

7. A "comment" line is one that has either a period (.), slash (/), or exclamation mark (!) as the first non-blank character. In addition, on any line, any input that follows an exclamation mark is taken as a comment.

Note

A Debye is 10^{-18} $cm^{3/2}$ $ergs^{1/2}$.

5.2. Including Transport Data in the Gas-phase Kinetics Input File

ANSYS Chemkin-Pro allows you to optionally include transport data within the *Gas-phase Kinetics* Input File. This is similar to the options available for thermodynamic data. This option can be used to supplement or replace transport data that may be provided in a separate file (e.g., *tran.dat*). In addition, this option may be particularly useful when reaction-rate constants are given in terms of the collision fre-

quency (see the description of the COLLEFF keyword in Table 3.7: Alphabetical Listing of Gas-phase Reaction Auxiliary Keywords (p. 43)). In such cases, the Lennard-Jones diameter, which is obtained from the transport data, is required for calculation of the collision frequency that is used to derive the reaction rate for those reactions. These are cases when transport data might not otherwise be required but the necessary data for specific species needed in the collision-frequency reactions may be included in the *Gas-phase Kinetics* Input File.

A full description of the syntax of this option is included in Transport Data (p. 38) .

5.3. Transport Data Included with CHEMKIN

Table 5.1: Species in *Transport* Database (p. 88) lists the species contained in the ANSYS Chemkin-Pro tran.dat file, which is included in every installation, as the corresponding data for each species.

Table 5.1: Species in *Transport* Database

Species Name	Geometry	ε/k_B	σ	μ	α	Z_{rot}
Al2Me6	2	471.	6.71	0.0	0.0	1.0
AlMe3	2	471.	5.30	0.0	0.0	1.0
AR	0	136.500	3.330	0.000	0.000	0.000
AR*	0	136.500	3.330	0.000	0.000	0.000
AS	0	1045.5	4.580	0.000	0.000	0.000
AS2	1	1045.5	5.510	0.000	0.000	1.000
ASH	1	199.3	4.215	0.000	0.000	1.000
ASH2	2	229.6	4.180	0.000	0.000	1.000
ASH3	2	259.8	4.145	0.000	0.000	1.000
AsH3	2	259.8	4.145	0.000	0.000	1.000
BCL3	2	337.7	5.127	0.000	0.000	1.000
C	0	71.400	3.298	0.000	0.000	0.000
C-SI3H6	2	331.2	5.562	0.000	0.000	1.000
C2	1	97.530	3.621	0.000	1.760	4.000
C2F4	2	202.6	5.164	0.000	0.000	1.000
C2F6	2	194.5	5.512	0.000	0.000	1.000
C2H	1	209.000	4.100	0.000	0.000	2.500
C2H2	1	209.000	4.100	0.000	0.000	2.500
C2H2OH	2	224.700	4.162	0.000	0.000	1.000
C2H3	2	209.000	4.100	0.000	0.000	1.000
C2H4	2	280.800	3.971	0.000	0.000	1.500
C2H5	2	252.300	4.302	0.000	0.000	1.500
C2H5OH	2	362.6	4.53	0.000	0.000	1.000
C2H6	2	252.300	4.302	0.000	0.000	1.500
C2N	1	232.400	3.828	0.000	0.000	1.000
C2N2	1	349.000	4.361	0.000	0.000	1.000

Species Name	Geometry	ε / k_B	σ	μ	α	Z_{rot}
C2O	1	232.400	3.828	0.000	0.000	1.000
C3H2	2	209.000	4.100	0.000	0.000	1.000
C3H3	1	252.000	4.760	0.000	0.000	1.000
C3H4	1	252.000	4.760	0.000	0.000	1.000
C3H4P	1	252.000	4.760	0.000	0.000	1.000
C3H6	2	266.800	4.982	0.000	0.000	1.000
C3H7	2	266.800	4.982	0.000	0.000	1.000
C3H8	2	266.800	4.982	0.000	0.000	1.000
C4H	1	357.000	5.180	0.000	0.000	1.000
C4H2	1	357.000	5.180	0.000	0.000	1.000
C4H2OH	2	224.700	4.162	0.000	0.000	1.000
C4H3	1	357.000	5.180	0.000	0.000	1.000
C4H4	1	357.000	5.180	0.000	0.000	1.000
C4H6	2	357.000	5.180	0.000	0.000	1.000
C4H8	2	357.000	5.176	0.000	0.000	1.000
C4H9	2	357.000	5.176	0.000	0.000	1.000
C4H9	2	357.000	5.176	0.000	0.000	1.000
C5H2	1	357.000	5.180	0.000	0.000	1.000
C5H3	1	357.000	5.180	0.000	0.000	1.000
C5H5OH	2	450.000	5.500	0.000	0.000	1.000
C6H2	1	357.000	5.180	0.000	0.000	1.000
C6H5	2	412.300	5.349	0.000	0.000	1.000
C6H5(L)	2	412.300	5.349	0.000	0.000	1.000
C6H5O	2	450.000	5.500	0.000	0.000	1.000
C6H6	2	412.300	5.349	0.000	0.000	1.000
C6H7	2	412.300	5.349	0.000	0.000	1.000
CF	1	94.2	3.635	0.000	0.000	1.000
CF2	2	108.0	3.977	0.000	0.000	1.000
CF3	2	121.0	4.320	0.000	0.000	1.000
CF4	2	134.0	4.662	0.000	0.000	1.000
CH	1	80.000	2.750	0.000	0.000	0.000
CH2	1	144.000	3.800	0.000	0.000	0.000
CH2(S)	1	144.000	3.800	0.000	0.000	0.000
CH2(SING)	1	144.000	3.800	0.000	0.000	0.000
CH2CHCCH	2	357.000	5.180	0.000	0.000	1.000
CH2CHCCH2	2	357.000	5.180	0.000	0.000	1.000
CH2CHCH2	2	260.000	4.850	0.000	0.000	1.000
CH2CHCHCH	2	357.000	5.180	0.000	0.000	1.000

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Species Name	Geometry	ε / k_B	σ	μ	α	Z_{rot}
CH2CHCHCH2	2	357.000	5.180	0.000	0.000	1.000
CH2CO	2	436.000	3.970	0.000	0.000	2.000
CH2F2	2	318.0	4.080	0.000	0.000	1.000
CH2HCO	2	436.000	3.970	0.000	0.000	2.000
CH2O	2	498.000	3.590	0.000	0.000	2.000
CH2OH	2	417.000	3.690	1.700	0.000	2.000
CH3	1	144.000	3.800	0.000	0.000	0.000
CH3CC	2	252.000	4.760	0.000	0.000	1.000
CH3CCCH2	2	357.000	5.180	0.000	0.000	1.000
CH3CCCH3	2	357.000	5.180	0.000	0.000	1.000
CH3CCH2	2	260.000	4.850	0.000	0.000	1.000
CH3CH2CCH	2	357.000	5.180	0.000	0.000	1.000
CH3CHCH	2	260.000	4.850	0.000	0.000	1.000
CH3CHO	2	436.000	3.970	0.000	0.000	2.000
CH3CO	2	436.000	3.970	0.000	0.000	2.000
CH3O	2	417.000	3.690	1.700	0.000	2.000
CH3OH	2	481.800	3.626	0.000	0.000	1.000
CH4	2	141.400	3.746	0.000	2.600	13.000
CH4O	2	417.000	3.690	1.700	0.000	2.000
CHF3	2	240.0	4.330	0.000	0.000	1.000
CL	0	130.8	3.613	0.000	0.000	1.000
CL-	0	130.8	3.613	0.000	0.000	1.000
CL2BNH2	2	337.7	5.127	0.000	0.000	1.000
CN	1	75.000	3.856	0.000	0.000	1.000
CN2	1	232.400	3.828	0.000	0.000	1.000
CNC	1	232.400	3.828	0.000	0.000	1.000
CNN	1	232.400	3.828	0.000	0.000	1.000
CO	1	98.100	3.650	0.000	1.950	1.800
CO2	1	244.000	3.763	0.000	2.650	2.100
DMG	2	675.8	5.22	0.000	0.000	1.000
E	0	850.	425.	0.000	0.000	1.000
F	0	80.000	2.750	0.000	0.000	0.000
F2	1	125.700	3.301	0.000	1.600	3.800
GA	0	2961.8	4.62	0.000	0.000	0.000
GACH3	2	972.7	4.92	0.000	0.000	1.000
GAH	1	335.5	4.24	0.000	0.000	1.000
GAME	2	972.7	4.92	0.000	0.000	1.000
GAME2	2	675.8	5.22	0.000	0.000	1.000

Species Name	Geometry	ε/k_B	σ	μ	α	Z_{rot}
GAME3	2	378.2	5.52	0.000	0.000	1.000
GaMe3	2	378.2	5.52	0.000	0.000	1.000
H	0	145.000	2.050	0.000	0.000	0.000
H2	1	38.000	2.920	0.000	0.790	280.000
H2ASCH3	2	408.0	4.73	0.000	0.000	1.000
H2C4O	2	357.000	5.180	0.000	0.000	1.000
H2CCCCH	2	357.000	5.180	0.000	0.000	1.000
H2CCCCH2	2	357.000	5.180	0.000	0.000	1.000
H2CCCH	2	252.000	4.760	0.000	0.000	1.000
H2CN	1	569.000	3.630	0.000	0.000	1.000
H2NO	2	116.700	3.492	0.000	0.000	1.000
H2O	2	572.400	2.605	1.844	0.000	4.000
H2O2	2	107.400	3.458	0.000	0.000	3.800
H2S	2	301.000	3.600	0.000	0.000	1.000
H2SISIH2	2	312.6	4.601	0.000	0.000	1.000
H3SISIH	2	312.6	4.601	0.000	0.000	1.000
HC2N2	1	349.000	4.361	0.000	0.000	1.000
HCCHCCH	2	357.000	5.180	0.000	0.000	1.000
HCCO	2	150.000	2.500	0.000	0.000	1.000
HCCOH	2	436.000	3.970	0.000	0.000	2.000
HCL	1	344.7	3.339	0.000	0.000	1.000
HCN	1	569.000	3.630	0.000	0.000	1.000
HCNO	2	232.400	3.828	0.000	0.000	1.000
HCO	2	498.000	3.590	0.000	0.000	0.000
HCO+	1	498.000	3.590	0.000	0.000	0.000
HE	0	10.200	2.576	0.000	0.000	0.000
HF	1	330.000	3.148	1.920	2.460	1.000
HF0	1	352.000	2.490	1.730	0.000	5.000
HF1	1	352.000	2.490	1.730	0.000	5.000
HF2	1	352.000	2.490	1.730	0.000	5.000
HF3	1	352.000	2.490	1.730	0.000	5.000
HF4	1	352.000	2.490	1.730	0.000	5.000
HF5	1	352.000	2.490	1.730	0.000	5.000
HF6	1	352.000	2.490	1.730	0.000	5.000
HF7	1	352.000	2.490	1.730	0.000	5.000
HF8	1	352.000	2.490	1.730	0.000	5.000
HNCO	2	232.400	3.828	0.000	0.000	1.000
HNNO	2	232.400	3.828	0.000	0.000	1.000

Note: PDF user guides
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Species Name	Geometry	ε / k_B	σ	μ	α	Z_{rot}
HNO	2	116.700	3.492	0.000	0.000	1.000
HNOH	2	116.700	3.492	0.000	0.000	1.000
HO2	2	107.400	3.458	0.000	0.000	1.000
HOCN	2	232.400	3.828	0.000	0.000	1.000
HSO2	2	252.000	4.290	0.000	0.000	1.000
I*C3H7	2	266.800	4.982	0.000	0.000	1.000
I*C4H9	2	357.000	5.176	0.000	0.000	1.000
K	0	850.	4.25	0.000	0.000	1.000
K+	0	850.	4.25	0.000	0.000	1.000
KCL	1	1989.	4.186	0.000	0.000	1.000
KH	1	93.3	3.542	0.000	0.000	1.000
KO	1	383.0	3.812	0.000	0.000	1.000
KO2	2	1213.	4.69	0.000	0.000	1.000
KOH	2	1213.	4.52	0.000	0.000	1.000
N	0	71.400	3.298	0.000	0.000	0.000
N*C3H7	2	266.800	4.982	0.000	0.000	1.000
N2	1	97.530	3.621	0.000	1.760	4.000
N2H2	2	71.400	3.798	0.000	0.000	1.000
N2H3	2	200.000	3.900	0.000	0.000	1.000
N2H4	2	205.000	4.230	0.000	4.260	1.500
N2O	1	232.400	3.828	0.000	0.000	1.000
NCN	1	232.400	3.828	0.000	0.000	1.000
NCNO	2	232.400	3.828	0.000	0.000	1.000
NCO	1	232.400	3.828	0.000	0.000	1.000
NH	1	80.000	2.650	0.000	0.000	4.000
NH2	2	80.000	2.650	0.000	2.260	4.000
NH3	2	481.000	2.920	1.470	0.000	10.000
NNH	2	71.400	3.798	0.000	0.000	1.000
NO	1	97.530	3.621	0.000	1.760	4.000
NO2	2	200.000	3.500	0.000	0.000	1.000
O	0	80.000	2.750	0.000	0.000	0.000
O(Si(OC2H5)3)2	2	522.7	5.25	0.000	0.000	1.000
O2	1	107.400	3.458	0.000	1.600	3.800
O3	2	180.000	4.100	0.000	0.000	2.000
OH	1	80.000	2.750	0.000	0.000	0.000
OSI(OC2H5)2	2	522.7	7.03	0.000	0.000	1.000
PH3	2	251.5	3.981	0.000	0.000	1.000
S	0	847.000	3.839	0.000	0.000	0.000

Species Name	Geometry	ε / k_B	σ	μ	α	Z_{rot}
S*C4H9	2	357.000	5.176	0.000	0.000	1.000
S2	1	847.000	3.900	0.000	0.000	1.000
SH	1	847.000	3.900	0.000	0.000	1.000
SI	0	3036.	2.910	0.000	0.000	0.000
Si(OC2H5)4	2	522.7	7.03	0.000	0.000	1.000
SI(OC2H5)4	2	522.7	7.03	0.000	0.000	1.000
Si(OH)(OC2H5)3	2	522.7	7.03	0.000	0.000	1.000
SI(OH)(OC2H5)3	2	522.7	7.03	0.000	0.000	1.000
SI(OH)2(OC2H5)2	2	522.7	6.35	0.000	0.000	1.000
Si(OH)2(OC2H5)2	2	522.7	6.35	0.000	0.000	1.000
SI(OH)3(OC2H5)	2	522.7	5.75	0.000	0.000	1.000
SI(OH)4	2	522.7	5.25	0.000	0.000	1.000
SI2	1	3036.	3.280	0.000	0.000	1.000
SI2H2	2	323.8	4.383	0.000	0.000	1.000
SI2H3	2	318.2	4.494	0.000	0.000	1.000
SI2H4	2	312.6	4.601	0.000	0.000	1.000
SI2H5	2	306.9	4.717	0.000	0.000	1.000
SI2H6	2	301.3	4.828	0.000	0.000	1.000
SI3	2	3036.	3.550	0.000	0.000	1.000
SI3H8	2	331.2	5.562	0.000	0.000	1.000
SIF	1	585.0	3.318	0.000	0.000	1.000
SIF3	2	309.6	4.359	0.000	0.000	1.000
SIF3NH2	2	231.0	4.975	0.000	0.000	1.000
SIF4	2	171.9	4.880	0.000	0.000	1.000
SIH	1	95.8	3.662	0.000	0.000	1.000
SIH2	2	133.1	3.803	0.000	0.000	1.000
SIH2(3)	2	133.1	3.803	0.000	0.000	1.000
SIH3	2	170.3	3.943	0.000	0.000	1.000
SIH3SIH2SIH	2	331.2	5.562	0.000	0.000	1.000
SIH4	2	207.6	4.084	0.000	0.000	1.000
SIHF3	2	180.8	4.681	0.000	0.000	1.000
SO	1	301.000	3.993	0.000	0.000	1.000
SO2	2	252.000	4.290	0.000	0.000	1.000
SO3	2	378.400	4.175	0.000	0.000	1.000
TMG	2	378.2	5.52	0.000	0.000	1.000

Note: PDF user guides
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Chapter 6: Description and Properties of Particles

Use of Particle Tracking to determine particle size distributions in a gas-particle flow requires identification of a condensed-phase material that may exist in a form that is dispersed within the gas-flow. In addition, you must specify certain properties of the particle "cloud" that will be tracked. This section describes the necessary input to the chemistry-set files, which are needed to establish these properties. Further discussions, of how kinetics rates may be specified to control the particle nucleation, growth, and transformation, are available in Chapter Particle Size-Distribution Tracking of the Chemkin-Pro Theory Manual .

Examples are available in the ANSYS Chemkin-Pro Tutorials Manual to illustrate how required information is presented to the Particle Tracking feature.

6.1. Description and Properties of the Particle Material

6.1.1. Dispersed Material

Within a reactor model that enables Particle Tracking, the simulation treats a particle population as a collection of tiny solid or liquid material pieces suspended in bulk gas. This dispersed material concept represents the fact that particles are in a condensed phase and also allows use of existing surface-kinetics capabilities to handle gas-particle interactions.

Since the particles represent a condensed-phase material, all particle-related definitions are included in the surface chemistry input file. To declare a dispersed material, the Surface Kinetics keyword MATERIAL must be provided at the top of the Surface Kinetics Input file. This allows assignment of a name to the surface material. This material can then be designated as a dispersed material (i.e., it will be tracked in particle form), using the keyword DISPERSED that follows the MATERIAL statement. For example,

Figure 6.1: Example of Dispersed Material Declaration

```
MATERIAL soot
DISPERSED
END
```

With this entry, the material "soot" will be recognized by ANSYS Chemkin-Pro as a dispersed material. Note that an END keyword is needed to close the DISPERSED keyword block, although at this time there is no additional information included in the block.

It is possible to have more than one type of particle co-exist in the same system, although currently the Particle Tracking equations do not consider interactions between different types of particles. Different types of particles are defined as different dispersed materials. Definitions of multiple dispersed or non-dispersed materials are separated by the MATERIAL keywords. For example, if a chemical system contains two types of particles, such that one is called soot and the other is called silicon, they should be declared in two separate MATERIAL blocks as illustrated in Figure 6.2: Example of Two Material Blocks (p. 96) .

Figure 6.2: Example of Two Material Blocks

```
MATERIAL soot
DISPERSED
END
REACTIONS
…
END
MATERIAL silicon
DISPERSED
END
REACTIONS
…
END
```

6.1.2. Particle Composition

One of the properties differentiating one type of particle from another is the chemical composition of the particle. The chemical composition of the particles is determined by the chemical composition of the sole bulk species specified for the dispersed material. There can only be one bulk species specified. This determines the "chemical unit" of the particle and this "chemical unit" for the initially formed condensed "species" in the material. This "chemical unit" can be a single atom, a group of atoms, or a chemical compound. ANSYS Chemkin-Pro identifies the "chemical unit" of the particle by the sole bulk species on the dispersed material. For example, Figure 6.3: Dispersed Graphite Material Declaration With Chemical Composition (p. 96) defines a particle type called "soot".

Figure 6.3: Dispersed Graphite Material Declaration With Chemical Composition

```
MATERIAL soot
DISPERSED
END
BULK/GRAPHITE/ C(B) /1.8/
END
THERMO
C(B)              121286C   1               S  0300.00   5000.00  1000.00      1
 0.14901664E+01 0.16621256E-02-0.06687204E-05 0.12908796E-09-0.09205334E-13    2
-0.07074018E+04-0.08717785E+02-0.06705661E+01 0.07181499E-01-0.05632921E-04    3
 0.02142298E-07-0.04168562E-11-0.07339498E+03 0.02601595E+02                   4
END
REACTIONS
…
END
```

The BULK declaration line indicates that the core of the "soot" particles consists of units of bulk species C(B) and the bulk density ρ_B of the particle core is 1.8 [gm/cm^3]. The actual chemical composition of C(B), the core of the "soot" particle, is a single carbon atom as it is defined in the Thermodynamic Data section that follows the BULK declaration.

Another example is given in Figure 6.4: Dispersed Silicon Dioxide Material Declaration With Chemical Composition (p. 96) , for a compound particle composed of silicon dioxide.

Figure 6.4: Dispersed Silicon Dioxide Material Declaration With Chemical Composition

```
MATERIAL silicon
DISPERSED
END
BULK/OXIDE/ SIO2(B) /2.533/
END
THERMO
SIO2(B)            72391SI  1O   2          S    298.00   2000.00 1000.00      1
 0.48925619E+01 0.41191629E-02-0.94570083E-07-0.80073115E-09 0.25433412E-12    2
```

```
-0.11005530E+06-0.23469570E+02 0.22325585E+01 0.12478522E-01-0.28715690E-05    3
-0.96847970E-08 0.62160411E-11-0.10962063E+06-0.10594849E+02                   4
END
REACTIONS
…
END
```

6.1.3. Particle Class

Since the Particle Tracking feature employs the method of moments to solve the size distribution, it is important to understand the concept of particle class and how this class concept is connected to surface reactions that describe particle nucleation and mass growth. We define the class of a particle by the number of bulk species in its core. The "soot" particle declared in Figure 6.4: Dispersed Silicon Dioxide Material Declaration With Chemical Composition (p. 96) provides an example. A "soot" particle of class 100 has a core consisting of 100 C(B) species regardless of whether or not other species and atoms might exist on the surface of the particle.

When a particle nucleus is created from gas-phase precursors, its class, that is, the inception class, is determined by the stoichiometric coefficient of the bulk species in the nucleation reaction. For example, the nucleation reaction in Figure 6.5: Nucleation Reaction Creating Particle Nuclei of Class 32 (p. 97) creates particle nuclei of class 32:

Figure 6.5: Nucleation Reaction Creating Particle Nuclei of Class 32

```
2A4 => 32C(B) + 20 H(se) + 28.72 open(se)        1.0E10   0.5     0.0
                NUCL
```

The syntax of the nucleation reaction will be discussed in a later section. A surface reaction resulting in a net gain in the number of bulk species increases the size of the particle and vice-versa.

6.1.4. Mass and Volume of an Individual Particle

The mass of a particle is computed by summing the masses of all bulk species molecules in the core. According to the particle class definition, the mass of a class *j* particle becomes

$$m_p(j) = j \times m_0 \tag{6.1}$$

The mass of a single bulk species molecule m_0 is assumed to be constant and can be calculated from

$$m_0 = W_B / N_{avo} \tag{6.2}$$

where W_B is the molar weight of the bulk species and $N_{avo} = 6.022 \times 10^{23} [\text{mole}^{-1}]$ is the Avogadro number. The volume of a class *j* particle can be calculated from its mass and bulk density of the particle core as

$$V_p(j) = m_p(j) / \rho_B = j \times m_0 / \rho_B \tag{6.3}$$

The bulk density of the particle core ρ_B has implicitly accounted for the effect of molecule packing inside the core and its value is given when the bulk species is declared. It thus can be seen that both particle mass and volume are proportional to its class. Up to this point, there is no assumption regarding the shape of the particles so Equation 6.1 (p. 97) to Equation 6.3 (p. 97) are generally applicable to particles of all shapes.

6.1.5. Diameter and Surface Area of an Individual Particle

However, in order to derive a characteristic length scale of a particle, it is necessary to make assumption about its geometric shape. Currently, we assume that all particles are spherical. Accordingly, the representative diameter of a class *j* particle can be written as

$$d_p(j)=d_j=\left(\frac{6}{\pi}\times V_p(j)\right)^{1/3}=\left(\frac{6m_0}{\pi\rho_B}\right)^{1/3}j^{1/3}=d_0\times j^{1/3} \tag{6.4}$$

The sphere-equivalent surface area of a class *j* particle is then given as

$$A_{s,p}(j)=\pi d_p^2(j)=\pi d_0^2\times j^{2/3}=A_{s,0}\times j^{2/3} \tag{6.5}$$

In the above equations,

$$d_0=\left(\frac{6m_0}{\pi\rho_B}\right)^{1/3} \tag{6.6}$$

and

$$A_{s,0}=\pi d_0^2 \tag{6.7}$$

are respectively the “unit” diameter and the “unit” surface area of the bulk species in particle core.

Chapter 7: Using the FITDAT Utility

FITDAT is a utility that produces the polynomial fitting coefficients required as input for each species defined in a Gas-phase Kinetics or Surface Kinetics input file. The program accepts a molecule description in the form of character-string keywords, followed by thermodynamic data in a variety of formats. It then performs a least-squares fitting procedure for thermodynamic data, and writes an output file (e.g. *fitdat.out*) that contains the fit results and information about the quality of the fit. The file may also contain error diagnostics. The default format for the fit results is polynomial fitting coefficients for each of two temperature-ranges, as expected by the Gas-phase Kinetics and Surface Kinetics Pre-processors. An optional output format is also available if more than two temperature-ranges are desired.

Details of the various input formats for the thermodynamic data are described in *FITDAT* Examples (p. 105). The first option is to input a table of specific heat, enthalpy, and entropy values as functions of temperature. Several formats are accepted, corresponding to those used by standard references for thermodynamic data. The second option is to input thermodynamic data in the form of polynomial fitting coefficients, which *FITDAT* will convert to the format used by ANSYS Chemkin-Pro. Again, several formats are accepted, corresponding to those used by standard compilations of thermodynamic data. The third option is to input the molecule's standard enthalpy, standard entropy, and vibrational frequencies, which are then used to estimate the thermodynamic properties.

The fit results can be cut and pasted directly into a thermodynamics data file, or a *Gas-phase Kinetics* or *Surface Kinetics* input file for use with ANSYS Chemkin-Pro. In addition to this output, *FITDAT* creates file(s) named *species_name.csv* (e.g. *H2.csv*) containing a table of comma-delimited data for each input species. These files facilitate visualization of evaluated fit results compared to the user's input data.

7.1. Running *FITDAT* from the User Interface

In the ANSYS Chemkin-Pro Interface, *FITDAT* is run from the Utility menu. To open the *FITDAT* panel, select the **Utility > Run 'FitDat' Polynomial Equation Fitting Utility...** menu option. The panel shown in Figure 7.1: Utilities—'Fitdat' Polynomial Equation Fitter (p. 100) will be displayed in the Working Area of the User Interface.

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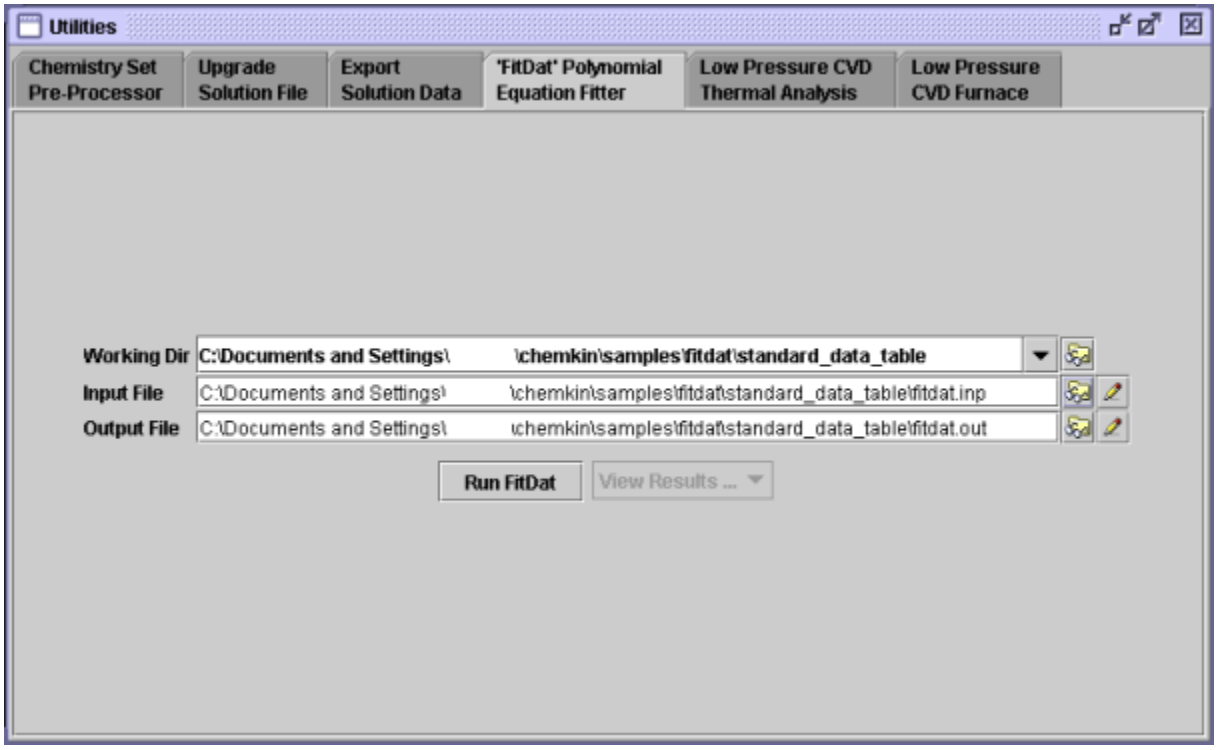
Figure 7.1: Utilities—'Fitdat' Polynomial Equation Fitter



The user must first assemble an input file that describes the fitting operation desired for the *FITDAT* session. The syntax of that input file is described in Keyword Syntax and Rules (p. 101) . Once the input file is assembled, *FITDAT* can be run by completing the following steps:

1. Use the **Working Dir** browse or pull-down menu tools to select a working directory. This is the directory where output files from the *FITDAT* run will be created.

2. Use the **Input File** browse or pull-down menu tools to select an input file. The syntax of the input file is described in Keyword Syntax and Rules (p. 101) .

3. Select an **Output File** name. Type a new name in the text box if you want to modify it from the default.

4. Use the **Run FitDat** button to execute the *FITDAT* utility.

5. Use the **View Results** button to examine the output file.

6. The user can import a *FITDAT species_name.csv* file into the ANSYS Chemkin-Pro Post-Processor to plot the fitting results. For more information about the Post-Processor, see the new Chemkin-Pro Visualization Manual .

7.2. Programming with FITDAT

The *FITDAT* Utility is written as a FORTRAN subroutine that is called from a driver routine, and is part of the ANSYS Chemkin-Pro library. We provide both C++ and FORTRAN driver routines. The driver routine performs the function of allocating total memory usage through definition of array sizes, as well as opening input and output files. *FITDAT* checks internally to ensure that the allocated work arrays are sufficiently large to process the input data. Users modifying the programs should be experienced with compiling and linking program files on their operating system and must have either a C++ or FORTRAN compiler installed.

7.3. Keyword Syntax and Rules

The *FITDAT* Utility input is in a Keyword format. On each input line, an identifying Keyword must appear first. For some Keywords only the Keyword itself is required, while for others, additional information is required. The order of the Keyword input is generally unimportant. The rules governing the syntax of the Keyword images are listed below:

Table 7.1: Summary of Rules for Keywords

Rule	Description
1	The first character-string in the line must be a keyword; the length of the character-string depends on keyword descriptions.
2	Any further input associated with the keyword can appear anywhere after the keyword, through column 100. The specific starting column is not important, as long as there is at least one space after the keyword.
3	When more than one piece of information is required, the order in which the information appears is unimportant.
4	When numbers are required as input, they may be stated in either integer, floating point, or scientific "E" format. The utility converts the numbers to the proper type. The double precision specifier is not recognized; however, conversion to double precision is done internally as necessary.
5	When more than one piece of information is required, the pieces are delimited by one or more blank spaces.

7.4. *FITDAT* Keywords

Table 7.2: *FITDAT* Keywords

Keyword	Definition			
SPEC	A species character-string symbol, to be used in the thermodynamic data and in an ANSYS Chemkin-Pro reaction mechanism, and in the name of the post-processing data file.			
	Parameters	Optional/Reqd.	Units	Examples
	Species	Required	--	SPEC **OH**
	Keyword Usage	Optional keyword. By default, this keyword is not used unless it can be determined from the data source.		
ELEM	The elemental composition of the species.			
	Parameters	Optional/Reqd.	Units	Examples
	Element	Required	--	ELEM **O** 1 ELEM **H**1
	Number of elements	Required	--	ELEM O **1** ELEM H **1**
	Keyword Usage	Optional keyword. By default, this keyword is not used unless it can be determined from the data source		
DIAG	The level of fitting procedure diagnostics printed to the output file. DIAG or DIAG 1 will print a summary of data vs. polynomial evaluation relative			

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Keyword	Definition			
	errors. DIAG 2 will print tables of input table vs. polynomial evaluations, as well as the summary of relative error.			
	Parameters	Optional/Reqd.	Units	Examples
	Diagnostic level	Optional	--	DIAG **2**
	Keyword Usage	Optional keyword. By default, no diagnostics are printed.		
NOTE	Print a 6-character legend to columns 19-24 of the output thermodynamic data. For example, NOTE 101602 notes the date of October 16, 2002, while NOTE Jan888 notes a JANAF data source.			
	Parameters	Optional/Reqd.	Units	Examples
	Legend	Required	--	NOTE **101602** NOTE **Jan888**
	Keyword Usage	Optional keyword. By default, no notes are printed.		
PHAS	The phase of the species, G (gas), L (liquid), or S (solid).			
	Parameters	Optional/Reqd.	Units	Examples
	Phase	Required	--	PHAS **G**
	Keyword Usage	Optional keyword. By default, the phase G is used unless it can be determined from data source.		
LINR	The linearity of the molecule; Y (molecule is linear) or N (no).			
	Parameters	Optional/Reqd.	Units	Examples
	Linearity	Required	--	LINR **Y**
	Keyword Usage	Optional keyword. By default, this keyword is not used unless it can be determined from the data source.		
TMIN	The minimum temperature requirement for the polynomial; if TMIN is lower than the starting temperature of input data, thermodynamic properties will be extrapolated at this point.			
	Parameters	Optional/Reqd.	Units	Examples
	Temperature	Required	K	TMIN **300**
	Keyword Usage	Optional keyword. By default, the minimum temperature is 300 K unless it can be determined from data source.		
TMAX	The maximum temperature requirement for the polynomial; if TMAX is greater than the ending temperature of input data, thermodynamic properties will be extrapolated at this point.			
	Parameters	Optional/Reqd.	Units	Examples
	Temperature	Required	K	TMAX **5000**

Keyword	Definition			
	Keyword Usage	Optional keyword. By default, the maximum temperature is 5000 K unless it can be determined from data source.		
TEMP	One or more temperatures dividing the ranges of the polynomial, at which the functional values are constrained; all TEMP values must be between TMIN and TMAX. Each TEMP given will result in a set of polynomial coefficients. If no TEMP is given, there will be one set of coefficients.			
	Parameters	Optional/Reqd.	Units	Examples
	Temperature or temperature range	Required	K	TEMP **1500** TEMP **1000 2000**
	Keyword Usage	Optional keyword. By default, this keyword is not used unless it can be determined from the data source.		
H298	Species' formation enthalpy at 298.15 K.			
	Parameters	Optional/Reqd.	Units	Examples
	Enthalpy	Required	kcal/mole	H298 **9.32**
	Keyword Usage	Optional keyword. By default, this keyword is not used unless it can be determined from the data source.		
NO298	Indicates that the *FITDAT* program should not try to constrain the species' formation enthalpy at the 298.15 K value. Normally the *FITDAT* program will attempt to exactly match the temperature fit at the 298.15 K point, but in some cases (e.g., the data point is not available) it may be desirable to remove this constraint.			
	Parameters	Optional/Reqd.	Units	Examples
		--	--	NO298
	Keyword Usage	Optional keyword. By default, the fit is constrained to exactly match the input value at 298.15 K.		
S298	Species' formation entropy at 298.15 K.			
	Parameters	Optional/Reqd.	Units	Examples
	Entropy	Required	cal/mole	S298 **43.88**
	Keyword Usage	Optional keyword. By default, this keyword is not used unless it can be determined from the data source.		
DATA	A table of data will follow, the format and contents of which depends on the data type given with this keyword.			
	Parameters	Optional/Reqd.	Calorie-based Units	Examples
	Type of data table	Required	--	DATA **CHEM** DATA **JANAF** DATA **NIST**

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Keyword	Definition			
				DATA **NASA**
	Keyword Usage	Optional keyword. By default, the DATA CHEM option is used.		
POLY	A set of polynomial data will follow, the format and contents of which depends on the polynomial type given with this keyword. The CHEM option will display ANSYS Chemkin-Pro-formatted polynomial records. The SHOM option will display Shomate polynomial records. The NASA option will display NASA-formatted polynomial records.			
	Parameters	Optional/Reqd.	Calorie-based Units	Examples
	Set of polynomial data	Required	--	POLY **CHEM** POLY **SHOM** POLY **NASA**
	Keyword Usage	Optional keyword. By default, the POLY CHEM option is used.		
VIBE	One or more species' vibrational frequency.			
	Parameters	Optional/Reqd.	Units	Examples
	Vibrational frequency	Required	cm^{-1}	VIBE 999.83
	Keyword Usage	Optional keyword.		
NPTS	Number of points to generate from TMIN to TMAX, when evaluating properties data from POLY or VIBE.			
	Parameters	Optional/Reqd.	Units	Examples
	Number of points	Required	--	NPTS **50**
	Keyword Usage	Optional keyword. By default, 100 points are generated.		
DELT	Temperature increment used from TMIN to TMAX, when evaluating properties data from POLY or VIBE.			
	Parameters	Optional/Reqd.	Units	Examples
	Temperature	Required	K	DELT **50**
	Keyword Usage	Optional keyword. By default, DELT value depends on the NPTS value.		
END	End of input, and start of the fitting process for the current species.			
	Keyword Usage	Required keyword.		

7.5. *FITDAT* Examples

This section discusses input files that allow *FITDAT* to provide thermodynamic data fitting coefficients using several different methods. These examples show NIST, Shomate, NASA, and other data formats (DATA CHEM Input Format (p. 105) through VIBE Input Format (p. 109)).

FITDAT is run from the ANSYS Chemkin-Pro Interface by selecting it from the **Utility** menu (see FITDAT Utility for Fitting Polynomials to Thermodynamic Data for more information). After running *FITDAT*, users may then launch the Chemkin-Pro Post-Processor using the **View > Graphical Post-processor** menu option. This action will actually result in a warning message and the display of a "Sample Plot", as *FITDAT* does not produce a typical solution file like other Chemkin-Pro problem and *FITDAT* results will therefore need to be plotted using the Import option in the Chemkin-Pro Post-Processor. The user selects the Import option from the Post-Processor's File menu. This opens a file browser to allow the user to select a *species_name.csv* file for plotting of fit results. After the file has been selected, further select the following items from the Select the Import File Format dialog: **Comma** radio button, Skip 2 lines of text (**Skip** slider control), and **Read column titles** check box.

7.5.1. DATA CHEM Input Format

This is an example of the minimum input required to fit default type of data, which is four columns consisting of temperature (K), and species properties C_p (cal/mole-K), S (cal/mole-K), and $H(T) - H(298)$ (kcal/mole). Defaults are `PHAS=G`, `TMIN=300`, and `TMAX=5000`, the first and last positive data points, but keywords may be used to supersede these values.

Figure 7.2: DATA CHEM Input File

```
SPEC OH
ELEM O 1
ELEM H 1
H298 9.32
TEMP 1500
DATA
0300.00  007.165  043.926  000.013
0400.00  007.087  045.974  000.725
     :
4900.00  009.232  065.778  038.571
5000.00  009.249  065.965  039.495
END
```

7.5.2. POLY CHEM Input Format

This is an example of the minimum input required to fit data evaluated from an existing ANSYS Chemkin-Pro -format polynomial; defaults `SPEC=OH`, `ELEM`, `PHAS=G` , `TMIN=300`, `TMAX=5000`, and `TEMP=1000` are obtained from the polynomial, and `H298` by an evaluation of the polynomial, but keywords may be used to supersede these values. This option might be used to generate fits for a different temperature range where the original data are no longer available.

Figure 7.3: POLY CHEM Input File

```
POLY CHEM
OH                121286O   1H   1          G  0300.00   5000.00  1000.00      1
 0.02882730E+02 0.10139743E-02-0.02276877E-05 0.02174683E-09-0.05126305E-14    2
 0.03886888E+05 0.05595712E+02 0.03637266E+02 0.01850910E-02-0.16761646E-05    3
 0.02387202E-07-0.08431442E-11 0.03606781E+05 0.13588605E+01
END
```

FITDAT evaluates the ANSYS Chemkin-Pro polynomial as described in Running *FITDAT* from the User Interface (p. 99) , to obtain thermodynamic properties for fitting. A table of NPTS temperatures from TMIN to TMAX will be used to evaluate the properties; keywords NPTS or DELT may be used to modify this phase.

7.5.3. DATA NIST Input Format

This is an example of the minimum input required to fit NIST-format data, which is 5 columns consisting of temperature (K), and species properties $C_p(\mathrm{cal/mole{\cdot}K})$, $S(\mathrm{cal/mole{\cdot}K})$, $-(G^o-H^o(298.15))/T(\mathrm{cal/mole{\cdot}K})$ and $H(T)-H(298)(\mathrm{kcal/mole})$. Input data can be obtained from the *NIST Chemistry WebBook[8] (p. 331)* , p. 124 using the following steps:

1. At the start of the NIST menu (http://webbook.nist.gov/chemistry/form-ser.html), choose **calorie-based units** in the toggle under question #3, when selecting the desired units for thermodynamic data.
2. Perform a **Formula Search** (e.g., search for OH).
3. Select **View Table** option under the Heat Capacity heading.
4. In the table view, highlight and copy the table text, then paste into a text file.

Defaults are PHAS=G, and TMIN=300, TMAX=6000, the first and last positive data points greater than 298, but keywords may be used to supersede these values.

Figure 7.4: DATA NIST Input File

```
SPEC OH
ELEM O 1
ELEM H 1
H298 9.318131
TEMP 1500.
DATA NIST
300. 7.16 43.95 43.91 0.01
400. 7.09 46.00 44.19 0.73
        :
5900. 9.41 67.53 59.42 47.89
6000. 9.43 67.69 59.55 48.83
END
```

7.5.4. POLY SHOM Input Format

This is an example of the minimum input required to convert a Shomate polynomial to ANSYS Chemkin-Pro format; The Shomate equations are given in Equation 7.1 (p. 107) through Equation 7.3 (p. 107) , where *t = Temperature(K)/1000*. Parameters (A, B, C, D, E, F, G, and H°f, 298) can be obtained from the *NIST Chemistry WebBook*.[8] (p. 331)

1. At the start of the NIST menu(http://webbook.nist.gov/chemistry/form-ser.html), choose **calorie-based units** in the toggle under question #3, when selecting the desired units for thermodynamic data.
2. Perform a **Formula Search** (e.g., search for OH).
3. Highlight and copy the table of parameters (including the heading row and the rows for the A , B , C , D , E , F , G parameters), then paste these into a text file.

Defaults are PHAS=G, TMIN=298, TMAX=6000, and TEMP=1000 are obtained from the Shomate data, and H298 by an evaluation of the polynomial, but keywords may be used to supersede the defaults.

Figure 7.5: POLY SHOM Input File

```
SPEC OH
ELEM O 1
ELEM H 1
POLY SHOM
Temperature (K) 298. - 1300. 1300. - 6000.
A 7.714551 6.870701
B -2.715801 1.126790
C 3.251781 -0.194724
D -0.919332 0.013085
E -0.000319 -0.656747
F 7.110691 6.313191
G 53.91451 51.17510
END
```

$$C_p = A + Bt + Ct^2 + Dt^3 + \frac{E}{t^2} \tag{7.1}$$

$$H - H(298) = At + \frac{Bt^2}{2} + \frac{Ct^3}{3} + \frac{Et^4}{4} - \frac{E}{t} + F - H(298) \tag{7.2}$$

$$S = A\ln(t) + Bt + \frac{Ct^2}{2} + \frac{Dt^3}{3} - \frac{E}{2t^2} + G \tag{7.3}$$

A table of NPTS temperatures from TMIN to TMAX will be used to evaluate the properties; keywords NPTS or DELT may be used to modify this process.

7.5.5. DATA NASA Input Format

This is an example of the minimum input required to fit NASA-format data, which is at least four columns consisting of temperature (K), and species properties C_p (cal/mole-K), H (T) - H (298) (kcal/mole), and S (cal/mole-K). NASA data can be obtained from the Properties From Coefficients (PFC) [8] (p. 331) program; request **calorie-based units**, and highlight, copy, and paste the resulting table into a text file. Defaults are PHAS=G , TMIN=300, TMAX=6000, the first and last positive data points, and H298 is the column 6 value at T=298.15, but keywords may be used to supersede the defaults.

Figure 7.6: DATA NASA Input File

```
SPEC OH
ELEM O 1
ELEM H 1
DATA NASA
!   THERMODYNAMIC FUNCTIONS CALCULATED FROM COEFFICIENTS FOR OH
!      T         Cp        H-H298        S      -(G-H298)/T      H        delta Hf     log K
!    deg-K   cal/mol-K    kcal/mol   cal/mol-K   cal/mol-K    kcal/mol    kcal/mol
      0         0.         -2.106       0.        INFINITE      6.803       8.853    INFINITE
     200        7.293      -0.707      41.035      44.572       8.202       8.877     -8.9035
     298.15     7.143       0.000      43.915      43.915       8.910
        :
        :
    5900        9.620      48.463      67.672      59.458      57.373       6.636      0.3749
    6000        9.625      49.425      67.834      59.596      58.335       6.573      0.3790
END
```

7.5.6. POLY NASA Input Format

This is an example of the minimum input required to convert a NASA polynomial[9] (p. 331) to Chemkin-Pro format. The equations defining polynomials are given in Equation 7.4 (p. 108) through Equation 7.6 (p. 108) . NASA polynomial data can be obtained from the Properties From Coefficients (PFC)[10] (p. 331), p. 124 and then highlighted, copied, and pasted into a text file. Defaults for SPEC, ELEM,

PHAS, TMIN, TMAX, TEMP, and H298 are obtained from the polynomial, but may be superseded by keyword usage.

Figure 7.7: POLY NASA Input File

```
POLY NASA
OH                D0(H-OH): Ruscic,2002. Gurvich,1978 pt1 p110 pt2 p37.
 3 g 4/02 O   1.00H   1.00    0.00    0.00    0.00 0     17.00734      37278.206
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8813.106
-1.998858990E+03 9.300136160E+01 3.050854229E+00 1.529529288E-03-3.157890998E-06
 3.315446180E-09-1.138762683E-12 0.000000000E+00 2.991214235E+03 4.674110790E+00
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8813.106
 1.017393379E+06-2.509957276E+03 5.116547860E+00 1.305299930E-04-8.284322260E-08
 2.006475941E-11-1.556993656E-15 0.000000000E+00 2.019640206E+04-1.101282337E+01
   6000.000 20000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8813.106
 2.847234193E+08-1.859532612E+05 5.008240900E+01-5.142374980E-03 2.875536589E-07
-8.228817960E-12 9.567229020E-17 0.000000000E+00 1.468393908E+06-4.023555580E+02
END
```

Figure 7.8: Format details for POLY NASA Input Files

```
line 1:       OH is species name
line 2:       3 is the number of temperature ranges
              5 sets of elemental composition, i.e., 'O 1.00' and 'H 1.00'
              0 in the next field indicates a gas
              17.00734 is the molecular weight
              37278.206 is H298 heat of formation, J/mol
line 3:       200-1000 is the first temperature range,
              7 is the number of Cp/R polynomial coefficients,
              -2,-1,0,1,2,3,4,0 are the T exponents for the coefficients,
              8813.106 is H(298)-H(0), J/mol
line 4:       a1 through a5 for temperatures 200-1000K
line 5:       a6 through a7 for temperatures 200-1000K, a8 (not used),
              integration constants b1, b2
lines 6-end:  same as 3-5, for more temperature ranges
```

The resulting non-dimensional thermodynamic properties are

$$\frac{C_p}{R} = a_1 T^{-2} + a_2 T^{-1} + a_3 + a_4 T + a_5 T^2 + a_6 T^3 + a_7 T^4 \tag{7.4}$$

$$\frac{H}{RT} = -a_1 T^{-2} + a_2 T^{-1} \ln(T) + a_3 + \frac{a_4 T}{2} + \frac{a_5 T^2}{3} + \frac{a_6 T^3}{4} + \frac{a_7 T^4}{5} + \frac{b_1}{T} \tag{7.5}$$

$$\frac{S}{R} = \frac{-a_1 T^{-2}}{2} - a_2 T^{-1} + a_3 \ln(T) + a_4 T + \frac{a_5 T^2}{2} + \frac{a_6 T^3}{3} + \frac{a_7 T^4}{4} + b_2 \tag{7.6}$$

A table of NPTS temperatures from TMIN to TMAX will be used to evaluate the properties; keywords NPTS or DELT may be used to modify this process.

7.5.7. DATA JANAF Input Format

This is an example of the minimum input required to fit JANAF-format data, which is at least five columns consisting of temperature (K), and species properties C_p (J/mole-K), S (J/mole-K), G (J/mole-K), and H (T) - H (298) (kJ/mole). Defaults SPEC=OH, PHAS=G , and ELEM are obtained from the CODE line, TMIN=300, TMAX=6000 are the first and last positive data points greater than 298, and H (298) (kJ/mole) is the column 6 value at T=298.15, but keywords may be used to supersede the defaults.

Figure 7.9: DATA JANAF Input File

```
DATA JANAF
```

```
!     Janaf table documentation:
!     Col 2-10:  Temperature (K)
!     Col 11-19: Heat Capacity, Cp (J/K-mole)
!     Col 20-29: Entropy, S (J/K-mole)
!     Col 30-39: Gibbs Free Energy, G (J/K-mole)
!     Col 40-51: Relative Enthalpy, H-H298 (kJ/mole)
!     Col 52-62: Enthalpy of Formation, Hf (kJ/mole)
!     Col 63-74: Gibbs Energy of Formation, Gf (kJ/mole)
!     Col 75-85: log (Equilibrium constant of formation), log(Keq(T))
!     Note: some of the above are in KJ and some in J.CODE =  300  H1O1(g)

CODE =  300  H1O1(g)

!Hydroxyl (OH)                                                          H O (g)
!                                                                       1 1
     0     0.        0.     INFINITE      -9.172     38.390      38.390   INFINITE
    25    29.487   106.145   447.063      -8.523     38.411      38.109    -79.625
    50    31.487   127.111   282.386      -7.764     38.391      37.805    -39.494
    75    32.719   140.171   232.937      -6.957     38.390      37.516
     :
     :
  5900    39.350   282.564   248.604     200.369     27.391     -39.860      0.353
  6000    39.423   283.226   249.175     204.308     27.019     -40.997      0.357

!PREVIOUS: June 1977 (1 atm)                          CURRENT: June 1977 (1 bar)
END
```

7.5.8. VIBE Input Format

This is an example of the minimum input required to fit vibrational frequency data. Defaults are PHAS=G, TMIN=300, TMAX=6000, and LINR=No (from the fact of more than one VIBE), but keywords may be used to supersede the defaults.

This method is provided for use in cases where little or no information is available in the literature about the molecule of interest. It contains a number of approximations:

1. Translational contributions to the heat capacity are treated classically via the equipartition function. This is generally a good assumption.

2. Rotational contributions to the heat capacity are treated classically via the equipartition function. This is a good assumption for most molecules at higher temperatures.

3. Hindered internal rotors are not explicitly treated, but rather approximated as vibrations. This is a less-good approximation.

In all cases, these approximations are more likely to break down at lower temperatures.

Figure 7.10: VIBE Input File

```
SPEC SIH2
ELEM SI 1
ELEM H 2
H298 58.0
S298 49.4
TEMP 1000
VIBE  999.83
VIBE 2011.69
VIBE 2001.72
END
```

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7.5.9. Example *FITDAT* Outputs

Figure 7.11: Example *fitdat.out* file (p. 110) shows the fitdat.out file that will be created if the `DATA  CHEM` input file discussed in DATA CHEM Input Format (p. 105) is run through the *FITDAT* utility.

Figure 7.11: Example *fitdat.out* file

```
        ************************************************************
        *                    CHEMKIN Release 4.0                   *
        *                     FITDAT Application                   *
        *         Thermodynamic properties fitting program.        *
        * Copyright 1997-2002 Reaction Design.  All Rights Reserved. *
        ************************************************************



            WORKING SPACE REQUIREMENTS
            PROVIDED         REQUIRED
  INTEGER             112            112
  REAL               9534           9534



  Reading keyword data...
  Setting SPEC name:                         OH
  Setting ELEM #  1:                         O   1
  Setting ELEM #  2:                         H   1
  Setting H298:                               9.320E+00 Kcal/mole
  Setting TEMP #  1:                          1.000E+03 K
  End of keyword input for species OH

 Species OH Fit:
 OH                      O   1H   1          G   300.000  5000.000 1000.00      1
  0.29446142E+01 0.91447172E-03-0.17338418E-06 0.95183610E-11 0.46042672E-15    2
  0.38598718E+04 0.52419727E+01 0.35069641E+01 0.12114174E-02-0.44383205E-05    3
  0.53991545E-08-0.19835349E-11 0.36200845E+04 0.18923732E+01                   4


  Reading keyword data...
  End of input file...
```

Figure 7.12: Example *fitdat.out* file with more than two temperature ranges (p. 110) shows example output that would result if the input discussed in DATA CHEM Input Format (p. 105) is modified to include polynomial coefficients for more than two temperature ranges (e.g., adding keyword line: `TEMP  2500`).

Figure 7.12: Example *fitdat.out* file with more than two temperature ranges

```
        ************************************************************
        *                     CHEMKIN Release 4.0                  *
        *                     FITDAT Application                   *
        *         Thermodynamic properties fitting program.        *
        * Copyright 1997-2002 Reaction Design.  All Rights Reserved. *
        ************************************************************



            WORKING SPACE REQUIREMENTS
            PROVIDED         REQUIRED
  INTEGER             112            112
  REAL               9534           9534



  Reading keyword data...
  Setting SPEC name:                         OH
  Setting ELEM #  1:                         O   1
```

```
 Setting ELEM #  2:                          H   1
 Setting H298:                                9.320E+00 Kcal/mole
 Setting TEMP #  1:                           1.000E+03 K
 Setting TEMP #  2:                           2.500E+03 K
 End of keyword input for species OH

Species OH Fit:
OH                      O   1H   1          G   300.000  5000.000              1
TEMP   300.000  1000.000  2500.000  5000.000
 0.31521126E+01 0.77090695E-03-0.15393767E-06 0.13363294E-10-0.27768811E-15
 0.36675921E+04 0.39045946E+01
 0.34408417E+01-0.28167277E-03 0.83197801E-06-0.34404565E-09 0.44913015E-13
 0.37077941E+04 0.26162167E+01
 0.37729215E+01-0.61576963E-03-0.15821000E-06 0.13103019E-08-0.61722943E-12
 0.35916670E+04 0.76556823E+00


 Reading keyword data...
 End of input file...
```

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Chapter 8: CHEMKIN Project Input: Keyword Syntax and Rules

In most cases, a Reactor Model input file is written by the ANSYS Chemkin-Pro Interface before a simulation run based on the Chemkin-Pro Project Input. The panel context and "bubble" help within the Interface provide basic guidance for setting up model-specific input parameters. However, in some cases users may want further information about a model parameter usage and in other cases they may want to assemble their own input files outside of the User Interface. For such cases, this chapter together with Reference Guide to Project Input Keywords (p. 115) and Alphabetical Listing of Project Input Keywords (p. 123) contain detailed information about input options for each Reactor Model. This chapter provides an overview of the syntax and rules for such parameter input.

User input information is generally written to a Reactor Model input file in "keyword" format. In this format, each input line starts with an identifying keyword. For some input, only the keyword itself is required, while others require one or more pieces of additional information. Many keywords have default values associated with them. If these default values are appropriate for the user's problem, then these keywords do not need to be included in the input file. In the case of restarts or continuation problems, some of the parameters can be changed from what was used in the previous solution. If these keywords are not included or not changed in the input keyword list for continuations or restarts, then the parameters will retain their former values. In the list of keywords that follow, we indicate whether or not each keyword may be changed on a restart from a previous solution. The order of the keyword input is not important. The general rules governing the syntax of the keyword lines are listed in Table 8.1: Summary of the Rules for Keywords (p. 113).

Note

Note that you can turn on or off the display of the "Keyword" associated with an ANSYS Chemkin-Pro Interface input parameter, using the modal option in the Preferences panel.

Table 8.1: Summary of the Rules for Keywords

Rule	Description
1	The first character-string in the line must be a keyword; the length of the character-string depends on keyword descriptions.
2	Any further input associated with the keyword can appear anywhere after the keyword, through column 80. The specific starting column is not important, as long as there is at least one space after the keyword.
3	When more than one piece of information is required, the order in which the information appears is important.
4	When numbers are required as input, they may be stated in integer, floating-point, or "E" format. ANSYS Chemkin-Pro converts the numbers to the proper type internally. The double precision specification D is not recognized; however, the double precision conversion will be done internally, as necessary.
5	When species names are required as input, they must appear exactly as they are specified in the *Gas-phase Kinetics* and *Surface Kinetics* input files.

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Rule	Description
6	When more than one piece of information is required, the pieces are delimited by one or more blank spaces.
7	If contradictory or duplicate keywords are input, ANSYS Chemkin-Pro uses the information that is last read. Under some circumstances, this will result in a warning printed to the output file.
8	A “comment” line is one that has either a period (.), slash (/), or exclamation mark (!) as the first non-blank character. In addition, on any Keyword line, any input that follows an exclamation mark is taken as a comment. All input lines, including comments, are printed to the output.
9	The keyword END must be the last input card. END keywords are required between sets of parameters for continuations.
10	If no parameter is given, then the keyword stands alone on the input line; keywords with parameters are demonstrated with examples.

Chapter 9: Reference Guide to Project Input Keywords

In this chapter, we group the available input reactor project input options (keywords) according to the Reactor Model with which they may be used. Note that many keywords can be used with several different Reactor Models and that there are a few cases where keywords that share the same name may have different meanings for different Reactor Models. General information about keyword syntax and rules is given in CHEMKIN Project Input: Keyword Syntax and Rules (p. 113). A detailed, alphabetical listing of all keywords is given in Alphabetical Listing of Project Input Keywords (p. 123). This chapter is meant to serve as a quick cross-reference to the more detailed information in Alphabetical Listing of Project Input Keywords (p. 123).

9.1. Closed 0-D Reactor Models

9.1.1. Internal Combustion HCCI Engine

The following keywords can be used to build an input file for a IC HCCI Engine Reactor Model:

ADAP, ADD, AEXT, AGGA, AGGB, AGGD, AGGE, AGGFD, AGGMN, AROP, ASEN, ASTEPS, ATLS, ATOL, AVALUE, AVAR, BETA, CAATQ, CLSC, CLSM, CMPR, CNTN, CNTT, COLR, CYBAR, DEG0, DELT, DIST, DTDEG, DTIGN, DTSV, EGRR, END, EPSR, EPSS, EPST, EQUI, FUEL, GFAC, GMHTC, GVEL, ICEN, ICHT, IPSR, KLIM, LODR, LOLR, MAXIT, MCUT, MMASS, NADAP, NCANG, NEWRUN, NMOM, NNEG, NOCG, NREV, NSOL, OXID, PNDE, PRDL, PRES, PRNT, PROE, PSBAR, PTM_SECTION_SIZEDEP_A0, PTM_SECTION_SIZEDEP_COLEFF, PTM_SECTION_SIZEDEP_DSTAR, PTM_SECTION_SIZEDEP_HAMAKER, PVFE, QEXP, QFUN, QLOS, QPRO, QRGEQ, REAC, RELAXC, RLGAS, RLMIX, ROP, RPM, RSTR, RTLS, RTOL, SCLM, SCLS,, SENT, SIZE, SOLUTION_TECHNIQUE, SSTT, STPT, TEMP, TEXP, TIFP, TIME, TLIM, TRAN, TRES, TRST, TSTR, TTIM, UIGN, UREF, USET, VOLC, VOLD, WENG, WOSP1, WOSP2, WOSP3, XMLI

9.1.2. Closed Homogeneous Batch Reactor

The following keywords can be used to build an input file for a Closed Homogeneous Reactor Model:

ADAP, ADD, AEXT, AFRA, AGGA, AGGB, AGGD, AGGE, AGGFD, AGGMN, AINT, AREA, AREAQ, AROP, ASEN, ASTEPS, ATLS, ATOL, AVALUE, AVAR, BETA, BLKEQ, BULK, CLSC, CLSM, CNTN, CNTT, COLR, CONP, CONV, COTV, DELT, DIST, DTIGN, DTSV, EGRR, END, ENRG, EPSG, EPSR, EPSS, EPST, EQUI, ETCH, FUEL, GFAC, GMHTC, HTC, HTRN, IPSR, IRET, ISTP, KLIM, MAXIT, MCUT, MMASS, NADAP, NEWRUN, NMOM, NNEG, NOCG, NSOL, OXID, PBDEN, PNDE, PPRO, PRES, PRNT, PROE, PTM_SECTION_SIZEDEP_A0, PTM_SECTION_SIZEDEP_COLEFF, PTM_SECTION_SIZEDEP_DSTAR, PTM_SECTION_SIZEDEP_HAMAKER, PVFE, QFUN, QLOS, QPRO, QRGEQ, QRSEQ, REAC, RELAXC, RLGAS, RLMIX, ROP, RSTR, RTLS, RTOL, SCLM, SCLS, SCOR, SENG, SENT, SFAC, SIZE, SOLUTION_TECHNIQUE, SSTT, STPT, SURF, TAMB, TEMP, TGIV, TIFP, TIME, TLIM, TPRO, TRAN, TRES, TRST, TSRF, TSTR, TTIM, UIGN, USET, VOL, VPRO, VTIM, WENG, XMLI

9.1.3. Closed Partially Stirred Reactor

The following keywords can be used to build an input file for a Closed PaSR Reactor Model:

ADAM, ATOL, BDF, CFL, CHEM, CLSE, CMIX, CTOL, CURL, DASP, DT, DT0, DTMX (transient), DTSV, END, EQUI, IEM, INIT, KOUT, MAXIT, MAXTIME, MIX, MIXT, NCFIT, NDPR, NNEG, NOJC, NPAR, PDF, PRES, QRGEQ,

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QRSEQ, RELAXC, RLGAS, RLMIX, RSTR, RTOL, SCAT, SIZE, SSMAXITER, TEMP, TIME, TRES, TRMAXITER, VOL, VPRO, WELL

9.1.4. Closed Plasma Reactor

The following keywords can be used to build an input file for a Closed Plasma Reactor Model:

ABSL, ADAP, AEXT, AFRA, AGGD, AGGE, AINT, AREA, AREAQ, AROP, ASEN, ASTEPS, ATIM, ATLM, ATLS, ATOL, AVALUE, AVAR, BETA, BLKEQ, BOHM, BPWR, BULK, CLSC, CLSM, CNTN, CNTT, CONP, COLR, CONV, DELT, DFAC, DIST, DTIGN, DTSV, ELSH, END, ENGE, ENRG, EPSG, EPSR, EPSS, EPST, ETCH, ETMP, GFAC, GMHTC, HTC, HTRN, IONE, IPSR, KLIM, MAXIT, MCUT, MMASS, NADAP, NEWRUN, NMOM, NNEG, NOCG, NSOL, PNDE, PPRO, PRES, PRNT, PROE, PVFE, PWRW, QFUN, QLOS, QLSE, QPRO, REAC, RELAXC, ROP, RSTR, RTIM, RTLM, RTLS, RTOL, SCLM, SCLS, SCOR, SENG, SENT, SFAC, SIZE, SOLUTION_TECHNIQUE, SSTT, STPT, SURF, TAMB, TEBND, TEMP, TGIV, TIFP, TIME, TION, TLIM, TPRO, TRAN, TRES, TRST, TSRF, TSTR, TTIM, USET, UIGN, VOL, VPRO, VTIM, WENG, WPRO, XMLI, XSDF, XSEK

9.1.5. Multi-Zone HCCI Engine Simulator

The following keywords can be used to build an input file for a Multi-Zone HCCI Engine Simulator:

ADAP, ADD, AEXT, AGGA, AGGB, AGGD, AGGE, AGGFD, AGGMN, AROP, ASEN, ASTEPS, ASWH, ATLS, ATOL, AVALUE, AVAR, BETA, CAATQ, CLSC, CLSM, CMPR, CNTN, CNTT, COLR, CYBAR, DEG0, DELT, DIST, DTDEG, DTIGN, DTSV, END, EPSR, EPSS, EPST, EQUI, FUEL, GFAC, GMHTC, GVEL, ICEN, ICHT, IPSR, KLIM, LODR, LOLR, MAXIT, MCUT, MMASS, MQAFR, MZMAS, NADAP, NCANG, NEWRUN, NMOM, NNEG, NOCG, NREV, NSOL, NZONE, OXID, PNDE, PRDL, PRES, PRNT, PROE, PSBAR, PVFE, QEXP, QFUN, QLOS, QPRO, QRGEQ, RELAXC, RLGAS, RLMIX, ROP, RPM, RSTR, RTLS, RTOL, SCLM, SCLS, SCOR, SENT, SIZE, SOLUTION_TECHNIQUE, SSTT, STPT, TEMP, TEXP, TIFP, TIME, TLIM, TRAN, TRES, TRST, TSTR, TSWH, TTIM, UIGN, UREF, USET, VOL, VOLC, VOLD, WENG, WOSP1, WOSP2, WOSP3, XEST, XMLI, ZONEAVG

9.1.6. SI Engine Zonal Simulator

The following keywords can be used to build an input file for an SI Engine Zonal Simulator:

ADAP, ADD, AEXT, AGGA, AGGB, AGGD, AGGE, AGGFD, AGGMN, AROP, ASEN, ASTEPS, ASWH, ATLS, ATOL, AVALUE, AVAR, BETA, CAAC, CAATQ, CAEC, CASC, CLSC, CLSM, CMPR, CNTN, CNTT, COLR, CYBAR, DEG0, DEGE, DELT, DIST, DTDEG, DTIGN, DTSV, END, EPSR, EPSS, EPST, SIZE, EQUI, FUEL, GFAC, GMHTC, GVEL, HSWC, HSWM, HSWT, ICEN, ICHT, IPSR, KLIM, LODR, LOLR, MAXIT, MCUT, MMASS, NADAP, NCANG, NEWRUN, NMOM, NNEG, NOCG, NREV, NSOL, OXID, PNDE, PRDL, PRES, PRNT, PROE, PSBAR, PVFE, QEXP, QFUN, QLOS, QPRO, QRGEQ, RELAXC, RLGAS, RLMIX, ROP, RPM, RSTR, RTLS, RTOL, SCLM, SCLS, SCOR, SENT, SIDR, SIKN, SIOA, SIZE, SOLUTION_TECHNIQUE, SSTT, STPT, TEMP, TEXP, TIFP, TIME, TLIM, TRAN, TRES, TRST, TSTR, TTIM, UIGN, UREF, USET, VOL, VOLC, VOLD, WENG, WOSP1, WOSP2, WOSP3, XEST, XMLI, ZONEAVG

9.2. Open 0-D Reactor Models

9.2.1. Perfectly Stirred Reactor

The following keywords can be used to build an input file for a PSR Reactor Model:

ABFR, ABSL, AEXT, AFRA, AGGA, AGGB, AGGD, AGGE, AGGFD, AGGMN, AINT, AREA, AREAQ, AROP, ASEN, ASTEPS, ATIM, ATLM, ATLS, ATOL, AVALUE, AVAR, BETA, BLKEQ, BULK, CLSC, CLSM, CNTN, CNTT, COLR, CPROD, DELT, DFAC, DIST, DTIGN, DTMN, DTMX (steady-state), DTSV, EGRR, END, ENRG, EPSG, EPSR, EPSS, EPST, EQUI, ETCH, FLRT, FPRO, FUEL, GFAC, GMHTC, HTC, HTRN, INLET, IPSR, IRET, ISTP, KLIM,

MAXIT, MAXTIME, MCUT, MMASS, NEWRUN, NJAC, NMOM, NNEG, NOCG, NOFT, NPSR, NSOL, OXID, PBDEN, PNDE, PNDI, PPRO, PRES, PRNT, PROD, PROE, PROI, PSURF, PTM_SECTION_SIZEDEP_A0, PTM_SECTION_SIZEDEP_COLEFF, PTM_SECTION_SIZEDEP_DSTAR, PTM_SECTION_SIZEDEP_HAMAKER, PVFE, PVFI, QFUN, QLOS, QPRO, QRGEQ, QRSEQ, QXCO (p. 281), QXRA (p. 281), REAC, RECY, RELAXC, RELT, RLGAS, RLMIX, ROP, RSTR, RTIM, RTLM, RTLS, RTOL, SCCM, SCCMPRO, SCLM, SCLS, SCOR, SENG, SENT, SFAC, SFLR, SIZE, SOLUTION_TECHNIQUE, SPOS, SSMAXITER, SSTT, STPT, STST, SURF, TAMB, TAU, TEMP, TGIV, TIFP, TIM1, TIM2, TIME, TINL, TJAC, TLIM, TPRO, TRAN, TRES, TRMAXITER, TRST, TSCCM, TSRF, TSTR, TTIM, UFAC, UIGN, USET, USEV (Restart), USEV (XMLI), USRIN, VOL, VPRO, VTIM, WENG, WPRO, XEST, XMLI, XMLS

9.2.2. Plasma Perfectly Stirred Reactor

The following keywords can be used to build an input file for a Plasma PSR Reactor Model:

ABSL, ADD, AEXT, AFRA, AGGA, AGGB, AGGD, AGGE, AGGFD, AGGMN, AINT, AREA, AREAQ, AROP, ASEN, ASTEPS, ATIM, ATLM, ATLS, ATOL, AVALUE, AVAR, BETA, BLKEQ, BOHM, BPWR, BULK, CLSC, CLSM, CNTN, CNTT, COLR, CPROD, DELT, DFAC, DIST, DTIGN, DTMN, DTMX (steady-state), DTSV, EGRR, ELSH, END, ENGE, EPSG, EPSR, EPSS, EPST, EQUI, ETCH, ETMP, FLRT, FPRO, FUEL, GFAC, GMHTC, HTC, HTRN, INLET, IONE, IPSR, IRET, ISTP, KLIM, MAXIT, MAXTIME, MCUT, MMASS, NEWRUN, NJAC, NMOM, NNEG, NOCG, NOFT, NPSR, NSOL, OXID, PNDE, PNDI, PPRO, PRES, PRNT, PROE, PROI, PSURF, PVFE, PVFI, PWRW, QFUN, QLSE, QPRO, QRGEQ, QRSEQ, QXCO (p. 281), QXRA (p. 281), REAC, RECY, RELAXC, RELT, ROP, RSTR, RTIM, RTLM, RTLS, RTOL, SCCM, SCCMPRO, SCLM, SCLS, SCOR, SENG, SENT, SFAC, SFLR, SIZE, SOLUTION_TECHNIQUE, SPOS, SSMAXITER, SSTT, STPT, STST, SURF, TAMB, TAU, TEBND, TEIN, TEMP, TGIV, TIFP, TIM1, TIM2, TIME, TINL, TION, TJAC, TLIM, TPRO, TRAN, TRES, TRMAXITER, TRST, TSCCM, TSRF, TSTR, TTIM, UFAC, UIGN, USET, USEV (Restart), USEV (XMLI), USRIN, VOL, VPRO, VTIM, WENG, WPRO, XEST, XMLI, XMLS, XSDF, XSEK

9.2.3. Partially Stirred Reactor

The following keywords can be used to build an input file for a PaSR Reactor Model:

ADAM, ATOL, BDF, CFL, CHEM, CMIX, CPROD, CURL, DASP, DT, DT0, DTMX (transient), DTSV, END, EQUI, FLRT, IEM, INIT, INLET, KOUT, MAXIT, MAXTIME, MIX, MIXT, NCFIT, NDPR, NEWRUN, NNEG, NOJC, NPAR, NPIN, PDF, PRES, REAC, RLGAS, RLMIX, RELAXC, RSTR, RTOL, SCAT, SIZE, SSMAXITER, TAU, TEMP, TIME, TINL, TRES, TRMAXITER, VOL, VPRO, WELL, XMLI, XMLS

9.3. Flow Reactor Models

9.3.1. Plug Flow Reactor

The following keywords can be used to build an input file for a PFR Reactor Model:

ABFR, ACHG, ADAP, ADD, ADIA, AFLO, AFRA, AINT, AREA, AREAF, AREAQ, AROP, ASEN, ASTEPS, ATLM, ATLS, ATOL, AVALUE, AVAR, BETA, BLKEQ, BULK, CLSC, CLSM, CNTN, CNTX, COLR, CPROD, DIST, DPRO, DTIGN, DX, DXMX, DXSV, EGRR, END, ENRG, EPSG, EPSR, EPSS, EPST, EQUI, ETCH, FLRT, FPRO, FUEL, GFAC, GMHTC, HTC, HTRN, IPSR, KLIM, MCUT, MMASS, MOMEN, NADAP, NEWRUN, NMOM, NNEG, NOCG, NSOL, OXID, PBDEN, PLUG, PNDE, PNDI, PPRO, PRES, PRNT, PROE, PROI, PSV, PTM_SECTION_NUM, PTM_SECTION_SIZEDEP_A0, PTM_SECTION_SIZEDEP_COLEFF, PTM_SECTION_SIZEDEP_DSTAR, PTM_SECTION_SIZEDEP_HAMAKER, PTM_SECTION_SN0, PTM_SECTION_SPACING, PTM_SECTION_TCOND, PTM_SECTIONAL, PVFE, PVFI, QFUN, QLOS, QPRO, QRGEQ, QRSEQ, RCHG, REAC, RLGAS, RLMIX, ROP, RSTR, RTIME, RTLM, RTLS, RTOL, SCCMPRO, SCLM, SCLS, SCOR, SENG, SFAC, SIZE, SSKIP, SSTT, SURF, TAMB, TEMP, TGIV, TIFP, TLIM, TPRO, TRST, TSRF, TSTP, TSTR, UIGN, USET, USEV (Restart), USEV (XMLI), VDOT, VDOTPRO, VEL, VIS, WENG, XEND, XMLI, XMLS, XRES, XSTR

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9.3.2. Plasma Plug Flow Reactor

The following keywords can be used to build an input file for a Plasma PFR Reactor Model:

ACHG, ADAP, ADIA, AFLO, AFRA, AINT, AREA, AREAF, AREAQ, AROP, ASEN, ASTEPS, ATLS, AVALUE, AVAR, BETA, BLKEQ, BOHM, BPWR, BULK, CLSC, CLSM, CNTN, CNTX, COLR, CPROD, DIAM, DIST, DPRO, DTIGN, DX, DXMX, DXSV, EGRR, ELSH, END, ENGE, ENRG, EPSG, EPSR, EPSS, EPST, EQUI, ETCH, ETMP, FLRT, FPRO, FUEL, GFAC, GMHTC, HTC, HTRN, IONE, IPSR, KLIM, MAXIT, MCUT, MMASS, MOMEN, NADAP, NEWRUN, NMOM, NNEG, NOCG, NSOL, OXID, PLUG, PNDE, PNDI, PPRO, PRES, PRNT, PROD, PROE, PROI, PSURF, PSV, PVFE, PVFI, PWRW, QFUN, QLOS, QLSE, QPRO, QRGEQ, QRSEQ, RCHG, REAC, RELAXC, ROP, RSTR, RTIME, RTLS, SCCMPRO, SCLM, SCLS, SCOR, SENG, SENT, SFAC, SIZE, SOLUTION_TECHNIQUE, SSKIP, SURF, TAMB, TEBND, TEMP, TGIV, TIFP, TION, TLIM, TPRO, TRST, TSRF, TSTP, TSTR, UIGN, USET, USEV (Restart), USEV (XMLI), VDOT, VDOTPRO, VELPRO, VIS, WENG, WPRO, XEND, XMLI, XMLS, XRES, XSDF, XSEK, XSTR

9.3.3. Planar Shear Flow

The following keywords can be used to build an input file for a Planar Shear Flow Reactor Model:

ABFR, AFLW, AFRA, ADIA, ATIM, ATLM, ATOL, BETA, BULK, CLSC, CLSM, CNTN, COLR, CPROD, DTMN, DTMX (steady-state), DX, DXMX, DXSV, END, FIXT, GASW, GFAC, GRAV, H0, HITE, HTRN, ICRD, IPSR, IRET, ISTP, KNMN, MAXIT, MAXTIME, MCUT, MIX, MORD, MULT, NEWRUN, NJAC, NMOM, NOCG, NOTP, NPTS, NSOL, PARP, PNDE, PNDI, PRES, PRNT, PROE, PROI, PVFE, PVFI, QLOS, QPRO, REAC, RLGAS, RLMIX, RELAXC, RSTR, RTIM, RTLM, RTOL, SFAC, SIZE, SLIP, SQRX, SSMAXITER, SSRX, STCH, STP0, SURF, SYMT, TDIF, TINF, TINL, TJAC, TPRO, TRMAXITER, TSPL, TSRF, TSTR, TWAB, TWPR, TWRE, TWST, UPROF, USET, USEV, UTRN, VCOR, VEL, VWALL, XEND, XMLI, XMLS, XRST, XTMP

9.3.4. Cylindrical Shear Flow

The following keywords can be used to build an input file for a Cylindrical Shear Flow Reactor Model:

ABFR, ADIA, AFRA, ATIM, ATLM, ATOL, BETA, BULK, CLSC, CLSM, COLR, CNTN, CPROD, DIST, DTMN, DTMX (steady-state), DX, DXMX, DXSV, END, GASW, GFAC, GRAV, H0, HITE, HTRN, ICRD, IPSR, IRET, ISTP, KNMN, MAXIT, MAXTIME, MCUT, MIX, MORD, MULT, NEWRUN, NJAC, NMOM, NOCG, NOTP, NPTS, NSOL, PARP, PNDE, PNDI, PRES, PRNT, PROE, PROI, PVFE, PVFI, QLOS, QPRO, REAC, RLGAS, RLMIX, RELAXC, RSTR, RTIM, RTLM, RTOL, SFAC, SIZE, SLIP, SQRX, SSMAXITER, SSRX, STCH, STP0, SURF, TDIF, TINF, TINL, TJAC, TPRO, TRMAXITER, TSPL, TSRF, TSTR, TWAB, TWPR, TWRE, TWST, UPROF, USET, USEV, UTRN, VCOR, VEL, VWALL, XEND, XMLI, XMLS, XRST, XTMP

9.3.5. Honeycomb Monolith Reactor

The Honeycomb Monolith Reactor Model is a special case of a general plug-flow reactor, where user input parameters describing the honeycomb geometry are used to automatically calculate the available surface area for gas-surface reactions. For details on the calculations performed for the Honeycomb Monolith Reactor Model, see Honeycomb Monolith Reactor Calculations of the Chemkin-Pro Theory Manual.

The following keywords can be used to build an input file for a Honeycomb Monolith Reactor Model:

ACHG, ADAP, ADIA, AEXT, AFLO, AFRA, AINT, AREA, AREAF, AREAQ, AROP, ASEN, ASTEPS, ATLS, ATOL, AVALUE, AVAR, BETA, BLKEQ, BULK, CLSC, CLSM, CNTN, CNTX, COLR, CPROD, DIAM, DIST, DPRO, DTIGN, DX, DXMX, DXSV, EGRR, END, ENRG, EPSG, EPSR, EPSS, EPST, EQUI, ETCH, FLRT, FPRO, FUEL, GFAC, GMHTC, HTC, HTRN, IPSR, KLIM, MAXIT, MCUT, MMASS, MOMEN, NADAP, NMOM, NNEG, NOCG, NSOL, OXID, PLUG, PNDE, PNDI, PPRO, PRES, PRNT, PROE, PROI, PSURF, PSV, PVFE, PVFI, QFUN, QLOS, QPRO,

QRGEQ, QRSEQ, RCHG, REAC, RLGAS, RLMIX, RELAXC, ROP, RSTR, RTIM, RTIME, RTLS, RTOL, SCCMPRO, SCLM, SCLS, SCOR, SENG, SENT, SFAC, SIZE, SOLUTION_TECHNIQUE, SSKIP, SSTT, SURF, TAMB, TEMP, TGIV, TIFP, TLIM, TPRO, TRST, TSRF, TSTP, TSTR, UIGN, USET, USEV (Restart), USEV (XMLI), VDOT, VDOTPRO, VEL, VIS, WENG, XEND, XMLI, XMLS, XRES, XSTR

9.4. Flame Simulators

9.4.1. Premixed Laminar Burner-stabilized Flame Simulator

The following keywords can be used to build an input file for a Premixed Laminar Burner-stabilized Flame Simulator:

AGGA, AGGB, AGGD, AGGE, AGGFD, AGGMN, APRO, ASEN, ATIM, ATOL, BURN, CDIF, CNTN, CPROD, CURV, DFAC, DIST, DTMN, DTMX (steady-state), EMPAR, END, ENRG, EPSS, FLRT, FLTB, FLT_PVSPEC, FLXB, GFAC, GRAD, GRID, HSEN, INTM, IRET, ISTP, JJRG, KOUT, MAXTIME, MIX, MSFX, MULT, NADP, NJAC, NOAGG, NOFT, NOTP (Reactor), NPTS, NSOL, NTOT, PENG, PFLR, PPRO, PRES, PRMN, PRNT, PROD, PSURF, PTM_SECTION_NUM, PTM_SECTION_SIZEDEP_A0, PTM_SECTION_SIZEDEP_COLEFF, PTM_SECTION_SIZEDEP_DSTAR, PTM_SECTION_SIZEDEP_HAMAKER, PTM_SECTION_SN0, PTM_SECTION_SPACING, PTM_SECTION_TCOND, PTM_SECTIONAL, QFUN, RACTV, RADGS, RADPT, REAC, RLGAS, RLMIX, RSTR, RTIM, RTOL, SCLM, SCLS, SENT, SFLR, SFMN, SGMAXIT, SGTOL, SIZE, SOLUTION_TECHNIQUE, SPOS, SSMAXITER, TBND, TDIF, TEMP, TGIV, TIM1, TIM2, TINF, TJAC, TPRO, TPROF, TRAN, TRCE, TRMAXITER, TSTR, TUNBURNT, USE_TPRO_GRID, USET, USEV (Restart), USEV (XMLI), UTRN, VCOR, WDIF, WMIX, XCEN, XEND, XIMN, XMLI, XMLS, XSTR

9.4.2. Flame Speed Simulator

The following keywords can be used to build an input file for a Flame Speed Simulator:

ASEN, ATIM, ATOL, CDIF, CNTN, CPROD, CURV, DFAC, DIST, DTMN, DTMX (steady-state), EMPAR, END, ENRG, EPSS, FLRT, FLTB, FLT_PVSPEC, FLXB, FREE, GFAC, GRAD, GRID, HSEN, INTM, IPSR, IRET, ISTP, JJRG, KOUT, MAXTIME, MIX, MSFX, MULT, NADP, NJAC, NOAGG, NOFT, NOTP (Reactor), NPTS, NSOL, NTOT, PENG, PFLR, PRES, PRMN, PRNT, PROD, PSURF, PTM_SECTION_NUM, PTM_SECTION_SIZEDEP_A0, PTM_SECTION_SIZEDEP_COLEFF, PTM_SECTION_SIZEDEP_DSTAR, PTM_SECTION_SIZEDEP_HAMAKER, PTM_SECTION_SN0, PTM_SECTION_SPACING, PTM_SECTION_TCOND, PTM_SECTIONAL, QFUN, RACTV, RADGS, RADPT, REAC, RLGAS, RLMIX, RSTR, RTIM, RTOL, SCLM, SCLS, SENT, SFLR, SFMN, SGMAXIT, SGTOL, SIZE, SOLUTION_TECHNIQUE, SPOS, SSMAXITER, TDIF, TEMP, TFIX, TIM1, TIM2, TINF, TJAC, TPRO, TPROF, TRAN, TRCE, TRMAXITER, TSTR, TUNBURNT, USET, USE_TPRO_GRID, USEV (Restart), USEV (XMLI), UTRN, VCOR, WDIF, WMIX, XCEN, XEND, XIMN, XMLI, XMLS, XSTR

9.4.3. Opposed-flow Flame Simulator

The following keywords can be used to build an input file for an Opposed-flow Flame Simulator:

AGGA, AGGB, AGGD, AGGE, AGGFD, AGGMN, AINL, ASEN, ATIM, ATOL, AXIS, CDIF, CNTN, CPROD, CURV, DFAC, DIST, DTMN, DTMX (steady-state), EMPAR, END, ENRG, EPSS, FLTB, GFAC, GRAD, GRID, HSEN, INLET, IPSR, IRET, ISTP, JJRG, KOUT, MAXTIME, MIX, MULT, NADP, NDPR, NJAC, NOAGG, NOFT, NOTP (Reactor), NPTS, NSOL, NTOT, PENG, PFLR, PLAN, PLAT, PPRO, PRES, PRNT, PROD, PSURF, PTM_SECTION_NUM, PTM_SECTION_SIZEDEP_A0, PTM_SECTION_SIZEDEP_COLEFF, PTM_SECTION_SIZEDEP_DSTAR, PTM_SECTION_SIZEDEP_HAMAKER, PTM_SECTION_SN0, PTM_SECTION_SPACING, PTM_SECTION_TCOND, PTM_SECTIONAL, QFUN, RACTV, RADGS, RADPT, REAC, RLGAS, RLMIX, RSTR, RTIM, RTOL, SENT, SFLR, SFMN, SGMAXIT, SGTOL, SIZE, SOLUTION_TECHNIQUE, SPOS, SSMAXITER, TDIF, TEMP, TGIV, TIM1, TIM2, TINF, TINL, TJAC, TMAX, TPRO, TRAN, TRMAXITER, TSRF, TSTR, UFAC, UINL, USET, UTRN, WDIF, WMIX, XCEN, XEND, XMLI, XMLS

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9.4.4. Premixed Laminar Burner-stabilized Stagnation Flow Flame Simulator

The following keywords can be used in addition to those listed in Opposed-flow Flame Simulator (p. 119), Opposed-flow Flame Simulator (p. 119), to build an input file for a Premixed Laminar Burner-stabilized Stagnation Flow Flame Simulator:

PTM_SECTION_NUM, PTM_SECTION_SIZEDEP_A0, PTM_SECTION_SIZEDEP_COLEFF, PTM_SECTION_SIZEDEP_DSTAR, PTM_SECTION_SIZEDEP_HAMAKER, PTM_SECTION_SN0, PTM_SECTION_SPACING, PTM_SECTION_TCOND, PTM_SECTIONAL, RLGAS, RLMIX, SCLM, SCLS, STAGNATION_FLAME, TINL

9.4.5. Flame-Extinction Simulator

The following keywords can be used in addition to those listed in Opposed-flow Flame Simulator (p. 119), Opposed-flow Flame Simulator (p. 119), to build an input file for a Flame-Extinction Simulator:

EXTINCTION, EXT_MAXTFRAC, EXT_METHOD, EXT_MINTFLAME, EXT_MINTFRAC, EXT_SAVEINT, EXT_STEPS, EXT_TSTEP, EXT_VFCNTRL, RLGAS, RLMIX, SCLM, SCLS

9.4.6. Diffusion Flamelet Generator

ATOL, ENDTIMEMAX, FLTB, IGRIDMETHOD_n, INLET, MIXFRACBIAS_FUEL, MIXFRACBIAS_OXID, NP_FUEL, NP_OXID, NPTS, NSTEPS_HIGH, NSTEPS_LOW, NTOT, PRES, REAC, RTOL, SSDR, SSDR_MAX, SSDR_MIN, TIME, TINL, TMAX, TPROFILE_n

9.5. CVD Reactors

9.5.1. Stagnation Flow CVD Reactor

The following keywords can be used to build an input file for a Stagnation Flow CVD Reactor Model:

AINL, ASEN, ATIM, ATOL, BULK, CDCT, CHEM, CNDT, CNDX, CNTN, COMP, COND, CPROD, CTOL, CURV, DELT, DFAC, DIST, DT0, DTMN, DTMX (steady-state), EMIS, EMSG, END, ENRG, EPSS, ETCH, FLAM, FLRT, FLUX, FPRO, GDOT, GFAC, GRAD, GRID, HSEN, INIT, INJM, INJS, INJT, INJW, INJX, INLET, INTM, IPSR, IRET, ISTP, JJRG, LINE, LPRT, MAXIT, MAXTIME, MIX, MORD, MULT, NADP, NEWRUN, NJAC, NOCH, NOFT, NONR, NOTP, NPTS, NSOL, NTOT, PRES, PRNT, PROD, PWRC, QDOT, QDTC, RADGS, RDSK, REAC, RELAXC, REOR, RLGAS, RLMIX, RRAD, RSTR, RTIM, RTOL, SCCM, SCCMPRO, SENT, SFAC, SFLR, SIZE, SPOS, SSMAXITER, STAG, STST, SURF, TBND, TDIF, TDSK, TEMP, TGIV, TIM1, TIM2, TIME, TINL, TJAC, TOFF, TPRO, TRAD, TRAN, TRCE, TRMAXITER, TSCCM, TSTR, TWAL, UFAC, UINL, USET, USEV (Restart), USEV (XMLI), VCOR, WMIX, WSRC, XCEN, XEND, XMLI, XMLS, XSRC, XSTR

9.5.2. Rotating Disk CVD Reactor

The following keywords can be used to build an input file for a Rotating Disk CVD Reactor Model:

AINL, ASEN, ATIM, ATOL, BULK, CDCT, CHEM, CNDT, CNDX, CNTN, COMP, COND, CPROD, CTOL, CURV, DELT, DFAC, DIST, DT0, DTMN, DTMX (steady-state), EMIS, EMSG, END, ENRG, EPSS, ETCH, FLAM, FLRT, FLUX, FPRO, GDOT, GFAC, GRAD, GRID, HSEN, INIT, INJM, INJS, INJT, INJW, INJX, INLET, INTM, IPSR, IRET, ISTP, JJRG, LINE, LPRT, MAXIT, MAXTIME, MIX, MORD, MULT, NADP, NEWRUN, NJAC, NOCH, NOFT, NONR, NOTP, NPTS, NSOL, NTOT, OINL, OMEG, PRES, PRNT, PROD, PWRC, QDOT, QDTC, RADGS, RDSK, REAC, RELAXC, REOR, RLGAS, RLMIX, RRAD, RSTR, RTIM, RTOL, SCCM, SCCMPRO, SENT, SFAC, SFLR, SIZE, SPOS, SSMAXITER, STST, SURF, TBND, TDIF, TDSK, TEMP, TGIV, TIM1, TIM2, TIME, TINL, TJAC, TOFF, TPRO, TRAD,

TRAN, TRCE, TRMAXITER, TSCCM, TSTR, TWAL, UFAC, UINL, USET, USEV (Restart), USEV (XMLI), VCOR, WMIX, WSRC, XCEN, XEND, XMLI, XMLS, XSRC, XSTR

9.6. Shock Tube Reactors

9.6.1. Normal Incident Shock

The following keywords can be used to build an input file for a Incident Shock Reactor Model:

ATOL, CNTN, CONC, DELT, DIA, DIST, END, INIT, IPSR, ISHK, ISKB, LGDT, NEWRUN, NSOL, P1A, P2A, RHO1, RHO2, RLGAS, RLMIX, RTOL, SIZE, T1, T2, TIME, TSTR, TSTR, USET, VISC, VSHK, XMLI

9.6.2. Normal Reflected Shock

The following keywords can be used to build an input file for a Reflected Shock Reactor Model:

ATOL, CNTN, CONC, DELT, DIST, END, INIT, IPSR, LGDT, NEWRUN, NSOL, P1A, P2A, P3A, RHO1, RHO2, RHO3, RLGAS, RLMIX, RSHK, RTOL, SIZE, T1, T2, T3, TIME, TSTR, TSTR, USET, VRS, VSHK, XMLI

9.7. Miscellaneous Reactor Models

9.7.1. Gas Mixer

The following keywords can be used to build an input file for a Gas Mixer Reactor Model:

ABSL, ATIM, ATOL, CNTN, CNTT, CPROD, DELT, DFAC, DIST, DTMN, DTMX (steady-state), DTSV, END, ENRG, FLRT, FPRO, GFAC, GMHTC, HTC, HTRN, INLET, IPSR, IRET, ISTP, MAXTIME, MMASS, NEWRUN, NJAC, NNEG, NOFT, NPSR, NSOL, PPRO, PRES, PRNT, QFUN, QLOS, REAC, RELT, RTIM, RTOL, SCCM, SCCMPRO, SCOR, SFAC, SFLR, SIZE, SPOS, SSMAXITER, STPT, STST, TAMB, TEMP, TGIV, TIM1, TIM2, TIME, TINL, TJAC, TPRO, TRAN, TRMAXITER, TSCCM, TSTR, TTIM, UFAC, USET, USEV, USRIN, VOL, VPRO, VTIM, WENG, XMLI, XMLS

9.7.2. Equilibrium

The following keywords can be used to build an input file for a Equilibrium Reactor Model:

CJ, CONX, CPROD, DIST, END, ENGY, ENTH, ENTR, FAZE, FREE, FROZ, IPSR, NEWRUN, NSOL, PEST, PH, PRES, PS, PV, REAC, RLGAS, RLMIX, SIZE, TEMP, TEST, TP, TS, TSTR, TV, USET, VH, VOL, VS, VU, XMLI

9.7.3. Mechanism Analyzer

The following keywords can be used to build an input file for a Mechanism Analyzer:

ALL, CARR, DIST, END, GEN, GRXN, GTHB, IPSR, LSCL, MAJ, NEWRUN, NONE, NSOL, PFAL, PHIA, PLOA, PNUM, PRES, SCOV, SIZE, SRXN, STCK, TBTH, TBTH, TDEL, TFAL, THIG, THRM, TLOW, TRAN, TSTR, TSUM, USET, XBTH, XMLI

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Chapter 10: Alphabetical Listing of Project Input Keywords

In this chapter we provide detailed information about the meaning and usage of each keyword entry that may be included as part of a Reactor Model input file. Reference Guide to Project Input Keywords (p. 115) provides a cross-referenced listing that shows which keywords are available for each Reactor Model, while CHEMKIN Project Input: Keyword Syntax and Rules (p. 113) provides general keyword syntax and rules. The following categorized lists of auxiliary keywords are provided:

- Table 3.4: Alphabetical Listing of REACTIONS-line Options for Gas-phase Kinetics Data (p. 39)
- Table 3.7: Alphabetical Listing of Gas-phase Reaction Auxiliary Keywords (p. 43)
- Table 4.3: Alphabetical Listing of REACTIONS-line Options for Surface Reaction Data (p. 66)
- Table 4.6: Alphabetical Listing of Surface Reaction Auxiliary Keywords (p. 72)

The alphabetical listing of keywords is distributed over the following sections:

10.1. Alphabetical Listing of Keywords [A-E]

Table 10.1: Alphabetical Listing of Keywords [A-E]

Keyword	Definition			
ABFR Solver	This keyword serves as a switch to turn on an empirical active surface area factor when surface reaction rates on the particle surface are calculated. The concept is that not all surface area (or sites) on the particle surface is active. The active surface area during the particle formation phase is found to be a function of total particle mass and gas temperature. The form and the model parameters of this empirical formulation are obtained by fitting predictions to measured data from premixed flames. By default this factor is turned off.			
	Parameters	Optional/Reqd.	Units	Examples
	--	--	--	ABFR
	Keyword Usage	Optional keyword. By default this factor is turned off.		
	Reactor Models	• Cylindrical Shear Flow Reactor • Planar Shear Flow Reactor • Perfectly-stirred Reactor (PSR) • Plug-flow Reactor (PFR)		

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Keyword	Definition			
ABSLSolver	This keyword is used to override the default value for the absolute perturbation in the solution variable used in the determination of the numerically derived Jacobian.			
	Parameters	Optional/Reqd.	Units	Examples
	Absolute perturbation	Required	--	ABSL **1.E-15**
	Keyword Usage	Optional keyword. By default, if the ATOL keyword is given, then the absolute perpetuation is set equal to the ATOL value. ATOL is not specified, then the absolute perturbation is set equal to the square root of the unit round-off error of the machine.		
	Reactor Models	• Closed Plasma Reactor • Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Plasma PSR		
ACHG Solver	Maximum absolute change in the surface site fractions (over one time step) for which the preliminary, fictitious transient equations can be considered to have converged to steady state. The convergence test is made against the sum of the ACHG value plus the product of RCHG multiplied by the old site-fraction value. Therefore, if ACHG is set to zero (by default) then only RCHG is used to control the convergence criteria.			
	Parameters	Optional/Reqd.	Units	Examples
	Absolute relative change	Required	--	ACHG **1.0E-7**
	Keyword Usage	Optional keyword. By default, only RCHG is used to determine convergence.		
	Reactor Models	• Honeycomb Reactor • Plasma Plug Flow Reactor • Plug Flow Reactor		
ADAM Solver	Flag indicating the implicit Adams method of the DVODE solver is used to integrate the equations.			
	Keyword Usage	Optional keyword. By default, the DASPK solver will be used.		
	Reactor Models	• Closed Partially Stirred Reactor (PaSR) • Partially Stirred Reactor (PaSR)		
ADAP Solver	Flag indicating the saving of additional adaptive points for improved resolution of the solution data (e.g., for post-processing and plotting) for transient simulations. ADAP is the default. ADAP inserts extra solution points when your solution is changing rapidly (e.g., a steep transient or engine ignition occurs).			

Keyword	Definition			
	How and when the points are inserted is controlled by the AVALUE, AVAR and ASTEPS keywords. The companion keyword, NADAP, can be used to turn off adaptive time-stepping during continuations, if desired.			
	Keyword Usage	Optional keyword. ADAP is the default.		
	Reactor Models	• Closed Plasma Reactor • Closed Homogeneous Reactor • Honeycomb Reactor • IC HCCI Engine Model • Multi-Zone HCCI Engine Simulator • Plasma Plug Flow Reactor • Plug Flow Reactor • SI Engine Zonal Simulator		
ADD Reactor or Inlet Property	Mole fractions of species that should be added to the inlet or initial composition but excluded from the equivalence-ratio calculation. This keyword is only valid when the equivalence-ratio option is used to specify the inlet or initial composition. These species do not enter into the equivalence ratio computations. One species is entered per line.			
	Parameters	Optional/Reqd.	Units	Examples
	Inlet stream name	**Optional (PSRs only)** If there is no stream name than the product species applies to the default or all defined streams.	--	ADD **mixture1** AR 0.2
	Species name	Required	--	ADD **AR** 0.2
	Additive fractions	Required	mole fractions	ADD AR **0.2**
	Keyword Usage	Optional keyword. By default, ADD is not used. But either REAC or EQUI / FUEL / OXID / CPROD is required for each inlet stream or to define initial conditions for a closed system.		

Keyword	Definition			
	Reactor Models	• Closed Homogeneous Batch Reactor • IC HCCI Engine • Plasma PSR • Plug Flow Reactor • SI Engine Zonal Simulator		
	Notes	• The ADD keywords must be changed as a set, not individually for a restart run. • The ADD keywords must be changed as a set, not individually for a continuation run.		
ADIA Reactor Property	Turns on the adiabatic wall condition for plug-flow or for planar, symmetric, shear-flow models. For planar, non-symmetric shear flow, an adiabatic wall is the default, but for symmetric (planar or cylindrical) shear-flow cases, the ADIA keyword is required for the adiabatic condition.			
	Keyword Usage	Optional keyword. By default, the specified (temperature) condition is used for shear-layer flow. The default behavior for plug-flow depends on the problem type; if the energy equation is being solved, the default is for adiabatic conditions.		
	Reactor Models	• Cylindrical Shear Flow Reactor • Honeycomb Reactor • Planar Shear Flow Reactor • Plasma Plug Flow Reactor • Plug Flow Reactor		
AEXT Reactor Property Profiles	External surface area (for 0-D Homogeneous systems) or surface area per unit length (for Plug Flow Models) used to control heat transfer to the external environment. AEXT is usually used to specify area profiles as a function of time (0-D Homogeneous systems) or distance (Plug Flow Models). However, if the AEXT value is only provided at a single point, then the surface area is assumed to be constant as a function of time (for transient 0-D Homogeneous systems) or distance (for Plug Flow Models). See also AREAQ.			
	Parameters	Optional/Reqd.	Units	Examples
	Time or Distance, depending on Reactor Model	Required	sec or cm	AEXT **0.0** 1.0
	External surface area or surface area per unit length,	Required	cm^2 or cm	AEXT 0.0 **1.0**

Keyword	Definition			
	depending on Reactor Model			
	Keyword Usage	Optional keyword. If not specified, the external area is assumed equal to the internal surface area (see AINT or AREA).		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Honeycomb Reactor • IC HCCI Engine • Perfectly Stirred Reactor (PSR) • Plasma PSR • SI Engine Zonal Simulator		
AFLO Reactor Property Profiles	Cross-sectional area profile as a function of distance. If only a single AFLO entry is provided, the cross-sectional area is assumed to be a constant at that specified value. See also AREAF and DIAM.			
	Parameters	Optional/Reqd.	Units	Examples
	Distance from inlet	Required	cm	AFLO **0.0** 1.0
	Cross-sectional area	Required	cm^2	AFLO 0.0 **1.0**
	Keyword Usage	Optional keyword. If none of DIAM, AFLO, or AREAF keywords are included, then an attempt will be made to use the GEOM user subroutine to determine the flow area.		
	Reactor Models	• Honeycomb Reactor • Plasma Plug Flow Reactor • Plug Flow Reactor		
AFLW Reactor Property	Fraction of the total lower wall surface area that corresponds to a surface material. For example, "AFLW WAFER 0.001" indicates that the material "WAFER" makes up 0.1% of the lower wall surface area. The material name must correspond to a material name declared in the *Surface Kinetics* input file or an error will occur.			
	Parameters	Optional/Reqd.	Units	Examples
	Surface material name	Required	--	AFLW **WAFER** 0.001
	Fraction of total surface area	Required	--	AFLW WAFER **0.001**
	Keyword Usage	Optional keyword. By default, 1.0 is used for all materials in all PSRs.		
	Reactor Models	• Non-symmetric Planar Shear Flow Reactor		

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<table>
<tr><th>Keyword</th><th>Definition</th></tr>
<tr><td>AFRA

Reactor Property</td><td>Fraction of the total surface area that corresponds to a surface material (see the multiple surface material capability under Surface Kinetics). For example, “AFRA WAFER 0.001” indicates that the material “WAFER” makes up 0.1% of the total reactor surface area. The material name must correspond to a material name declared in the Surface Kinetics input file or an error will occur.
<table>
<tr><th>Parameters</th><th>Optional/Reqd.</th><th>Units</th><th>Examples</th></tr>
<tr><td>Surface material name</td><td>Optional</td><td>--</td><td>AFRA WAFER 0.001</td></tr>
<tr><td>Fraction of total surface area</td><td>Required</td><td>--</td><td>AFRA WAFER 0.001</td></tr>
<tr><td>Reactor number (PSR clusters only)</td><td>Optional

If no number is given, the keyword is assumed to apply to all reactors in a cluster.</td><td>--</td><td>AFRA WAFER 0.001 2</td></tr>
<tr><td>Keyword Usage</td><td colspan="3">Optional keyword. By default, 1.0 is used for all materials in all PSRs.</td></tr>
<tr><td>Reactor Models</td><td colspan="3">• Closed Homogeneous Batch Reactor
• Closed Plasma Reactor
• Cylindrical Shear Flow Reactor
• Honeycomb Reactor
• Perfectly Stirred Reactor (PSR)
• Planar Shear Flow Reactor
• Plasma Plug Flow Reactor
• Plasma PSR
• Plug Flow Reactor</td></tr>
</table></td></tr>
<tr><td>AGGA

Reactor Property</td><td>The pre-exponential factor of the Arrhenius-like expression for characteristic fusion time.
<table>
<tr><th>Parameters</th><th>Optional/Reqd.</th><th>Units</th><th>Examples</th></tr>
<tr><td>Material name</td><td>Required</td><td>--</td><td>AGGA SOOT 1.0E10</td></tr>
</table></td></tr>
</table>

Keyword	Definition			
	Pre-exponential factor	Required	sec	AGGA **C(B) 1.0E7**
	Keyword Usage	Optional keyword. By default, the pre-exponential factor is 1.0E-30.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Diffusion or Premixed Opposed-flow Flame • IC HCCI Engine • Multi-Zone HCCI Engine Simulator • Perfectly Stirred Reactor (PSR) • Plasma PSR • Premixed Laminar Burner-stabilized Flame • SI Engine Zonal Simulator		
AG-GB Reactor Property	The temperature exponent of the Arrhenius-like expression for characteristic fusion time.			
	Parameters	Optional/Reqd.	Units	Examples
	Material name	Optional	--	AGGB SOOT 1.0
	Temperature exponent	Required		AGGB **C(B) 0.5**
	Keyword Usage	Optional keyword. By default, the temperature exponent is 0.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Diffusion or Premixed Opposed-flow Flame • IC HCCI Engine • Multi-Zone HCCI Engine Simulator • Perfectly Stirred Reactor (PSR) • Plasma PSR • Premixed Laminar Burner-stabilized Flame • SI Engine Zonal Simulator		
AG-GD	The exponent of the primary particle diameter in the Arrhenius-like expression for characteristic fusion time.			

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Keyword	Definition			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	Primary particle name	Optional	--	AGGD C(B) 1.0
	Keyword Usage	Optional keyword. By default, the primary particle diameter is 1.0.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Diffusion or Premixed Opposed-flow Flame • IC HCCI Engine • Multi-Zone HCCI Engine Simulator • Perfectly Stirred Reactor (PSR) • Plasma PSR • Premixed Laminar Burner-stabilized Flame • SI Engine Zonal Simulator		
AGGE Reactor Property	The activation temperature of the Arrhenius-like expression for characteristic fusion time.			
	Parameters	Optional/Reqd.	Units	Examples
	Material name	Required	--	AGGE **SOOT** 0.0
	Activation temperature	Required	K	AGGE C(B) **800**
	Keyword Usage	Optional keyword. By default, the activation temperature is 0.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Diffusion or Premixed Opposed-flow Flame • IC HCCI Engine • Multi-Zone HCCI Engine Simulator • Perfectly Stirred Reactor (PSR) • Plasma PSR • Premixed Laminar Burner-stabilized Flame • SI Engine Zonal Simulator		
AGGFD	The fractal dimension of the aggregate.			

Keyword	Definition			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	Material name	Required	--	AGGFD **SOOT 1.0E3.0**
	Fractal dimension	Required	--	AGGFD **C(B) 1.8**
	Keyword Usage	Optional keyword. By default, the fractal dimension is 3.0.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Diffusion or Premixed Opposed-flow Flame • IC HCCI Engine • Multi-Zone HCCI Engine Simulator • Perfectly Stirred Reactor (PSR) • Plasma PSR • Premixed Laminar Burner-stabilized Flame • SI Engine Zonal Simulator		
AGGMN Reactor Property	The threshold value to include the sintering effect in particle aggregation. For the Moments Method, this indicates the ratio of the collision to the fusion time scale, whereas for the Sectional Method, this indicates the minimum value of the characteristic fusion time.			
	Parameters	Optional/Reqd.	Units	Examples
	Material name	Required	--	AGGMN **SOOT** 1.0E10
	Threshold	Required	-- (Moments)sec (Sectional)	AGGMN SOOT **1.0E-4**
	Keyword Usage	Optional keyword. By default, the threshold is 1.0E-3 for the Moments Method and 1.0E-06 for the Sectional Method.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Diffusion or Premixed Opposed-flow Flame • IC HCCI Engine • Multi-Zone HCCI Engine Simulator • Perfectly Stirred Reactor (PSR) • Plasma PSR • Premixed Laminar Burner-stabilized Flame		

Keyword	Definition			
		• SI Engine Zonal Simulator		
AINL Inlet Property	The radial velocity spreading rate. At the inlet $x = L$, $v/r =$ AINL.			
	Parameters	Optional/Reqd.	Units	Examples
	Radial velocity divided by radius	Required	1/sec	AINL **2.3**
	Keyword Usage	Optional keyword. By default, the radial velocity spreading rate is 0.0.		
	Reactor Models	• Diffusion or Premixed Opposed-flow Flame • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
	Notes	• Supersedes previous **AFUE** and **AOXI** keywords.		
AINT Reactor Property Profiles	Internal surface area (for 0-D Homogeneous systems) or surface area per unit length (for Plug Flow models) that is considered active for surface chemistry. AINT is usually used to specify area profiles as a function of time (0-D Homogeneous systems) or distance (Plug Flow models). However, if the AINT value is only provided at a single point, then the surface area is assumed to be constant as a function of time (for transient 0-D Homogeneous systems) or distance (for Plug Flow models). See also AREA.			
	Parameters	Optional/Reqd.	Units	Examples
	Time or distance, depending on Reactor Model	Required	sec or cm	AINT **0.0** 1.0
	Internal surface area or area per unit length, depending on Reactor Model	Required	cm2 or cm	AINT 0.0 **1.0**
	Keyword Usage	Optional keyword. If not specified, the internal surface area is determined based on the hydraulic diameter for a plug-flow, as specified through AFLO, AREAF, or DIAM keywords. For 0-D Homogenous systems, a value of 0.0 is assumed by default.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Honeycomb Reactor • Perfectly Stirred Reactor (PSR) • Plasma PSR • Plasma Plug Flow Reactor		

<table>
<tr><th>Keyword</th><th colspan="4">Definition</th></tr>
<tr><td></td><td></td><td colspan="3">• Plug Flow Reactor</td></tr>
<tr><td rowspan="3">ALL

Output</td><td colspan="4">Turns default output on for all of Surftherm's tables.</td></tr>
<tr><td>Keyword Usage</td><td colspan="3">Optional keyword. By default, the all output will be printed. See also NONE.</td></tr>
<tr><td>Reactor Models</td><td colspan="3">• Mechanism Analyzer</td></tr>
<tr><td rowspan="7">APRO

Reactor Property Profiles</td><td colspan="4">Use of the APRO keyword(s) allow the user to specify a piece-wise linear profile as a function of distance for the stream-tube area. The stream-tube area is given relative to the burner area and is therefore dimensionless. Each input provides a pair and the x coordinates must be in ascending order. For example, APRO 0.1 1.2 assigns a relative area of 1.2 at a position 0.1 cm from the burner surface.</td></tr>
<tr><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td>x-coordinates</td><td>Required</td><td>cm</td><td>APRO 0.1 1.2</td></tr>
<tr><td>Relative area</td><td>Required</td><td>dimensionless</td><td>APRO 0.1 1.2</td></tr>
<tr><td>Keyword Usage</td><td colspan="3">Optional keyword. By default, the area ratio is constant at 1.0.</td></tr>
<tr><td>Reactor Models</td><td colspan="3">• Premixed Laminar Burner-stabilized Flame</td></tr>
<tr><td>Notes</td><td colspan="3">• This keyword can be changed for a restart run.</td></tr>
<tr><td rowspan="5">AREA

Reactor Property</td><td colspan="4">The total internal surface area (for 0-D homogeneous reactors) or surface area per unit length (for plug-flow) in the reactor. The internal surface area represents the area available for surface chemistry. See also AINT.</td></tr>
<tr><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td>Total surface area or surface area per unit length, depending on Reactor Model</td><td>Required</td><td>cm^2
or cm</td><td>AREA 200</td></tr>
<tr><td>Reactor number (PSR clusters only)</td><td>Optional

If no number is given, the keyword is assumed to apply to all reactors in a cluster.</td><td>--</td><td>AREA 200 1</td></tr>
<tr><td>Keyword Usage</td><td colspan="3">Optional keyword. By default, the total surface area is set to 0.0 for 0-D homogeneous reactor models and is</td></tr>
</table>

<table>
<tr><th>Keyword</th><th colspan="4">Definition</th></tr>
<tr><td></td><td></td><td colspan="3">determined based on the hydraulic diameter (set using DIAM, AREAF, AFLO) for plug-flow.</td></tr>
<tr><td></td><td>Reactor Models</td><td colspan="3">• Closed Homogeneous Batch Reactor
• Closed Plasma Reactor
• Honeycomb Reactor
• Perfectly Stirred Reactor (PSR)
• Plasma PSR
• Plasma Plug Flow Reactor
• Plug Flow Reactor</td></tr>
<tr><td>AREAF

Reactor Property</td><td colspan="4">The total cross-sectional flow area. See also AFLO.</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td></td><td>Cross-sectional flow area</td><td>Required</td><td>cm^2</td><td>AREAF 200</td></tr>
<tr><td></td><td>Keyword Usage</td><td colspan="3">Optional keyword. Either DIAM or AREAF must be set, unless the user has implemented the GEOM user subroutine.</td></tr>
<tr><td></td><td>Reactor Models</td><td colspan="3">• Honeycomb Reactor
• Plasma Plug Flow Reactor
• Plug Flow Reactor</td></tr>
<tr><td>AREAQ

Reactor Property</td><td colspan="4">The total external surface area (for 0-D homogeneous reactors) or surface area per unit length (for plug-flow) in the reactor. The external surface area represents the area available for heat transfer to the external environment. See also AEXT.</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td></td><td>Total surface area or surface area per unit length, depending or Reactor Model</td><td>Required</td><td>cm^2
or cm</td><td>AREAQ 200</td></tr>
<tr><td></td><td>Reactor number (PSR clusters only)</td><td>Optional

If no number is given, the keyword is assumed to apply to all</td><td>--</td><td>AREAQ 200 1</td></tr>
</table>

Keyword	Definition			
		reactors in a cluster.		
	Keyword Usage	Optional keyword. By default, the total external surface are is set equal to the internal surface area (AREA, AINT), unless AREAQ or AEXT are included.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Honeycomb Reactor • Perfectly Stirred Reactor (PSR) • Plasma PSR • Plasma Plug Flow Reactor • Plug Flow Reactor		
AROP Output	Determine the rate-of-production coefficients for all species and print results to the diagnostic output file of the reactor simulation.			
	Keyword Usage	Optional keyword. By default, no rate-of-production values are printed.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Honeycomb Reactor • IC HCCI Engine • Perfectly Stirred Reactor (PSR) • Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor • SI Engine Zonal Simulator		
	Notes	• This keyword can be added but not removed from a continuation run.		
ASEN Output	Calculate the first-order, A-factor sensitivity coefficients (i.e., with respect to the gas-phase and surface chemistry rate constants) for species fractions and for other dependent variables in the system. Sensitivity results will be included in the XML Solution File. For 0-D and Plug Flow systems, sensitivity results will also be printed to the diagnostic output file.			
	Parameters	Optional/Reqd.	Units	Examples

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Keyword	Definition			
	String indicating for which variables sensitivity coefficients will be saved or printed. The string is a space-delimited list containing species names and any one of the following: ALL, AVEL, RVEL, CVEL, FLRT, or TEMP (see Notes)	Optional If no string is given, then ALL is assumed.	--	ASEN **H2O** ASEN **TEMP**
	Keyword Usage	Optional keyword. By default, no sensitivity coefficients are computed or printed. See also SENG.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Diffusion or Premixed Opposed-flow Flame • Honeycomb Reactor • IC HCCI Engine • Perfectly Stirred Reactor (PSR) • Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor • SI Engine Zonal Simulator • Stagnation Flow CVD Reactor		
	Notes	• This keyword can be added but not removed from a continuation run. • See also EPSS, EPSG, EPST, SENG, and HSEN for other sensitivity options The optional parameter strings are defined as follows: • ALL: all species and all other dependent variables in the solution		

<table>
<tr><th>Keyword</th><th colspan="4">Definition</th></tr>
<tr><td></td><td></td><td colspan="3">• AVEL: axial velocity (Plug Flow, Diffusion or Premixed Opposed-flow Flames, Rotating Disk, and Stagnation Flow CVD Reactors only)
• CVEL: circumferential velocity (Rotating Disk and Stagnation Flow CVD Reactors only)
• RVEL: radial velocity (Diffusion or Premixed Opposed-flow Flames, Rotating Disk, and Stagnation Flow CVD Reactors only)
• FLRT: mass flow rate (Premixed Laminar Flame-speed Calculation only)
• TEMP: gas temperature</td></tr>
<tr><td>ASTEPS

Output</td><td colspan="4">Uses the integrator steps to adaptively insert extra solution data points in addition to those specified by the DTSV option whenever the solver takes the number of integration steps specified by this option. The default is 20, the value used if no argument is provided. The purpose of the ASTEPS keyword is to ensure that during a transient solution, sufficient solution data points are available around the time of a fast transient, for example a rapidly increasing temperature, so that an accurate analysis of the problem is possible (to allow a good plotting resolution).</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td></td><td>Integration steps</td><td>Option-al.</td><td>--</td><td>ASTEPS 20</td></tr>
<tr><td></td><td>Keyword Usage</td><td colspan="3">Optional keyword. By default ASTEPS is set to 20.</td></tr>
<tr><td></td><td>Reactor Models</td><td colspan="3">• Closed Homogeneous Reactor
• Closed Plasma Reactor
• Honeycomb Reactor
• IC HCCI Engine
• Multi-Zone HCCI Engine Simulator
• Perfectly Stirred Reactor (PSR)
• Plasma Plug Flow Reactor
• Plasma PSR
• Plug Flow Reactor
• SI Engine Zonal Simulator</td></tr>
<tr><td></td><td>Notes</td><td colspan="3">• For further details, see the description of DTSV.</td></tr>
</table>

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<table>
<tr><th>Keyword</th><th>Definition</th></tr>
<tr><td>AS-WH

Reactor Property</td><td>Crank angle at which the simulation switches from fixed-temperature condition to using energy equation with Woschni correlation as the heat transfer model. By default the energy equation is used starting at zero crank angle.
<table>
<tr><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td>Crank angle in degrees.</td><td>Required</td><td>degree</td><td>ASWH 5.0</td></tr>
<tr><td>Keyword Usage</td><td colspan="3">Optional keyword.</td></tr>
<tr><td>Reactor Models</td><td colspan="3">• Multi-Zone HCCI Engine Simulator
• SI Engine Zonal Simulator</td></tr>
</table></td></tr>
<tr><td>ATIM

Solver</td><td>Absolute tolerance for convergence of Newton iteration as it is used in the pseudo time stepping procedure for steady-state problems employing the Twopnt solver. Since we are not seeking accuracy in a transient solution, this convergence criteria typically does not need to be as stringent as for the Newton iteration on the actual steady-state solution.
<table>
<tr><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td>Absolute tolerance</td><td>Required</td><td>--</td><td>ATIM 1.E-6</td></tr>
<tr><td>Keyword Usage</td><td colspan="3">Optional keyword. By default, the absolute tolerance is 1.E-9. See also RTIM.</td></tr>
<tr><td>Reactor Models</td><td colspan="3">• Closed Plasma Reactor
• Cylindrical Shear Flow Reactor
• Diffusion or Premixed Opposed-flow Flame
• Honeycomb Reactor
• Non-reactive Gas Mixer
• Perfectly Stirred Reactor (PSR)
• Planar Shear Flow Reactor
• Plasma PSR
• Premixed Laminar Burner-stabilized Flame
• Premixed Laminar Flame-speed Calculation
• Rotating Disk CVD Reactor
• Stagnation Flow CVD Reactor</td></tr>
<tr><td>Notes</td><td colspan="3">• For a precise definition, see the description of ATOL.</td></tr>
</table></td></tr>
<tr><td>ATLM

Solver</td><td>ATOL is used for all variables.
<table>
<tr><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td>Tolerance</td><td>Required</td><td>--</td><td>ATLM 1.0E-6</td></tr>
</table></td></tr>
</table>

Keyword	Definition			
	Keyword Usage	ATOL.		
	Reactor Models	• Closed Plasma Reactor • Cylindrical Shear Flow Reactor • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma PSR		
ATLS Solver	Absolute tolerance used by the transient DASPK solver, as an indicator of the accuracy desired in the solution for the sensitivity coefficients only. Generally, the sensitivity coefficients need not be solved to a great degree of accuracy, so these tolerances could be lower than the tolerances placed on the physical variables.			
	Parameters	Optional/Reqd.	Units	Examples
	Absolute tolerance	Required	--	ATLS **1.E-3**
	Keyword Usage	Optional keyword. By default, the absolute tolerance is 1.E-5.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Honeycomb Reactor • IC HCCI Engine • Perfectly Stirred Reactor (PSR) • Plasma PSR • Plasma Plug Flow Reactor • Plug Flow Reactor • SI Engine Zonal Simulator		
ATOL Solver	Absolute tolerance used by the solvers as an indicator of the accuracy desired in the physical solution. Typically ATOL should be less than the smallest meaningful value of a species mass fraction.			
	Parameters	Optional/Reqd.	Units	Examples
	Absolute tolerance	Required	--	ATOL **1.E-9**
	Keyword Usage	Optional keyword. The default values are: CVD, Partially Stirred Reactor (PaSR), Plug Flow Reactor, Shear Flow Reactor: 1.E-8 Open 0-D Reactors run in steady-state mode, Opposed-flow Flame, Premixed Laminar		

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Keyword	Definition	
		Burner-stabilized Flame, Premixed Laminar Flame-speed Calculation: 1.E-9 Normal Incident Shock, Normal Reflected Shock: 1.E-10 Closed 0-D Reactors and Open 0-D Reactors run in transient mode: 1.E-20 See also RTOL.
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Partially Stirred Reactor (PaSR) • Closed Plasma Reactor • Cylindrical Shear Flow Reactor • Diffusion or Premixed Opposed-flow Flame • Honeycomb Reactor • IC HCCI Engine • Non-reactive Gas Mixer • Normal Incident Shock • Normal Reflected Shock • Opposed-flow Flame • Partially Stirred Reactor (PaSR) • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma PSR • Plug Flow Reactor • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor • SI Engine Zonal Simulator • Stagnation Flow CVD Reactor
AVALUE Output	Uses the integrator steps to adaptively insert extra solution data points in addition to those specified by the DTSV option whenever the variable specified by the AVAR keyword moves by ±*x* since the last time an extra data point was generated.	

<table>
<tr><th>Keyword</th><th>Definition</th></tr>
<tr><td></td><td>You must specify a value for AVALUE; there is no default and you must also specify the AVAR keyword. The purpose of the AVALUE keyword is to ensure that during a transient solution, sufficient solution data points are available around the time of a fast transient, for example a rapidly increasing temperature, so that an accurate analysis of the problem is possible (to allow plotting a resolution).
<table>
<tr><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td>Integration steps</td><td>Required</td><td>--</td><td>AVALUE 10</td></tr>
<tr><td>Keyword Usage</td><td colspan="3">Optional keyword. AVAR is required.</td></tr>
<tr><td>Reactor Models</td><td colspan="3">• Closed Plasma Reactor
• Closed Homogeneous Reactor
• Honeycomb Reactor
• IC HCCI Engine Model
• Multi-Zone HCCI Engine Simulator
• Perfectly Stirred Reactor (PSR)
• Plasma Plug Flow Reactor
• Plasma PSR
• Plug Flow Reactor
• SI Engine Zonal Simulator</td></tr>
<tr><td>Notes</td><td colspan="3">• See also ASTEPS and AVAR is required when AVALUE is used.</td></tr>
</table></td></tr>
<tr><td>AV-
AR

Output</td><td>Determines which variable is used for the AVALUE keyword. Parameter <string> should be “temperature” or the name of a particular species to serve as the time-stepping monitor species.There is no default species value. AVAR is required when the AVALUE keyword is used.
<table>
<tr><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td>String</td><td>Required</td><td>--</td><td>AVALUE temperature

AVALUE CH4</td></tr>
<tr><td>Keyword Usage</td><td colspan="3">Optional keyword.</td></tr>
<tr><td>Reactor Models</td><td colspan="3">• Closed Plasma Reactor
• Closed Homogeneous Reactor
• Honeycomb Reactor
• IC HCCI Engine Model
• Multi-Zone HCCI Engine Simulator</td></tr>
</table></td></tr>
</table>

Keyword	Definition			
		• Perfectly Stirred Reactor (PSR) • Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor • SI Engine Zonal Simulator		
AX-IS Reactor Property	Use a radial, axisymmetric coordinate system.			
	Keyword Usage	Optional keyword. By default, the coordinate system is radially axisymmetric.		
	Reactor Models	• Diffusion or Premixed Opposed-flow Flame		
BDF Solver	Flag indicating the backward differentiation formulas of the DVODE solver is used to integrate the equations.			
	Keyword Usage	Optional keyword. By default, the DASPK solver will be used.		
	Reactor Models	• Closed Partially Stirred Reactor (PaSR) • Partially Stirred Reactor (PaSR)		
BDUR Solver	Specifies the value of the "duration of combustion," Dq_c, in the Wiebe function. Dq_c must be greater than 0.			
	Parameters	Optional/Reqd.	Units	Examples
	Duration of combustion in number of crank angles	Required	degree	BDUR 45.6
	Keyword Usage	Optional keyword.		
	Reactor Models	• SI Engine Zonal Simulator		
BEFF Solver	Specifies the mass fraction of the fresh fuel-air charge being consumed by the premixed flame, i.e., the combustion efficiency. The combustion efficiency must be > 0.0 and $\leq$ 1.0 and is set to 1.0 (complete combustion) by default.			
	Parameters	Optional/Reqd.	Units	Examples
	Combustion efficiency	Optional	--	BEFF 0.85
	Keyword Usage	Optional keyword.		
	Reactor Models	• SI Engine Zonal Simulator		
BETA Reactor Property	This is a combined correction factor to the coalescent collision between particles. The van der Waals forces can enhance the collision frequency while non-coalescent collision can reduce the frequency. The default value is 1.0, i.e., van der Waals effect is off and collisions are 100% coalescent.			

Keyword	Definition			
	Parameters	Optional/Reqd.	Units	Examples
	Material name	Required	--	BETA **C(B)** 0.9
	Enhance factor	Required	--	BETA C(B) **0.9**
	Keyword Usage	Optional keyword.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Cylindrical Shear Flow Reactor • Honeycomb Monolith Reactor • IC HCCI Engine • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma PSR • Plasma Plug Flow Reactor • Plug Flow Reactor • SI Engine Zonal Simulator		
BINI Solver	Specifies the value of the "duration of combustion," q_c, in the Wiebe function.			
	Parameters	Optional/Reqd.	Units	Examples
	Start of combustion crank angle	Required	degree	BINI -15.3
	Keyword Usage	Optional keyword.		
	Reactor Models	• SI Engine Zonal Simulator		
BLKEQ Reactor Property	Toggle to turn on or off solution of bulk activities for bulk species.			
	Parameters	Optional/Reqd.	Units	Examples
	String "on" or "off" to turn on or off solution of the bulk-species equations	Required	--	BLKEQ **ON** BLKEQ **OFF**
	Keyword Usage	Optional keyword. By default, bulk-activity equations are solved when there is more than one bulk species in one or more bulk phases on a material. Otherwise the bulk activities are presumed constant at their initial value.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor		

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<table>
<tr><th>Keyword</th><th>Definition</th></tr>
<tr><td></td><td></td><td>• Honeycomb Reactor
• Perfectly Stirred Reactor (PSR)
• Plasma Plug Flow Reactor
• Plasma PSR
• Plug Flow Reactor</td></tr>
<tr><td>BLTK

Reactor Property</td><td colspan="3">Specifies a boundary-layer thickness. When BLTK is declared, a parabolic velocity profile is specified with a zero velocity at each wall increasing to the velocity specified by VEL at a distance of BLTK from the wall. A flat (constant) velocity profile is used for distances greater than BLTK from the wall. In addition, if the initial gas temperature differs from the initial surface temperature the application linearly interpolates the gas-phase temperature profile between the wall temperature and the bulk gas temperature over the distance BLTK.</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td></td><td>Boundary-layer thickness</td><td>Required</td><td>cm</td><td>BLTK 0.05</td></tr>
<tr><td></td><td>Keyword Usage</td><td colspan="2">Optional keyword. By default, the boundary-layer thickness is set to 0 and a full parabolic velocity is assumed.</td></tr>
<tr><td></td><td>Reactor Models</td><td colspan="2">• Cylindrical Shear Flow Reactor
• Planar Shear Flow Reactor</td></tr>
<tr><td>BP-WR

Reactor Property</td><td colspan="3">RF bias power at a specified material. The energy that the ions gain in the sheath is estimated as this power divided by the total ion current to that material as calculated in the plasma-reactor model. For example, “BPWR material1 200” specifies an applied bias of 200 W to the material boundary, material1. The ion energy gain calculated from the sheath model results in a reduced effective power deposition to the electrons (unless ELSH is also specified), as described in Homogeneous 0-D Reactor Models of the Chemkin-Pro Theory Manual .</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td></td><td>Material name</td><td>Optional

If there is no material name than the multiplier applies to all materials.</td><td>--</td><td>BPWR material1 200 1</td></tr>
<tr><td></td><td>RF bias power</td><td>Required</td><td>watts</td><td>BPWR 200</td></tr>
<tr><td></td><td>Reactor number (PSR clusters only)</td><td>Optional</td><td>--</td><td>BPWR material1 200 1</td></tr>
</table>

Keyword	Definition			
		If no number is given, the profile described by the first two values is assumed to apply to all reactors in a cluster.		
	Keyword Usage	Optional keyword. By default, the RF bias power is set to 0.0.		
	Reactor Models	• Closed Plasma Reactor • Plasma PSR • Plasma Plug Flow Reactor		
BULK Reactor Property	The estimated or initial bulk species activities. This is required input for bulk species in bulk phases that are being etched. For example, BULK Ga(d) 1.0 assigns the estimated activity of 1.0 to the Ga(d) bulk phase species.			
	Parameters	Optional/Reqd.	Units	Examples
	Bulk species name	Required	--	BULK **Ga(d)**1.0
	Bulk activity	Required	--	BULK Ga(d) **1.0**
	Keyword Usage	Required keyword. The bulk activity should be specified for bulk species. By default, the initial or estimated bulk species activities are 0.0.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Cylindrical Shear Flow Reactor • Honeycomb Reactor • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor		

Keyword	Definition			
		• Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
	Notes	• The sum of all estimated bulk phase activities for each bulk phase n should equal one. If they do not sum to one, they will be normalized to one, and a warning message will be printed in the diagnostic output. • See also: ETCH keyword. • Formerly **ACT** keyword for some reactor models in previous ANSYS Chemkin-Pro versions.		
BURN Reactor Property	Indicates a burner-stabilized flame problem type, with specified inlet flow rates.			
	Keyword Usage	Required keyword.		
	Reactor Models	• Premixed Laminar Burner-stabilized Flame		
	Notes	• The problem-type can be changed for a restart run. • See also FREE.		
CAAC Output	The crank angle at 50% mass burned and is also referred as the anchoring angle. This is one of the three crank angle parameters required to construct the Wiebe function profile that will pass these three crank angles at their corresponding burned mass fractions. By default, this angle marks when half of the original mass is burned. All three crank angles, CASC , CAAC , and CAEC must be provided.			
	Parameters	Optional/Reqd.	Units	Examples
	Crankangle at 50% mass burned	Required	degree	**CAAC 8.1**
	Keyword Usage	Optional keyword.		
	Reactor Models	• SI Engine Zonal Simulator		
CAATQ Output	Calculates the crank angle for the specified amount of total heat release. The crank angle for 10% and 50% of total heat release will be calculated by default.			
	Parameters	Optional/Reqd.	Units	Examples
	Percentage of total heat release	Required	percent	**CAATQ 90**
	Keyword Usage	Optional keyword.		
	Reactor Models	• IC HCCI Engine • Multi-Zone HCCI Engine Simulator • SI Engine Zonal Simulator		
CAEC Output	The crank angle at 90% mass burned. This is one of the three crank angle parameters required to construct the Wiebe function profile that will pass these three crank angles at their corresponding burned mass fractions. By default, this			

<table>
<tr><th>Keyword</th><th>Definition</th></tr>
<tr><td></td><td>angle marks when 90% of the original mass is burned. All three crank angles, CASC , CAAC , and CAEC must be provided.
<table>
<tr><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td>Crankangle at 90% mass burned</td><td>Required</td><td>degree</td><td>CAEC 23.0</td></tr>
<tr><td>Keyword Usage</td><td colspan="3">Optional keyword.</td></tr>
<tr><td>Reactor Models</td><td colspan="3">• SI Engine Zonal Simulator</td></tr>
</table></td></tr>
<tr><td>CARR

Reactor Property</td><td>Specify the named species as the carrier gas. This keyword is used to identify the species in calculating binary diffusion coefficients for tables and for non-dimensionalizations that require a binary diffusion coefficient.
<table>
<tr><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td>Species name</td><td>Optional</td><td>--</td><td>CARR H2</td></tr>
<tr><td>Species number</td><td>Optional</td><td>--</td><td>CARR 3</td></tr>
<tr><td>Keyword Usage</td><td colspan="3">Optional keyword. The default is to use the gas species with the largest mole fraction (from the XBTH input) in the bath-gas composition. If the gas-phase bath-gas composition is not specified, the default is to use the first species in the mechanism.</td></tr>
<tr><td>Reactor Models</td><td colspan="3">• Mechanism Analyzer</td></tr>
</table></td></tr>
<tr><td>CASC

Output</td><td>The crank angle at 10% mass burned. This is one of the three crank angle parameters required to construct the Wiebe function profile that will pass these three crank angles at their corresponding burned mass fractions. By default, this angle marks when 10% of the original mass is burned. All three crank angles, CASC , CAAC , and CAEC must be provided.
<table>
<tr><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td>Crankangle at 10% mass burned</td><td>Required</td><td>degree</td><td>CASC -15.4</td></tr>
<tr><td>Keyword Usage</td><td colspan="3">Optional keyword.</td></tr>
<tr><td>Reactor Models</td><td colspan="3">• SI Engine Zonal Simulator</td></tr>
</table></td></tr>
<tr><td>CD-CT

Reactor Property</td><td>Include conduction through the substrate in the energy balance. Inclusion of this keyword requires specification of a substrate thickness (CNDX). This value is used only if the disk temperature is being calculated from an energy balance by including keyword RADB . See Equation 14.18 of the Chemkin-Pro Theory Manual .
<table>
<tr><td>Keyword Usage</td><td>Optional keyword. By default, conduction through the substrate is not included.</td></tr>
<tr><td>Reactor Models</td><td>• Rotating Disk CVD Reactor

• Stagnation Flow CVD Reactor</td></tr>
</table></td></tr>
<tr><td>CDIF

Solver</td><td>Use central differencing on convective terms in the equations.</td></tr>
</table>

Keyword	Definition			
	Keyword Usage	Optional keyword. By default, windward differencing is used.		
	Reactor Models	• Diffusion or Premixed Opposed-flow Flame • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation		
CFL Reactor Property	The Courant-Friedrichs-Lewy (CFL) number for the convective process; this parameter limits the fraction of particles whose properties can be set to the inlet conditions per time step.			
	Parameters	Optional/Reqd.	Units	Examples
	CFL number	Required	--	CFL **1.0**
	Keyword Usage	Optional keyword. By default, the CFL number is 0.5.		
	Reactor Models	• Closed Partially Stirred Reactor (PaSR) • Partially Stirred Reactor (PaSR)		
CHEM Reactor Property	Specifies that gas-phase chemistry will be included in the calculations.			
	Keyword Usage	Optional keyword. This option is used to reactivate the chemical kinetics if the NOCH option was in effect for the previous calculation for CVD Reactors. For PaSRs, the default is to neglect chemistry and do a mixing calculation only.		
	Reactor Models	• Closed Partially Stirred Reactor (PaSR) • Partially Stirred Reactor (PaSR) • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
CJ Problem Type	Chapman-Jouguet detonation. In this case, H, S, V, and T contain the unburned state and TEST gives the burned temperature estimate.			
	Keyword Usage	Optional keyword. The user must include exactly one problem-type keyword		
	Reactor Models	• Chemical and Phase Equilibrium Calculations		
CLSC Reactor Property	Defines a critical particle class under which the oxidation process starts to affect (reduce) the particle number density. This parameter is only used by the particle burnout model and has no effect on particle formation and growth. The default value is the minimum particle class plus the maximum class change due to surface reaction.			
	Parameters	Optional/Reqd.	Units	Examples
	Material name	Required	--	CLSC **CARBON** 40
	Critical particle class	Required	--	CLSC CARBON **40**

Keyword	Definition			
	Keyword Usage	Optional keyword. The default value is the minimum particle class plus the maximum class change due to surface reaction.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Cylindrical Shear Flow Reactor • Honeycomb Monolith Reactor • IC HCCI Engine • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma PSR • Plasma Plug Flow Reactor • Plug Flow Reactor • SI Engine Zonal Simulator		
CLSE Reactor Property	Flag indicating the reactor is a closed system, i.e., mass flow rate is zero.			
	Keyword Usage	Required Keyword.		
	Reactor Models	• Closed Partially Stirred Reactor (PaSR)		
CLSM Reactor Property	Defines the smallest particle class that can exist in the system. This parameter is only used by the particle burnout model and has no effect on particle formation and growth. The default value is the smallest inception class defined by the nucleation reactions.			
	Parameters	Optional/Reqd.	Units	Examples
	Material name	Required	--	CLSM **CARBON** 32
	Minimum particle class	Required	--	CLSM CARBON **32**
	Keyword Usage	Optional keyword. The default value is the smallest inception class defined by the nucleation reactions.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Cylindrical Shear Flow Reactor • Honeycomb Monolith Reactor • IC HCCI Engine • Perfectly Stirred Reactor (PSR)		

Keyword	Definition			
		• Planar Shear Flow Reactor • Plasma PSR • Plasma Plug Flow Reactor • Plug Flow Reactor • SI Engine Zonal Simulator		
CMIX Reactor Property	The controlling parameter for the modified Curl's and the IEM models for a PaSR.			
	Parameters	Optional/Reqd.	Units	Examples
	Time ratio for scalar mixing (Equation 9.1 of the Chemkin-Pro Theory Manual *)*	Required	--	CMIX **1.0**
	Keyword Usage	Required keyword, unless WELL keyword is included.		
	Reactor Models	• Closed Partially Stirred Reactor (PaSR) • Partially Stirred Reactor (PaSR)		
CM-PR Reactor Property	Engine compression ratio. The compression ratio is defined as the maximum total volume in the cylinder (clearance volume plus swept volume) divided by the clearance volume.			
	Parameters	Optional/Reqd.	Units	Examples
	Engine compression ratio	Required	--	CMPR **10**
	Keyword Usage	Optional keyword. By default, the ratio is 15.		
	Reactor Models	• IC HCCI Engine • SI Engine Zonal Simulator		
CNDT Reactor Property	The back-side temperature of the substrate for use in calculation of conduction losses. This value is used only if the disk temperature is being calculated from an energy balance by including keywords RADB and CDCT . See Equation 14.18 of the Chemkin-Pro Theory Manual .			
	Parameters	Optional/Reqd.	Units	Examples
	Back-side temperature	Required	K	CNDT **350.**
	Keyword Usage	Optional keyword. By default, the back-side temperature is 300.		
	Reactor Models	• Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		

<table>
<tr><th>Keyword</th><th colspan="4">Definition</th></tr>
<tr><td>CNDX

Reactor Property</td><td colspan="4">The thickness of the substrate for calculation of conduction losses. This value is used only if the disk temperature is being calculated from an energy balance by including keywords RADB and CDCT . See Equation 14.18 of the Chemkin-Pro Theory Manual .</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td></td><td>Substrate thickness</td><td>Required</td><td>cm</td><td>CNDX 0.03</td></tr>
<tr><td></td><td>Keyword Usage</td><td colspan="3">Optional keyword. By default, the substrate thickness is 0.0.</td></tr>
<tr><td></td><td>Reactor Models</td><td colspan="3">• Rotating Disk CVD Reactor
• Stagnation Flow CVD Reactor</td></tr>
<tr><td>CNTN

Reactor Property</td><td colspan="4">Inclusion of this keyword causes ANSYS Chemkin-Pro to expect keywords for another problem to follow the END keyword. The following problem uses the solution of the previous problem as its initial guess. This capability is very similar to that provided by RSTR. However, in the case of CNTN , several related problems can be solved by one job submission, without having to manipulate the XML Solution File. The solutions resulting from CNTN keywords are written sequentially to one XML Solution File.</td></tr>
<tr><td></td><td>Keyword Usage</td><td colspan="3">Optional keyword. By default, no continuation is expected.</td></tr>
<tr><td></td><td>Reactor Models</td><td colspan="3">• Closed Homogeneous Batch Reactor
• Closed Plasma Reactor
• Cylindrical Shear Flow Reactor
• Honeycomb Reactor
• IC HCCI Engine
• Non-reactive Gas Mixer
• Normal Incident Shock
• Normal Reflected Shock
• Opposed-flow Flame Simulator
• Perfectly Stirred Reactor (PSR)
• Planar Shear Flow Reactor
• Plasma Plug Flow Reactor
• Plasma PSR
• Plug Flow Reactor
• Premixed Laminar Burner-stabilized Flame</td></tr>
</table>

Keyword	Definition			
		• Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor Using Steady-state Solver • SI Engine Zonal Simulator • Stagnation Flow CVD Reactor Using Steady-state Solver		
CNTT Reactor Property	This will cause the starting time of the continuation calculation to be equal to the end time of the last solution.			
	Keyword Usage	Optional keyword. By default, the starting time of a continuation is set to zero.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • IC HCCI Engine • Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Plasma PSR • SI Engine Zonal Simulator		
CNTX Reactor Property	This will cause the starting distance of the continuation calculation to be equal to the end distance of the last solution. This keyword is used for Plug Flow Reactors in place of CNTT.			
	Keyword Usage	Optional keyword. By default, the starting distance of a continuation is set to zero.		
	Reactor Models	• Honeycomb Reactor • Plasma Plug Flow Reactor • Plug Flow Reactor		
COLR Reactor Property	This flag indicates the collision formulation to be used to calculate the collision rate among particles. Three types of collision formulations are available: free molecular regime (=0), continuum regime (=1), and transition regime (=3). The collision rate in the transition regime is obtained as the harmonic mean of the collision rates of free-molecular regime and continuum regime. By default, formulation for free-molecular collision is used.			
	Parameters	Optional/Reqd.	Units	Examples
	Material name	Required	--	COLR **C(B)**1
	Collision regime	Required	--	BETA C(B) **1**
	Keyword Usage	Optional keyword. By default, the formulation for the free-molecular regime is used (0).		
	Reactor Models	• Closed Homogeneous Batch Reactor		

Keyword	Definition			
		• Closed Plasma Reactor • Cylindrical Shear Flow Reactor • Honeycomb Monolith Reactor • IC HCCI Engine • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma PSR • Plasma Plug Flow Reactor • Plug Flow Reactor • SI Engine Zonal Simulator		
COMP Reactor Property	The boundary condition used at the inlet boundary for the gas species equations will be that of a fixed gas composition, as specified by the REAC keywords.			
	Keyword Usage	Optional keyword. By default, a flux balance is solved at the inlet (see keyword FLUX).		
	Reactor Models	• Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
CONC Output	If this keyword is used, the printed output will appear in molar concentration (mole/cc) rather than mole fraction.			
	Keyword Usage	Optional keyword. By default, mole fractions are printed.		
	Reactions	• Normal Incident Shock • Normal Reflected Shock		
COND Reactor Property	The thermal conductivity of the substrate in SI units, for use in calculation of conduction losses. This value is used only if the disk temperature is being calculated from an energy balance by including keywords RADB and CDCT . See Equation 14.18 of the Chemkin-Pro Theory Manual .			
	Parameters	Optional/Reqd.	Units	Examples
	Thermal conductivity	Required	W/cm K	COND **2.1**
	Keyword Usage	Optional keyword. By default, the thermal conductivity is 1.38.		
	Reactor Models	• Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		

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Keyword	Definition			
CONP Problem Type	A transient solution will be obtained with the pressure held constant. The equations solved are those of a constant pressuresystem and the energy equation will be solved.			
	Keyword Usage	Optional keyword. By default, a constant pressure problem is assumed.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor		
CONV Problem Type	A transient solution will be obtained with the volume held constant. The equations solved are those of a constant volume system and the energy equation will be solved. In this case, the pressure is allowed to float.			
	Keyword Usage	Optional keyword. By default, a constant pressure problem is assumed.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor		
CONX Reactor Property	This keyword is used to specify a constant (constrained) mole fraction for a species. For example, CONX H2 0.1 will fix the fraction of hydrogen in the mixture to be 0.1.			
	Parameters	Optional/Reqd.	Units	Examples
	Species name	Required	--	CONX **H2**0.1
	Mole fraction of the species	Required	mole fraction	CONX H2 **0.1**
	Keyword Usage	Optional keyword. By default, composition equilibrium is determined for all species.		
	Reactor Models	• Chemical and Phase Equilibrium Calculations		
COTV Problem Type	• A transient solution will be obtained with the • temperature and • volume held • constant at the initial values. In this case, the pressure is allowed to float.			
	Keyword Usage	Optional keyword. By default, a constant pressure is assumed.		
	Reactor Models	• Closed Homogeneous Batch Reactor		
CPROD Inlet or Reactor Property	One of these CPROD inputs must appear for each complete-combustion product species when the equivalence ratio option is used (EQUI) for an inlet stream or for the initial conditions of a closed system.			
	Parameters	Optional/Reqd.	Units	Examples

Keyword	Definition			
	Inlet stream name (PSRs only)	Optional If there is no stream name than the product species will be used for all defined inlet streams.	--	CPROD **mixture1** CO2 CPROD **mixture1** H2O
	Species name	Required	--	CPROD H2OCPROD **CO2**
	Keyword Usage	Required keyword when EQUI option is used for an inlet stream or for the initial conditions in a reactor. The specified group of complete-combustion product species must include all of the elements contained in the fuel and oxidizer species. The products must also be "saturated" species. See the ANSYS Chemkin-Pro Tutorials Manual for more information.		
	Reactor Models	• Chemical and Phase Equilibrium Calculations • Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Cylindrical Shear Flow Reactor • Diffusion or Premixed Opposed-flow Flame • Honeycomb Reactor • IC HCCI Engine • Non-reactive Gas Mixer • Partially Stirred Reactor (PaSR) • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor		

Keyword	Definition			
		• Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
	Notes	• The CPROD keywords must be changed as a set, not individually for a restart run. • The CPROD keywords must be changed as a set, not individually for continuation run.		
CTOL Reactor Property	Criterion for determining when steady state is reached using a transient solver for Partially Stirred Reactors. The required parameter sets the normalized slope of mean density change in time $\left(d\overline{\rho}/dt\right)$. The default number of time points used to determine the slope is 100; this value can be changed with the keyword NCFIT.			
	Parameters	Optional/Reqd.	Units	Examples
	Normalized slope of mean density	Required	--	CTOL **1.0E-3**
	Keyword Usage	Optional keyword. By default, the program does not check for the steady state.		
	Reactor Models	• Closed Partially Stirred Reactor (PaSR) • Partially Stirred Reactor (PaSR)		
CTOL Solver	Criterion for determining when steady-state is reached by a transient solver for CVD Reactors. The steady state is reached when the normalized absolute values of all time derivatives are less than CTOL.			
	Parameters	Optional/Reqd.	Units	Examples
	Steady-state criterion	Required	--	CTOL **1.0E-2**
	Keyword Usage	Optional keyword. By default, the criterion is 1.0E-4.		
	Reactor Models	• Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
CURL Reactor Property	Flag indicating that the modified Curl's model will be used to simulate the molecular mixing within the computational particle.			
	Keyword Usage	Optional keyword. By default, a well mixed model is assumed.		
	Reactor Models	• Closed Partially Stirred Reactor (PaSR) • Partially Stirred Reactor (PaSR)		

Keyword	Definition			
CURV Solver	Parameter that controls the degree of mesh adaptation based on the second derivative, or curvature, in the solution. A reasonable value is usually between about 0.1 and 1.0, where no adaptation based on curvature is specified with 1.0.			
	Parameters	Optional/Reqd.	Units	Examples
	Normalized curvature parameter	Required	--	CURV **0.7**
	Keyword Usage	Optional keyword. By default, the curvature parameter is set to 0.5.		
	Reactor Models	• Diffusion or Premixed Opposed-flow Flame • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
	Notes	• This keyword can be changed for a restart run. • Steady-state 1-D Solution Methods of the Chemkin-Pro Theory Manual for more information.		
CY-BAR Reactor Property	The cylinder head area to bore-area ratio.			
	Parameters	Optional/Reqd.	Units	Examples
	Ratio of cylinder head area to bore area.	Required	None	CYBAR **1.2**
	Keyword Usage	Optional keyword. Default = 1.0.		
	Reactor Models	• IC HCCI Engine • Multi-zone HCCI Engine • SI Engine Zonal Simulator		
	Notes	• CYBAR should be > 1.0.		
DASP Solver	Flag indicating the DASPK solver is used to integrate the transient equations.			
	Keyword Usage	Optional keyword. By default, the DASPK solver will be used.		
	Reactor Models	• Closed Partially Stirred Reactor (PaSR) • Partially Stirred Reactor (PaSR)		
DEG0	The starting crank angle for the transient IC HCCI Engine model, in degrees.			

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Keyword	Definition			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	Crank angle	Required	degrees	DEG0 **45**
	Keyword Usage	Optional keyword. By default, this starting angle is 180 degrees.		
	Reactor Models	• IC HCCI Engine • SI Engine Zonal Simulator		
DE-GE Output	The ending crank angle for the IC engine simulation. Normally, this is the same as the crank angle at Exhaust Valve Open (EVO).			
	Parameters	Optional/Reqd.	Units	Examples
	Crankangle at end of simulation	Required	degree	**CAAC 120.5**
	Keyword Usage	Optional keyword.		
	Reactor Models	• IC HCCI Engine • Multi-zone HCCI Engine • SI Engine Zonal Simulator		
DELT Solver	The time interval for solution printing to the diagnostic text output file, for the transient solver. Note that the number of time points written to the diagnostic output file is equal to the value given by TIME divided by DELT.			
	Parameters	Optional/Reqd.	Units	Examples
	Time interval	Required	sec	DELT **1.0E-4**
	Aurora Usage	Optional keyword. By default, the value of the maximum solver timestep (STPT) is used.		
	Spin Usage	Optional keyword. By default, this is a required keyword for a transient calculation.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • IC HCCI Engine • Non-reactive Gas Mixer • Normal Incident Shock • Normal Reflected Shock • Perfectly Stirred Reactor (PSR) • Plasma PSR • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		

Keyword	Definition			
		• SI Engine Zonal Simulator		
	Notes	• Backwards compatible with **DT** from previous versions.		
DFAC Solver	Factor by which to divide the time step in the steady-state solver, *Twopnt*'s, time stepping procedure when necessary, i.e., when the current time step does not converge.			
	Parameters	Optional/Reqd.	Units	Examples
	Division factor	Required	--	DFAC **1.5**
	Keyword Usage	Optional keyword. By default, the division factor is set to 2.2.		
	Reactor Models	• Closed Plasma Reactor • Diffusion or Premixed Opposed-flow Flame • Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Plasma PSR • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
DIA Reactor Property	Shock-tube diameter, used for boundary layer corrections.			
	Parameters	Optional/Reqd.	Units	Examples
	Tube diameter	Required	cm	DIA **2.0**
	Keyword Usage	Optional keyword. By default, the tube diameter is set to 1.0.		
	Reactor Models	• Normal Incident Shock		
DIAM Reactor Property	Tube diameter or hydraulic diameter, where the diameter is constant along the channel. See also DPRO, AREAF, AFLO and user subroutine GEOM.			
	Parameters	Optional/Reqd.	Units	Examples
	Tube diameter	Required	cm	DIAM **5.3**
	Keyword Usage	Optional keyword. The user must specify DIAM, DPRO, AREAF, or AFLO, unless the GEOM user routine is to be used.		
	Reactor Models	• Honeycomb Reactor • Plasma Plug Flow Reactor • Plug Flow Reactor		

<table>
<tr><th>Keyword</th><th>Definition</th></tr>
<tr><td>DIST

XMLI</td><td>This keyword is valid with the XMLI option, when the XML Solution File that is used for initialization or restart contains data as a function of axial distance (e.g. from Shear-layer Flow or Plug Flow). In this case, select the values to use in initialization or restart as those corresponding to the distance that is closest to (greater than or equal to) the specified distance.
<table>
<tr><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td>Axial distance</td><td>Required</td><td>cm</td><td>DIST 5.0</td></tr>
<tr><td>Keyword Usage</td><td colspan="3">Optional keyword. By default, uses the data from the last axial distance found in the XML Solution File.</td></tr>
<tr><td>Reactor Models</td><td colspan="3">• Chemical and Phase Equilibrium Calculations
• Closed Homogeneous Batch Reactor
• Closed Plasma Reactor
• Cylindrical Shear Flow Reactor
• Diffusion or Premixed Opposed-flow Flame
• Honeycomb Reactor
• IC HCCI Engine
• Mechanism Analyzer
• Non-reactive Gas Mixer
• Normal Incident Shock
• Normal Reflected Shock
• Perfectly Stirred Reactor (PSR)
• Planar Shear Flow Reactor
• Plasma Plug Flow Reactor
• Plasma PSR
• Plug Flow Reactor
• Premixed Laminar Burner-stabilized Flame
• Premixed Laminar Flame-speed Calculation
• Rotating Disk CVD Reactor
• SI Engine Zonal Simulator
• Stagnation Flow CVD Reactor</td></tr>
</table></td></tr>
<tr><td>DPRO</td><td>Hydraulic diameter or tube diameter as a function of distance. See also DIAM, AREAF, AFLO, and user subroutine GEOM.</td></tr>
</table>

Keyword	Definition			
Reactor Property Profiles	Parameters	Optional/Reqd.	Units	Examples
	Distance from inlet	Required	cm	DPRO **0.0**1.0
	Hydraulic diameter	Required	cm	DPRO 0.0 **1.0**
	Keyword Usage	Optional keyword. The user must enter DIAM, DPRO, AREAF, or AFLO, unless user subroutine GEOM is to be used.		
	Reactor Models	• Honeycomb Reactor • Plasma Plug Flow Reactor • Plug Flow Reactor		
DT Reactor Property	The time step size of the Monte Carlo simulation.			
	Parameters	Optional/Reqd.	Units	Examples
	Time step	Required	sec	DT **1.0E-4**
	Keyword Usage	Required keyword.		
	Reactor Models	• Closed Partially Stirred Reactor (PaSR) • Partially Stirred Reactor (PaSR)		
DT0 Solver	The initial time step size used by the transient solver.			
	Parameters	Optional/Reqd.	Units	Examples
	Initial time step size	Required	sec	DT0 **1.0E-4**
	Keyword Usage	Optional keyword. By default, the initial time step size is set to 1.0E-6.		
	Reactor Models	• Closed Partially Stirred Reactor (PaSR) • Partially Stirred Reactor (PaSR) • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
	Notes	• Backwards compatible with H0 keyword.		
DTDEG Solver	The maximum time step in terms of crank angle that may be taken by the DASPK solver for the transient IC HCCI Engine model, in degrees. If DTDEG is specified, then it will overwrite the time step value specified by STPT.			
	Parameters	Optional/Reqd.	Units	Examples
	Time step	Required	degrees	DTDEG **30**
	Keyword Usage	Optional keyword. By default, this time step is value of STPT.		
	Reactor Models	• IC HCCI Engine • SI Engine Zonal Simulator		

Keyword	Definition			
	Notes	• See also: STPT keyword.		
DTIGN Output	Temperature threshold used to determine when ignition has occurred and allow printing of ignition delay times. The ignition temperature will be the initial temperature plus this value. Only applicable when you are solving the energy equation with the transient solver.			
	Parameters	Optional/Reqd.	Units	Examples
	Ignition temperature delta	Required	K	DTIGN **200**
	Keyword Usage	Optional keyword. See also TLIM .		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Honeycomb Monolith Reactor • IC HCCI Engine • Perfectly Stirred Reactor (PSR) • Plasma PSR • Plasma Plug Flow Reactor • Plug Flow Reactor • SI Engine Zonal Simulator		
DTMN Solver	Minimum time step tolerated in the steady-state solver, *Twopnt* 's time stepping algorithm before flagging an error condition.			
	Parameters	Optional/Reqd.	Units	Examples
	Minimum time step	Required	sec	DTMN **1.E-9**
	Keyword Usage	Optional keyword. By default, the minimum time step is 1.E-10.		
	Reactor Models	• Cylindrical Shear Flow Reactor • Diffusion or Premixed Opposed-flow Flame • Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Plasma PSR • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor • Planar Shear Flow Reactor		

<table>
<tr><th>Keyword</th><th colspan="4">Definition</th></tr>
<tr><td></td><td></td><td colspan="3">• Premixed Laminar Burner-stabilized Flame
• Premixed Laminar Flame-speed Calculation</td></tr>
<tr><td>DTMX

(steady-state) Solver</td><td colspan="4">Maximum time step allowed in Twopnt 's time-stepping algorithm. When this value is reached, the time step size will no longer be increased and time stepping will continue with a fixed time step.</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td></td><td>Maximum time step</td><td>Required</td><td>sec</td><td>DTMX 1.E-3</td></tr>
<tr><td></td><td>Keyword Usage</td><td colspan="3">Optional keyword. By default, the maximum time step is 1.E-2.</td></tr>
<tr><td></td><td>Reactor Models</td><td colspan="3">• Cylindrical Shear Flow Reactor
• Diffusion or Premixed Opposed-flow Flame
• Non-reactive Gas Mixer
• Perfectly Stirred Reactor (PSR)
• Planar Shear Flow Reactor
• Plasma PSR
• Premixed Laminar Burner-stabilized Flame
• Premixed Laminar Flame-speed Calculation
• Rotating Disk CVD Reactor
• Stagnation Flow CVD Reactor</td></tr>
<tr><td>DTMX

(transient) Solver</td><td colspan="4">Maximum time step used internally by the solver in transient calculations. DTMX determines the largest time-step the transient solver can take at one time and thereby controls the resolution for interpolation of specified time-profiles.</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td></td><td>Maximum time step</td><td>Required</td><td>sec</td><td>DTMX 1.E-3</td></tr>
<tr><td></td><td>Keyword Usage</td><td colspan="3">Optional keyword. By default, the maximum time step is 1.E-4.</td></tr>
<tr><td></td><td>Reactor Models</td><td colspan="3">• Closed Partially Stirred Reactor (PaSR)
• Partially Stirred Reactor (PaSR)</td></tr>
<tr><td>DTSV

Output or Solver</td><td colspan="4">Controls the time interval for data to be written to the XML Solution File (e.g., XMLdata.zip). Note that the number of time points written to the XML Solution File is equal to the value given by TIME divided by DTSV.</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td></td><td>Time interval for solution saving</td><td>Required</td><td>sec</td><td>DTSV 1.0E-5</td></tr>
</table>

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Keyword	Definition			
	Keyword Usage	Optional keyword. By default, the value of the STPT keyword is used.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • IC HCCI Engine • Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Plasma PSR • Closed Partially Stirred Reactor (PaSR) • Partially Stirred Reactor (PaSR) • SI Engine Zonal Simulator		
DX Output or Solver	Distance interval for printing the solution to the diagnostic output file.			
	Parameters	Optional/Reqd.	Units	Examples
	Distance interval	Required	cm	DX **0.25.**
	Keyword Usage	Optional keyword. By default, the distance interval is the value of the DXMX is used, or XEND divided by 100 if DXMX is not available.		
	Reactor Models	• Cylindrical Shear Flow Reactor • Honeycomb Reactor • Planar Shear Flow Reactor • Plasma Plug Flow Reactor • Plug Flow Reactor		
DXMX Solver	The maximum distance step that can be used internally by the transient solver. DXMX determines the largest step that the solver can take at one time and thereby controls the resolution for interpolation of specified spatial-profiles. See also DX and DXSV.			
	Parameters	Optional/Reqd.	Units	Examples
	Distance interval	Required	cm	DXMX **0.1**
	Keyword Usage	Optional keyword. By default, If either DX or DXSV are specified, then DXMX is set to the smallest of these values. If neither DX nor DXSV are specified, then DXMX is set to the value of XEND divided by 100.		
	Reactor Models	• Cylindrical Shear Flow Reactor • Honeycomb Reactor		

<table>
<tr><th>Keyword</th><th colspan="4">Definition</th></tr>
<tr><td></td><td></td><td colspan="3">• Planar Shear Flow Reactor
• Plasma Plug Flow Reactor
• Plug Flow Reactor</td></tr>
<tr><td>DXSV

Solver</td><td colspan="4">Controls the distance interval for data to be written to the XML Solution File (e.g., XMLdata.zip). The number of points written to the XML Solution File is equal to the value given by XEND divided by DXSV.</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td></td><td>Distance interval</td><td>Required</td><td>cm</td><td>DXSV 0.1</td></tr>
<tr><td></td><td>Keyword Usage</td><td colspan="3">Optional keyword. By default, the value of DXMX is used.</td></tr>
<tr><td></td><td>Reactor Models</td><td colspan="3">• Cylindrical Shear Flow Reactor
• Honeycomb Reactor
• Planar Shear Flow Reactor
• Plasma Plug Flow Reactor
• Plug Flow Reactor</td></tr>
<tr><td>EGRR

Reactor or Inlet Property</td><td colspan="4">Specifies the EGR rate for an inlet stream or for the initial conditions in a closed reactor.</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td></td><td>EGR ratio</td><td>Optional</td><td>None</td><td>EGRR 0.2</td></tr>
<tr><td></td><td>Keyword Usage</td><td colspan="3">Optional keyword. EGR rate can be used in any reactor model as a feature on input or initial composition panels. EGR specification can be activated when Equivalence ratio option is used to specify inlet or initial composition. Leaving the EGR Rate box empty will use no EGR, but use diluants if specified on the Added Species tab. When EGR Rate is specified, the composition on the Added Species tab is used as the EGR composition. The sum of all the fractions on the Added Species tab should be 1.0 when EGR Rate is specified. If the sum is less than 1, Chemkin will automatically normalize the EGR composition.</td></tr>
<tr><td></td><td>Reactor Models</td><td colspan="3">• Closed Homogeneous Batch Reactor
• IC HCCI Engine
• Perfectly Stirred Reactor (PSR)
• Honeycomb Reactor
• Plasma Plug Flow Reactor
• Plasma PSR</td></tr>
</table>

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Keyword	Definition			
		• Plug Flow Reactor		
ELSH Reactor Property	Specified energy loss to ions in the sheath for each ion lost at a specified material. The energy that the ions gain in the sheath is typically assumed to be the sheath voltage, which can be described as a multiplier of kT_e. The value given here is the value of the multiplier. For example, "ELSH material1 5.0" would result in an ion energy gain of $5kT_e$ as it crossed the sheath near the material material1. This energy gain for the ions results in a reduced effective power deposition to the electrons, as described in Plasma Systems of the Chemkin-Pro Theory Manual .			
	Parameters	Optional/Reqd.	Units	Examples
	Material name	Optional If there is no material name then the multiplier applies to all materials.	--	ELSH **material1**5.0 1
	Multiplier value	Required	--	ELSH **5.0**
	Reactor number (PSR clusters only)	Optional If no number is given, values are assumed to apply to all reactors in a cluster.	--	ELSH material1 5.0 **1**
	Keyword Usage	Optional keyword. By default, the multiplier is set to 0.0, when no ELSH keyword is included.		
	Reactor Models	• Closed Plasma Reactor • Plasma Plug Flow Reactor • Plasma PSR		
EMIS Reactor Property	The emissivity of the disk. This value is used only if the disk temperature is being calculated from an energy balance by including keyword RADB . See Equation 14.18 of the Chemkin-Pro Theory Manual .			
	Parameters	Optional/Reqd.	Units	Examples
	Emissivity	Required	--	EMIS **0.9**

Keyword	Definition			
	Keyword Usage	Optional keyword. By default, the emissivity is 0.85.		
	Reactor Models	• Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
EMPAR Reactor Property	This keyword provides the value of the model parameter C_{part} for computing the overall emissivity of the named particle cloud as given in Equation 12.21 in the Chemkin-Pro Theory Manual .			
	Parameters	Optional/Reqd.	Units	Examples
	Material name	Required	--	EMPAR soot 700
	Model coefficient	Required	$m^{-1}K^{-1}$	EMPAR soot **700**
	Keyword Usage	Optional keyword. The default value is 700 ($m^{-1}K^{-1}$).		
	Reactor Models	• Diffusion or Premixed Opposed-flow Flame • Burner-stabilized Pre-mixed Flame • Premixed Laminar Flame-speed Calculation		
EMSG Reactor Property Profiles	Approximation of the temperature-dependent emissivity of the gas-mixture, used to calculate a radiation-loss term in the gas energy equation. The radiation is calculated between the gas and the disk (using the gas temperature) and between the gas and the inlet (using the inlet temperature). The EMSG keyword provides temperature, emissivity pairs for the gas mixture.			
	Parameters	Optional/Reqd.	Units	Examples
	Temperature	Required	K	EMSG **2000**0.03
	Emissivity	Required	--	EMSG 2000 **0.03**
	Keyword Usage	Optional keyword. By default, no gas radiation loss is included in the energy equation.		
	Reactor Models	• Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
END Reactor Property	This keyword signifies the end of the input data for a given reactor description. It must appear after each set of data when continuation jobs are indicated using the CNTN keyword.			
	Keyword Usage	Required keyword.		
	Reactor Models	• Chemical and Phase Equilibrium Calculations • Closed Homogeneous Batch Reactor • Closed Partially Stirred Reactor (PaSR) • Closed Plasma Reactor • Cylindrical Shear Flow Reactor • Diffusion or Premixed Opposed-flow Flame		

<table>
<tr><th>Keyword</th><th>Definition</th></tr>
<tr><td></td><td></td><td>
• Honeycomb Reactor
• IC HCCI Engine
• Mechanism Analyzer
• Non-reactive Gas Mixer
• Normal Incident Shock
• Normal Reflected Shock
• Partially Stirred Reactor (PaSR)
• Perfectly Stirred Reactor (PSR)
• Planar Shear Flow Reactor
• Plasma Plug Flow Reactor
• Plasma PSR
• Plug Flow Reactor
• Premixed Laminar Burner-stabilized Flame
• Premixed Laminar Flame-speed Calculation
• Rotating Disk CVD Reactor
• SI Engine Zonal Simulator
• Stagnation Flow CVD Reactor
</td></tr>
<tr><td>END-TIMEMAX

Reactor Property</td><td colspan="2">Since the physical time required to reach steady-state normally increases with decreasing values of SSDR, the integration time is increased by the factor SSDR_nominal/currentSSDR for SSDR values smaller than the nominal. The maximum value for the end-time is limited to the value specified by this control.</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td></td><td>Maximum value of end time</td><td>Optional</td><td>s</td><td>ENDTIMEMAX 1.0E+05</td></tr>
<tr><td></td><td>Keyword Usage</td><td colspan="2">Optional keyword. The default value for the Diffusion Flamelet Generator is 1.0E+05</td></tr>
<tr><td></td><td>Reactor Models</td><td colspan="2">• Diffusion Flamelet Generator</td></tr>
<tr><td>ENGE

Reactor Property</td><td colspan="2">Solve the electron energy equation. The user must still specify a temperature (see ETMP), which provides the initial guess or initial value for the electron temperature.</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td></td><td>Reactor number (PSR clusters only)</td><td>Optional</td><td>--</td><td>ENGE 2</td></tr>
</table>

Keyword	Definition			
		If no number is given, values are assumed to apply to all reactors in a cluster.		
	Keyword Usage	Optional keyword. By default, the electron energy equation is not solved.		
	Reactor Models	• Closed Plasma Reactor • Plasma PSR • Plasma Plug Flow Reactor		
	Notes	• ENGE must be specified when electrons are present for all PSRs.		
ENGY Reactor Property	Specifies the starting internal energy for the initial mixture.			
	Parameters	Optional/Reqd.	Units	Examples
	Energy	Required	erg/g	ENGY **1.5E9**
	Keyword Usage	Optional keyword. The user must specify two state variables and the composition to define the initial mixture.		
	Reactor Models	• Chemical and Phase Equilibrium Calculations		
EN-RG Problem Type	Solve the energy equation to determine the gas temperature.			
	Parameters	Optional/Reqd.	Units	Examples
	Reactor number (PSR clusters only)	Optional If no number is given, the keyword is assumed to apply to all reactors in a cluster.	--	ENRG **2**
	Keyword Usage	Optional keyword. Either TGIV or ENRG must be specified in most cases. For closed homogeneous		

<table>
<tr><th>Keyword</th><th colspan="4">Definition</th></tr>
<tr><td></td><td></td><td colspan="3">systems, ICEN, CONP, CONV, or COTV can be specified instead. For Premixed Flamespeed Calculations, ENRG is required.</td></tr>
<tr><td></td><td>Reactor Models</td><td colspan="3">• Closed Homogeneous Batch Reactor
• Closed Plasma Reactor
• Diffusion or Premixed Opposed-flow Flame
• Honeycomb Reactor
• Non-reactive Gas Mixer
• Perfectly Stirred Reactor (PSR)
• Plasma Plug Flow Reactor
• Plasma PSR
• Plug Flow Reactor
• Premixed Laminar Flame-speed Calculation
• Premixed Laminar Burner-stabilized Flame
• Rotating Disk CVD Reactor
• Stagnation Flow CVD Reactor</td></tr>
<tr><td></td><td>Notes</td><td colspan="3">• The user must still specify an initial or initial estimate of the gas temperature or temperature profile. See also: TEMP or TPRO keyword.
• For steady-state reactor models, this initial temperature is used in solving the intermediate fixed-temperature problem and is an initial guess for the solution of the full problem including the energy equation.
• Inclusion of the keywords CONP, CONV, or ICEN, will also indicate that the energy equation should be solved.for closed homogeneous systems.</td></tr>
<tr><td rowspan="5">ENTH

Reactor Property</td><td colspan="4">Specifies the starting enthalpy for the initial mixture.</td></tr>
<tr><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td>Enthalpy</td><td>Required</td><td>erg/g</td><td>ENTH 1.5E9</td></tr>
<tr><td>Keyword Usage</td><td colspan="3">Optional keyword. The user must specify two state variables and the composition to define the initial mixture.</td></tr>
<tr><td>Reactor Models</td><td colspan="3">• Chemical and Phase Equilibrium Calculations</td></tr>
</table>

Keyword	Definition			
ENTR Reactor Property	Specifies the starting entropy for the initial mixture.			
	Parameters	Optional/Reqd.	Units	Examples
	Entropy	Required	erg/(g · K)	ENTR **7.0E7**
	Keyword Usage	Optional keyword. The user must specify two state variables and the composition to define the initial mixture.		
	Reactor Models	• Chemical and Phase Equilibrium Calculations		
EPSG Output	Threshold value for the first-order sensitivity coefficients for the growth rates of all bulk phases with respect to the rate constants. Coefficients below this value are neither printed to the diagnostic output file nor saved in the XML Solution File.			
	Parameters	Optional/Reqd.	Units	Examples
	Threshold value	Required	--	EPSG **.01**
	Keyword Usage	Optional keyword. By default, the threshold value for bulk phases is set to 0.001.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Honeycomb Reactor • Perfectly Stirred Reactor (PSR) • Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor		
	Notes	• This keyword can be added but not removed from a continuation run.		
EPSR Output	Threshold value for the rate-of-production coefficients. Coefficients below this value are neither printed to the diagnostic output file nor saved in the XML Solution File.			
	Parameters	Optional/Reqd.	Units	Examples
	Threshold value	Required	--	EPSR **.02**
	Keyword Usage	Optional keyword. By default, the threshold value for rate-of-production coefficients is set to 0.01.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Honeycomb Reactor • IC HCCI Engine		

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<table>
<tr><th>Keyword</th><th colspan="4">Definition</th></tr>
<tr><td></td><td></td><td colspan="3">• Perfectly Stirred Reactor (PSR)
• Plasma Plug Flow Reactor
• Plasma PSR
• Plug Flow Reactor
• SI Engine Zonal Simulator</td></tr>
<tr><td></td><td>Notes</td><td colspan="3">• This keyword can be added but not removed from a continuation run.</td></tr>
<tr><td>EPSS

Output</td><td colspan="4">Threshold value for the first-order sensitivity coefficients for the species with respect to the rate constants. Coefficients below this value are neither printed to the diagnostic output file nor saved in the XML Solution File.</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td></td><td>Threshold value</td><td>Required</td><td>--</td><td>EPSS .01</td></tr>
<tr><td></td><td>Keyword Usage</td><td colspan="3">Optional keyword. By default, the threshold value for species is set to 0.001.</td></tr>
<tr><td></td><td>Reactor Models</td><td colspan="3">• Closed Homogeneous Batch Reactor
• Closed Plasma Reactor
• Diffusion or Premixed Opposed-flow Flame
• Honeycomb Reactor
• IC HCCI Engine
• Perfectly Stirred Reactor (PSR)
• Plasma Plug Flow Reactor
• Plasma PSR
• Plug Flow Reactor
• Premixed Laminar Burner-stabilized Flame
• Premixed Laminar Flame-speed Calculation
• Rotating Disk CVD Reactor
• SI Engine Zonal Simulator
• Stagnation Flow CVD Reactor</td></tr>
<tr><td></td><td>Notes</td><td colspan="3">• This keyword can be added but not removed from a continuation run.</td></tr>
</table>

Keyword	Definition			
EPST Output	Threshold value for the first-order sensitivity coefficients for the gas temperature with respect to the rate constants. Coefficients below this value are neither printed to the diagnostic output file nor saved in the XML Solution File.			
	Parameters	Optional/Reqd.	Units	Examples
	Threshold value	Required	--	EPST **.01**
	Keyword Usage	Optional keyword. By default, the threshold value for gas temperature is set to 0.001.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Honeycomb Reactor • IC HCCI Engine • Perfectly Stirred Reactor (PSR) • Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor • SI Engine Zonal Simulator		
	Notes	• This keyword can be added but not removed from a continuation run.		
EQRX Solver	Specifies that the products from the premixed flame will be estimated by equilibrium calculation with constant enthalpy and pressure in the 2-zone SI Engine simulation. By default, equilibrium calculation is used to obtain gas product composition from the premixed flame.			
	Parameters	Optional/Reqd.	Units	Examples
	--	Optional	--	EQRX
	Keyword Usage	Optional keyword.		
	Reactor Models	• SI Engine Zonal Simulator		
EQUI Reactor Property	Flag indicating that equilibrium composition will be calculated. The chemical state of the statistical event particles will be determined by the corresponding equilibrium states instead of by time integration of the chemical source terms.			
	Keyword Usage	Optional keyword. By default, chemistry is neglected and a mixing-only calculation is performed. See also CHEM.		
	Reactor Models	• Closed Partially Stirred Reactor (PaSR) • Partially Stirred Reactor (PaSR) • SI Engine Zonal Simulator		

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Keyword	Definition			
EQUI Reactor or Inlet Property	Specifies the air/fuel equivalence ratio for an inlet stream or for the initial conditions in a closed reactor.			
	Parameters	Optional/Reqd.	Units	Examples
	Inlet stream name (for open systems only)	Optional If there is no stream name than the air/fuel equivalence ratio applies to the default or all defined streams.	--	EQUI **mixture1** 1.1
	Air / fuel equivalence ratio	Required	--	EQUI **1.1**
	Keyword Usage	Optional keyword. Either REAC or EQUI keywords are required for each inlet stream or to specify the initial conditions of a closed reactor. When EQUI is included, FUEL / OXID / CPROD keywords must also be supplied.		
	Reactor Models	• Closed Homogeneous Batch Reactor • IC HCCI Engine • Perfectly Stirred Reactor (PSR) • Honeycomb Reactor • Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor		
ETCH Reactor Property	Inclusion of this keyword indicates that a given bulk phase is expected to be etched instead of grown or deposited. This option changes the form of the equations to be solved for the bulk phase composition, as described in Bulk Species Equations During Etch of the Chemkin-Pro Theory Manual .			
	Parameters	Optional/Reqd.	Units	Examples
	Bulk phases	Optional Required if there is more than one	--	ETCH **BULK1**

Keyword	Definition			
		bulk phase		
	Reactor number (PSR clusters only)	Optional If no number is given, the keyword is assumed to apply to all reactors in a cluster.	--	ETCH BULK1 **2**
	Keyword Usage	Optional keyword. By default, the names of the unnamed *Surface Kinetics* bulk phases is: BULK1, BULK2, etc.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Honeycomb Reactor • Perfectly Stirred Reactor (PSR) • Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
	Notes	• When the keyword ETCH is supplied for a bulk phase, it is required that bulk activities (see BULK) are also included for each bulk-phase species in that phase that is etched.		
ET-MP Reactor Property	The electron temperature in the reactor. This value is used as the initial estimate of the electron temperature for steady-state iteration (when ENGE is included), or as the initial electron temperature value for transient simulations.			
	Parameters	Optional/Reqd.	Units	Examples
	Electron temperature	Required	K	ETMP **33000.**
	Reactor number (PSR clusters only)	Optional	--	ETMP 33000. **1**

Keyword	Definition			
		If no number is given, values are assumed to apply to all reactors in a cluster.		
	Keyword Usage	Optional keyword. By default, the electron temperature is the same as the gas temperature.		
	Reactor Models	• Closed Plasma Reactor • Plasma PSR • Plasma Plug Flow Reactor		
EXTINCTION Reactor Property	Indicates extinction problem type.			
	Keyword Usage	Required keyword.		
	Reactor Models	• Extinction of Diffusion or Premixed Opposed-flow Flame		
EXT_MAXTFRAC Reactor Property	The fraction multiplying the current T maximum that is used to constrain the flame toward extinction. The extinction simulator finds the location at which T = maximum temperature fraction * (Current maximum temperature — Inlet temperature). Temperature at this location is successively decreased by the user-specified temperature step size until it reaches T = minimum temperature fraction * (Current maximum temperature — Inlet temperature). A new location is then selected using the maximum temperature fraction. This process is repeated until the desired number of steps is reached or until the flame is effectively extinguished.			
	Parameters	Optional/Reqd.	Units	Examples
	Maximum Temperature Fraction	Required	--	EXT_MAXTFRAC **0.8**
	Keyword Usage	Required. The default value is 10.8.		
	Reactor Models	• Extinction of Diffusion or Premixed Opposed-flow Flame		
	Notes	• Also see keyword EXT_MINTFRAC .		
EXT_METHOD Reactor Property	Specifies the type of control technique to be used in extinction simulation.			
	Parameters	Optional/Reqd.	Units	Examples
	BOOLEAN	Required	--	EXT_METHOD **0**

Keyword	Definition			
	Keyword Usage	Optional. By default, the value is 0 which indicates 1-point control. The other possible choice is 1 which indicates 2-point control.		
	Reactor Models	• Extinction of Diffusion or Premixed Opposed-flow Flame		
EXT _MINTFLAME Reactor Property	If the maximum temperature in any solution obtained in the extinction simulation is below this value, the extinction simulator will stop assuming that there is no flame.			
	Parameters	Optional/Reqd.	Units	Examples
	Minimum Flame Temperature	Required	K	EXT_MINTFLAME **1500**
	Keyword Usage	Optional. The default value is 11500.		
	Reactor Models	• Extinction of Diffusion or Premixed Opposed-flow Flame		
	Notes	• This option is useful to avoid computing solutions beyond extinction point.		
EXT _MINTFRAC Reactor Property	The fraction multiplying the current T maximum that is used to constrain the flame toward extinction. The extinction simulator finds the location at which T = maximum temperature fraction * (Current maximum temperature — Inlet temperature). Temperature at this location is successively decreased by the user-specified temperature step size until it reaches T = minimum temperature fraction * (Current maximum temperature — Inlet temperature). A new location is then selected using the maximum temperature fraction. This process is repeated until the desired number of steps is reached or until the flame is effectively extinguished			
	Parameters	Optional/Reqd.	Units	Examples
	Minimum Temperature Fraction	Required	--	EXT_MINTFRAC **0.2**
	Keyword Usage	Required. The default value is 10.2.		
	Reactor Models	• Extinction of Diffusion or Premixed Opposed-flow Flame		
	Notes	• Also see keyword EXT_MAXTFRAC .		
EXT _SAVEINT Reactor Property	Frequency of saving solution in extinction simulation.			
	Parameters	Optional/Reqd.	Units	Examples
	Saving frequency	Required	--	EXT_SAVEINT **10**
	Keyword Usage	Optional. The default value is 10.		
	Reactor Models	• Extinction of Diffusion or Premixed Opposed-flow Flame		
	Notes	• Since extinction problems are numerically intensive, it may be prudent to save solutions frequently. The input value of this keyword indicates the number of solutions are found before an opposed-flow solution is saved in the process of marching towards the extinction point. (A new		

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Keyword	Definition			
		extinction simulation can be started by using the restart facility.).		
EXT _STEPS Reactor Property	Number of times opposed flow solution is computed in search of the extinction point.			
	Parameters	Optional/Reqd.	Units	Examples
	Solution steps	Required	--	EXT_STEPS **100**
	Keyword Usage	Optional. The default value is 100.		
	Reactor Models	• Extinction of Diffusion or Premixed Opposed-flow Flame		
EXT _TSTEP Reactor Property	Temperature step by which temperature at control point is decreased in extinction simulator.			
	Parameters	Optional/Reqd.	Units	Examples
	Temperature step	Required	K	EXT_TSTEP **5**
	Keyword Usage	Optional. Default value is 5.		
	Reactor Models	• Extinction of Diffusion or Premixed Opposed-flow Flame		
EXT _VFCNTRL Reactor Property	Specifies how to constrain nozzle velocities in extinction simulation.			
	Parameters	Optional/Reqd.	Units	Examples
	BOOLEAN	Required	--	EXT_VFCNTRL **1**
	Keyword Usage	Required. The default value is 1 which indicates that momentum of the two jets should be balanced. This creates the stagnation plane in the middle. The other option is 0 which indicates that the magnitude of velocity from both nozzles is the same.		
	Reactor Models	• Extinction of Diffusion or Premixed Opposed-flow Flame		
	Notes	• This option can only be used for 1-point control. For a 2-point control, it is ignored if specified.		

10.2. Alphabetical Listing of Keywords [F-O]

Table 10.2: Alphabetical Listing of Keywords [F-O]

Keyword	Definition	
FAZE Reactor Property	Specifies a fixed-phase constraint on the equilibrium calculation. Species that are initially in the gas phase will remain in the gas phase and species that are originally in a condensed phase (i.e., bulk species) will remain in that condensed phase. If there is only one phase in the chemistry set, the phase constraint has no effect.	
	Keyword Usage	Optional keyword. By default, phase equilibrium as well as composition equilibrium is determined.
	Reactor Models	• Chemical and Phase Equilibrium Calculations

Keyword	Definition			
FIXT Reactor Property	Specifies a fixed-temperature boundary condition on the upper wall (only used for non-symmetric cartesian coordinates).			
	Parameters	Optional/Reqd.	Units	Examples
	Temperature	Optional, if a temperature is not specified, the value of the inlet gas temperature will be used (TINL)	K	FIXT **400**
	Keyword Usage	Optional keyword. By default, a zero temperature gradient is enforced if FIXT is omitted (adiabatic upper wall)		
	Reactor Models	• Planar Shear Flow Reactor		
FLAM Reactor Property	Position and fixed-temperature value for calculating strained, lifted flames. In this case, the inlet gas velocity is calculated (rather than fixed) based on a fixed location of the flame front. The flame front location is specified by giving a location and value of a temperature (above the inlet temperature value) to fix at this position.			
	Parameters	Optional/Reqd.	Units	Examples
	Flame position	Required	cm	FLAM **0.5**700.
	Temperature	Required	K	FLAM 0.5 **700.**
	Keyword Usage	Optional keyword. By default, no temperature is fixed in the calculation.		
	Reactor Models	• Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
FLRT Inlet Property	The mass flow rate into the reactor for an optionally specified inlet stream. For Premixed Laminar Flame calculations, this is mass flux at the inlet (mass flow rate per area) and there is no option for inlet stream name.			
	Parameters	Optional/Reqd.	Units	Examples
	Inlet stream name (Not valid for Premixed Laminar Flames)	Optional If there is no stream name then the mass flow rate	--	FLRT **secondary_air** 0.13

Keyword	Definition			
		applies to the default or to all defined streams.		
	Mass flow rate or Mass flux (for Premixed Laminar Flames)	Required	g/sec g/(cm^2 · sec)	FLRT secondary_air **0.13** FLRT 0.04
	Keyword Usage	**PFRs and Monolith Reactors:** Flow specification via one of VEL, VDOT, VDOTPRO SCCM SCCMPRO FLRT, or FPRO is required. PSRs and PaSRs: Optional keyword. If none of TAU, FLRT/FPRO, SCCM/SCCMPRO are specified or are nonzero, then a closed-system is assumed. FLRT/FPRO or SCCM/SCCMPRO is required for each INLET stream defined. Premixed Laminar Flames: Required keyword. Stagnation Flow CVD Reactors: FLRT / FPRO or SCCM / SCCMPRO or UINL is required for each inlet stream defined. Rotating Disk CVD Reactors: Optional keyword.		
	Reactor Models	• Honeycomb Monolith Reactor • Non-reactive Gas Mixer • Partially Stirred Reactor (PaSR) • Perfectly Stirred Reactor (PSR) • Plasma PFR • Plasma PSR • Plug Flow Reactor • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
FLT_PVSPEC Reactor Property	Species name and its mass-fraction weighting factor to be used in the calculation of the rate-of-progress variable when generating flamelet tables (for premixed flames).			
	Parameters	Optional/Reqd.	Units	Examples
	Species name	Required	--	FLT_PVSPEC **CO2**1.2
	Mass-fraction weighting factor	Required	--	FLT_PVSPEC CO2 **1.2**

<table>
<tr><th>Keyword</th><th colspan="4">Definition</th></tr>
<tr><td></td><td>Keyword Usage</td><td colspan="3">Required keyword when generating flamelet table.</td></tr>
<tr><td></td><td>Reactor Models</td><td colspan="3">• Rotating Disk CVD Reactor
• Stagnation Flow CVD Reactor</td></tr>
<tr><td>FLTB

Output</td><td colspan="4">Export one-dimensional flamelet tables in the standard flamelet format to the specified file. The file will be created in the working directory.</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td></td><td>Flamelet table filename</td><td>Required</td><td>--</td><td>FLTB flamelet.txt</td></tr>
<tr><td></td><td>Keyword Usage</td><td colspan="3">Optional keyword. By default, no flamelet table is exported. The name of the flamelet table file generated is FileName_1.FileExt (where FileName is the user-provided name; FileName= flamelet and FileExt=txt in the example given here.) When continuations are used, the filename is appended with “_n” where n is the continuation number+1 . For extinction studies, the flamelet files are generated based on input “Step Interval for Saving (EXT_SAVEINT)”. Thus, “ _n” in the flamelet filename generated in the extinction study indicates the (total steps/EXT_SAVEINT).</td></tr>
<tr><td></td><td>Reactor Models</td><td colspan="3">• - Opposed-flow Flame Simulator</td></tr>
<tr><td>FLUX

Reactor Property</td><td colspan="4">This keyword indicates that a flux balance will determine the mass fractions of the species at the inlet (rather than a fixed composition). If FLUX is specified, the REAC keywords are used to determine the convective mass flux in, which is balanced against diffusive fluxes to dynamically determine the inlet gas composition. See Equation 14.21 of the Chemkin-Pro Theory Manual .</td></tr>
<tr><td></td><td>Keyword Usage</td><td colspan="3">Optional keyword. By default, a flux balance is solved at the inlet. See also COMP.</td></tr>
<tr><td></td><td>Reactor Models</td><td colspan="3">• Rotating Disk CVD Reactor
• Stagnation Flow CVD Reactor</td></tr>
<tr><td>FLXB

Reactor Property</td><td colspan="4">Use extrapolation to obtain species mass fractions at the outflow (or hot) boundary. By default, PREMIX assumes all species have zero mass fraction gradients at the outflow boundary. However, for pollutant species such as NO, their concentrations are still growing in the post flame region so that their mass fraction profiles have positive gradients at the outflow boundary. The extrapolation boundary condition provides a proper outflow treatment when mass fraction gradients are not zero at the outflow boundary.</td></tr>
<tr><td></td><td>Keyword Usage</td><td colspan="3">Optional keyword. By default, zero mass fraction gradient is used as outflow boundary condition</td></tr>
<tr><td></td><td>Reactor Models</td><td colspan="3">• Premixed Laminar Burner-stabilized Flame
• Premixed Laminar Flame-speed Calculation</td></tr>
</table>

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Keyword	Definition			
FPRO Inlet Property Profiles	Used to specify a transient profile or function of mass flow rate vs. time for an inlet stream. The profile specified will be interpolated linearly from the FPRO points provided.			
	Parameters	Optional/Reqd.	Units	Examples
	Inlet stream name	Optional If there is no stream name then the reactant and mole fraction apply to all streams.	--	FPRO **purge** 0.19 29.0
	Time	Required	sec (cm for flow reactors)	FPRO **0.19**29.0
	Flow rate	Required	g/sec	FPRO 0.19 **29.0**
	Keyword Usage	**PFRs and Monolith Reactors:** Flow specification via one of VEL, VDOT, VDOTPRO SCCM SCCMPRO FLRT, or FPRO is required. PSRs and PaSRs: Optional keyword. If none of TAU, FLRT / FPRO, SCCM / SCCMPRO are specified or are nonzero, then a closed-system is assumed. FLRT / FPRO or SCCM / SCCMPRO is required for each INLET stream defined. Premixed Laminar Flames: Required keyword. Stagnation Flow CVD Reactors: FLRT / FPRO or SCCM / SCCMPRO or UINL is required for each inlet stream defined. Rotating Disk CVD Reactors: Optional keyword.		
	Reactor Models	• Honeycomb Monolith Reactor. • Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Plasma PFR • Plasma PSR • Plug Flow Reactor (PFR) • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		

Keyword	Definition			
FREE Reactor Property	Specifies that the equilibrium species composition will be calculated. See also FROZ.			
	Keyword Usage	Optional keyword. By default, the composition will be calculated.		
	Reactor Models	• Chemical and Phase Equilibrium Calculations		
FREE Reactor Property	Specifies the problem type, which will be to solve for a freely propagating flame to determine flame speed.			
	Keyword Usage	Required keyword.		
	Reactor Models	• Premixed Laminar Flame-speed Calculation		
	Notes	• The problem-type can be changed for a restart run. See also BURN.		
FROZ Reactor Property	Specifies that species composition will be frozen or fixed during the equilibrium calculation. See also FREE.			
	Keyword Usage	Optional keyword. By default, the composition will be calculated.		
	Reactor Models	• Chemical and Phase Equilibrium Calculations		
FUEL Inlet or Reactor Property	Defines the fuel mole fraction composition for an inlet stream in an open system or for the initial conditions in a closed system, when an equivalence ratio is specified (EQUI). It must be followed by a species name and then the mole fraction. One of these FUEL inputs must appear for each fuel species, which are used to determine the inlet composition based on an equivalence-ratio calculation. Any given species can participate simultaneously as a fuel, oxidizer, or product. The sum of all the fuel mole fractions should equal one. If it does not, a warning message will be printed and the mole fractions will be normalized so the sum does equal one.			
	Parameters	Optional/Reqd.	Units	Examples
	Inlet stream name (PSRs only)	Optional If there is no stream name than the fuel mole fraction compassion applies to the default or all defined streams.	--	FUEL **mixture1** C2H2 0.5
	Species name	Required	--	FUEL **C2H2**0.5

Keyword	Definition			
	Fuel fraction	Required	mole fractions	FUEL C2H2 **0.5**
	Keyword Usage	Required keyword when EQUI option is used for an inlet stream or for the initial conditions in a reactor.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Honeycomb Reactor • IC HCCI Engine • Perfectly Stirred Reactor • Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor • SI Engine Zonal Simulator		
	Notes	• The mole fractions are of the fuel itself, not for the entire composition. • The FUEL keywords must be changed as a set, not individually for a restart run. • The FUEL keywords must be changed as a set, not individually for continuation run.		
GASW Reactor Property	Estimated gas-phase mole fractions at the wall boundaries, which may be helpful to aid in convergence. The sum of all the GASW values should equal one. However, if they do not, a cautionary message will be printed and the mole fractions will be normalized so the sum does equal one. The actual gas mole fractions at each wall at the initial condition of the boundary-layer calculation will be calculated via the *Twopnt* procedure (unless the NOTP keyword appears).			
	Parameters	Optional/Reqd.	Units	Examples
	Gas species name	Required	--	GASW **SIH2**1.0E-4
	Mole fraction of gas species	Required	mole fractions	GASW SIH2 **1.0E-4**
	Keyword Usage	Optional keyword. By default, values given by the REAC keyword will be used.		
	Reactor Models	• Cylindrical Shear Flow Reactor • Planar Shear Flow Reactor		
GDOT Reactor Property	This keyword may be used to specify explicitly the net surface production rates of gas-phase species at the substrate, instead of using *Surface Kinetics*. In order to use this option, the *Surface Kinetics* input file must be empty, which means that the number of surface reactions, surface site species and bulk species must all be zero in the *Surface Kinetics* input file.			

Keyword	Definition			
	Parameters	Optional/Reqd.	Units	Examples
	Species name	Required	--	GDOT **H** -1.3E-7
	Net surface production rate	Required	mole/cm^{2}sec	GDOT H **-1.3E-7**
	Keyword Usage	Optional keyword. By default, the net surface production rate is 0.0.		
	Reactor Models	• Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
GEN Output	Controls the printing of general information about the chemistry set. It also controls the printing of summary tables about the reaction thermodynamics. The ALL option produces all of the general information tables. NONE will suppress this output. If only GEN is given on the input line, ALL is assumed (the default). The GEN information is printed by default unless explicitly turned off.			
	Parameters	Optional/Reqd.	Units	Examples
	ALL option	Optional	--	GEN **ALL**
	NONE option	Optional	--	GEN **NONE**
	Keyword Usage	Optional keyword. By default, the table output is determined by the ALL or NONE keyword.		
	Reactor Models	• Mechanism Analyzer		
GFAC Reactor Property	This keyword specifies that the rates of all gas-phase reactions will be multiplied (scaled) by the factor GFAC. This option is sometimes useful if convergence difficulties are encountered due to unusually large reaction rates. Using GFAC, the problem can first be first solved with artificially reduced reaction rates, which then can be increased in subsequent continuations or restarts until GFAC is one. In addition, setting GFAC and SFAC to zero for a perfectly stirred reactor simulation, enables the Non-reactive Gas Mixer Reactor Model.			
	Parameters	Optional/Reqd.	Units	Examples
	Multiplier value	Required	--	GFAC **2.0**
	Reactor number (PSR clusters only)	Optional If no number is given, values are assumed to apply to all reactors in a cluster.	--	GFAC 2.0 **1**
	Keyword Usage	**General**: Optional keyword. By default, the multiplier value is set to 1.0.		

<table>
<tr><th>Keyword</th><th colspan="4">Definition</th></tr>
<tr><td></td><td></td><td colspan="3">Non-reactive Mixer: Required keyword, must be set to 0.0 to enable this Reactor Model.</td></tr>
<tr><td></td><td>Reactor Models</td><td colspan="3">• Closed Homogeneous Batch Reactor
• Closed Plasma Reactor
• Cylindrical Shear Flow Reactor
• Diffusion or Premixed Opposed-flow Flame
• Honeycomb Reactor
• IC HCCI Engine
• Non-reactive Gas Mixer
• Perfectly Stirred Reactor (PSR)
• Planar Shear Flow Reactor
• Plasma Plug Flow Reactor
• Plasma PSR
• Plug Flow Reactor
• Premixed Laminar Burner-stabilized Flame
• Premixed Laminar Flame-speed Calculation
• Rotating Disk CVD Reactor
• SI Engine Zonal Simulator
• Stagnation Flow CVD Reactor</td></tr>
<tr><td>GMHTC

Reactor Property</td><td colspan="4">The reactor wall temperature will be obtained by solving energy conservation equation for the reactor wall. It uses the heat transfer coefficient between the inner wall surface and the gas mixture inside the reactor specified by GMHTC. The initial wall temperature is the surface temperature. When this option is used, all the external heat fluxes, i.e., heat loss to the environment and heat exchange between the reactors in a network, are applied to the wall energy equation instead of the gas phase energy equation. The heat generated by the surface reactions will also be included in the wall energy equation.</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td></td><td>Material name</td><td>Option-al.

If no material is specified,</td><td>--</td><td>GMHTC material10.1</td></tr>
</table>

Keyword	Definition			
		the same value will be used for all materials.		
	Heat transfer coefficient	Required	cal/(cm^2-K-sec)	GMHTC **0.1**
	Reactor number (PSR clusters only)	**Option-al.** If no number is given, the keyword is assumed to apply to all reactors in a cluster.	--	GMHTC material1 0.1 **1**
	Keyword Usage	Optional keyword. This keyword must be used with MMASS . By default, the wall energy equation will not be solved and the reactor wall temperature is equal to the gas temperature in the reactor unless the surface temperature is specified.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Honeycomb Monolith Reactor • IC HCCI Engine • Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Plasma PSR • Plasma Plug Flow Reactor • Plug Flow Reactor • SI Engine Zonal Simulator		
GRAD Reactor Property	Parameter that controls the degree of mesh adaptation based on the maximum first derivative, or gradient in the solution. A reasonable value is usually between about 0.1 and 1.0, where no adaptation based on gradient is specified with 1.0.			
	Parameters	Optional/Reqd.	Units	Examples

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Keyword	Definition			
	Gradient of mesh adaptation	Required	--	GRAD **0.5**
	Keyword Usage	Optional keyword. By default, the gradient is set to 0.1.		
	Reactor Models	• Diffusion or Premixed Opposed-flow Flame • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
	Notes	• This keyword can be changed for a restart or continuation run. • Steady-state 1-D Solution Methods of the Chemkin-Pro Theory Manual for more information.		
GRAV Reactor Property	The value of the acceleration of gravity. The buoyancy term can only be included in the boundary-layer equations if gravity acts parallel to the principal flow direction. Thus, GRAV 980 may be used to describe flow vertically upward, or GRAV -980 for flow downward. Omitting this keyword neglects the buoyancy term.			
	Parameters	Optional/Reqd.	Units	Examples
	Acceleration of gravity	Required	cm/sec^2	GRAV **-980**
	Keyword Usage	Optional keyword. By default, the acceleration of gravity.is zero.		
	Reactor Models	• Cylindrical Shear Flow Reactor • Planar Shear Flow Reactor		
GRID Reactor Property Profiles	Specifies a point on an initial grid. Up to NTOT of these GRID inputs can be included. Each GRID entry contains the spatial coordinate of a mesh point. The GRID keywords are a grouped list and the grid coordinates must appear in ascending order.			
	Parameters	Optional/Reqd.	Units	Examples
	mesh point coordinate	Required	cm	GRID **0.0**
	Keyword Usage	Optional keyword. If no GRID keywords are included, the grid will have equally spaced grid points based on the value of NPTS.		
	Reactor Models	• Diffusion or Premixed Opposed-flow Flame • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation		

<table>
<tr><th>Keyword</th><th colspan="4">Definition</th></tr>
<tr><td></td><td colspan="4">• Rotating Disk CVD Reactor
• Stagnation Flow CVD Reactor</td></tr>
<tr><td>GRXN
Output</td><td colspan="4">Prints out a table of reaction rates and other pertinent information for each gas-phase reaction. The ALL option is the default and produces tables for every gas-phase reaction. The NONE option suppresses output for all of the reactions. If reaction information is desired for only certain reactions, they may be optionally specified by their number (given in the Pre-processor output) or by typing an exact duplicate of the reaction expression (see example input).</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td></td><td>ALL option</td><td>Optional, default is ALL</td><td>--</td><td>GRXN ALL</td></tr>
<tr><td></td><td>NONE option</td><td>Optional, default is ALL</td><td>--</td><td>GRXN NONE</td></tr>
<tr><td></td><td>Gas reaction number list</td><td>Optional, default is ALL</td><td>--</td><td>GRXN 2 5</td></tr>
<tr><td></td><td>Gas reaction expression</td><td>Optional, default is ALL</td><td>--</td><td>GRXN CH4+H<=>CH3+H2</td></tr>
<tr><td></td><td>Keyword Usage</td><td colspan="3">Optional keyword. By default, the table output is determined by the ALL or NONE keyword.</td></tr>
<tr><td></td><td>Reactor Models</td><td colspan="3">• Mechanism Analyzer</td></tr>
<tr><td>GTHB
Output</td><td colspan="4">Create an extra table of the reaction rates for those reactions that involve third bodies. This option employs the bath-gas composition (specified by the XBTH keyword) to yield effective reaction rates. The ALL option is the default and produces tables for every gas-phase reaction. The NONE option suppresses output for all of the reactions. If reaction information is desired for only certain reactions, they may be optionally specified by their number (given in the Pre-processor output) or by typing an exact duplicate of the reaction expression (see example input).</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td></td><td>ALL option</td><td>Optional, default is ALL</td><td>--</td><td>GTHB ALL</td></tr>
<tr><td></td><td>NONE option</td><td>Optional, de-</td><td>--</td><td>GTHB NONE</td></tr>
</table>

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Keyword	Definition			
		fault is ALL		
	Gas reaction number list	**Optional, default is ALL**	--	GTHB **2 5**
	Gas reaction expression	**Optional, default is ALL**	--	GTHB **2H+M<=>H2+M**
	Keyword Usage	Optional keyword. By default, the table output is determined by the ALL or NONE keyword.		
	Reactor Models	• Mechanism Analyzer		
GVEL Reactor Property	Activate the Woschni correlation for the average cylinder gas velocity. This keyword can only be used in conjunction with the ICHT keyword. Internal Combustion Engine Model of the Chemkin-Pro Theory Manual .			
	Parameters	Optional/Reqd.	Units	Examples
	C_{11} *in the average gas velocity correlation*	Required	--	GVEL **2.28** 0.308 0.324 0
	C_{12} *parameter in the Woschni correlation*	Required	cm/(sec · K)	GVEL 2.28 **0.308** 0.324 0
	C_{2} *parameter in the Woschni correlation*	Required		GVEL 2.28 0.308 **0.324** 0
	Ratio of swirl velocity to mean piston speed	Required	--	GVEL 2.28 0.308 0.324 **0**
	Keyword Usage	Optional keyword. By default, the setting is GVEL 1 0 0 0.		
	Reactor Models	• IC HCCI Engine • SI Engine Zonal Simulator		
HITE Reactor Property	The channel height (for cartesian coordinates), or the reactor radius (cylindrical coordinates), or distance between the channel wall and the symmetry line for a symmetric planar channel.			
	Parameters	Optional/Reqd.	Units	Examples
	Channel height or radius	Required	cm	HITE **2.0**
	Keyword Usage	Required keyword.		
	Reactor Models	• Cylindrical Shear Flow Reactor		

<table>
<tr><th>Keyword</th><th colspan="4">Definition</th></tr>
<tr><td></td><td></td><td colspan="3">• Planar Shear Flow Reactor</td></tr>
<tr><td rowspan="5">H0

Solver</td><td colspan="4">The initial distance step size used by the transient solver.</td></tr>
<tr><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td>Initial time step size</td><td>Required</td><td>cm</td><td>H0 1.0E-4</td></tr>
<tr><td>Keyword Usage</td><td colspan="3">Optional keyword. By default, the initial time step size is set to 1.0E-6.</td></tr>
<tr><td>Reactor Models</td><td colspan="3">• Cylindrical Shear Flow Reactor

• Planar Shear Flow Reactor</td></tr>
<tr><td rowspan="4">HP

Problem Type</td><td colspan="4">Constant pressure and enthalpy constraints.</td></tr>
<tr><td>Keyword Usage</td><td colspan="3">Optional keyword. Exactly one problem type keyword must be included.</td></tr>
<tr><td>Reactor Models</td><td colspan="3">• Chemical and Phase Equilibrium Calculations</td></tr>
<tr><td>Notes</td><td colspan="3">• PH keyword is equivalent.</td></tr>
<tr><td rowspan="6">HSEN

Output</td><td colspan="4">Calculate the first-order, heat-of-formation sensitivity coefficients (i.e., with respect to the gas-phase and surface species heats of formation) for species fractions and for other dependent variables in the system. Sensitivity results will be included in the XML Solution File.</td></tr>
<tr><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td>String indicating for which variables sensitivity coefficients will be saved or printed. The string is a space-delimited list containing species names and any one of the following: ALL, AVEL, RVEL, CVEL, FLRT, or TEMP (see Notes)</td><td>Optional

If no string is given, then ALL is assumed.</td><td>--</td><td>HSEN OH

HSEN TEMP</td></tr>
<tr><td>Keyword Usage</td><td colspan="3">Optional keyword. By default, no sensitivity coefficients are computed or printed.</td></tr>
<tr><td>Reactor Models</td><td colspan="3">• Diffusion or Premixed Opposed-flow Flame

• Premixed Laminar Burner-stabilized Flame

• Premixed Laminar Flame-speed Calculation

• Rotating Disk CVD Reactor

• Stagnation Flow CVD Reactor</td></tr>
</table>

Keyword	Definition			
	Notes	• This keyword can be added but not removed from a continuation or restart run • See also EPSS, EPSG, EPST, SENG, and HSEN for other sensitivity options The optional parameter strings are defined as follows: • ALL: all species and all other dependent variables in the solution • AVEL: axial velocity (Plug Flow, Diffusion or Premixed Opposed-flow Flames, Rotating Disk, and Stagnation Flow CVD Reactors only) • CVEL: circumferential velocity (Rotating Disk and Stagnation Flow CVD Reactors only) • RVEL: radial velocity (Diffusion or Premixed Opposed-flow Flames, Rotating Disk, and Stagnation Flow CVD Reactors only) • FLRT: mass flow rate (Premixed Laminar Flame-speed Calculation only) • TEMP: gas temperature		
HSWC Reactor Property	Specifies the crank angle when the entire wall heat loss will be switched from the unburned zone to the burned zone. HSWM , HSWT , and HSWC are mutually exclusive.			
	Parameters	Optional/Reqd.	Units	Examples
	Crank angle	Required	degree	HSWC **-0.4**
	Keyword Usage	Optional keyword.		
	Reactor Models	• SI Engine Zonal Simulator		
HSWT Reactor Property	Specifies the burned mass fraction value at which the entire wall heat loss will be switched from the unburned zone to the burned zone. HSWM , HSWT , and HSWC are mutually exclusive.			
	Parameters	Optional/Reqd.	Units	Examples
	Temperature	Required	K	HSWM **0.05**
	Keyword Usage	Optional keyword.		
	Reactor Models	• SI Engine Zonal Simulator		
HSWM Reactor Property	Specifies the burned mass fraction value at which the entire wall heat loss will be switched from the unburned zone to the burned zone. HSWM , HSWT , and HSWC are mutually exclusive.			
	Parameters	Optional/Reqd.	Units	Examples

Keyword	Definition			
	Burned mass fraction	Required	--	HSWM **973.15**
	Keyword Usage	Optional keyword.		
	Reactor Models	• SI Engine Zonal Simulator		
HTC Reactor Property	The overall, per-area, heat-transfer coefficient for convective or conductive heat transfer out of the system. This keyword is only relevant when the energy equation is being solved.			
	Parameters	Optional/Reqd.	Units	Examples
	Material name	**Optional.** If no material is specified, the same value will be used for all materials.	--	HTC **material1** 1.E-4
	Heat transfer coefficient	Required	cal/(cm^2-K-sec)	HTC material1 **1.E-4**
	Reactor number (PSR clusters only)	**Optional.** If no number is given, the keyword is assumed to apply to all reactors in a cluster.	--	HTC material1 1.E-4 **1**
	Keyword Usage	Optional keyword. This keyword must be used with TAMB. By default, the heat loss from the reactor will be zero. See also QLOS and QPRO .		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Honeycomb Monolith Reactor • Non-reactive Gas Mixer		

<table>
<tr><th>Keyword</th><th colspan="4">Definition</th></tr>
<tr><td></td><td colspan="4">Perfectly Stirred Reactor (PSR)
Plasma PSR
Plasma Plug Flow Reactor
Plug Flow Reactor</td></tr>
<tr><td>HTRN

Reactor Property</td><td colspan="4">The heat transfer coefficient and ambient temperature for specification of the heat loss from the reactor along the external surface area, at an optionally specified surface material. This keyword is only relevant when the energy equation is being solved.</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td></td><td>Material name (0-D and Plug Flow systems only)</td><td>Optional

If no material is specified, the same value will be used for all materials.</td><td>--</td><td>HTRN material1 1.E-4 298</td></tr>
<tr><td></td><td>Heat transfer coefficient</td><td>Required</td><td>cal/(cm^2. K . sec)</td><td>HTRN 1.E-4 298

HTRN 1.E-4</td></tr>
<tr><td></td><td>Ambient temperature (0-D and Plug Flow systems only)</td><td>Required</td><td>K</td><td>HTRN 1.E-4 298</td></tr>
<tr><td></td><td>Reactor number (PSR clusters only)</td><td>Optional

If no number is given, the keyword is assumed to apply to all reactors in a cluster.</td><td>--</td><td>HTRN material1 1.E-4 298 1</td></tr>
<tr><td></td><td>Keyword Usage</td><td colspan="3">Optional keyword. By default, the heat loss from the reactor will be zero. See also QLOS and QPRO.</td></tr>
<tr><td></td><td>Reactor Models</td><td colspan="3">Closed Homogeneous Batch Reactor</td></tr>
</table>

<table>
<tr><th>Keyword</th><th colspan="4">Definition</th></tr>
<tr><td></td><td colspan="4">Closed Plasma Reactor
Cylindrical Shear Flow Reactor
Honeycomb Reactor
Non-reactive Gas Mixer
Perfectly Stirred Reactor (PSR)
Planar Shear Flow Reactor
Plasma Plug Flow Reactor
Plasma PSR
Plug Flow Reactor</td></tr>
<tr><td>ICEN

Reactor Property</td><td colspan="4">The transient IC HCCI Engine model will be implemented. The solution will be obtained with the volume as a function of time, where the function of time is determined by an engine model that defines the volume as a function of user-specified engine parameters. The equations solved are those of a specified volume function of time, but the user does not need to provide a subroutine or volume vs. time profile for this calculation. This problem type is only allowed for closed (zero flow-rate) systems.</td></tr>
<tr><td></td><td>Keyword Usage</td><td colspan="3">Optional keyword. By default, a constant pressure, constant volume, steady-state problem is assumed.</td></tr>
<tr><td></td><td>Reactor Models</td><td colspan="3">IC HCCI Engine</td></tr>
<tr><td></td><td>Notes</td><td colspan="3">See also: CMPR, VOLC, RPM, and LOLR keywords.
SI Engine Zonal Simulator</td></tr>
<tr><td>ICHT

Reactor Property</td><td colspan="4">Convective heat transfer correlation for the transient IC HCCI Engine model, using the following generalized convective heat transfer correlation: $\mathrm{Nu}_h = a\mathrm{Re}^b\mathrm{Pr}^c$. Where Nu_h is the Nusselt number for heat transfer, Re is the Reynolds number, and Pr is the Prandtl number. For more information on the usage of these parameters, see Internal Combustion Engine Model of the Chemkin-Pro Theory Manual .</td></tr>
<tr><td></td><td colspan="4"><table>
<tr><th>Parameters</th><th>Optional/Reqd.</th><th>Units</th><th>Examples</th></tr>
<tr><td>The value a in heat transfer correlation</td><td>Required</td><td>dimensionless</td><td>ICHT .035.5 .33 10. 350.</td></tr>
<tr><td>The value b in heat transfer correlation</td><td>Required</td><td>dimensionless</td><td>ICHT .035 .5.33 100 350.</td></tr>
<tr><td>The value c in heat transfer correlation</td><td>Required</td><td>dimensionless</td><td>ICHT .035 .5 .33 10. 350.</td></tr>
<tr><td>Bore diameter</td><td>Required</td><td>cm</td><td>ICHT .0350.5 .33 10. 350.</td></tr>
</table></td></tr>
</table>

Keyword	Definition			
	Wall temperature	Required	K	ICHT .035 .5 .33 10. **350.**
	Keyword Usage	Optional keyword. By default, an adiabatic (zero heat loss) condition is assumed. See also GVEL for Woschni correlation extensions.		
	Reactor Models	• IC HCCI Engine • SI Engine Zonal Simulator		
ICRD Reactor Model or Reactor Property	Flag to specify coordinate system, which determines the Reactor Model and symmetry assumptions for shear-layer flow.			
	Parameters	Optional/Reqd.	Units	Examples
	Coordinate flag indicating Planar Shear Flow Reactor, with, non-symmetric boundary conditions	Required	--	ICRD **PLAN**
	Coordinate flag indicating Planar Shear Flow Reactor, assuming symmetry with respect to the center axis	Required	--	ICRD **SYMC**
	Coordinate flag indicating Cylindrical Shear Flow Reactor, using radial coordinates	Required	--	ICRD **RAD**
	Keyword Usage	Required keyword.		
	Reactor Models	• Cylindrical Shear Flow Reactor • Planar Shear Flow Reactor		
	Notes	• Only one-half of the physical domain is used for the radial or symmetric channel case, and the lower boundary is the symmetry line		
IEM Reactor Property	Flag indicating that the interaction-by-exchange-with-the-mean (IEM) model will be used to simulate the molecular mixing within the computational particle.			
	Keyword Usage	Optional keyword. By default, a well mixed model is assumed.		
	Reactor Models	• Closed Partially Stirred Reactor (PaSR) • Partially Stirred Reactor (PaSR)		

Keyword	Definition			
IGRIDMETHOD_n Reactor Property	Choice for the initial grid profile. Integer *n* can be 1, 2, or 3 and mean uniform grid, biased grid, and read from an input file, respectively. In general, the uniform grid is not very useful and a biased grid should be used. The bias is created with respect to the location of the stoichiometric mixture fraction.			
	Keyword Usage	Required keyword. The default value is IGRIDMETHOD_2, indicating a biased grid.		
	Reactor Models	• Diffusion Flamelet Generator		
INIT Reactor Property	The initial gas mole fraction of the given species in the reactor for a transient simulation. There may be as many INIT lines as there are species in the problem.			
	Parameters	Optional/Reqd.	Units	Examples
	Species name	Required	--	INIT **N2**0.79
	Gas fraction	Required	Mole fraction	INIT N2 **0.79**
	Keyword Usage	Optional keyword. By default, if no INIT entries are made, the inlet gas properties will be used. When some INIT entries are present, species not explicitly entered are taken as having a mole fraction of 0.		
	Reactor Models	• Closed Partially Stirred Reactor (PaSR) • Partially Stirred Reactor (PaSR) • Normal Incident Shock • Normal Reflected Shock • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
INJM Reactor Property	Total mass flow rate of the injected gas. See Equation 14.5 of the Chemkin-Pro Theory Manual .			
	Parameters	Optional/Reqd.	Units	Examples
	Mass flow rate	Required	$g/(cm^2 \cdot sec)$	INJM **0.15**
	Keyword Usage	Required keyword when INJS is used; otherwise it is ignored.		
	Reactor Models	• Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
INJS Reactor Property	Injection of gas species at a location along the axis of symmetry can be included using one or more INJS keywords. The injection is specified as a spatially distributed Gaussian source. INJM is the total mass flow, i.e., the spatial integral of the mass flow function. This source term will be added to Equation 14.5 of the Chemkin-Pro Theory Manual . INJS specifies the species composition of the injected flow, in mole fractions.			

Keyword	Definition			
	Parameters	Optional/Reqd.	Units	Examples
	Species name	Required	--	INJS **H2**0.5
	Species composition	Required	mole fractions	INJS H2 **0.5**
	Keyword Usage	Optional keyword. By default, there is no mass injection along the flow axis.		
	Reactor Models	• Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
INJT Reactor Property	Temperature of the injected gas.			
	Parameters	Optional/Reqd.	Units	Examples
	Temperature	Required	K	INJT **300.**
	Keyword Usage	Optional keyword. By default, no enthalpy is added to the energy equation with the injected gas. If INJS is not included, this keyword will be ignored.		
	Reactor Models	• Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
INJW Reactor Property	Half-width of the Gaussian gas-injection source. See Equation 14.5 of the Chemkin-Pro Theory Manual .			
	Parameters	Optional/Reqd.	Units	Examples
	Half-width	Required	cm	INJW **0.07**
	Keyword Usage	Optional keyword. By default, the width is 0.0. Keyword is ignored unless INJS is present.		
	Reactor Models	• Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
INJX Reactor Property	Height above the disk which is the center of the Gaussian-shaped injection source. See Equation 14.5 of the Chemkin-Pro Theory Manual .			
	Parameters	Optional/Reqd.	Units	Examples
	Height	Required	cm	INJX **0.6**
	Keyword Usage	Optional keyword. By default, the height is 0.0. Keyword is ignored unless INJS is present.		
	Reactor Models	• Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
INLET Reactor Property	Specification of a reactor inlet stream. Specify an optional name for the stream and a reactor number. For each INLET stream defined, you must also specify the corresponding inlet temperature (TINL), composition (REAC), or set of EQUI / OXID / FUEL / CPROD / ADD), and flow rate (FLRT or SCCM).			
	Parameters	Optional/Reqd.	Units	Examples

Keyword	Definition			
	Inlet stream name	Required	--	INLET **secondary_air**2
	Reactor number (PSR clusters only)	Optional If no number is given, values are assumed to apply to all reactors in a cluster.	--	INLET secondary_air **2**
	Keyword Usage	Optional keyword. If no streams are defined, the program will assume there is a single inlet for the first reactor in series or that the system is a single closed reactor (if FLRT, SCCM and TAU are not defined).		
	Reactor Models	• Diffusion or Premixed Opposed-flow Flame • Non-reactive Gas Mixer • Partially Stirred Reactor (PaSR) • Perfectly Stirred Reactor (PSR) • Plasma PSR • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
	Notes	• This keyword can not be changed for a restart or continuation run.		
INTM Reactor Property	The estimated peak mole fractions values for "intermediate" species. One of these INTM inputs should appear for each intermediate species desired. It is usually better to estimate values somewhat higher than those that are actually present in the flame. For example, INTM HO2 0.001 gives an estimate fraction of 0.001 for the intermediate HO2. Any given species can participate simultaneously as a reactant, intermediate, or product.			
	Parameters	Optional/Reqd.	Units	Examples
	Species name	Required	--	INTM **HO2**0.001
	Estimated fraction	Required	mole fraction	INTM HO2 **0.001**
	Keyword Usage	Optional keyword. By default, the estimated fraction is set to 0 unless the user has set a minimum threshold to a non-zero value on the Reactor panel (see XIMN to set a non-zero threshold value).		

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<table>
<tr><th>Keyword</th><th colspan="4">Definition</th></tr>
<tr><td></td><td>Reactor Models</td><td colspan="3">• Premixed Laminar Burner-stabilized Flame
• Premixed Laminar Flame-speed Calculation
• Rotating Disk CVD Reactor
• Stagnation Flow CVD Reactor</td></tr>
<tr><td></td><td>Notes</td><td colspan="3">• See Starting Estimates of the Chemkin-Pro Theory Manual for more information.</td></tr>
<tr><td>IONE

Reactor Property</td><td colspan="4">Specified energy loss to ions in the sheath for each ion lost at a specified material. The energy that the ions gain in the sheath is specified in electron Volts. For example, “IONE material1 30” would result in an ion energy gain of 30 eV as it crossed the sheath near the material material1. This energy gain for the ions results in a reduced effective power deposition to the electrons (unless ELSH is also specified), as described in Electron Energy Equation for Plasma Systems of the Chemkin-Pro Theory Manual .</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td></td><td>Material name</td><td>Optional

If there is no material name than the specified energy loss applies to all materials.</td><td>--</td><td>IONE material1 30 1</td></tr>
<tr><td></td><td>Specified energy loss</td><td>Required</td><td>eV</td><td>IONE 30</td></tr>
<tr><td></td><td>Reactor number (PSR clusters only)</td><td>Optional

If no number is given, values are assumed to apply to all reactors in a cluster.</td><td>--</td><td>IONE material1 30 1</td></tr>
<tr><td></td><td>Keyword Usage</td><td colspan="3">Optional keyword. By default, the ion energy is determined by the ELSH keyword.</td></tr>
</table>

<table>
<tr><th>Keyword</th><th colspan="4">Definition</th></tr>
<tr><td></td><td>Reactor Models</td><td colspan="3">• Closed Plasma Reactor
• Plasma Plug Flow Reactor
• Plasma PSR</td></tr>
<tr><td>IPSR

XMLI</td><td colspan="4">Use this keyword to specify which PSR to use for the initialization (XMLI), when more than one PSR is stored on the XML Solution File that is used for initialization (i.e. on XMLdata.zip).</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td></td><td>PSR number</td><td>Required</td><td>--</td><td>IPSR 2</td></tr>
<tr><td></td><td>Keyword Usage</td><td colspan="3">Optional keyword. By default, the last PSR saved in the XML Solution File is used.</td></tr>
<tr><td></td><td>Reactor Models</td><td colspan="3">• Chemical and Phase Equilibrium Calculations
• Closed Homogeneous Batch Reactor
• Closed Plasma Reactor
• Cylindrical Shear Flow Reactor
• Diffusion or Premixed Opposed-flow Flame
• Honeycomb Reactor
• IC HCCI Engine
• Mechanism Analyzer
• Non-reactive Gas Mixer
• Normal Incident Shock
• Normal Reflected Shock
• Perfectly Stirred Reactor (PSR)
• Planar Shear Flow Reactor
• Plasma Plug Flow Reactor
• Plasma PSR
• Plug Flow Reactor
• Premixed Laminar Burner-stabilized Flame
• Premixed Laminar Flame-speed Calculation
• Rotating Disk CVD Reactor
• SI Engine Zonal Simulator</td></tr>
</table>

Keyword	Definition			
		• Stagnation Flow CVD Reactor		
IRET Solver	Number of time steps to be taken in *Twopnt*'s pseudo time stepping algorithm before increasing the time step.			
	Parameters	Optional/Reqd.	Units	Examples
	Number of time steps	Required	--	IRET **200**
	Keyword Usage	Optional keyword. By default, the number of times steps is set to 25 or 50 depending on the Reactor Model (See Notes below).		
	Reactor Models	• Cylindrical Shear Flow Reactor • Diffusion or Premixed Opposed-flow Flame • Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Plasma PSR • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
	Notes	• Default value is 25 for PSRs and 50 for all other reactors listed above.		
ISHK Problem Type	Inclusion of this keyword designates an incident shock problem without boundary layer correction.			
	Keyword Usage	Required keyword. Either ISHK or ISKB must be included to indicate a Normal Incident Shock problem type. See also RSHK.		
	Reactor Models	• Normal Incident Shock		
ISKB Problem Type	Inclusion of this keyword designates an incident shock problem with boundary layer correction.			
	Keyword Usage	Required keyword. Either ISHK or ISKB must be included to indicate a Normal Incident Shock problem type. See also RSHK.		
	Reactor Models	• Normal Incident Shock		
ISTP	specifies the number of initial pseudo time steps that are taken by the steady-state TWOPNT solver, prior to attempting a Newton iteration. Normally, the Newton			

<table>
<tr><th>Keyword</th><th>Definition</th></tr>
<tr><td>Solver</td><td>iteration will be attempted first, with time steps invoked only if the Newton iteration fails. Nevertheless, there may be circumstances where initial time stepping is desirable. The time step size is specified with the TIM1 or TIM2 keyword. The ISTP keyword only applies to the first grid network, not the subsequently refined ones. If need to find a steady state solution via pure time integration, please refer to the TRAN option.
<table>
<tr><th>Parameters</th><th>Optional/Reqd.</th><th>Units</th><th>Examples</th></tr>
<tr><td>Number of initial time steps</td><td>Required</td><td>--</td><td>ISTP 100</td></tr>
<tr><td>Keyword Usage</td><td colspan="3">Optional keyword. By default, the number of initial time steps is set to 0.</td></tr>
<tr><td>Reactor Models</td><td colspan="3">• Cylindrical Shear Flow Reactor
• Diffusion or Premixed Opposed-flow Flame
• Non-reactive Gas Mixer
• Perfectly Stirred Reactor (PSR)
• Planar Shear Flow Reactor
• Plasma PSR
• Premixed Laminar Burner-stabilized Flame
• Premixed Laminar Flame-speed Calculation
• Rotating Disk CVD Reactor
• Stagnation Flow CVD Reactor</td></tr>
</table></td></tr>
<tr><td>JJRG

Restart</td><td>On continuations or restarts, the number of mesh points can be reduced. Twopnt itself does not remove grid points. Therefore, on a sequence of continuation problems the number of grid points can grow because the region where they are needed may change. JJRG thus provides a capability to remove grid points. The old solution is adaptively interpolated onto a new grid of JJRG points. When JJRG is added, its effect is carried over to the subsequent continuations, if any. Often this is not desired. To prevent its operation, JJRG can be set to a high value, such as the maximum number of grid-points. The reduction of grid points then does not happen since JJRG does not add grid-points.
<table>
<tr><th>Parameters</th><th>Optional/Reqd.</th><th>Units</th><th>Examples</th></tr>
<tr><td>Number of mesh points</td><td>Required</td><td>--</td><td>JJRG 40</td></tr>
<tr><td>Keyword Usage</td><td colspan="3">Optional keyword. By default, the number of grid points will be the same as in the previous solution.</td></tr>
<tr><td>Reactor Models</td><td colspan="3">• Diffusion or Premixed Opposed-flow Flame
• Premixed Laminar Burner-stabilized Flame
• Premixed Laminar Flame-speed Calculation</td></tr>
</table></td></tr>
</table>

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Keyword	Definition			
		• Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
KLIM Output	Calculate the ignition delay as the time when the fraction of the specified species reaches its maximum value. Only applicable when you are solving the energy equation with transient solver.			
	Parameters	Optional/Reqd.	Units	Examples
	Species name	Required	--	KLIM **OH**
	Keyword Usage	Optional keyword. See also TIFP .		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Honeycomb Monolith Reactor • IC HCCI Engine • Perfectly Stirred Reactor (PSR) • Plasma PSR • Plasma Plug Flow Reactor • Plug Flow Reactor • SI Engine Zonal Simulator		
KNMN Reactor Property	The minimum Knudsen number, above which the wall slip-velocity model will be used.			
	Parameters	Optional/Reqd.	Units	Examples
	Minimum Knudsen number	Required	--	KNMN **10**
	Keyword Usage	Optional keyword. It is relevant only when the slip velocity model is used. See also SLIP .		
	Reactor Models	• Cylindrical Shear Flow Reactor • Planar Shear Flow Reactor		
KOUT Output	List of species names whose mass fractions will be printed to the diagnostic output file for Premixed or Opposed-flow Flames or to the *history.plt* file for PaSRs. A maximum number of 5 species can be included on a single line.			
	Parameters	Optional/Reqd.	Units	Examples
	List of species names	Required	--	KOUT **H2 O2 H2O H OH**
	Keyword Usage	Optional keyword. By default, none of the species fractions are printed.		
	Reactor Models	• Diffusion or Premixed Opposed-flow Flame		

<table>
<tr><th>Keyword</th><th colspan="4">Definition</th></tr>
<tr><td></td><td></td><td colspan="3">• Closed Partially Stirred Reactor (PaSR)
• Partially Stirred Reactor (PaSR)
• Premixed Laminar Burner-stabilized Flame
• Premixed Laminar Flame-speed Calculation</td></tr>
<tr><td rowspan="5">LG-DT

Solver</td><td colspan="4">Controls the time interval for data to be written to the XML Solution File (e.g., XMLdata.zip) using a logarithmic time scale.</td></tr>
<tr><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td>Logarithmic time-step</td><td>Required</td><td>ALOG10(sec)</td><td>LGDT 1.0</td></tr>
<tr><td>Keyword Usage</td><td colspan="3">Optional keyword. If neither DTSV nor LGDT are set, then the time step used is ending time minus the beginning time, divided by 100.</td></tr>
<tr><td>Reactor Models</td><td colspan="3">• Normal Incident Shock
• Normal Reflected Shock</td></tr>
<tr><td rowspan="3">LINE

Reactor Property</td><td colspan="4">An indicator that a linear profile is used for the initial gas species distribution along the reactor center line. For Opposed-flow Flames, the mole fractions vary linearly from one inlet to the other, with inlet values forming the end points. For transient CVD Reactors, the mole fractions vary linearly from the inlet values, specified by keyword REAC, to the INIT value at the surface.</td></tr>
<tr><td>Keyword Usage</td><td colspan="3">Optional keyword. By default, a plateau profile is used for Opposed-flow Flames (PLAT). For transient CVD Reactors, the default initial gas species profiles are assumed axially uniform with mole fractions specified by INIT ; the keyword is ignored for steady-state CVD Reactor simulations.</td></tr>
<tr><td>Reactor Models</td><td colspan="3">• Rotating Disk CVD Reactor
• Stagnation Flow CVD Reactor</td></tr>
<tr><td rowspan="5">LO-DR

Reactor Property</td><td colspan="4">Piston offset to crank radius ratio.</td></tr>
<tr><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td>Ratio of piston offset to crank radius.</td><td>Required</td><td>None</td><td>LODR 0.1</td></tr>
<tr><td>Keyword Usage</td><td colspan="3">Optional keyword. Default = 0.0.</td></tr>
<tr><td>Reactor Models</td><td colspan="3">• IC HCCI Engine
• Multi-zone HCCI Engine
• SI Engine Zonal Simulator</td></tr>
</table>

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Keyword	Definition			
	Notes	• The absolute value of LODR must be less than the value of LOLR minus 1.0: |LODR| < (LOLR - 1).		
LOLR Reactor Property	Ratio of the length of the engine connecting rod to the crank radius.			
	Parameters	Optional/Reqd.	Units	Examples
	Connection rod to crank radius ratio	Required	--	LOLR **5.**
	Keyword Usage	Optional keyword. By default, this ratio is 33.3.		
	Reactor Models	• IC HCCI Engine • SI Engine Zonal Simulator		
LPRT Output	Printing control LPRT turns on extensive printing that provides information on rates of progress of individual surface reactions. This can be informative in understanding the surface reaction behavior.			
	Keyword Usage	Optional keyword. By default, there is no extended printing of surface rate information.		
	Reactor Models	• Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
LSCL Reactor Property	Sets the length scale (cm) for the calculation of gas and surface Damkohler numbers.			
	Parameters	Optional/Reqd.	Units	Examples
	Length scale	Required	cm	LSCL **3.**
	Keyword Usage	Optional keyword. By default, the length scale is 1 cm.		
	Reactor Models	• Mechanism Analyzer		
LUMP-TO Reactor Property	This is an optional approach to species mass conservation closure. In this case, the selected species is assumed to be a diluent and its fraction is set to one minus the sum of all others			
	Parameters	Optional/Reqd.	Units	Examples
	Species name	Required	--	LUMPTO AR
	Keyword Usage	Optional keyword.		
	Reactor Models	• Cylindrical Shear Flow Reactor • Planar Shear Flow Reactor		
MAJ Reactor Property	Sets the "Major Species". This is only used to calculate an effective diffusion coefficient when non-dimensionalizing the reaction rate constants.			
	Parameters	Optional/Reqd.	Units	Examples
	Species name	Optional	--	MAJ **CH4**
	Species number	Optional	--	MAJ **1**

Keyword	Definition			
	Keyword Usage	Optional keyword. The default is to use the gas species with the second largest mole fraction (from the XBTH input) in the bath-gas composition. If the gas-phase bath-gas composition is not specified, the default is to use the second species in the mechanism.		
	Reactor Models	• Mechanism Analyzer		
MAXIT Solver	Controls the maximum number of iterations the integrator solver can take per step to solve the transient problem. The default is 4 and you should increase this value to give the integrator greater chance to solve your problem if it is very hard to solve (stiff or very nonlinear or discontinuous) or if the run fails with a "nonlinear solver failed to converge repeatedly" message.			
	Parameters	Optional/Reqd.	Units	Examples
	Iteration number	Required	--	MAXIT 10
	Keyword Usage	Optional keyword.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Partially Stirred Reactor • Closed Plasma Reactor • Cylindrical Shear Flow Reactor • Honeycomb Reactor • IC HCCI Engine • Multi-Zone HCCI Engine Simulator • Partially Stirred Reactor (PaSR) • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor • Rotating Disk CVD Reactor • SI Engine Zonal Simulator • Stagnation Flow CVD Reactor			
MAX-TIME Solver	The maximum number times the steady state solver TWOPNT will use its pseudo-time stepping algorithm. You may need to increase this value for very stiff problems to allow TWOPNT to find a solution by letting it switch between steady state searching and time stepping more than 100 times.			

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Keyword	Definition			
	Parameters	Optional/Reqd.	Units	Examples
	Maximum steady state iterations	Optional	--	MAXTIME **200**
	Keyword Usage	Optional keyword. By default, the maximum number of time stepping operations is 100.		
	Reactor Models	• Cylindrical Shear Flow Reactor • Diffusion or Premixed Opposed-flow Flame • Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma PSR • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
	Notes	• SSMAXITER must be >=1.		
MCUT Reactor Property	Minimum number of particles required to "switch on" the surface rate calculations (coagulation and surface reaction). The default value is 1 [particles/cm^3].			
	Parameters	Optional/Reqd.	Units	Examples
	Material name	Required	--	MCUT **C(B)** 100
	Cutoff number density	Required	particles/cm^3	MCUT C(B) **100**
	Keyword Usage	Optional keyword.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Cylindrical Shear Flow Reactor • Honeycomb Monolith Reactor • IC HCCI Engine • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma PSR		

Keyword	Definition			
		• Plasma Plug Flow Reactor • Plug Flow Reactor • SI Engine Zonal Simulator		
MIX Reactor Property	Use a mixture-average model for calculating the transport coefficients and diffusion fluxes.			
	Keyword Usage	Optional keyword. By default, mixture-averaged transport is used.		
	Reactor Models	• Cylindrical Shear Flow Reactor • Diffusion or Premixed Opposed-flow Flame • Planar Shear Flow Reactor • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
MIX Reactor Property	Flag indicating a mixing-only problem, where chemistry will be ignored.			
	Keyword Usage	Optional keyword. This is the default. See also CHEM and EQUI.		
	Reactor Models	• Closed Partially Stirred Reactor (PaSR) • Partially Stirred Reactor (PaSR)		
MIX-FRAC-BI-AS_FUEL Reactor Property	Bias factor for the grid on the fuel side, that is, between the mixture fraction equal to its stoichiometric mixture fraction and 1. A value greater than unity should be given and it means more grid points near the stoichiometric mixture fraction.			
	Parameters	Optional/Reqd.	Units	Examples
	Bias factor for grid	**Required for corresponding grid choice.**	--	MIXFRACBIAS_FUEL **1.2**
	Keyword Usage	Required keyword.		
	Reactor Models	• Diffusion Flamelet Generator		
MIX-FRAC-BI-AS_OX-ID	Bias factor for the grid on the oxidizer side, that is, between the mixture fraction equal to its stoichiometric mixture fraction and 0. A value greater than unity should be given and it means more grid points near the stoichiometric mixture fraction.			
	Parameters	Optional/Reqd.	Units	Examples

Keyword	Definition			
Reactor Property	*Bias factor for grid*	**Required for corresponding grid choice.**	--	MIXFRACBIAS_OXID **1.2**
	Keyword Usage	Required keyword.		
	Reactor Models	• Diffusion Flamelet Generator		
MIXT Reactor Property	The characteristic time of the mixing process in the reactor.			
	Parameters	Optional/Reqd.	Units	Examples
	Characteristic time	Required	sec	MIXT **1.0E-3**
	Reactor Models	• Closed Partially Stirred Reactor (PaSR) • Partially Stirred Reactor (PaSR)		
MLMT Solver	Specifies the minimum value of gas mass in the zones. By default, the minimum zone mass is set to 10^{-6} g.			
	Parameters	Optional/Reqd.	Units	Examples
	Value of the b parameter	Optional	--	MLMT 1.0E-5
	Keyword Usage	Optional keyword.		
	Reactor Models	• SI Engine Zonal Simulator		
MMASS MMASS	The reactor wall temperature will be obtained by solving energy conservation equation for the reactor wall. It uses the thermal mass of the reactor wall and the heat transfer coefficient between the inner wall surface and the gas mixture inside the reactor. MMASS specifies the thermal mass of the reactor wall.			
	Parameters	Optional/Reqd.	Units	Examples
	Material name	**Optional.** If no material is specified, the same value will be used for all materials.	--	MMASS **material1** 500
	Thermal mass	Required	cal/K	MMASS **500**
	Reactor number (PSR clusters only)	**Optional.** If no number is given, the keyword is	--	MMASS material1.500 **1**

Keyword	Definition			
		assumed to apply to all reactors in a cluster.		
	Keyword Usage	Optional keyword. This keyword must be used with GMHTC . For Plug Flow Reactors the unit of thermal mass is cal/(cm-K).		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Honeycomb Monolith Reactor • IC HCCI Engine • Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Plasma PSR • Plasma Plug Flow Reactor • Plug Flow Reactor • SI Engine Zonal Simulator		
MOMEN Reactor Property	Turn on or off solution of the momentum equation for a plug-flow simulation.			
	Parameters	Optional/Reqd.	Units	Examples
	String "ON" or "OFF" to toggle the momentum equation	Required	--	MOMEN **ON** MOMEN OFF
	Keyword Usage	Optional keyword. By default, the momentum equation is solved (ON).		
	Reactor Models	• Honeycomb Reactor • Plasma Plug Flow Reactor • Plug Flow Reactor		
MORD Solver	Maximum order of integration used by the transient solver.			
	Parameters	Optional/Reqd.	Units	Examples
	Maximum order of integration	Required	--	MORD **3**
	Keyword Usage	Optional keyword. By default, the maximum order of integration is 5.		

Keyword	Definition			
	Reactor Models	• Cylindrical Shear Flow Reactor • Planar Shear Flow Reactor • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
MQA-FR Reactor Property	The external heat transfer (heat loss) area fraction of each zone.			
	Parameters	Optional/Reqd.	Units	Examples
	Area fraction	Required	--	MQAFR 0.15 4
	Zone number	Required	--	MQAFR 0.15 4
	Keyword Usage	Optional keyword.		
	Reactor Models	• Multi-Zone HCCI Engine Simulator		
MS-FX Reactor Property	Use a new discretization scheme for convective flux terms. In some cases, the original discretization scheme might not conserve species fluxes across the flame zone. With this new scheme, species mass fluxes are always conserved. Since accurate mass fluxes require fine resolution of species profiles, this new scheme in general incurs more grid points and longer run time than the original scheme does.The differences between major species solutions obtained by these two schemes are subtle.			
	Keyword Usage	Optional keyword. By default, the original discretization scheme is used.		
	Reactor Models	• Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation		
MULT Reactor Property	Use full multicomponent model for the transport coefficients and diffusion fluxes. See also MIX.			
	Keyword Usage	Optional keyword. By default, mixture-averaged transport is used.		
	Reactor Models	• Cylindrical Shear Flow Reactor • Diffusion or Premixed Opposed-flow Flame • Planar Shear Flow Reactor • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
MZMAS	Specifies zone mass fractions. MZM will compute the exact zone volumes at the beginning of the simulation. Use either VOL or MZMAS to set up the initial zone volumes: An error will be issued if both keywords are used in the same input file.			

<table>
<tr><th>Keyword</th><th colspan="4">Definition</th></tr>
<tr><td rowspan="5">Reactor Property</td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td>zone mass fraction</td><td>Required</td><td></td><td>MZMAS 0.2 7</td></tr>
<tr><td>zone number</td><td>Required</td><td></td><td>MZMAS 0.2 7</td></tr>
<tr><td>Keyword Usage</td><td colspan="3">Optional keyword.</td></tr>
<tr><td>Reactor Models</td><td colspan="3">• Multi-Zone HCCI Engine Simulator</td></tr>
<tr><td rowspan="3">NADAP

Solver</td><td colspan="4">Turns off the saving of adaptive points (see ADAP, which is the default). NADAP is provided to turn off adaptive points during a con tin uta ti on run if they have already been turned on with ADAP.</td></tr>
<tr><td>Keyword Usage</td><td colspan="3">Optional keyword. By default, ADAP is the default in the ANSYS Chemkin-Pro user interface and NADAP is the default for the command line.</td></tr>
<tr><td>Reactor Models</td><td colspan="3">• Closed Plasma Reactor
• Closed Homogeneous Reactor
• Honeycomb Reactor
• IC HCCI Engine Model
• Multi-Zone HCCI Engine Simulator
• Plasma Plug Flow Reactor
• Plug Flow Reactor
• SI Engine Zonal Simulator</td></tr>
<tr><td rowspan="6">NADP

Reactor Property</td><td colspan="4">Number of mesh points that Twopnt can add at one time during each grid refinement.</td></tr>
<tr><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td>Number of mesh points</td><td>Required</td><td>--</td><td>NADP 2</td></tr>
<tr><td>Keyword Usage</td><td colspan="3">Optional keyword. By default, no maximum is set for the number of points that can be added at once by the Twopnt solver.</td></tr>
<tr><td>Reactor Models</td><td colspan="3">• Diffusion or Premixed Opposed-flow Flame
• Premixed Laminar Burner-stabilized Flame
• Premixed Laminar Flame-speed Calculation
• Rotating Disk CVD Reactor
• Stagnation Flow CVD Reactor</td></tr>
<tr><td>Notes</td><td colspan="3">• This keyword can not be changed on a continuation or restart run.</td></tr>
</table>

Note: PDF user guides no longer in Chemkin-Pro install after release 19.0

Keyword	Definition			
NCANG Reactor Property	Run the simulation for 180 degrees of crank angle (0.5 revolution). If the "starting crank angle" (DEG0) is set to 180 degrees, the simulation will stop at crank angle = 360 (=180+180) degrees (i.e., top dead center). Use one of TIME , NREV , or NCANG to set the simulation time. The last keyword (of the three) in the input file takes effect.			
	Parameters	Optional/Reqd.	Units	Examples
	number_of_crank_angles	Required	degrees	NCANG **180**
	Keyword Usage	Optional keyword.		
	Reactor Models	• IC HCCI Engine • SI Engine Zonal Simulator		
NCFIT Reactor Property	Optional number of time points used to determine the slope when used in conjunction with keyword CTOL.			
	Parameters	Optional/Reqd.	Units	Examples
	Number of time points	Required	--	NCFIT **100**
	Keyword Usage	Optional keyword. NCFIT is only used in conjunction with CTOL.		
		• Closed Partially Stirred Reactor (PaSR) • Partially Stirred Reactor (PaSR)		
	Notes	Default value is 100.		
ND-PR Output or Solver	Frequency of output printing during time integration, given as the number of time steps.			
	Parameters	Optional/Reqd.	Units	Examples
	Print frequency	Required	--	NDPR **50**
	Keyword Usage	Optional keyword. By default, the print frequency is at every 1 time step.		
	Reactor Models	• Closed Partially Stirred Reactor (PaSR) • Diffusion or Premixed Opposed-flow Flame • Partially Stirred Reactor (PaSR)		
NE-WRUN Reactor Property	Inclusion of this keyword causes ANSYS Chemkin-Pro to expect keywords for another problem to follow the END keyword. The following problem does not use the solution of the previous problem as its initial guess. This capability is quite different to that provided by CNTN . The solutions resulting from NEWRUN keywords are written sequentially to one XML Solution File.			
	Keyword Usage	Optional keyword. By default, no new run is expected.		
	Reactor Models	• Chemical and Phase Equilibrium Calculations • Closed Homogeneous Batch Reactor		

<table>
<tr><th>Keyword</th><th colspan="4">Definition</th></tr>
<tr><td></td><td colspan="4">Closed Plasma Reactor
Cylindrical Shear Flow Reactor
Honeycomb Monolith Reactor
IC HCCI Engine
Mechanism Analyzer
Non-reactive Gas Mixer
Normal Incident Shock
Normal Reflected Shock
Partially Stirred Reactor
Perfectly Stirred Reactor (PSR)
Planar Shear Flow Reactor
Plasma PSR
Plasma Plug Flow Reactor
Plug Flow Reactor
Rotating Disk CVD Reactor Using Transient Solver
SI Engine Zonal Simulator
Stagnation Flow CVD Reactor Using Transient Solver</td></tr>
<tr><td rowspan="5">NINT-G-STEPS

Reactor Property</td><td colspan="4">The number of internal steps that the solver can take. When the integration time is too long and/or the system of equations is too stiff, the solver may take many internal time steps. This control acts as a check to avoid long, infinite, or hung processes. The simulator may take a corrective action (such as trying a few more steps or declare failure and/or provide diagnostic information).</td></tr>
<tr><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td>Maximum value of SSDR</td><td>Optional</td><td>--</td><td>NINTGSTEPS 10000</td></tr>
<tr><td>Keyword Usage</td><td colspan="3">Optional keyword. The default value for the Diffusion Flamelet Generator is 5000.</td></tr>
<tr><td>Reactor Models</td><td colspan="3">• Diffusion Flamelet Generator</td></tr>
<tr><td rowspan="3">NJAC

Solver</td><td colspan="4">For the steady-state Twopnt solver, specifies the maximum number of Newton steps that can be taken in solving the steady state problem before a new Jacobian is evaluated. If NJAC=1, then a full Newton method will result.</td></tr>
<tr><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td>Retirement age</td><td>Required</td><td>--</td><td>NJAC 20</td></tr>
</table>

<table>
<tr><th>Keyword</th><th colspan="4">Definition</th></tr>
<tr><td></td><td>Keyword Usage</td><td colspan="3">Optional keyword. By default, the retirement age is set at 20.</td></tr>
<tr><td></td><td>Reactor Models</td><td colspan="3">• Cylindrical Shear Flow Reactor
• Diffusion or Premixed Opposed-flow Flame
• Non-reactive Gas Mixer
• Perfectly Stirred Reactor (PSR)
• Planar Shear Flow Reactor
• Plasma PSR
• Premixed Laminar Burner-stabilized Flame
• Premixed Laminar Flame-speed Calculation
• Rotating Disk CVD Reactor
• Stagnation Flow CVD Reactor</td></tr>
<tr><td>NMOM

Reactor Property</td><td colspan="4">Number of moments used in the simulation for tracking particle size distribution. MINMO(=3) $\leq$ NMOM $\leq$ MAXMO(=6). If NMOM = 6, then 6 moments of the size distribution function are solved, from the 0^{th} moment to the 5^{th} moment.</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td></td><td>Number of moments</td><td>Required</td><td>--</td><td>NMOM 6</td></tr>
<tr><td></td><td>Keyword Usage</td><td colspan="3">Optional keyword. Default is the MINMO value.</td></tr>
<tr><td></td><td>Reactor Models</td><td colspan="3">• Closed Homogeneous Batch Reactor
• Closed Plasma Reactor
• Cylindrical Shear Flow Reactor
• Honeycomb Monolith Reactor
• IC HCCI Engine
• Perfectly Stirred Reactor (PSR)
• Planar Shear Flow Reactor
• Plasma PSR
• Plasma Plug Flow Reactor
• Plug Flow Reactor
• SI Engine Zonal Simulator</td></tr>
</table>

Keyword	Definition			
NNEG Solver	Flag instructing transient solver to try to constrain all components of the solution vector to be non-negative. This is usually unnecessary, but it may help to use this keyword if negative solution components appear to be causing problems in convergence.			
	Keyword Usage	Optional keyword. By default, the solution is not constrained and is not usually necessary.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Partially Stirred Reactor (PaSR) • Closed Plasma Reactor • Honeycomb Reactor • IC HCCI Engine • Non-reactive Gas Mixer • Partially Stirred Reactor (PaSR) • Perfectly Stirred Reactor (PSR) • Plasma PSR • Plasma Plug Flow Reactor • Plug Flow Reactor • SI Engine Zonal Simulator		
	Notes	• NNEG can be added to but cannot be removed from a continuation run.		
NO-AGG Reactor Property	Turns off particle aggregation effect. Particle aggregation is included by default in the Particle Tracking module.			
	Parameters	Optional/Reqd.	Units	Examples
	Material name	Required	--	NOAGG **SOOT**
	Keyword Usage	Optional keyword.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Diffusion or Premixed Opposed-flow Flame • IC HCCI Engine • Multi-Zone HCCI Engine Simulator • Perfectly Stirred Reactor (PSR) • Plasma PSR		

Keyword	Definition	
		• Premixed Laminar Burner-stabilized Flame
NOCG Reactor Property	Exclude coagulation of particles.	
	Keyword Usage	Optional keyword.
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Cylindrical Shear Flow Reactor • Honeycomb Monolith Reactor • IC HCCI Engine • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma PSR • Plasma Plug Flow Reactor • Plug Flow Reactor • SI Engine Zonal Simulator
NOCH Reactor Property	This keyword specifies that the rates of all gas-phase reactions will be set to zero, regardless of the values specified in the *Gas-phase Kinetics* input.	
	Keyword Usage	Optional keyword. By default, gas chemistry is turned on. See also CHEM.
	Reactor Models	• Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor
NOFT Solver or Reactor Property	For steady-state cases, when this keyword is specified and an energy equation is being solved, the intermediate solution at a fixed temperature will be skipped. In this case, solution to the energy and species equations will be attempted simultaneously from the user-specified initial guess.	
	Keyword Usage	Optional keyword. By default, the fixed temperature solution is obtained before adding the energy equation.
	Reactor Models	• Diffusion or Premixed Opposed-flow Flame • Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Plasma PSR • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation

Keyword	Definition			
		• Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
	Notes	• See also, ENRG and ENGE keywords.		
NO-JC Solver	Flag indicating the non-stiff Adams method (no Jacobian) of the DVODE solver is used to integrate the equations.			
	Keyword Usage	Optional keyword. By default, the DASPK solver will be used.		
	Reactor Models	• Closed Partially Stirred Reactor (PaSR) • Partially Stirred Reactor (PaSR)		
NONE Output	Turns default output off for all of *Surftherm* 's tables. One can use this keyword in combination with another keyword below, to turn on output from only a few features. This keyword will also turn off all previously specified output from keywords given before it.			
	Keyword Usage	Optional keyword. By default, the ALL output will be printed.		
	Reactor Models	• Mechanism Analyzer		
NONR Reactor Property	This keyword specifies that the non-reacting problem will not be solved as the first stage in the solution of the full problem.			
	Keyword Usage	Optional keyword. By default, the non-reacting problem is solved first.		
	Reactor Models	• Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
NOTP Reactor Property	Exclude thermophoresis of particles.			
	Parameters	Optional/Reqd.	Units	Examples
	Material name	Required	--	NOTP **SOOT**
	Keyword Usage	Optional keyword. By default, thermophoresis of particles is excluded.		
	Reactor Models	• Diffusion or Premixed Opposed-flow Flame • Opposed-flow Flame • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation		
NOTP Solver	Do not solve for the initial gas-phase and surface concentrations at the walls using the *Twopnt* procedure.			
	Keyword Usage	Optional keyword. By default, the initial *Twopnt* procedure is solved.		

Keyword	Definition			
	Reactor Models	• Cylindrical Shear Flow Reactor • Planar Shear Flow Reactor		
NPAR Reactor Property	The number of statistical events (particles) used by the Monte Carlo process to form the stochastic ensemble.			
	Parameters	Optional/Reqd.	Units	Examples
	Number of particles	Required	--	NPAR **1000**
	Keyword Usage	Required keyword.		
	Reactor Models	• Closed Partially Stirred Reactor (PaSR) • Partially Stirred Reactor (PaSR)		
NP_FUEL Reactor Property	Number of points on the fuel side, that is, between the mixture fraction equal to its stoichiometric mixture fraction and 1.			
	Parameters	Optional/Reqd.	Units	Examples
	Number of grid points	**Required for corresponding grid choice**	--	NP_FUEL **11**
	Keyword Usage	Required keyword.		
	Reactor Models	• Diffusion Flamelet Generator		
NP_OXID Reactor Property	Number of points on the oxidizer side, that is, between the mixture fraction equal to its stoichiometric mixture fraction and 0.			
	Parameters	Optional/Reqd.	Units	Examples
	Number of grid points	**Required for corresponding grid choice**	--	NP_OXID **11**
	Keyword Usage	Required keyword.		
	Reactor Models	• Diffusion Flamelet Generator		
NPIN Reactor Property	The minimum number of event particles in the reactor whose properties will be replaced by those of the inlet mixture per time step.			
	Parameters	Optional/Reqd.	Units	Examples
	Number of particles	Required	--	NPIN **5**
	Keyword Usage	Optional keyword. By default, the minimum number of the event particles is 2.		
	Reactor Models	• Partially Stirred Reactor (PaSR)		
NPSR	Number of perfectly stirred reactors (PSRs) or zones in a reactor cluster.			

Keyword	Definition			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	Number of reactors or zones	Required	--	NPSR **5**
	Keyword Usage	Optional keyword. By default, the number of PSRs is set to 1.		
		• Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Plasma PSR		
NPTS Reactor Property	The number of initial mesh points. The inclusion of NPTS will generate an equi-spaced mesh of NPTS points across the domain, in the axial direction for Flames and CVD Reactors, and in the cross-flow direction for Shear Flow Reactors. The user can also specify an initial non-uniform mesh using the keyword GRID, in which case the NPTS input is not needed.			
	Parameters	Optional/Reqd.	Units	Examples
	Number of mesh points	Required	--	NPTS **50**
	Keyword Usage	Optional keyword. By default, the number of initial mesh points is set to 6.		
	Reactor Models	• Cylindrical Shear Flow Reactor • Diffusion or Premixed Opposed-flow Flame • Planar Shear Flow Reactor • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
NREV Reactor Property	The number of revolutions of the crank used to determine the end time of the simulation. Fractional values are acceptable.			
	Parameters	Optional/Reqd.	Units	Examples
	Number of revolutions	Required	--	NREV **1**
	Keyword Usage	Optional keyword. Either NREV or TIME must be specified.		
	Reactor Models	• IC HCCI Engine • SI Engine Zonal Simulator		
	Notes	• On a restart, the number of crank revolutions will be determined from the value of TIME.		

Note: PDF user guides no longer in Chemkin-Pro install after release 19.0

<table>
<tr><th>Keyword</th><th>Definition</th></tr>
<tr><td>NSOL

XMLI</td><td>Use this keyword to specify which solution to use for the initialization (XMLI) or restart (RSTR), when more than one solution is stored on the XML Solution File that is used for the restart or initialization (e.g., on XMLdata.zip).
<table>
<tr><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td>Solution used</td><td>Required</td><td>--</td><td>NSOL 3</td></tr>
<tr><td>Keyword Usage</td><td colspan="3">Optional keyword. By default, the last solution saved in the XML Solution File.</td></tr>
<tr><td>Reactor Models</td><td colspan="3">• Chemical and Phase Equilibrium Calculations
• Closed Homogeneous Batch Reactor
• Closed Plasma Reactor
• Cylindrical Shear Flow Reactor
• Diffusion or Premixed Opposed-flow Flame
• Honeycomb Reactor
• IC HCCI Engine
• Mechanism Analyzer
• Non-reactive Gas Mixer
• Normal Incident Shock
• Normal Reflected Shock
• Perfectly Stirred Reactor (PSR)
• Planar Shear Flow Reactor
• Plasma Plug Flow Reactor
• Plasma PSR
• Plug Flow Reactor
• Premixed Laminar Burner-stabilized Flame
• Premixed Laminar Flame-speed Calculation
• Rotating Disk CVD Reactor
• SI Engine Zonal Simulator
• Stagnation Flow CVD Reactor</td></tr>
</table></td></tr>
<tr><td>NSTEPS_HIGH

Reactor Property</td><td>Number of steps to be taken to reach the specified maximum value of SSDR (SSDR_max). The simulator somputes the new SSDR to be taken on a subsequent step as SSDR used in previous step + fixedStepSize where the fixedStepSize = (SSDR_max - SSDR_Nominal)/NSTEP_High. For example, if the specified nominal</td></tr>
</table>

<table>
<tr><th>Keyword</th><th>Definition</th></tr>
<tr><td></td><td>and maximum values are 1 and 21, respectively, then 5 steps will yield the constant size to be 4 and result in the sequence of SSDR values as {1, 5, 9, 13, 17, 21}.

Continuations to the maximum value can be turned off by setting this input to 0.
<table>
<tr><th>Parameters</th><th>Optional/Reqd.</th><th>Units</th><th>Examples</th></tr>
<tr><td>Number of steps to maximum SSDR</td><td>Required</td><td>--</td><td>NSTEPS_HIGH 5</td></tr>
<tr><td>Keyword Usage</td><td colspan="3">Required keyword.</td></tr>
<tr><td>Reactor Models</td><td colspan="3">• Diffusion Flamelet Generator</td></tr>
</table></td></tr>
<tr><td>NSTEPS_LOW

Reactor Property</td><td>Number of steps to be taken to reach the specified minimum value of SSDR. The simulator computes the new SSDR to be used on a subsequent step as a constantFactor * SSDR_Used_in_previous step. That is, NSTEP_LOW* log(constantFactor) = log(SSDR_min/SSDR_nominal). For example, if the specified nominal and minimum values are 1 and 0.001, respectively, then 3 steps will yield the constant factor to be 0.1 and result in the sequence of SSDR values as {1, 0.1, 0.01, 0.001}.

Continuations to the minimum value can be turned off by setting this input to 0.
<table>
<tr><th>Parameters</th><th>Optional/Reqd.</th><th>Units</th><th>Examples</th></tr>
<tr><td>Number of steps to maximum SSDR</td><td>Required</td><td>--</td><td>NSTEPS_HIGH 5</td></tr>
<tr><td>Keyword Usage</td><td colspan="3">Required keyword.</td></tr>
<tr><td>Reactor Models</td><td colspan="3">• Diffusion Flamelet Generator</td></tr>
</table></td></tr>
<tr><td>NTOT

Reactor Property</td><td>Maximum number of grid points allowed during mesh adaptation.
<table>
<tr><th>Parameters</th><th>Optional/Reqd.</th><th>Units</th><th>Examples</th></tr>
<tr><td>Number of grid points</td><td>Required</td><td>--</td><td>NTOT 200</td></tr>
<tr><td>Keyword Usage</td><td colspan="3">Optional keyword. The default maximum number of grid points is 100 for: Rotating Disk CVD Reactor, Stagnation Flow CVD Reactor; 250 for Diffusion or Premixed Opposed-flow Flame, Premixed Laminar Burner-stabilized Flame, Premixed Laminar Flame-speed Calculation.</td></tr>
<tr><td>Reactor Models</td><td colspan="3">• Diffusion or Premixed Opposed-flow Flame

• Premixed Laminar Burner-stabilized Flame

• Premixed Laminar Flame-speed Calculation

• Rotating Disk CVD Reactor

• Stagnation Flow CVD Reactor</td></tr>
</table></td></tr>
</table>

Keyword	Definition			
	Notes	• This keyword can not be changed on a restart or continuation run. • In previous versions, **NMAX** keyword was used.		
NZONE Reactor Property	Specifies the number of zones to be used in the multi-zone simulation. This keyword MUST be used with the ICEN keyword or an error will be issued. The default value is 1 (= single zone model). The multi-zone model will be turned on when NZONE > 1.			
	Parameters	Optional/Reqd.	Units	Examples
	Number of zones	Required	--	NZONE **5**
	Keyword Usage	Optional keyword.		
	Reactor Models	• Multi-Zone HCCI Engine Simulator		
OINL Reactor Property	The inlet-gas spin rate. At the inlet $x=L$, v/r = OINL.			
	Parameters	Optional/Reqd.	Units	Examples
	Inlet-gas spin rate	Required	rpm	OINL **100**
	Keyword Usage	Optional keyword. By default, the inlet-gas spin rate is 0.0.		
	Reactor Models	• Rotating Disk CVD Reactor		
OMEG Problem Type and Reactor Property	The disk rotation rate; also specifies the Rotating Disk CVD Reactor model.			
	Parameters	Optional/Reqd.	Units	Examples
	Disk rotation rate	Required	rpm	OMEG **1000**
	Keyword Usage	Required keyword. See also STAG.		
	Reactor Models	• Rotating Disk CVD Reactor		
OX-ID Inlet or Reactor Property	Defines the oxidizer mole fraction composition for an inlet stream in an open system, or for the initial conditions in a closed system, when an equivalence ratio is specified (EQUI). It must be followed by a species name and then the mole fraction. One of these OXID inputs must appear for each oxidizer species, which are used to determine the inlet composition based on an equivalence-ratio calculation (EQUI). Any given species can participate simultaneously as a fuel, oxidizer, or product. The sum of all the oxidizer mole fractions should equal one. If it does not, a warning message will be printed and the mole fractions will be normalized so the sum does equal one.			
	Parameters	Optional/Reqd.	Units	Examples
	Inlet stream name (PSRs only)	Optional If there is no stream name than the oxidizer mole	--	OXID **mixture1** O2 0.5

Keyword	Definition			
		fraction composition applies to the default or all defined streams.		
	Species name	Required	--	OXID **O2** 0.5
	Fuel fraction	Required	mole fractions	OXID O2 **0.5**
	Keyword Usage	Required keyword when EQUI option is used for an inlet stream or for the initial conditions in a reactor.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Honeycomb Reactor • IC HCCI Engine • Perfectly Stirred Reactor • Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor • SI Engine Zonal Simulator		
	Notes	• The mole fractions are of the oxidizer itself, not for the entire composition. • The OXID keywords must be changed as a set, not individually for a restart run. • The OXID keywords must be changed as a set, not individually for continuation run.		

10.3. Alphabetical Listing of Keywords [P-S]

Table 10.3: Alphabetical Listing of Keywords [P-S]

Keyword	Definition			
P1A Reactor Property	Pressure before the incident shock.			
	Parameters	Optional/Reqd.	Units	Examples
	Pressure	Required	atm	P1A **1.0**
	Keyword Usage	Optional Keyword. The shock velocity and any two of temperature, pressure, or density must be specified		

Keyword	Definition			
		for conditions before the incident shock. See also T1 and RHO1 .		
	Reactor Models	• Normal Incident Shock • Normal Reflected Shock		
P2A Reactor Property	Pressure after the incident shock.			
	Parameters	Optional/Reqd.	Units	Examples
	Pressure	Required	atm	P2A **2.3**
	Keyword Usage	Optional Keyword. Any two of temperature, pressure, or density must be specified for conditions after the incident shock. See also T2 and RHO2 .		
	Reactor Models	• Normal Incident Shock • Normal Reflected Shock		
P3A Reactor Property	Pressure after the reflected shock, given as p_5 in the equations.			
	Parameters	Optional/Reqd.	Units	Examples
	Pressure	Required	atm	P3A **2.3**
	Keyword Usage	Optional Keyword. Any two of temperature, pressure, or density must be specified for conditions before the reflected shock. See also T3 and RHO3 .		
	Reactor Models	• Normal Reflected Shock		
PARP Output	Partial-pressures of the gas-phase species will be used in the diagnostic output file.			
	Keyword Usage	Optional keyword. By default, mass fractions are printed, not partial pressures.		
	Reactor Models	• Cylindrical Shear Flow Reactor • Planar Shear Flow Reactor		
PB-DEN Output	This keyword resets all bulk species densities defined in the surface mechanism to the value given by this keyword.			
	Parameters	Optional/Reqd.	Units	Examples
	material_name	Required	None	PBDEN **ligA** 2.15
	bulk_density	Required	g/cm^3	PBDEN ligA **2.15**
	Keyword Usage	Optional keyword.		
	Reactor Models	• Closed Homogeneous Reactor • Perfectly Stirred Reactor (PSR) • Plug Flow Reactor (PFR)		

Keyword	Definition			
PDF Output	Request the probability distribution of a scalar to be output to a *pdf.plt* file. Any number of PDF entries is allowed.			
	Parameters	Optional/Reqd.	Units	Examples
	Scalar (temperature or species name)	Required	--	PDF **T**
	Keyword Usage	Optional keyword. By default, no PDF is printed.		
	Reactor Models	• Closed Partially Stirred Reactor (PaSR) • Partially Stirred Reactor (PaSR)		
PENG Reactor Property	Include the energy conservation equation for particles.			
	Keyword Usage	Optional keyword.		
	Reactor Models	• Opposed-flow Flame • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation		
PEST Reactor Property	Specifies an estimate of the equilibrium pressure.			
	Parameters	Optional/Reqd.	Units	Examples
	Pressure	Required	atm	PEST **1.1**
	Keyword Usage	Optional keyword. May help convergence to the equilibrium pressure, or assure an appropriate equilibrium pressure is calculated when a second, trivial solution exists.		
	Reactor Models	• Chemical and Phase Equilibrium Calculations		
PFAL Output	Analyze the pressure fall-off of a gas phase reaction, i.e., creates a table of reaction rates versus total gas pressure at a constant temperature. The ALL option is the default and produces tables for every gas-phase reaction. The NONE option suppresses output for all of the reactions. If reaction information is desired for only certain reactions, they may be optionally specified by their number (given in the Pre-processor output) or by typing an exact duplicate of the reaction expression (see example input).			
	Parameters	Optional/Reqd.	Units	Examples
	ALL option	**Optional, default is ALL**	--	PFAL **ALL**
	NONE option	**Optional, default is ALL**	--	PFAL **NONE**
	Gas reaction number list	**Optional, de-**	--	PFAL **2 5**

Keyword	Definition			
		fault is ALL		
	Gas reaction expression	**Optional, default is ALL**	--	PFAL **2CH3(+M)<=>C2H6(+M)**
	Keyword Usage	Optional keyword. By default, the table output is determined by the ALL or NONE keyword.		
	Reactor Models	• Mechanism Analyzer		
PFLR Reactor Property	Set the minimum bounds of the particle moments to a slightly negative number to allow the solver more room to search for a solution.			
	Parameters	Optional/Reqd.	Units	Examples
	Minimum bound	Required	--	**PFLR -1.0d-06**
	Keyword Usage	Optional keyword.		
	Reactor Models	• Opposed-flow Flame • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation		
PH Problem Type	Constant pressure and enthalpy constraints.			
	Keyword Usage	Optional keyword. Exactly one problem type keyword must be included.		
	Reactor Models	• Chemical and Phase Equilibrium Calculations		
	Notes	HP keyword is equivalent.		
PHIA Reactor Property	Set the upper limit of the pressure range (in atmospheres) in tables where the gas pressure is varied.			
	Parameters	Optional/Reqd.	Units	Examples
	Pressure	Required	atm	PHIA **2.**
	Keyword Usage	Optional keyword. By default, the pressure is 1.315789 atm (1000 Torr).		
	Reactor Models	• Mechanism Analyzer		
	Notes	• **In previous versions, keyword PHIG was used with units of Torr**		
PLAN Reactor Property	Use a planar coordinate system, which is appropriate for a Tsuji burner configuration.			
	Keyword Usage	Optional keyword. By default, the coordinate system is radial and axisymmetric.		
	Reactor Models	• Diffusion or Premixed Opposed-flow Flame		

Keyword	Definition			
PLAT Reactor Property	Use a plateau profile to set up initial solution estimates, rather than a linear profile.			
	Keyword Usage	Optional keyword. By default, the plateau profile is used.		
	Reactor Models	• Diffusion or Premixed Opposed-flow Flame		
PLOA Reactor Property	Set the lower limit of the pressure range (in atmospheres) in tables where the gas pressure is varied.			
	Parameters	Optional/Reqd.	Units	Examples
	Pressure	Required	atm	PLOA **1.0**
	Keyword Usage	Optional keyword. By default, the pressure is 0.001315789 atm (1 Torr)		
	Reactor Models	• Mechanism Analyzer		
	Notes	• **In previous versions, keyword PLOW was used with units of Torr**		
PLUG Reactor Property	Indicates that plug-flow equations will be solved and that the Reactor Model will be one of the family of Plug Flow Reactors.			
	Keyword Usage	Required keyword.		
	Reactor Models	• Honeycomb Reactor • Plasma Plug Flow Reactor • Plug Flow Reactor		
PNDE Reactor Property	Assigns the initial (or estimate for steady-state calculations) number density of the particle consisting of the designated bulk species. The default value is 0. The reactor number is optional. When no reactor number is given, the same initial number density will apply to all reactors in the network. If neither PVFE nor PROE is given, the initial/estimate values of the moments are computed as $M_0 = \mathrm{PNDE}$ $M_i = \left(\Delta C_{\mathrm{nuc1}}\right) \times M_{i-1} \quad 1 < i \leq \mathrm{NMOM}$			
	Parameters	Optional/Reqd.	Units	Examples
	Material name	Required	--	PNDE **C(B)** 1.0E10 4
	Number density	Required	particles/cm^3	PNDE C(B) **1.0E10** 4
	Reactor number	Optional	--	PNDE C(B) 1.0E10 **4**
	Keyword Usage	Optional keyword. The default value is value for the number density is 0.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor		

<table>
<tr><th>Keyword</th><th colspan="4">Definition</th></tr>
<tr><td></td><td colspan="4">Cylindrical Shear Flow Reactor
Honeycomb Monolith Reactor
IC HCCI Engine
Perfectly Stirred Reactor (PSR)
Planar Shear Flow Reactor
Plasma PSR
Plasma Plug Flow Reactor
Plug Flow Reactor
SI Engine Zonal Simulator</td></tr>
<tr><td>PNDI

Inlet Property</td><td colspan="4">Assigns the number density of the particle consisting of the designated material name to the named inlet stream. The default value is 0. The stream name is optional if there is only one inlet.</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td></td><td>Stream name</td><td>Optional if only one inlet.</td><td>--</td><td>PNDI exhaust C(B) 1.0E12</td></tr>
<tr><td></td><td>Material name</td><td>Required</td><td>--</td><td>PNDI exhaust C(B) 1.0E12</td></tr>
<tr><td></td><td>Mass density</td><td>Required</td><td>particles/cm^3</td><td>PNDI exhaust C(B) 1.0E12</td></tr>
<tr><td></td><td>Keyword Usage</td><td colspan="3">Optional keyword. The default value for the mass density is 0.</td></tr>
<tr><td></td><td>Reactor Models</td><td colspan="3">Cylindrical Shear Flow Reactor
Honeycomb Monolith Reactor
Perfectly-stirred Reactor (PSR)
Planar Shear Flow Reactor
Plasma PSR
Plasma Plug Flow Reactor
Plug-flow Reactor (PFR)</td></tr>
<tr><td>PNUM

Reactor Property</td><td colspan="4">Set the total number of pressure entries in tables where the gas pressure is varied. The default is 10. Note that the changes in the pressure are determined on a logarithmic scale.</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
</table>

Keyword	Definition			
	Number of pressures	Required	--	PNUM **10**
	Keyword Usage	Optional keyword. By default, the number of pressures is 10.		
	Reactor Models	• Mechanism Analyzer		
PPRO Reactor Property Profiles	Reactor pressure profile specified as a function of time for transient 0-D homogeneous systems or as a function of distance for Plug Flow Reactors.			
	Parameters	Optional/Reqd.	Units	Examples
	Time or Distance value, depending on Reactor Model	Required	sec or cm	PPRO **1.0E-4** 1.0
	Pressure	Required	atm	PPRO 1.0E-4 **1.0**
	Reactor number (PSR clusters only)	Optional If no number is given, the profile described by the first two values is assumed to apply to all reactors in a cluster.	--	PPRO 1.0E-4 1.0 **1**
	Keyword Usage	Optional keyword. By default, no profile is provided.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Diffusion or Premixed Opposed-flow Flame • Honeycomb Reactor • Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor		

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Keyword	Definition			
PRDL Reactor Property	The Prandlt number used in the generalized heat transfer correlation.			
	Parameters	Optional/Reqd.	Units	Examples
	Prandlt number	Required	--	PRDL **0.77**
	Keyword Usage	Optional keyword. By default, the value is 0.7.		
	Reactor Models	• IC HCCI Engine • SI Engine Zonal Simulator		
PRES Reactor Property	The reactor pressure in atmospheres. Depending on the Reactor Model and problem type, the pressure specified can serve as the pressure constraint (for constant-pressure problems), as an initial guess for pressure (for steady-state problems where pressure is a variable), or as the initial reactor pressure (for transient cases where pressure is a variable). For the Mechanism Analyzer, this is the bath-gas pressure.			
	Parameters	Optional/Reqd.	Units	Examples
	Reactor pressure	Required	atm	PRES **1.0**
	Reactor number (PSR clusters only)	Optional If no number is given, the keyword is assumed to apply to all reactors in a cluster.	--	PRES 1.0 **1**
	Keyword Usage	Required keyword in most cases. Optional keyword only for Mechanism Analyzer, where the default is 1 atm.		
	Reactor Models	• Chemical and Phase Equilibrium Calculations • Closed Homogeneous Batch Reactor • Closed Partially Stirred Reactor (PaSR) • Closed Plasma Reactor • Cylindrical Shear Flow Reactor • Diffusion or Premixed Opposed-flow Flame • Honeycomb Reactor • IC HCCI Engine		

<table>
<tr><th>Keyword</th><th colspan="4">Definition</th></tr>
<tr><td></td><td></td><td colspan="3">• Mechanism Analyzer
• Non-reactive Gas Mixer
• Partially Stirred Reactor (PaSR)
• Perfectly Stirred Reactor (PSR)
• Planar Shear Flow Reactor
• Plasma Plug Flow Reactor
• Plasma PSR
• Plug Flow Reactor
• Premixed Laminar Burner-stabilized Flame
• Premixed Laminar Flame-speed Calculation
• Rotating Disk CVD Reactor
• SI Engine Zonal Simulator
• Stagnation Flow CVD Reactor</td></tr>
<tr><td></td><td>Notes</td><td colspan="3">• In previous version, PRMT was an alternate keyword that allowed pressure input in millitorr units, for 0-D homogeneous and plug-flow systems only.
• In previous versions, this was PBTH for the Mechanism Analyzer.</td></tr>
<tr><td>PRMN

Reactor Property</td><td colspan="4">Minimum mole fraction value applied to the estimated values of the flame products, when the (default) equilibrium is used to determine product estimates. Ignored in the case that PROD2 keywords are present.</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td></td><td>Product fraction</td><td>Required</td><td>mole fractions</td><td>PRMN 1.0E-10</td></tr>
<tr><td></td><td>Keyword Usage</td><td colspan="3">Optional keyword. By default, the flame product fraction is set to 0.</td></tr>
<tr><td></td><td>Reactor Models</td><td colspan="3">• Premixed Laminar Burner-stabilized Flame
• Premixed Laminar Flame-speed Calculation</td></tr>
<tr><td>PRNT

Output</td><td colspan="4">Printing control. “PRNT 0” provides printed output for only the solution (plus sensitivity coefficients and rates-of-production coefficients, when requested). “PRNT 1” provides an additional summary of the iteration path from the solver. “PRNT 2” includes printing at every stage of the Twopnt solver’s Newton iteration and time stepping procedure. More printing is sometimes helpful when diagnosing problems and trying to adjust the input parameters to optimize convergence.</td></tr>
</table>

<table>
<tr><th>Keyword</th><th>Definition</th></tr>
<tr><td></td><td>However, since the increased printing requires more function evaluations to show how the solution is progressing, the computer time increases with increased printing.
<table>
<tr><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td>Print control number</td><td>Required</td><td>--</td><td>PRNT 1</td></tr>
<tr><td>Keyword Usage</td><td colspan="3">Optional keyword. By default, the print control is set to 1.</td></tr>
<tr><td>Reactor Models</td><td colspan="3">• Closed Homogeneous Batch Reactor
• Closed Plasma Reactor
• Cylindrical Shear Flow Reactor
• Diffusion or Premixed Opposed-flow Flame
• Honeycomb Reactor
• IC HCCI Engine
• Non-reactive Gas Mixer
• Perfectly Stirred Reactor (PSR)
• Planar Shear Flow Reactor
• Plasma Plug Flow Reactor
• Plasma PSR
• Plug Flow Reactor
• Premixed Laminar Burner-stabilized Flame
• Premixed Laminar Flame-speed Calculation
• Rotating Disk CVD Reactor
• SI Engine Zonal Simulator
• Stagnation Flow CVD Reactor</td></tr>
</table></td></tr>
<tr><td>PROD

Reactor Property</td><td>Estimated values of the gas-phase mole fractions at the far end of the domain (i.e., the deposition surface for CVD reactors or the burned state at XEND for Premixed Laminar Flames) or in the middle of the flame (for Opposed-flow Flames). The sum of the product mole fractions should equal to 1.0; if they do not, then a warning message will be printed to the diagnostic output file and the mole fractions will be normalized so that they do sum to one.
<table>
<tr><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td>Species name</td><td>Required</td><td>--</td><td>PROD H2O 0.5</td></tr>
<tr><td>Mole fraction</td><td>Required</td><td>--</td><td>PROD H2O 0.5</td></tr>
</table></td></tr>
</table>

Keyword	Definition			
	Keyword Usage	Optional keyword. If PROD2 keywords are not provided, then an equilibrium calculation will be used to determine the estimated product composition (see also PRMN).		
	Reactor Models	• Diffusion or Premixed Opposed-flow Flame • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
	Notes	• Any given species may simultaneously be included as a reactant (REAC), intermediate (INTM), and product (PROD2). • The PROD2 keywords must be changed as a set, not individually for a restart run. • The PROD2 keywords must be changed as a set, not individually for continuation run.		
PROE Reactor Property	Assigns the initial (or estimate for steady-state calculations) number density of the particle consisting of the designated material name. The default value is 0. The reactor number is optional. When no reactor number is given, the same initial particle mass density will apply to all reactors in the network. The PROE keyword must be used in conjunction with the PNDE keyword and is mutually exclusive to keyword PVFE. When both PNDE and PROE are given, the moments are calculated as $M_0 = \mathrm{PNDE}$ $M_1 = \frac{\mathrm{PROE}}{m_0}$ $M_i = \left(\Delta C_{\mathrm{nuc1}}\right) \times M_{i-1} \quad 1 < i \leq \mathrm{NMOM}$ where m_0 is the mass of a material name molecule and ρ_B is the mass density of the bulk material.			
	Parameters	Optional/Reqd.	Units	Examples
	Material name	Required	--	PROE **C(B)** 1.0E-10 1
	Mass density	Required	$\mathrm{gm/cm^3}$	PROE C(B) **1.0E-10** 1
	Reactor number	Optional	--	PROE C(B) 1.0E-10 **1**
	Keyword Usage	Optional keyword. The default value for the mass density is 0. PNDE keyword required. Cannot be used with PVFE.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor		

<table>
<tr><th>Keyword</th><th colspan="4">Definition</th></tr>
<tr><td></td><td colspan="4">Cylindrical Shear Flow Reactor
Honeycomb Monolith Reactor
IC HCCI Engine
Perfectly Stirred Reactor (PSR)
Planar Shear Flow Reactor
Plasma PSR
Plasma Plug Flow Reactor
Plug Flow Reactor
SI Engine Zonal Simulator</td></tr>
<tr><td>PROI

Inlet Property</td><td colspan="4">Assigns the mass density of the particle consisting of the designated material name to the named inlet stream. The default value is 0. The stream name is optional if there is only one inlet. The PROI keyword must be used in conjunction with the PNDI keyword and is mutually exclusive to keyword PVFI.</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td></td><td>Stream name</td><td>Optional if there is only one inlet.</td><td>--</td><td>PROI EGR C(B) 1.0E-10</td></tr>
<tr><td></td><td>Material name</td><td>Required</td><td>--</td><td>PROI EGR C(B) 1.0E-10</td></tr>
<tr><td></td><td>Number density</td><td>Required</td><td>gm/cm^3</td><td>PROI EGR C(B) 1.0E-10</td></tr>
<tr><td></td><td>Keyword Usage</td><td colspan="3">Optional keyword. Must be used with PNDI. Cannot be used with PVFI. The default value for the number density is 0.</td></tr>
<tr><td></td><td>Reactor Models</td><td colspan="3">Cylindrical Shear Flow Reactor
Honeycomb Monolith Reactor
Perfectly-stirred Reactor (PSR)
Planar Shear Flow Reactor
Plasma PSR
Plasma Plug Flow Reactor
Plug-flow Reactor (PFR)</td></tr>
<tr><td>PS

Problem Type</td><td colspan="4">Constant pressure and entropy constraints.</td></tr>
<tr><td></td><td>Keyword Usage</td><td colspan="3">Optional keyword. Exactly one problem-type keyword must be included.</td></tr>
</table>

Keyword	Definition			
	Reactor Models	• Chemical and Phase Equilibrium Calculations		
	Notes	• SP keyword.is equivalent.		
PS-BAR Reactor Property	The piston head area to bore area ratio.			
	Parameters	Optional/Reqd.	Units	Examples
	Ratio of piston head area to bore area.	Required	None	PSBAR **1.1**
	Keyword Usage	Optional keyword. Default = 1.0.		
	Reactor Models	• IC HCCI Engine • Multi-zone HCCI Engine • SI Engine Zonal Simulator		
	Notes	PSBAR should be > 1.0.		
PSURF Inlet Property	Initial surface coverage on particles by the surface site species in the inlet flow.			
	Parameters	Optional/Reqd.	Units	Examples
	Stream name	**Optional if there is only one inlet.**	--	PSURF **inlet1** C(S) 0.1
	Surface species name	Required	--	PSURF inlet1 **C(S)** 0.1
	Surface coverage	Required	--	PSURF inlet1 C(S) **0.1**
	Keyword Usage	Optional keyword		
	Reactor Models	• Honeycomb Reactor • Opposed-flow Flame • Perfectly Stirred Reactor (PSR) • Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation		
PSV Solver	Pseudo-velocity for use in modifying the surface species equations for improved convergence. This pseudo-convection term is incorporated into the surface site fraction equations in order to convert algebraic equations to differential equations. The value of the PSV should be small enough such that it has no effect on the			

Keyword	Definition			
	solution results, but large enough to affect the convergence behavior. If not supplied, then the unmodified equations are used. The modified equations are sometimes helpful in reaching steady-state conditions for problems with stiff surface chemistry (e.g. catalytic combustion), but should not be used if no convergence problems are encountered. A recommended value to try for PSV would be about 1/10th of the inlet velocity, but the simulation should be repeated with smaller or larger values to make sure that it has no effect on the solution.			
	Parameters	Optional/Reqd.	Units	Examples
	Pseudo-velocity	Required	cm/sec	PSV **10.**
	Keyword Usage	Optional keyword. By default, the value is set to 10* ATOL.		
	Reactor Models	• Honeycomb Reactor • Plasma Plug Flow Reactor • Plug Flow Reactor		
PTM_SECTION_NUM Reactor Property	The number of sections to use for the specified material.			
	Parameters	Optional/Reqd.	Units	Examples
	Material name	Required	--	PTM_SECTION_NUM **SOOT** 30
	Number of sections	Required	--	PTM_SECTION_NUM **SOOT** 30
	Keyword Usage	Required when the Sectional Model is used.		
	Reactor Models	• Opposed-flow Flame • Plug Flow Reactor • Premixed Laminar Burner Stabilized Flame • Premixed Laminar Burner Stabilized Stagnation Flame • Premixed Laminar Flame Speed Calculator		
PTM_SECTION_SIZEDEP_A0 Reactor Property	Tanh function constant that is used to blend lower and upper bounds of collision efficiency.			
	Parameters	Optional/Reqd.	Units	Examples
	Material name	Required	None	PTM_SECTION_SIZEDEP_A0 **SOOT** 5
	A0	Required	None	PTM_SECTION_SIZEDEP_A0 SOOT **5**
	Keyword Usage	Optional keyword. Default size is 7.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Internal Combustion Engine • Perfectly Stirred Reactor (PSR)		

<table>
<tr><th>Keyword</th><th colspan="4">Definition</th></tr>
<tr><td></td><td></td><td colspan="3">• Diffusion or Premixed Opposed Flow Flame
• Plug Flow Reactor
• Premixed Laminar Burner Stabilized Flame
• Premixed Laminar Burner Stabilized Stagnation Flame
• Premixed Laminar Flame Speed Calculator</td></tr>
<tr><td rowspan="5">PTM_SECTION_SIZEDEP_COLEFF

Reactor Property</td><td colspan="4">Use size-dependent collision efficiency for particles .</td></tr>
<tr><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td>Material name</td><td>Required</td><td>None</td><td>PTM_SECTION_SIZEDEP_COLEFF
SOOT</td></tr>
<tr><td>Keyword Usage</td><td colspan="3">Optional keyword. Not used by default.</td></tr>
<tr><td>Reactor Models</td><td colspan="3">• Closed Homogeneous Batch Reactor
• Internal Combustion Engine
• Perfectly Stirred Reactor (PSR)
• Diffusion or Premixed Opposed Flow Flame
• Plug Flow Reactor
• Premixed Laminar Burner Stabilized Flame
• Premixed Laminar Burner Stabilized Stagnation Flame
• Premixed Laminar Flame Speed Calculator</td></tr>
<tr><td rowspan="5">PTM_SECTION_SIZEDEP_DSTAR

Reactor Property</td><td colspan="4">Limit diameter for size-dependent collision efficiency.</td></tr>
<tr><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td>Material name</td><td>Required</td><td>None</td><td>PTM_SECTION_SIZEDEP_DSTAR
SOOT 13-06</td></tr>
<tr><td>Diameter</td><td>Required</td><td>None</td><td>PTM_SECTION_SIZEDEP_DSTAR
SOOT 13-06</td></tr>
<tr><td>Keyword Usage</td><td colspan="3">Optional keyword. No default value is given and must be specified by user when using size-dependent collision efficiency. For soot simulation, the value generally ranges from 10 to 20 nm.</td></tr>
<tr><td>Reactor Models</td><td colspan="3">• Closed Homogeneous Batch Reactor
• Internal Combustion Engine
• Perfectly Stirred Reactor (PSR)
• Diffusion or Premixed Opposed Flow Flame
• Plug Flow Reactor</td></tr>
</table>

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<table>
<tr><th>Keyword</th><th>Definition</th></tr>
<tr><td></td><td></td><td>• Premixed Laminar Burner Stabilized Flame
• Premixed Laminar Burner Stabilized Stagnation Flame
• Premixed Laminar Flame Speed Calculator</td></tr>
<tr><td>PTM_SECTION_SIZEDEP_HAMAKER

Reactor Property</td><td colspan="2">Hamaker constant for computing potential well depth when using size-dependent deposition efficiency for particles.</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td></td><td>Material name</td><td>Required</td><td>None</td><td>PTM_SECTION_SIZEDEP_HAMAKER SOOT 5e-13</td></tr>
<tr><td></td><td>Diameter</td><td>Required</td><td>None</td><td>PTM_SECTION_SIZEDEP_HAMAKER SOOT 5e-13</td></tr>
<tr><td></td><td>Keyword Usage</td><td colspan="2">Optional keyword. Default value is 7e-13 erg.</td></tr>
<tr><td></td><td>Reactor Models</td><td colspan="2">• Closed Homogeneous Batch Reactor
• Internal Combustion Engine
• Perfectly Stirred Reactor (PSR)
• Diffusion or Premixed Opposed Flow Flame
• Plug Flow Reactor
• Premixed Laminar Burner Stabilized Flame
• Premixed Laminar Burner Stabilized Stagnation Flame
• Premixed Laminar Flame Speed Calculator</td></tr>
<tr><td>PTM_SECTION_SN0

Reactor Property</td><td colspan="3">Number of “atoms” in the smallest section for the specified material. When etching reactions are present, the number of sectional atoms parameter needs to be unity. When only growth is present, the user can give some higher value to avoid calculations for smaller particles that will never be present. However, this value must not be greater than the number of atoms in the smallest nucleating particle.</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td></td><td>Material name</td><td>Required</td><td>--</td><td>PTM_SECTION_SN0
SOOT 1</td></tr>
<tr><td></td><td>Number of sectional “atoms”</td><td>Required</td><td>--</td><td>PTM_SECTION_SN0
SOOT 1</td></tr>
<tr><td></td><td>Keyword Usage</td><td colspan="2">Required when the Sectional Model is used.</td></tr>
<tr><td></td><td>Reactor Models</td><td colspan="2">• Opposed-flow Flame
• Plug Flow Reactor
• Premixed Laminar Burner Stabilized Flame
• Premixed Laminar Burner Stabilized Stagnation Flame</td></tr>
</table>

Keyword	Definition			
		• Premixed Laminar Flame Speed Calculator		
PTM_SECTION_SPACING Reactor Property	Geometric spacing factor to be used for sections.			
	Parameters	Optional/Reqd.	Units	Examples
	Material name	Required	--	PTM_SECTION_SPACING CARBON 2.0
	Geometric spacing factor	Required	--	PTM_SECTION_SPACING CARBON 2.0
	Keyword Usage	Required when the Sectional Model is used.		
	Reactor Models	• Opposed-flow Flame • Plug Flow Reactor • Premixed Laminar Burner Stabilized Flame • Premixed Laminar Burner Stabilized Stagnation Flame • Premixed Laminar Flame Speed Calculator		
PTM_SECTION_TCOND Reactor Property	Thermal conductivity of particle material. This is a required input when any of the flame models are using the Sectional Model with thermophoresis.			
	Parameters	Optional/Reqd.	Units	Examples
	Material name	Required	--	PTM_SECTION_TCOND CARBON 2.0E+05
	Thermal conductivity of "material"	Required	erg/s-cm-K	PTM_SECTION_TCOND CARBON 2.0E+05
	Keyword Usage	Required when the Sectional Model with thermophoresis is used.		
	Reactor Models	• Opposed-flow Flame • Plug Flow Reactor • Premixed Laminar Burner Stabilized Flame • Premixed Laminar Burner Stabilized Stagnation Flame • Premixed Laminar Flame Speed Calculator		
PTM_SECTIONAL Reactor Property	Signals that sectional model is to be used. This is a required keyword when the Sectional Model is used.			
	Keyword Usage	Required when the Sectional Model is used.		
	Reactor Models	• Opposed-flow Flame • Plug Flow Reactor • Premixed Laminar Burner Stabilized Flame		

<table>
<tr><th>Keyword</th><th colspan="4">Definition</th></tr>
<tr><td></td><td colspan="2"></td><td colspan="2">• Premixed Laminar Burner Stabilized Stagnation Flame
• Premixed Laminar Flame Speed Calculator</td></tr>
<tr><td rowspan="4">PV

Problem Type</td><td colspan="4">Constant pressure and volume constraints.</td></tr>
<tr><td colspan="2">Keyword Usage</td><td colspan="2">Optional keyword. Exactly one problem-type keyword must be included.</td></tr>
<tr><td colspan="2">Reactor Models</td><td colspan="2">• Chemical and Phase Equilibrium Calculations</td></tr>
<tr><td colspan="2">Notes</td><td colspan="2">• VP keyword is equivalent.</td></tr>
<tr><td>PVFE

Reactor Property</td><td colspan="4">Assigns the initial (or estimate for steady state calculations) number density of the particle consisting of the designated material name. The default value is 0. The reactor number is optional. When no reactor number is given, the same initial particle volume fraction will apply to all reactors in the network. The PVFE keyword must be used in conjunction with the PNDE keyword and is mutually exclusive to keyword PROE. When both PNDE and PVFE are given, the moments are calculated as
$$M_0 = \mathrm{PNDE}$$
$$M_1 = \frac{\rho_B \times \mathrm{PVFE}}{m_0}$$
$$M_i = \left(\Delta C_{\mathrm{nuc1}}\right) \times M_{i-1} \quad 1 < i \leq \mathrm{NMOM}$$
where m_0 is the mass of a material name molecule and ρ_B is the mass density of the bulk material.</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td></td><td>Material name</td><td>Required</td><td>--</td><td>PVFE C(B) 1.0E-10 4</td></tr>
<tr><td></td><td>Volume fraction</td><td>Required</td><td>cm^3 /cm^3</td><td>PVFE C(B) 1.0E-10 4</td></tr>
<tr><td></td><td>Reactor number</td><td>Optional</td><td>--</td><td>PVFE C(B) 1.0E-10 4</td></tr>
<tr><td></td><td colspan="2">Keyword Usage</td><td colspan="2">Optional keyword. The default value is value for the volume fraction is 0. PNDE keyword required.</td></tr>
<tr><td></td><td colspan="2">Reactor Models</td><td colspan="2">• Closed Homogeneous Batch Reactor
• Closed Plasma Reactor
• Cylindrical Shear Flow Reactor
• Honeycomb Monolith Reactor
• IC HCCI Engine
• Perfectly Stirred Reactor (PSR)
• Planar Shear Flow Reactor
• Plasma PSR</td></tr>
</table>

<table>
<tr><th>Keyword</th><th colspan="4">Definition</th></tr>
<tr><td></td><td></td><td colspan="3">• Plasma Plug Flow Reactor
• Plug Flow Reactor
• SI Engine Zonal Simulator</td></tr>
<tr><td>PVFI

Inlet Property</td><td colspan="4">Assigns the volume fraction of the particle consisting of the designated material name to the named inlet stream. The default value is 0. The stream name is optional if there is only one inlet. The PVFI keyword must be used in conjunction with the PNDI keyword and is mutually exclusive to keyword PROI.</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td></td><td>Stream name</td><td>Optional if there is only one inlet.</td><td>--</td><td>PVFI mixture1 C(B) 1.0E--9</td></tr>
<tr><td></td><td>Material name</td><td>Required</td><td>--</td><td>PVFI mixture1 C(B) 1.0E-9</td></tr>
<tr><td></td><td>Number density</td><td>Required</td><td>cm^3 /cm^3</td><td>PVFI mixture1 C(B) 1.0E-9</td></tr>
<tr><td></td><td>Keyword Usage</td><td colspan="3">Optional keyword. Must be used with PNDI. Cannot be used with PROI. The default value for the number density is 0.</td></tr>
<tr><td></td><td>Reactor Models</td><td colspan="3">• Cylindrical Shear Flow Reactor
• Honeycomb Monolith Reactor
• Perfectly-stirred Reactor (PSR)
• Planar Shear Flow Reactor
• Plasma PSR
• Plasma Plug Flow Reactor
• Plug-flow Reactor (PFR)</td></tr>
<tr><td>PWRC

Reactor Property</td><td colspan="4">The power being supplied to heat the deposition surface or disk. This value is used only if the disk temperature is being calculated from an energy balance by including keyword RADB . See Equation 14.18 of the Chemkin-Pro Theory Manual .</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td></td><td>Power</td><td>Required</td><td>cal/(cm^2 . sec)</td><td>PWRC 15.E7</td></tr>
<tr><td></td><td>Keyword Usage</td><td colspan="3">Optional keyword. By default, the power is 0.0.</td></tr>
<tr><td></td><td>Reactor Models</td><td colspan="3">• Rotating Disk CVD Reactor</td></tr>
</table>

Keyword	Definition			
		• Stagnation Flow CVD Reactor		
PWRW Reactor Property	Total power deposition to the plasma.			
	Parameters	Optional/Reqd.	Units	Examples
	Total power deposition	Required	Watts	PWRW **1000.**
	Reactor number (PSR clusters only)	Optional If no number is given, the value is assumed to apply to all reactors in a cluster.	--	PWRW 1000. **1**
	Keyword Usage	Required keyword.		
	Reactor Models	• Closed Plasma Reactor • Plasma Plug Flow Reactor • Plasma PSR		
QDOT Reactor Property	The power being supplied to heat the gas as a spatially distributed Gaussian heat source. QDOT is the total power, i.e., the spatial integral of the heat source function. See Equation 14.14 of the Chemkin-Pro Theory Manual .			
	Parameters	Optional/Reqd.	Units	Examples
	Power	Required	erg/(cm^2 . sec)	QDOT **1.0E7**
	Keyword Usage	Optional keyword. By default, the power is 0.0.		
	Reactor Models	• Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
QDTC Reactor Property	The power being supplied to heat the gas as a spatially distributed Gaussian heat source. QDTC is the total power, i.e., the spatial integral of the heat source function. See Equation 14.14 of the Chemkin-Pro Theory Manual .			
	Parameters	Optional/Reqd.	Units	Examples
	Power	Required	cal/(cm^2 . sec)	QDTC **1.0E7**
	Keyword Usage	Optional keyword. By default, the power is 0.0.		

Keyword	Definition			
	Reactor Models	• Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
QEXP Reactor Property	Specifies the gas chemistry heat release rate that defines the start of the expansion period. This keyword will take effect only when the gas heat release equation is solved (activated by keyword: QRGEQ).			
	Parameters	Optional/Reqd.	Units	Examples
	heat_release_rate	Required	cal/sec	QEXP **0.5**
	Keyword Usage	Optional keyword. Default is 0.1 cal/sec.		
	Reactor Models	• Multi-Zone HCCI Simulator • IC HCCI Engine • SI Engine Zonal Simulator		
QFUN Reactor Property User Subroutine	Reactor heat loss will be given as a specified function of time (for 0-D homogeneous reactors) or as a function of distance (for Plug Flow Reactors), through a user-programmed subroutine. FUNCTION PSQFUN (LENIQ, LENRQ, IQFUN, RQFUN) must be provided to specify the heat loss and linked to the application program. See the Application Programming Interface Manual for details on how to work with user subroutines.			
	Keyword Usage	Optional keyword. By default, the value there is no heat loss from the reactor. The units returned from the user subroutine must be in erg/sec. See also QPRO.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Diffusion or Premixed Opposed-flow Flame • Honeycomb Reactor • IC HCCI Engine • Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • SI Engine Zonal Simulator		

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<table>
<tr><th>Keyword</th><th colspan="4">Definition</th></tr>
<tr><td></td><td>Notes</td><td colspan="3">• See also QPRO as an alternate way to specify heat-loss as a function of time.
• Keywords QFUN, QLOS and QPRO are mutually exclusive.</td></tr>
<tr><td>QLOS

Reactor Property</td><td colspan="4">The heat loss or heat flux from the reactor to the external environment at an optionally specified surface material. The units are for a total heat loss for 0-D homogeneous reactors, or for heat flux per area for all channel-flow reactors (Plug Flow Reactor, Honeycomb Reactor, Plasma Plug Flow Reactor, and Shear Flow Reactors). This option is only relevant when the energy equation is being solved.</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td></td><td>Material name (for 0-D homogeneous and plug-flow reactors only)</td><td>Optional

If no material is specified, the value will be used for all materials.</td><td>--</td><td>QLOS material1 50</td></tr>
<tr><td></td><td>Heat loss or Heat flux (depending on Reactor Model)</td><td>Required</td><td>cal/sec or cal/cm2-s</td><td>QLOS 50</td></tr>
<tr><td></td><td>Reactor number (PSR clusters only)</td><td>Optional

If no number is given, the keyword is assumed to apply to all reactors in a cluster.</td><td>--</td><td>QLOS material1 50 1</td></tr>
<tr><td></td><td>Keyword Usage</td><td colspan="3">Optional keyword. By default, there is no heat loss from the reactor. See also QPRO, HTRN, and QFUN.</td></tr>
<tr><td></td><td>Reactor Models</td><td colspan="3">• Closed Homogeneous Batch Reactor
• Closed Plasma Reactor
• Cylindrical Shear Flow Reactor
• Honeycomb Reactor</td></tr>
</table>

<table>
<tr><th>Keyword</th><th colspan="4">Definition</th></tr>
<tr><td></td><td colspan="4">IC HCCI Engine
Non-reactive Gas Mixer
Planar Shear Flow Reactor
Plasma Plug Flow Reactor
Plug Flow Reactor
Perfectly Stirred Reactor (PSR)
SI Engine Zonal Simulator</td></tr>
<tr><td>QLSE

Reactor Property Profiles</td><td colspan="4">This is an additional energy loss term for the electrons that may be introduced to account for inelastic collisional losses that are not already included explicitly in the Gas-phase Kinetics reaction mechanism. Energy loss values are specified here as a function of electron temperature and are given per ionization event to be consistent with the work of Lee, et al.[11] (p. 331) For example, “QLSE 34800. 100.” would represent an electron energy loss of 100 eV/ionization event for an electron temperature of 34800 K (3.0 eV).</td></tr>
<tr><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td colspan="2">Examples</td></tr>
<tr><td>Energy loss</td><td>Required</td><td>eV</td><td colspan="2">QLSE 34800. 100.</td></tr>
<tr><td>Electron temperature</td><td>Required</td><td>K</td><td colspan="2">QLSE 34800. 100.</td></tr>
<tr><td>Keyword Usage</td><td colspan="4">Optional keyword. By default, the additional energy loss term is 0.0.</td></tr>
<tr><td>Reactor Models</td><td colspan="4">Closed Plasma Reactor
Plasma Plug Flow Reactor
Plasma PSR</td></tr>
<tr><td>QPRO

Reactor Property Profiles</td><td colspan="4">The heat loss profile or heat flux profile from the reactor to the external environment at an optionally specified surface material, given as a piece-wise linear function of time or distance. Each QPRO entry represents a point in a piecewise-linear profile. The units are for a total heat loss vs. time for 0-D homogeneous reactors, or for heat flux per area vs. distance for all channel-flow reactors (Plug Flow Reactor, Honeycomb Reactor, Plasma Plug Flow Reactor, and Shear Flow Reactors). This option is only relevant when the energy equation is being solved.</td></tr>
<tr><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td colspan="2">Examples</td></tr>
<tr><td>Time or Distance value (depending on Reactor Model)</td><td>Required</td><td>sec or cm</td><td colspan="2">QPRO 1.0E-4 10.0</td></tr>
<tr><td>Heat loss or Heat flux (depending on Reactor Model)</td><td>Required</td><td>cal/sec or cal/cm2-sec</td><td colspan="2">QPRO 1.0E-4 10.0</td></tr>
</table>

Keyword	Definition			
	Reactor number (PSR clusters only)	Optional If no number is given, the profile described by the first two values is assumed to apply to all reactors in a cluster.	--	QPRO 1.0E-4 10.0 **1**
	Keyword Usage	Optional keyword. By default, there is no heat loss from the reactor. See also QLOS, HTRN, and QFUN.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Cylindrical Shear Flow Reactor • Honeycomb Reactor • IC HCCI Engine • Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma PSR • Plasma Plug Flow Reactor • Plug Flow Reactor • SI Engine Zonal Simulator		
QRGEQ Output	Solve a separate equation that integrates the heat release due to gas-phase reactions to obtain a more accurate heat-release profile. If this option is not checked, only local heat release rates will be reported at each saved or printed time steps. Only applicable when you are solving the energy equation with transient solver.			
	Parameters	Optional/Reqd.	Units	Examples
	Keyword Usage	Optional keyword. By default, the heat release integration equation is not solved.		

Keyword	Definition			
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Honeycomb Monolith Reactor • IC HCCI Engine • Perfectly Stirred Reactor (PSR) • Plasma PSR • Plasma Plug Flow Reactor • Plug Flow Reactor • SI Engine Zonal Simulator		
QRSEQ Output	Solve a separate equation that integrates the heat release due to surface reactions to obtain a more accurate heat-release profile. If this option is not checked, only local heat release rates will be reported at each saved or printed time steps. Only applicable when you are solving the energy equation with transient solver.			
	Parameters	Optional/Reqd.	Units	Examples
	Keyword Usage	Optional keyword. By default, the heat release integration equation is not solved.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Honeycomb Monolith Reactor • IC HCCI Engine • Perfectly Stirred Reactor (PSR) • Plasma PSR • Plasma Plug Flow Reactor • Plug Flow Reactor		
QXCO Recycling	This keyword defines the heat-transfer coefficient and the heat-transfer surface area for thermal conductive/convective heat flux between the two specified reactors in a reactor cluster. The direction of the heat flux will come from the higher-temperature reactor to the lower-temperature reactor. This keyword is only relevant when the ENRG keyword is used and when there are multiple reactors in a cluster.			
	Parameters	Optional/Reqd.	Units	Examples
	Reactor Number	Required	--	QXCO **3** 6 1.0E-3 1000.
	Reactor Number	Required	--	QXCO 3 **6** 1.0E-3 1000.

Keyword	Definition			
	Heat-transfer coefficient	Required	cal/(cm^2 · sec · K)	QXCO 3 6 **1.0E-3** 1000.
	Heat-transfer surface area	Required	cm^2	QXCO 3 6 1.0E-3 **1000.**
	Keyword Usage	Optional keyword. By default, there is no heat exchange between reactors.		
	Reactor Models	• Perfectly Stirred Reactor (PSR) • Plasma PSR		
	Notes	• The order of the two reactor numbers that define the heat connection is not important. • This parameter is used in conjunction with the external surface area (AREAQ or AEXT).		
QXRA Recycling	This keyword defines the thermal emissivity/absorptivity and the heat-transfer surface area for thermal radiative flux between the two specified reactors in a reactor cluster. The direction of the heat flux will come from the higher-temperature reactor to the lower-temperature reactor. This keyword is only relevant when the ENRG keyword is used and when there are more than one reactor in a cluster.			
	Parameters	Optional/Reqd.	Units	Examples
	Reactor Number	Required	--	QXRA **2** 3 0.1 1000.
	Reactor Number	Required	--	QXRA 2 **3** 0.1 1000.
	Emissivity/absorptivity	Required	--	QXRA 2 3 **0.1** 1000.
	Heat-transfer surface area	Required	cm^2	QXRA 2 3 0.1 **1000.**
	Keyword Usage	Optional keyword. By default, there is no heat exchange between reactors. Note that the order of the two reactor numbers that define the heat connection is un-important.		
	Reactor Models	• Perfectly Stirred Reactor (PSR) • Plasma PSR		
	Notes	• The order of the two reactor numbers that define the heat connection is not important. • This parameter is used in conjunction with the external surface area (AREAQ or AEXT).		
RACTV Reactor Property	By default, when the gas-phase thermal radiation calculation is on, contributions from all major radiating species (such as CO_2, H_2 O, CO, and CH_4) will not be included. A major radiating species is a species of which the absorption coefficient			

Keyword	Definition			
	is available to the application. This keyword allows the user to include the contribution of a major species in the radiation heat loss calculation.			
	Parameters	Optional/Reqd.	Units	Examples
	Species symbol	Required	--	RACTV CO
	Keyword Usage	Optional keyword.		
	Reactor Models	• Diffusion or Premixed Opposed-flow Flame • Burner-stabilized Pre-mixed Flame • Premixed Laminar Flame-speed Calculation		
RADB Reactor Property	Use an energy balance to determine the disk or susceptor (deposition surface) temperature. If RADB is specified, TDSK is used as the initial guess for the susceptor temperature.			
	Keyword Usage	Optional keyword. By default, the susceptor temperature is fixed as TDSK.		
	Reactor Models	• Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
RADGS Reactor Property	Turns on the radiation heat loss term in the gas energy equation. The optional model number indicates which thermal radiation model will be employed to calculate the radiation intensity.			
	Parameters	Optional/Reqd.	Units	Examples
	Reactor number	Required	--	RADGS **0**
	Keyword Usage	Currently, the optically-thin limit model is the only model implemented and hence is the default model. The model number for the optically-thin limit model is 0.		
	Reactor Models	• Diffusion or Premixed Opposed-flow Flame • Burner-stabilized Pre-mixed Flame • Premixed Laminar Flame-speed Calculation		
RADPT Reactor Property	Allows radiative heat loss contribution from particulates associated with the named material to be included independently.			
	Parameters	Optional/Reqd.	Units	Examples
	Material Name	Required	--	RADPT **CO**
	Reactor Models	• Diffusion or Premixed Opposed-flow Flame • Burner-stabilized Pre-mixed Flame • Premixed Laminar Flame-speed Calculation		

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Keyword	Definition			
RCHG Solver	Maximum relative change in the surface site fractions (over one time step) for which the initial fictitious transient equations that establish the initial surface site fractions can be considered to have converged to steady state.			
	Parameters	Optional/Reqd.	Units	Examples
	Maximum relative change	Required	--	RCHG **1.0E-3**
	Keyword Usage	Optional keyword. By default, the maximum relative change is set to 1.0E-6.		
	Reactor Models	• Honeycomb Reactor • Plasma Plug Flow Reactor • Plug Flow Reactor		
RDSK Reactor Property	Ratio of the substrate radius to the separation distance between it and the upper radiating disk. This is used in calculating a surface radiation balance. RRAD is used only if the disk temperature is being calculated by including keyword RADB . See Equation 14.18 of the Chemkin-Pro Theory Manual .			
	Parameters	Optional/Reqd.	Units	Examples
	Ratio of substrate	Required	--	RDSK **3.0**
	Keyword Usage	Optional keyword. This is keyword is required only when RRAD and RADB are included.		
	Reactor Models	• Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
REAC Inlet or Reactor Property	Mole fraction of the reagent gases entering the reactor for an inlet stream or for the initial conditions in a closed system. For example, REAC fuel1 C2H2 0.5, would indicate that acetylene has a mole fraction of 0.5 in the inlet stream named fuel1. The sum of all the reactant mole fractions should equal to one. However, if they do not the fractions will be normalized so that they do sum to one, and a warning message will be printed to the output file.			
	Parameters	Optional/Reqd.	Units	Examples
	Inlet stream name (for PSRs and CVD Reactors only)	Optional If there is no stream name than the reactant and mole fraction apply to all streams.	--	REAC **fuel1** C2H2 0.5
	Species name	Required	--	REAC **C2H2** 0.5

Keyword	Definition			
	Reactant fraction	Required	mole fractions	REAC C2H2 **0.5**
	Keyword Usage	Required keyword, except in cases where an equivalence ratio option is used (EQUI).		
	Reactor Models	• Chemical and Phase Equilibrium Calculations • Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Cylindrical Shear Flow Reactor • Diffusion or Premixed Opposed-flow Flame • Honeycomb Reactor • IC HCCI Engine • Non-reactive Gas Mixer • Partially Stirred Reactor (PaSR) • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
	Notes	• The REAC keywords must be changed as a set, not individually for a restart run. • The REAC keywords must be changed as a set, not individually for continuation run.		
RECY Recycling	For a cluster of reactors (NPSR > 1), specifies recycling or routing of a mass flow from one reactor to another and the fractional flow associated with this stream.			
	Parameters	Optional/Reqd.	Units	Examples
	Reactor Number, from which the flow originates	Required	--	RECY **2** 1 0.3

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Keyword	Definition			
	Reactor Number, to which the flow is transferred	Required	--	RECY 2 **1** 0.3
	Percent that will be recycled from Reactor 2 back into Reactor 1	Required	--	RECY 2 1 **0.3**
	Keyword Usage	Optional keyword. By default all flow out of a reactor in will flow into the next reactor in the series (e.g. RECY 1 2 1.0 and RECY 2 3 1.0 for a three-reactor system). If recycle loops are defined, then the effective "recycling" from the upstream into the downstream reactor will be one minus the sum of the recycle streams out of the upstream reactor into other reactors.		
	Reactor Models	• Perfectly Stirred Reactor (PSR) • Plasma PSR		
RELAXC Solver	Controls the convergence method used for transient runs. When applied, it uses a relaxed scheme whereby the integrator solver tries harder to achieve a solution at each time, but occasionally may result in increased time to solve your problem or numerical instabilities. Therefore, you should use this only if your transient run fails with a "nonlinear solver failed to converge repeatedly" message or you believe your problem is very stiff, highly nonlinear or discontinuous.			
	Keyword Usage	Optional keyword.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Partially Stirred Reactor • Closed Plasma Reactor • Cylindrical Shear Flow Reactor • Honeycomb Reactor • IC HCCI Engine • Multi-Zone HCCI Engine Simulator • Partially Stirred Reactor (PaSR) • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor		

Keyword	Definition			
		• Rotating Disk CVD Reactor • SI Engine Zonal Simulator • Stagnation Flow CVD Reactor		
RELT Solver	This keyword is used to override the default value for the relative perturbation in the solution variable used in the determination of the numerically derived Jacobian.			
	Parameters	Optional/Reqd.	Units	Examples
	Relative perturbation	Required	--	RELT **1.E-15**
	Keyword Usage	Optional keyword. By default, the relative perturbation is set equal to the square root of the unit round-off error of the machine.		
	Reactor Models	• Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Plasma PSR		
RE-OR Reactor Property	The option may be used when the TRCE option is in effect. Using TRCE, the conservation equation for the last species in the gas-phase and each surface and bulk phase is not solved: the last species concentration (mass fraction or site fraction) is chosen so that the fractions sum to one. The REOR option causes TRCE to choose dynamically and locally (at each mesh point and in each phase) the species of largest concentration and not solve its conservation equation.			
	Keyword Usage	Optional keyword. By default, the last species in each phase is chosen.		
	Reactor Models	• Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
RHO1 Reactor Property	Mass density before the incident shock.			
	Parameters	Optional/Reqd.	Units	Examples
	Mass density	Required	gm/cm^3	RHO1 **1.E-4**
	Keyword Usage	Optional keyword. The shock velocity and any two of temperature, pressure, or density must be specified for conditions before the incident shock. See also T1 and P1A .		
	Reactor Models	• Normal Incident Shock • Normal Reflected Shock		
RHO2	Mass density after the incident shock.			

Keyword	Definition			
Reactor Property	Parameters	Optional/Reqd.	Units	Examples
	Mass density	Required	g/cm^3	RHO2 **1.E-4**
	Keyword Usage	Optional keyword. Any two of temperature, pressure, or density must be specified for conditions after the incident shock. See also T2 and P2A .		
	Reactor Models	• Normal Incident Shock • Normal Reflected Shock		
RHO3 Reactor Property	Mass density after the reflected shock.			
	Parameters	Optional/Reqd.	Units	Examples
	Mass density	Required	g/cm^3	RHO3 **1.E-4**
	Keyword Usage	Optional keyword. Any two of temperature, pressure, or density must be specified for conditions after the reflected shock. See also T3 and P3A .		
	Reactor Models	• Normal Reflected Shock		
RL-GAS Reactor Property	This optional keyword is used to turn the real gas model on or off. Setting the option value to 1 will activate the real gas model if the gas reaction mechanism contains the real gas data. A value of 0 = turn OFF the real gas model and 1= turn ON the model.			
	Parameters	Optional/Reqd.	Units	Examples
	Enabled	Required	g/cm^3	RLGAS **1**
	Keyword Usage	Optional keyword. By default, the real gas model is turned OFF.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Partially Stirred Reactor • Cylindrical Shear Flow Reactor • Diffusion or Premixed Opposed-flow Flame • Flame-Extinction Simulator • Honeycomb Reactor • IC HCCI Engine • Multi-Zone HCCI Engine Simulator • Normal Incident Shock • Normal Reflected Shock		

<table>
<tr><th>Keyword</th><th colspan="4">Definition</th></tr>
<tr><td></td><td></td><td colspan="3">• Partially Stirred Reactor (PaSR)
• Perfectly Stirred Reactor (PSR)
• Planar Shear Flow Reactor
• Plug Flow Reactor
• Rotating Disk CVD Reactor
• SI Engine Zonal Simulator
• Stagnation Flow CVD Reactor</td></tr>
<tr><td rowspan="5">RL-MIX

Reactor Property</td><td colspan="4">This optional keyword will activate the selected real gas mixing rule if the real gas model is turned on (by RLGAS). A value of 0 = use the Van der Waals mixing rule and 1 = use the pseudocritical method (see Real Gas Data (p. 36)).</td></tr>
<tr><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td>Method</td><td>Required</td><td>None</td><td>RLMIX 0</td></tr>
<tr><td>Keyword Usage</td><td colspan="3">Optional keyword. By default, the van der Waals method will be applied.</td></tr>
<tr><td>Reactor Models</td><td colspan="3">• Closed Homogeneous Batch Reactor
• Closed Partially Stirred Reactor
• Cylindrical Shear Flow Reactor
• Diffusion or Premixed Opposed-flow Flame
• Flame-Extinction Simulator
• Honeycomb Reactor
• IC HCCI Engine
• Multi-Zone HCCI Engine Simulator
• Normal Incident Shock
• Normal Reflected Shock
• Partially Stirred Reactor (PaSR)
• Perfectly Stirred Reactor (PSR)
• Planar Shear Flow Reactor
• Plug Flow Reactor
• Rotating Disk CVD Reactor
• SI Engine Zonal Simulator</td></tr>
</table>

Keyword	Definition			
		• Stagnation Flow CVD Reactor		
ROP Output	Inclusion of this keyword causes the rate-of-production coefficients to be printed for specified species. The keyword must be followed by one or more names of species. If any ROP keywords are used, all the rate-of-production coefficients will be computed and written to the XML Solution File (e.g., XMLdata.zip). However, only those specified by the ROP keyword will be printed in the diagnostic output file. More than one species may be entered per line. If the line is blank after the ROP keyword, then all rate-of-production contributions are computed and written to the XML Solution File, but none are printed.			
	Keyword Usage	Optional keyword. By default, no rate-of-production values are computed.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Honeycomb Reactor • IC HCCI Engine • Perfectly Stirred Reactor (PSR) • Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor • SI Engine Zonal Simulator		
	Notes	• This keyword can be added but not removed from a continuation run. • Rates of production can be calculated for other Reactor Models through the graphical ANSYS Chemkin-Pro Post-processor		
RPM Reactor Property	Revolutions per minute of the engine crank arm.			
	Parameters	Optional/Reqd.	Units	Examples
	Revolutions per minute	Required	rpm	RPM **1200**
	Keyword Usage	Optional keyword. By default, the rpm is 1500.		
	Reactor Models	• IC HCCI Engine • SI Engine Zonal Simulator		
RRAD Reactor Property	Ratio of the upper radiating disk radius to the separation distance between it and the lower substrate. This is used in calculating a surface radiation balance. RRAD is used only if the disk temperature is being calculated by including keyword RADB . See Equation 14.18 of the Chemkin-Pro Theory Manual .			

Keyword	Definition			
	Parameters	Optional/Reqd.	Units	Examples
	Ratio of the upper radiating disk	Required	--	RRAD **3.0**
	Keyword Usage	Required keyword only if RADB and RDSK are included.		
	Reactor Models	• Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
RSHK Problem Type	Inclusion of this keyword designates a reflected shock problem.			
	Keyword Usage	Required keyword. See also ISHK.		
	Reactor Models	• Normal Reflected Shock		
RSTR Cluster Property	Inclusion of this keyword causes ANSYS Chemkin-Pro to read a solution off the XML Solution File (e.g., XMLdata.zip) and begin iteration or integration on the current reactor conditions from this solution.			
	Keyword Usage	Optional keyword. By default, a solution is started from the user-specified conditions and no XML Solution File is used.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Partially Stirred Reactor (PaSR) • Closed Plasma Reactor • Cylindrical Shear Flow Reactor • Diffusion or Premixed Opposed-flow Flame • Honeycomb Reactor • IC HCCI Engine • Partially Stirred Reactor (PaSR) • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor • SI Engine Zonal Simulator		

Keyword	Definition			
		• Stagnation Flow CVD Reactor		
RTIM Solver	Relative tolerance for convergence of Newton iteration as it is used in the pseudo time stepping procedure for steady-state problems employing the *Twopnt* solver. Since we are not seeking accuracy in a transient solution, this convergence criteria typically does not need to be as stringent as for the Newton iteration on the actual steady-state solution.			
	Parameters	Optional/Reqd.	Units	Examples
	Absolute tolerance	Required	--	RTIM **1.E-3**
	Keyword Usage	Optional keyword. By default, the relative tolerance is 1.E-4. See also ATIM.		
	Reactor Models	• Closed Plasma Reactor • Cylindrical Shear Flow Reactor • Diffusion or Premixed Opposed-flow Flame • Honeycomb Reactor • Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma PSR • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
	Notes	• For a more precise definition, see the description of RTOL.		
RTIME Reactor Property	Turn on or off solution of the residence-time equation for a plug-flow simulation.			
	Parameters	Optional/Reqd.	Units	Examples
	String "ON" or "OFF" to toggle the momentum equation	Required	--	RTIME **ON** RTIME OFF
	Keyword Usage	Optional keyword. By default, the residence-time equation is solved (ON).		
	Reactor Models	• Honeycomb Reactor • Plasma Plug Flow Reactor • Plug Flow Reactor		

<table>
<tr><th>Keyword</th><th>Definition</th></tr>
<tr><td>RTLM

Solver</td><td>A different relative tolerance can be assigned to moment variables in steady-state calculations. By default, the same relative tolerance given by RTOL is used for all variables.
<table>
<tr><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td>Tolerance</td><td>Required</td><td>--</td><td>RTLM 1.0E-4</td></tr>
<tr><td>Keyword Usage</td><td colspan="3">Optional keyword. By default, the absolute tolerance is determined by RTOL.</td></tr>
<tr><td>Reactor Models</td><td colspan="3">• Closed Plasma Reactor
• Cylindrical Shear Flow Reactor
• Perfectly Stirred Reactor (PSR)
• Planar Shear Flow Reactor
• Plasma PSR</td></tr>
</table></td></tr>
<tr><td>RTLS

Solver</td><td>Relative tolerance used by the transient solver, DASPK, as an indicator of the accuracy desired in the solution for the sensitivity coefficients only. Generally, the sensitivity coefficients need not be solved to a great degree of accuracy, so these tolerances should be lower than the tolerances placed on the physical variables.
<table>
<tr><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td>Relative tolerance</td><td>Required</td><td>--</td><td>RTLS 1.E-2</td></tr>
<tr><td>Keyword Usage</td><td colspan="3">Optional keyword. By default, the relative tolerance is 1.E-5.</td></tr>
<tr><td>Reactor Models</td><td colspan="3">• Closed Homogeneous Batch Reactor
• Closed Plasma Reactor
• Honeycomb Reactor
• IC HCCI Engine
• Perfectly Stirred Reactor (PSR)
• Plasma PSR
• Plasma Plug Flow Reactor
• Plug Flow Reactor
• SI Engine Zonal Simulator</td></tr>
</table></td></tr>
<tr><td>RTOL

Solver</td><td>Relative tolerance used by the solver to determine convergence and as an indicator of the accuracy desired in the physical solution. In general the value of RTOL roughly corresponds to the number of significant digits that should be expected from a solution. A typical value should be between 10-3 and 10-6, which would provide roughly three to six significant digits.</td></tr>
</table>

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Keyword	Definition			
	Parameters	Optional/Reqd.	Units	Examples
	Relative tolerance	Required	--	RTOL **1.E-3**
	Keyword Usage	Optional keyword. The default values are: Open 0-D Reactors run in steady-state mode, Opposed-flow Flame, Premixed Laminar Burner-stabilized Flame, Premixed Laminar Flame-speed Calculation, Shear Flow Reactor: 1.E-4 Normal Incident Shock, Normal Reflected Shock, Plug Flow Reactor, Partially Stirred Reactor (PaSR), CVD: 1.E-6 Closed 0-D Reactors and Open 0-D Reactors run in transient mode: 1.E-8 See also ATOL.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Partially Stirred Reactor (PaSR) • Closed Plasma Reactor • Cylindrical Shear Flow Reactor • Diffusion or Premixed Opposed-flow Flame • Honeycomb Reactor • IC HCCI Engine • Non-reactive Gas Mixer • Normal Incident Shock • Normal Reflected Shock • Opposed-flow Flame • Partially Stirred Reactor (PaSR) • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma PSR • Plug Flow Reactor • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor		

<table>
<tr><th>Keyword</th><th colspan="4">Definition</th></tr>
<tr><td></td><td></td><td colspan="3">• SI Engine Zonal Simulator
• Stagnation Flow CVD Reactor</td></tr>
<tr><td rowspan="5">SCAT

Output</td><td colspan="4">Request the scatter plot of a scalar to be output to the file scatter.plt.</td></tr>
<tr><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td>Scalar (temperature or species name)</td><td>Required</td><td>--</td><td>SCAT CH4</td></tr>
<tr><td>Keyword Usage</td><td colspan="3">Optional keyword. By default, no scatter plot is printed.</td></tr>
<tr><td>Reactor Models</td><td colspan="3">• Closed Partially Stirred Reactor (PaSR)
• Partially Stirred Reactor (PaSR)</td></tr>
<tr><td rowspan="6">SCCM

Inlet Property</td><td colspan="4">The volumetric flow rate into the reactor for an optionally specified inlet stream, in standard cubic centimeters per minute assuming that the inlet temperature is 298.15 K and the inlet pressure is 1 atm unless a different value for TSCCM is provided.</td></tr>
<tr><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td>Inlet stream name</td><td>Optional

If there is no stream name than the volumetric flow rate applies to the default or all defined streams.</td><td>--</td><td>SCCM secondary_air
300</td></tr>
<tr><td>Equivalent volumetric flow rate at standard conditions</td><td>Required</td><td>standard cm ^{3} /min</td><td>SCCM secondary_air
300</td></tr>
<tr><td>Keyword Usage</td><td colspan="3">PSRs and PaSRs: Optional keyword. If none of TAU, FLRT / FPRO, SCCM / SCCMPRO are specified or are nonzero, then a closed-system is assumed. FLRT / FPRO or SCCM / SCCMPRO is required for each INLET stream defined.

Stagnation Flow CVD Reactors: FLRT / FPRO or SCCM / SCCMPRO or UINL is required for each inlet stream defined.

Rotating Disk CVD Reactors: Optional keyword.</td></tr>
</table>

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<table>
<tr><th>Keyword</th><th colspan="4">Definition</th></tr>
<tr><td></td><td>Reactor Models</td><td colspan="3">• Non-reactive Gas Mixer
• Perfectly Stirred Reactor (PSR)
• Plasma PSR
• Rotating Disk CVD Reactor
• Stagnation Flow CVD Reactor</td></tr>
<tr><td>SCCMPRO

Inlet Property Profiles</td><td colspan="4">Used to specify a transient profile or function of mass flow rate vs. time for an inlet stream, in standard cubic centimeters per minute assuming that the inlet temperature is 298.15 K and the inlet pressure is 1 atm unless a different standard temperature (TSCCM) is entered. The profile specified will be interpolated linearly from the SCCMPRO points provided.</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td></td><td>Inlet stream name</td><td>Optional

If no stream name is given, the profile described by the reactant and mole fraction is assumed to apply to all reactors in a cluster.</td><td>--</td><td>SCCMPRO purge 0.19 300</td></tr>
<tr><td></td><td>Time</td><td>Required</td><td>sec (cm for flow reactors)</td><td>SCCMPRO 0.19 300</td></tr>
<tr><td></td><td>Equivalent volumetric flow rate at standard conditions</td><td>Required</td><td>standard cm^3 /min</td><td>SCCMPRO 0.19 300</td></tr>
<tr><td></td><td>Keyword Usage</td><td colspan="3">PFRs and Monolith Reactors: Flow specification via one of VEL, VDOT, VDOTPRO SCCM SCCMPRO FLRT, or FPRO is required.

PSRs and PaSRs: Optional keyword. If none of TAU, FLRT / FPRO, SCCM / SCCMPRO are specified or are</td></tr>
</table>

<table>
<tr><th>Keyword</th><th colspan="4">Definition</th></tr>
<tr><td></td><td></td><td colspan="3">nonzero, then a closed-system is assumed. FLRT / FPRO or SCCM / SCCMPRO is required for each INLET stream defined.

Stagnation Flow CVD Reactors: FLRT / FPRO or SCCM / SCCMPRO or UINL is required for each inlet stream defined.

Rotating Disk CVD Reactors: Optional keyword.</td></tr>
<tr><td></td><td>Reactor Models</td><td colspan="3">• Honeycomb Monolith Reactor
• Non-reactive Gas Mixer
• Perfectly Stirred Reactor (PSR)
• Plasma PFR
• Plasma PSR
• Plug Flow Reactor
• Rotating Disk CVD Reactor
• Stagnation Flow CVD Reactor</td></tr>
<tr><td>SCLM

Reactor Property</td><td colspan="4">Scaling factor for the particles moments (moments method) or number density (sectional method). A non-unity value for this parameter changes the units of the (internal) solution variable for particle moments or number density. For example, setting it to 1.0E+06 results in micro-moles whereas setting it to 1.0E+09 means that it is nano-moles. A value of 1 would mean that the unit should be moles. A recommended value for typical problems is 1.0E+12. Such scaling helps preserve the positivity of the solution during numerical computation.</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td></td><td>Scaling factor</td><td>Required</td><td>--</td><td>SCLM 1.0E+12</td></tr>
<tr><td></td><td>Keyword Usage</td><td colspan="3">Optional keyword.</td></tr>
<tr><td></td><td>Reactor Models</td><td colspan="3">• Closed Homogeneous Batch Reactor
• Closed Plasma Reactor
• Flame-Extinction Simulator
• Honeycomb Monolith Reactor
• IC HCCI Engine
• Multi-Zone HCCI Engine Simulator
• Opposed-flow Flame
• Perfectly Stirred Reactor (PSR)
• Plasma Plug Flow Reactor</td></tr>
</table>

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<table>
<tr><th>Keyword</th><th colspan="4">Definition</th></tr>
<tr><td></td><td></td><td colspan="3">• Plasma PSR
• Plug Flow Reactor
• Premixed Laminar Burner-stabilized Flame
• Premixed Laminar Flame-speed Calculation
• SI Engine Zonal Simulator
• Stagnation Flow Flame Simulator</td></tr>
<tr><td rowspan="6">SCLS

Reactor Property</td><td colspan="4">Scaling factor for the particle surface species concentrations. A non-unity value for this parameter changes the units of the (internal) solution variable for particle surface species. For example, setting it to 1.0E+06 results in micro-moles whereas setting it to 1.0E+09 means that it is nano-moles. A value of 1 would mean that the unit should be moles. A recommended value for typical problems is 1.0E+12. Such scaling helps preserve the positivity of the solution during numerical computation.</td></tr>
<tr><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td>Scaling factor</td><td>Required</td><td>--</td><td>SCLS 1.0E+12</td></tr>
<tr><td>Keyword Usage</td><td colspan="3">Optional keyword.</td></tr>
<tr><td>Reactor Models</td><td colspan="3">• Closed Homogeneous Batch Reactor
• Closed Plasma Reactor
• Flame-Extinction Simulator
• Honeycomb Monolith Reactor
• IC HCCI Engine
• Multi-Zone HCCI Engine Simulator
• Opposed-flow Flame
• Perfectly Stirred Reactor (PSR)
• Plasma Plug Flow Reactor
• Plasma PSR
• Plug Flow Reactor
• Premixed Laminar Burner-stabilized Flame
• Premixed Laminar Flame-speed Calculation
• SI Engine Zonal Simulator
• Stagnation Flow Flame Simulator</td></tr>
</table>

<table>
<tr><th>Keyword</th><th colspan="4">Definition</th></tr>
<tr><td>SCOR

Solver</td><td colspan="4">Flag instructing that the transient solver, DASPK will use staggered corrector method to solve sensitivity equations. The staggered corrector method is the sensitivity method that was used in previous versions of ANSYS Chemkin-Pro and is mainly provided for backwards compatibility. It is generally slower than the default sensitivity method in Chemkin-Pro (which is the staggered direct method) but sometimes can be more stable and robust than the staggered direct method.</td></tr>
<tr><td></td><td>Keyword Usage</td><td colspan="3">Optional keyword. By default, DASPK uses staggered corrector method to solve sensitivity equations.</td></tr>
<tr><td></td><td>Reactor Models</td><td colspan="3">• Closed Homogeneous Batch Reactor
• Closed Plasma Reactor
• Honeycomb Reactor
• IC HCCI Engine
• Non-reactive Gas Mixer
• Perfectly Stirred Reactor (PSR)
• Plasma PSR
• Plasma Plug Flow Reactor
• Plug Flow Reactor
• SI Engine Zonal Simulator</td></tr>
<tr><td></td><td>Notes</td><td colspan="3">• SCOR can be changed for a continuation run, but it cannot be removed from one.</td></tr>
<tr><td>SCOV

Output</td><td colspan="4">Analyze the coverage dependence of a surface reaction, i.e., create a table of effective reaction rates versus temperature. Surface coverage is assumed to be that of the bath-gas composition. The ALL option is the default and produces tables for every surface reaction. The NONE option suppresses output for all of the reactions. If reaction information is desired for only certain reactions, they may be optionally specified by their number (given in the Pre-processor output) or by typing an exact duplicate of the reaction expression (see example input).</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td></td><td>ALL option</td><td>Optional, default is ALL</td><td>--</td><td>SCOV ALL</td></tr>
<tr><td></td><td>NONE option</td><td>Optional, default is ALL</td><td>--</td><td>SCOV NONE</td></tr>
<tr><td></td><td>Surface reaction number list</td><td>Optional, de-</td><td>--</td><td>SCOV 2 5</td></tr>
</table>

Keyword	Definition			
		fault is ALL		
	Surface reaction expression	**Option-al, de-fault is ALL**	--	SCOV **CH(S)+H<=>C(S,R)+H2**
	Keyword Usage	Optional keyword. By default, the table output is determined by the ALL or NONE keyword.		
	Reactor Models	• Mechanism Analyzer		
SENG Output	Inclusion of this keyword causes the calculation of the first-order sensitivity coefficients, with respect to the gas-phase and surface chemistry rate constants, for the growth rate of all bulk phases. Growth-rate sensitivities will be included in the printed output and the XML Solution File (e.g., XMLdata.zip).			
	Keyword Usage	Optional keyword. By default, no sensitivity coefficients are computed. See also ASEN.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Honeycomb Reactor • Perfectly Stirred Reactor (PSR) • Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor		
	Notes	• This keyword can be added but not removed from a continuation run.		
SENT Output	Calculate and store sensitivity coefficients for gas temperature with respect to reaction A-factors.See ASEN.			
	Keyword Usage	Optional keyword. By default, no sensitivity coefficients are computed or printed. Same as ASEN TEMP.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Honeycomb Reactor • IC HCCI Engine • Multi-Zone HCCI Engine Simulator • Perfectly Stirred Reactor (PSR) • Plasma Plug Flow Reactor		

<table>
<tr><th>Keyword</th><th colspan="4">Definition</th></tr>
<tr><td></td><td colspan="4">Plasma PSR
Plug Flow Reactor
Opposed-flow Flame
Premixed Laminar Burner-stabilized Flame
Premixed Laminar Flame-speed Calculation
Rotating Disk CVD Reactor
SI Engine Zonal Simulator
Stagnation Flow CVD Reactor</td></tr>
<tr><td>SFAC

Reactor Property</td><td colspan="4">This keyword specifies that the rates of all surface reactions will be multiplied (scaled) by the factor SFAC. This option is sometimes useful if convergence difficulties are encountered due to unusually large reaction rates. The problem would be first solved with artificially reduced reaction rates, which then can be increased in subsequent continuations or restarts until SFAC is one.</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td></td><td>Multiplier value</td><td>Required</td><td>--</td><td>SFAC 2.0</td></tr>
<tr><td></td><td>Reactor number
(PSR clusters only)</td><td>Optional

If no number is given, value is assumed to apply to all reactors in a cluster.</td><td>--</td><td>SFAC 2.0 1</td></tr>
<tr><td></td><td>Keyword Usage</td><td colspan="3">Optional keyword. By default, the multiplier value is set to 1.0.</td></tr>
<tr><td></td><td>Reactor Models</td><td colspan="3">Closed Homogeneous Batch Reactor
Closed Plasma Reactor
Cylindrical Shear Flow Reactor
Honeycomb Reactor
Non-reactive Gas Mixer
Perfectly Stirred Reactor (PSR)
Planar Shear Flow Reactor</td></tr>
</table>

<table>
<tr><th>Keyword</th><th>Definition</th></tr>
<tr><td></td><td></td><td>• Plasma Plug Flow Reactor
• Plasma PSR
• Plug Flow Reactor
• Rotating Disk CVD Reactor
• Stagnation Flow CVD Reactor</td></tr>
<tr><td>SFLR
Solver</td><td colspan="2">Sometimes during the solution procedure some of the very small gas-phase mass fractions, surface site fractions, or bulk species fractions may be calculated as a slightly negative number. No solution component will be allowed to drop below the floor value specified by SFLR.</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td></td><td>Minimum bounds on the solution variables</td><td>Required</td><td>--</td><td>SFLR -1.E-5</td></tr>
<tr><td></td><td>Keyword Usage</td><td colspan="2">Optional keyword. By default, the minimum bounds on the solution variables is set to -1.E-4</td></tr>
<tr><td></td><td>Reactor Models</td><td colspan="2">• Diffusion or Premixed Opposed-flow Flame
• Non-reactive Gas Mixer
• Perfectly Stirred Reactor (PSR)
• Plasma PSR
• Rotating Disk CVD Reactor
• Stagnation Flow CVD Reactor
• Premixed Laminar Burner-stabilized Flame
• Premixed Laminar Flame-speed Calculation</td></tr>
<tr><td>SFMN
Solver</td><td colspan="3">Set the minimum bounds of the surface species concentration to a slightly negative number to allow the solver more room to search for a solution.</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td></td><td>Minimum bound</td><td>Required</td><td>--</td><td>SFMN -1.0d-06</td></tr>
<tr><td></td><td>Keyword Usage</td><td colspan="2">Optional keyword. Usable only with Particle Tracking.</td></tr>
<tr><td></td><td>Reactor Models</td><td colspan="2">• Opposed-flow Flame
• Premixed Laminar Burner-stabilized Flame
• Premixed Laminar Flame-speed Calculation</td></tr>
<tr><td>SGMAXIT
Solver</td><td colspan="3">This controls the maximum number of iterations the segregated solver can take per step to solve the problem. The default is 100 and you may increase this value to give the solver greater chance to solve your problem if it is very hard to solve.</td></tr>
</table>

Keyword	Definition			
	Parameters	Optional/Reqd.	Units	Examples
	Scaling factor	Required	--	SGMAXIT 100
	Keyword Usage	Optional keyword.		
	Reactor Models	• Diffusion or Premixed Opposed-flow Flame • Opposed-flow Flame • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation		
SG-TOL Solver	Absolute tolerance criterion on gas-phase mole fractions in segregated scheme.			
	Parameters	Optional/Reqd.	Units	Examples
	Absolute tolerance	Required	--	SGTOL 1.0E-10
	Keyword Usage	Optional keyword. The default value is 1E-10.		
	Reactor Models	• Diffusion or Premixed Opposed-flow Flame • Opposed-flow Flame • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation		
SIDR Solver	Turns on the multi-zone SI Engine Zonal simulation with gas-phase chemistry de-activated. The number of zones is set to 2 by default. SIKN and SIDR are mutually exclusive.			
	Parameters	Optional/Reqd.	Units	Examples
	Number of zones	Required	--	SIDR 2
	Keyword Usage	Optional keyword.		
	Reactor Models	• SI Engine Zonal Simulator		
SIKN Solver	Turns on the multi-zone SI Engine Zonal simulation with gas-phase chemistry activated. The number of zones is set to 2 by default.SIKN and SIDR are mutually exclusive.			
	Parameters	Optional/Reqd.	Units	Examples
	Number of zones	Required	--	SIKN 2
	Keyword Usage	Optional keyword.		
	Reactor Models	• SI Engine Zonal Simulator		
SIOA Reactor Property	Specifies the crank angle when the SI Engine Zonal Simulator properties will be saved to the XML solution file.			
	Parameters	Optional/Reqd.	Units	Examples
	crank_angle	Required	degree	SIOA **5.1**
	Keyword Usage	Optional keyword.		
	Reactor Models	• SI Engine Zonal Simulator		

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Keyword	Definition			
SIZE Output	Use this keyword to set the data block size in bytes for the XML Solution File (e.g., *XMLdata.zip*). Changing this value may affect the performance of the XML parsing routines in the graphical ANSYS Chemkin-Pro Post-processor.			
	Parameters	Optional/Reqd.	Units	Examples
	Data block size	Required	bytes	SIZE **10000000**
	Keyword Usage	Optional keyword. By default, the data block size is 10 MB.		
	Reactor Models	• Chemical and Phase Equilibrium Calculations • Closed Homogeneous Batch Reactor • Closed Partially Stirred Reactor (PaSR) • Closed Plasma Reactor • Cylindrical Shear Flow Reactor • Diffusion or Premixed Opposed-flow Flame • Honeycomb Reactor • IC HCCI Engine • Mechanism Analyzer • Non-reactive Gas Mixer • Normal Incident Shock • Normal Reflected Shock • Partially Stirred Reactor (PaSR) • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor • SI Engine Zonal Simulator • Stagnation Flow CVD Reactor		

<table>
<tr><th>Keyword</th><th colspan="4">Definition</th></tr>
<tr><td>SLIP

Reactor Property</td><td colspan="4">Use the slip velocity model to calculate axial velocity at wall when Knudsen number is large. The model calculates the axial velocity at wall as $U_{wall}=C\cdot L\cdot\left(\frac{2-\Sigma_v}{\Sigma_v}\right)\cdot\frac{dU}{dy}$ where L is the characteristic length, U is the axial velocity, C is the multiplier, Σ_v is the tangential momentum accommodation coefficient.</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td></td><td>Multiplier</td><td>Required</td><td>--</td><td>SLIP 3.0 0.9</td></tr>
<tr><td></td><td>Tangential momentum accommodation coefficient</td><td>Required</td><td>--</td><td>SLIP 3.0 0.9</td></tr>
<tr><td></td><td>Keyword Usage</td><td colspan="3">Optional keyword. By default, the slip velocity model is not used.</td></tr>
<tr><td></td><td>Reactor Models</td><td colspan="3">• Cylindrical Shear Flow Reactor
• Planar Shear Flow Reactor</td></tr>
<tr><td>SOLUTION

_TECHNIQUE
Solver</td><td colspan="4">Controls the underlying solution technique. Previous versions of ANSYS Chemkin-Pro use an older and generally less robust solution method. By default, solution_technique is set to 1, which means the new and generally more robust (and for larger mechanisms often faster) technique is used. Setting solution_technique to 0 uses the older method and you should only use this if you are having convergence issues with CHEMKIN-Pro and are confident you do not have any problems with your mechanism or problem specification.</td></tr>
<tr><td></td><td>Keyword Usage</td><td colspan="3">Optional keyword. By default, SOLUTION_TECHNIQUE is set to 1.</td></tr>
<tr><td></td><td>Reactor Models</td><td colspan="3">• Closed Homogeneous Batch Reactor
• Closed Plasma Reactor
• Honeycomb Reactor
• IC HCCI Engine
• Multi-Zone HCCI Engine Simulator
• Perfectly Stirred Reactor (PSR)
• Plasma Plug Flow Reactor
• Plasma PSR
• Plug Flow Reactor
• Opposed-flow Flame
• Premixed Laminar Burner-stabilized Flame
• Premixed Laminar Flame-speed Calculation
• SI Engine Zonal Simulator</td></tr>
</table>

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Keyword	Definition			
SP Problem Type	Constant pressure and entropy constraints.			
	Keyword Usage	Optional keyword. Exactly one problem-type keyword must be included.		
	Reactor Models	• Chemical and Phase Equilibrium Calculations		
	Notes	• PS keyword.is equivalent.		
SPOS Solver	This keyword provides a (small positive) number that will replace any negative species mass or site fractions. The replacement is made after every successful sequence of time steps, upon adding mesh points, and on restart or continuation. SPOS is often helpful in starting difficult problems when the initial guess is far from the solution. SPOS attempts to force the transient solution away from nonphysical regions that may otherwise be entered due to bad initial conditions and badly conditioned systems.			
	Parameters	Optional/Reqd.	Units	Examples
	Species mass fraction	Required	--	SPOS **1.E-14**
	Keyword Usage	Optional keyword. By default, no substitution is made for negative fractions during solution for all Reactor Models except for Opposed-flow Flames, where the default value is 1.E-10.		
	Reactor Models	• Diffusion or Premixed Opposed-flow Flame • Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Plasma PSR • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
SQRX Solver	A pseudo wall thermal conductivity to allow surface enthalpy production to "overflow" in the downstream direction. This keyword is useful when the reactor model fails to converge repeatedly because of stiff surface chemistry and the reactor wall temperature is not fixed. The overall enthalpy of the reactor is still conserved because this pseudo wall enthalpy flux is included in the energy equation.			
	Parameters	Optional/Reqd.	Units	Examples
	Pseudo conductivity	Required	--	SQRX **0.001**
	Keyword Usage	Optional keyword. By default, no thermal conduction in wall is considered.		
	Reactor Models	• Cylindrical Shear Flow Reactor		

<table>
<tr><th>Keyword</th><th>Definition</th></tr>
<tr><td></td><td></td><td>• Planar Shear Flow Reactor</td></tr>
<tr><td>SRXN

Output</td><td colspan="2">Prints out a table of reaction rates and other pertinent information for a surface reaction. The ALL option is the default and produces tables for every surface reaction. The NONE option suppresses output for all of the reactions. If reaction information is desired for only certain reactions, they may be optionally specified by their number (given in the Pre-processor output) or by typing an exact duplicate of the reaction expression (see example input).</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td></td><td>ALL option</td><td>Optional, default is ALL</td><td>--</td><td>SRXN ALL</td></tr>
<tr><td></td><td>NONE option</td><td>Optional, default is ALL</td><td>--</td><td>SRXN NONE</td></tr>
<tr><td></td><td>Surface reaction number list</td><td>Optional, default is ALL</td><td>--</td><td>SRXN 2 5</td></tr>
<tr><td></td><td>Surface reaction expression</td><td>Optional, default is ALL</td><td>--</td><td>SRXN CH(S)+H<=>C(S,R)+H2</td></tr>
<tr><td></td><td>Keyword Usage</td><td colspan="3">Optional keyword. By default, the table output is determined by the ALL or NONE keyword.</td></tr>
<tr><td></td><td>Reactor Models</td><td colspan="3">• Mechanism Analyzer</td></tr>
<tr><td>SSDR

Reactor Property</td><td colspan="4">The nominal value of the Stoichiometric Scalar Dissipation Rate (SSDR). The first flamelet will be computed for this value.</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td></td><td>Nominal value of SSDR</td><td>Required</td><td>1/s</td><td>SSDR 1.0</td></tr>
<tr><td></td><td>Keyword Usage</td><td colspan="3">Optional keyword.</td></tr>
<tr><td></td><td>Reactor Models</td><td colspan="3">• Diffusion Flamelet Generator</td></tr>
<tr><td>SSDR_MAX

Reactor Property</td><td colspan="4">The maximum value of the Stoichiometric Scalar Dissipation Rate (SSDR). After computing a flamelet for the nominal value (specified by keyword SSDR), continuations to SSDR_MAX are done in a number of steps as specified by keyword NSTEP_HIGH.</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td></td><td>Maximum value of SSDR</td><td>Optional</td><td>1/s</td><td>SSDR_MAX 100</td></tr>
<tr><td></td><td>Keyword Usage</td><td colspan="3">Optional keyword.</td></tr>
</table>

Keyword	Definition			
	Reactor Models	• Diffusion Flamelet Generator		
SS-DR_MIN Reactor Property	The minimum value of the Stoichiometric Scalar Dissipation Rate (SSDR). After computing a flamelet for the nominal value (specified by keyword SSDR), continuations to SSDR_MIN are done in a number of steps as specified by keyword NSTEP_LOW.			
	Parameters	Optional/Reqd.	Units	Examples
	Minimum value of SSDR	Optional	1/s	SSDR_MIN **0.001**
	Keyword Usage	Optional keyword.		
	Reactor Models	• Diffusion Flamelet Generator		
SSKIP Solver	Skip the initial surface site fraction calculation.			
	Keyword Usage	Optional keyword. By default, an initial solution is performed to determine the surface site fractions holding the reagent gas species constant.		
	Reactor Models	• Honeycomb Monolith Reactor • Plasma Plug Flow Reactor • Plug Flow Reactor		
SS-MAX-ITER Solver	The maximum number of iterations per steady state search, in the steady-state solver TWOPNT. This is the maximum number of iterations that are allowed each time TWOPNT searches to find the steady state solution. Typically you will not need to change this maximum because TWOPNT will revert to its time stepping algorithm and then re-try searching for the steady state.			
	Parameters	Optional/Reqd.	Units	Examples
	Maximum steady state iterations	Optional	--	SSMAXITER **120**
	Keyword Usage	Optional keyword. By default, the maximum number of iterations is 100.		
	Reactor Models	• Cylindrical Shear Flow Reactor • Diffusion or Premixed Opposed-flow Flame • Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma PSR • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor		

Keyword	Definition			
		• Stagnation Flow CVD Reactor		
	Notes	• SSMAXITER must be >=1.		
SS-RX Solver	A pseudo diffusivity for surface species to allow them to diffuse along the wall surface in the downstream direction. This keyword is useful when the reactor model fails to converge repeatedly because of stiff surface chemistry and the reactor wall temperature is fixed. The overall mass and element conservations of the reactor are still satisfied because pseudo surface species fluxes are included in the surface species equations.			
	Parameters	Optional/Reqd.	Units	Examples
	Pseudo conductivity	Required	--	SSRX **0.0001**
	Keyword Usage	Optional keyword. By default, no surface species flux on wall is considered.		
	Reactor Models	• Cylindrical Shear Flow Reactor • Planar Shear Flow Reactor		
	Notes	• Typically, the value of SSRX should be kept under 0.01.		
SSTT Solver	Inclusion of this keyword indicates that the local sensitivity analysis will be performed instead of the integrated sensitivity analysis for transient or plug-flow calculations. This may be helpful in speeding up calculations of sensitivity, but we caution that the local sensitivity is less accurate than the integrated sensitivity.			
	Keyword Usage	Optional keyword. By default, the integrated sensitivity analysis will be performed for transient calculations when sensitivity data is requested.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Honeycomb Reactor • IC HCCI Engine • Perfectly Stirred Reactor (PSR) • Plasma PSR • Plasma Plug Flow Reactor • Plug Flow Reactor • SI Engine Zonal Simulator		
	Notes	• SSTT can be added to a continuation run, but it cannot be removed from one.		
STAG	Specify a Stagnation Flow CVD Reactor model.			

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Keyword	Definition			
Problem Type	**Keyword Usage**	Required keyword. See also OMEG. If the keyword STAG is given and the spin rate OMEG is nonzero, then this inconsistent input will generate an error. A stagnation-point flow can also be specified by using "OMEG 0".		
	Reactor Models	• Stagnation Flow CVD Reactor		
STAG-NA-TION _FLAME Problem Type	Indicates Burner-stabilized Stagnation Flow problem type.			
	Keyword Usage	Required keyword.		
	Reactor Models	• Premixed Laminar Burner-stabilized Stagnation Flow Flame Simulator		
STCH Reactor Property	Parameter to produce a non-uniform grid. For cartesian coordinates the initial grid location for a node J is X(J)=A*(J-1)**STCH, where A=HITE/(NPTS-1)**STCH, HITE is the reactor height, and NPTS is the total number of grid nodes. If STCH=1, a uniform grid is produced. For STCH > 1, the grid is more tightly spaced at the lower boundary (cartesian-coordinates) or at the outer boundary (cylindrical coordinates), and consequently the grid is more widely spaced at the other boundary.			
	Parameters	Optional/Reqd.	Units	Examples
	Cartesian coordinates	Required	--	STCH **1.2**
	Keyword Usage	Optional keyword. By default, the program is set to 1.		
	Reactor Models	• Cylindrical Shear Flow Reactor • Planar Shear Flow Reactor		
STCK Output	Analyzes the forward and reverse surface reaction's sticking coefficient, if applicable. The ALL option is the default and produces tables for every surface reaction with a sticking-coefficient formulation. The NONE option suppresses output for all of the reactions. If reaction information is desired for only certain reactions, they may be optionally specified by their number (given in the Pre-processor output) or by typing an exact duplicate of the reaction expression (see example input).			
	Parameters	Optional/Reqd.	Units	Examples
	ALL option	**Optional, default is ALL**	--	STCK **ALL**
	NONE option	**Optional, default is ALL**	--	STCK **NONE**
	Surface reaction number list	**Optional, de-**	--	STCK **2 5**

Keyword	Definition			
		fault is ALL		
	Surface reaction expression	**Option-al, de-fault is ALL**	--	STCK **CH(S)+H<=>C(S,R)+H2**
	Keyword Usage	Optional keyword. By default, the table output is determined by the ALL or NONE keyword.		
	Reactor Models	• Mechanism Analyzer		
STP0 Solver	Initial time step size used by the steady-state solver *Twopnt* during the initial calculation for the surface conditions at the inlet.			
	Parameters	Optional/Reqd.	Units	Examples
	Initial time step	Required	cm	STP0 **1.0E-7**
	Keyword Usage	Optional keyword. By default, the initial time step is 1.0E-6.		
	Reactor Models	• Cylindrical Shear Flow Reactor • Planar Shear Flow Reactor		
STPT Solver	The maximum internal time step for the solver in transient calculations. STPT determines the largest time-step the transient solver can take at one time and thereby controls the resolution for interpolation of specified time-profiles.			
	Parameters	Optional/Reqd.	Units	Examples
	Time step	Required	sec	STPT **1.0E-4**
	Aurora Usage	Optional keyword. If not specified, then If either DELT or DTSV are specified, STPT is set to the smallest of these values. If neither DELT nor DTSV are specified, then STPT is set to the value of the end time divided by 100.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • IC HCCI Engine • Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Plasma PSR • SI Engine Zonal Simulator		
	Notes	• See also: DELT and DTSV keywords.		
STST	The solution will be obtained using a steady-state calculation (with the solver *Twopnt*) rather than a transient calculation (using the solver DASPK).			

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<table>
<tr><th>Keyword</th><th colspan="4">Definition</th></tr>
<tr><td rowspan="3">Reactor Property</td><td>Keyword Usage</td><td colspan="3">Optional keyword. By default, a steady-state calculation is performed.</td></tr>
<tr><td>Reactor Models</td><td colspan="3">• Non-reactive Gas Mixer
• Perfectly Stirred Reactor (PSR)
• Plasma PSR
• Rotating Disk CVD Reactor
• Stagnation Flow CVD Reactor</td></tr>
<tr><td>Notes</td><td colspan="3">• Exclusive toggle with TRAN.</td></tr>
<tr><td rowspan="8">SURF

Reactor Property</td><td colspan="4">Initial values (transient) or estimates (steady-state) for the surface site fraction values for the surface species on each surface site type (surface phase).</td></tr>
<tr><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td>Surface species name</td><td>Required</td><td>--</td><td>SURF Ga(s) 0.001</td></tr>
<tr><td>Surface fractions</td><td>Required</td><td>site fractions</td><td>SURF Ga(s) 0.001</td></tr>
<tr><td>Keyword Usage</td><td colspan="3">Optional keyword. By default, the initial or estimated surface-site fractions are 0.0.</td></tr>
<tr><td>Reactor Models</td><td colspan="3">• Closed Homogeneous Batch Reactor
• Closed Plasma Reactor
• Cylindrical Shear Flow Reactor
• Honeycomb Reactor
• Perfectly Stirred Reactor (PSR)
• Planar Shear Flow Reactor
• Plasma Plug Flow Reactor
• Plasma PSR
• Plug Flow Reactor
• Rotating Disk CVD Reactor
• Stagnation Flow CVD Reactor</td></tr>
<tr><td>Notes</td><td colspan="3">• The sum of the site fractions should equal one for each surface site type (phase). However, if they do not, a cautionary message will be printed and the site fractions for each surface site type will be normalized so the sum does equal one.</td></tr>
</table>

Keyword	Definition	
SYMT Reactor Property	Keyword for temperature boundary condition on the upper wall (only used for non-symmetric cartesian coordinates). The upper wall temperature is set equal to the bottom wall temperature if SYMT is specified.	
	Keyword Usage	Optional keyword. By default, an adiabatic top wall is used.
	Reactor Models	• Planar Shear Flow Reactor

10.4. Alphabetical Listing of Keywords [T-Z]

Table 10.4: Alphabetical Listing of Keywords [T-Z]

Keyword	Definition			
T1 Reactor Property	Temperature before the incident shock.			
	Parameters	Optional/Reqd.	Units	Examples
	Temperature	Required	K	T1 **300.**
	Keyword Usage	Optional keyword. The shock velocity and any two of temperature, pressure, or density must be specified for conditions before the incident shock. See also P1A and RHO1 .		
	Reactor Models	• Normal Incident Shock • Normal Reflected Shock		
T2 Reactor Property	Temperature after the incident shock.			
	Parameters	Optional/Reqd.	Units	Examples
	Temperature	Required	K	T2 **1500.**
	Keyword Usage	Optional keyword. Any two of temperature, pressure, or density must be specified for conditions after the incident shock. See also RHO2 and P2A .		
	Reactor Models	• Normal Incident Shock • Normal Reflected Shock		
T3 Reactor Property	Temperature after the reflected shock, given as T_5 in the equations.			
	Parameters	Optional/Reqd.	Units	Examples
	Temperature	Required	K	T2 **1500.**
	Keyword Usage	Optional keyword. Any two of temperature, pressure, or density must be specified for conditions after the reflected shock. See also RHO3 and P3A .		
	Reactor Models	• Normal Reflected Shock		
TAMB Reactor Property	Ambient temperature for convective or conductive heat transfer out of the system. This keyword is only relevant when the energy equation is being solved.			
	Parameters	Optional/Reqd.	Units	Examples

Keyword	Definition			
	Material name	**Optional.** If no material is specified, the same value will be used for all materials.	--	TAMB **material1** 298
	Ambient temperature	Required	K	TAMB **298**
	Reactor number (PSR clusters only)	**Optional.** If no number is given, the keyword is assumed to apply to all reactors in a cluster.	--	TAMB material1 298 **1**
	Keyword Usage	Optional keyword. This keyword must be used with HTC .		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Honeycomb Monolith Reactor • Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Plasma PSR • Plasma Plug Flow Reactor • Plug Flow Reactor		
TAU Reactor Property	The nominal residence time of the gas in the reactor when flow is present.			
	Parameters	Optional/Reqd.	Units	Examples
	Nominal residence time	Required	sec	TAU **1.E-3**
	Reactor number (PSR clusters only)	Optional	--	TAU 1.E-3 **1**

Keyword	Definition			
		If no number is given, the keyword is assumed to apply to all reactors in a cluster.		
	Keyword usage	PSRs: Optional keyword. If none of TAU, FLRT / FPRO, SCCM / SCCMPRO are specified or are nonzero, then a closed-system is assumed. FLRT / FPRO or SCCM / SCCMPRO is required for each INLET stream defined. PaSRs: Optional keyword. Unless the CLSE keyword is used, any two of FLRT, STPT and reactor volume (VOL) are required.		
	Reactor Models	• Partially Stirred Reactor (PaSR) • Perfectly Stirred Reactor (PSR) • Plasma PSR		
TBND Solver	The upper boundary for gas temperature. Setting TBND to the upper limit of thermodynamic data can prevent the *Gas-phase Kinetics* Pre-processor from getting erratic thermal data by extrapolating the fitting polynomials.			
	Parameters	Optional/Reqd.	Units	Examples
	Upper boundary	Required	K	TBND 10000.
	Keyword Usage	Optional keyword. By default, the upper boundary is 5000.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Diffusion of Premixed Opposed-flow Flame • Honeycomb Reactor • Perfectly Stirred Reactor (PSR) • Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor • Premixed Laminar Burner-stabilized Flame		

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<table>
<tr><th>Keyword</th><th colspan="4">Definition</th></tr>
<tr><td></td><td colspan="4">• Premixed Laminar Flame-speed Calculation
• Rotating Disk CVD Reactor
• Stagnation Flow CVD Reactor</td></tr>
<tr><td>TBTH

Reactor Property</td><td colspan="4">Set the bath gas temperature in Kelvin. This temperature is used wherever a single temperature is needed. The default is 298.15 K.</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td></td><td>Bath gas temperature</td><td>Required</td><td>K</td><td>TBTH 900.</td></tr>
<tr><td></td><td>Keyword Usage</td><td colspan="3">Optional keyword. By default, the bath gas temperature is 298.15.</td></tr>
<tr><td></td><td>Reactor Models</td><td colspan="3">• Mechanism Analyzer</td></tr>
<tr><td>TDIF

Reactor Property</td><td colspan="4">Include thermal diffusion (Soret effect) in the transport calculations.</td></tr>
<tr><td></td><td>Keyword Usage</td><td colspan="3">Optional keyword. By default, thermal diffusion is not included.</td></tr>
<tr><td></td><td>Reactor Models</td><td colspan="3">• Cylindrical Shear Flow Reactor
• Diffusion or Premixed Opposed-flow Flame
• Planar Shear Flow Reactor
• Premixed Laminar Burner-stabilized Flame
• Premixed Laminar Flame-speed Calculation
• Rotating Disk CVD Reactor
• Stagnation Flow CVD Reactor</td></tr>
<tr><td>TDEL

Reactor Property</td><td colspan="4">Set the temperature increment in all tables where the temperature is varied.</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td></td><td>Temperature</td><td>Required</td><td>K</td><td>TDEL 200.</td></tr>
<tr><td></td><td>Keyword Usage</td><td colspan="3">Optional keyword. By default, the temperature step is 100 K.</td></tr>
<tr><td></td><td>Reactor Models</td><td colspan="3">• Mechanism Analyzer</td></tr>
<tr><td>TDSK

Reactor Property</td><td colspan="4">Temperature of the deposition surface. This is a constant value taken as a boundary condition, unless the keyword RADB is given, indicating that the susceptor or disk temperature is calculated from an energy balance. If RADB is specified, TDSK is taken as the initial guess for the susceptor temperature.</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td></td><td>Surface temperature</td><td>Required</td><td>K</td><td>TDSK 1200</td></tr>
<tr><td></td><td>Keyword Usage</td><td colspan="3">Required keyword.</td></tr>
</table>

<table>
<tr><th>Keyword</th><th colspan="4">Definition</th></tr>
<tr><td></td><td>Reactor Models</td><td colspan="3">• Rotating Disk CVD Reactor
• Stagnation Flow CVD Reactor</td></tr>
<tr><td>TEBND

Reactor Property</td><td colspan="4">The upper boundary for electron temperature. Can be useful for preventing non-plasma solutions in steady state problems.</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td></td><td>Upper boundary</td><td>Required</td><td>K</td><td>TEBND 8000</td></tr>
<tr><td></td><td>Keyword Usage</td><td colspan="3">Optional keyword. By default, the upper boundary is 200000 K (roughly 20 eV).</td></tr>
<tr><td></td><td>Reactor Models</td><td colspan="3">• Closed Plasma Reactor
• Plasma PSR
• Plasma Plug Flow Reactor</td></tr>
<tr><td>TEIN

Inlet Property</td><td colspan="4">Electron temperature in the inlet stream. For most cases, there are no free electrons in the inlet stream, in which case the electron inlet temperature is not used.</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td></td><td>Electron temperature</td><td>Required</td><td>K</td><td>TEIN 300.</td></tr>
<tr><td></td><td>Keyword Usage</td><td colspan="3">Optional keyword. By default, the electrons have the same temperature as the inlet gas.</td></tr>
<tr><td></td><td>Reactor Models</td><td colspan="3">• Plasma PSR</td></tr>
<tr><td>TEMP

Reactor Property</td><td colspan="4">The reactor gas temperature. Depending on the Reactor Model and problem type, this is either the user-supplied temperature constraint (TGIV), an initial estimate of the temperature (ENRG), or the initial reactor temperature (for transient cases). See also TPRO.</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td></td><td>Reactor gas temperature</td><td>Required</td><td>K</td><td>TEMP 1000.</td></tr>
<tr><td></td><td>Reactor number (PSR clusters only)</td><td>Optional
If no number is given, the keyword is assumed to apply to all reactors in a cluster.</td><td>--</td><td>TEMP 1000. 1</td></tr>
<tr><td></td><td>Keyword Usage</td><td colspan="3">Required keyword.</td></tr>
</table>

<table>
<tr><th>Keyword</th><th colspan="4">Definition</th></tr>
<tr><td></td><td>Reactor Models</td><td colspan="3">• Chemical and Phase Equilibrium Calculations
• Closed Homogeneous Batch Reactor
• Closed Partially Stirred Reactor (PaSR)
• Closed Plasma Reactor
• Diffusion or Premixed Opposed-flow Flame
• Honeycomb Reactor
• IC HCCI Engine
• Non-reactive Gas Mixer
• Partially Stirred Reactor (PaSR)
• Perfectly Stirred Reactor (PSR)
• Plasma Plug Flow Reactor
• Plasma PSR
• Plug Flow Reactor
• Premixed Laminar Burner-stabilized Flame
• Premixed Laminar Flame-speed Calculation
• Rotating Disk CVD Reactor
• SI Engine Zonal Simulator
• Stagnation Flow CVD Reactor</td></tr>
<tr><td></td><td>Notes</td><td colspan="3">• In previous versions, TINI keyword was used for some Reactor Models.</td></tr>
<tr><td>TEST

Reactor Property</td><td colspan="4">Specifies an estimate of the equilibrium temperature.</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td></td><td>Temperature</td><td>Required</td><td>K</td><td>TEST 2000</td></tr>
<tr><td></td><td>Keyword Usage</td><td colspan="3">Optional keyword. May help convergence to the equilibrium temperature, or assure an appropriate equilibrium temperature is calculated when a second, trivial solution exists (e.g., for adiabatic flame-temperature calculations).</td></tr>
<tr><td></td><td>Reactor Models</td><td colspan="3">• Chemical and Phase Equilibrium Calculations</td></tr>
<tr><td>TEXP</td><td colspan="4">Specifies the average/cylinder temperature that defines the start of the expansion period. This keyword has a lower priority than QEXP .</td></tr>
</table>

<table>
<tr><th>Keyword</th><th>Definition</th></tr>
<tr><td>Reactor Property</td><td>
<table>
<tr><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td>temperature</td><td>Required</td><td>K</td><td>TEXP 1150.0</td></tr>
<tr><td>Keyword Usage</td><td colspan="3">Optional keyword. Default = 1000K.</td></tr>
<tr><td>Reactor Models</td><td colspan="3">• Multi-Zone HCCI Simulator
• IC HCCI Engine
• SI Engine Zonal Simulator</td></tr>
</table>
</td></tr>
<tr><td>TFAL

Output</td><td>Analyze the fall-off of a gas-phase reaction with respect to changes in the temperature, i.e., create a table of reaction rates versus temperature at a constant pressure. The pressure and gas composition are assumed to be that of the bath gas. The ALL option is the default and produces tables for every gas-phase reaction. The NONE option suppresses output for all of the reactions. If reaction information is desired for only certain reactions, they may be optionally specified by their number (given in the Pre-processor output) or by typing an exact duplicate of the reaction expression (see example input).
<table>
<tr><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td>ALL option</td><td>Optional, default is ALL</td><td>--</td><td>TFAL ALL</td></tr>
<tr><td>NONE option</td><td>Optional, default is ALL</td><td>--</td><td>TFAL NONE</td></tr>
<tr><td>Gas reaction number list</td><td>Optional, default is ALL</td><td>--</td><td>TFAL 2 5</td></tr>
<tr><td>Gas reaction expression</td><td>Optional, default is ALL</td><td>--</td><td>TFAL 2CH3(+M)<=>C2H6(+M)</td></tr>
<tr><td>Keyword Usage</td><td colspan="3">Optional keyword. By default, the table output is determined by the ALL or NONE keyword.</td></tr>
<tr><td>Reactor Models</td><td colspan="3">• Mechanism Analyzer</td></tr>
</table>
</td></tr>
<tr><td>TFIX

Reactor Property</td><td>When solving a freely propagating adiabatic flame (FREE), the problem is posed in a flame-fixed coordinate system. In this case the flame speed becomes an eigenvalue. Therefore, an additional constraint is required. We choose to supply this additional condition by fixing the temperature at one point in the flame, and this input allows the specification of that fixed temperature. Given the fixed temperature, the flame position is determined from the initial temperature profile as specified by the TPRO or TPROF inputs. If the fixed temperature is not one of the temperatures specified in the input, then a linear interpolation of the</td></tr>
</table>

<table>
<tr><th>Keyword</th><th>Definition</th></tr>
<tr><td></td><td>temperature profile to determine the position of TFIX is used and a mesh point added at that point.
<table>
<tr><th>Parameters</th><th>Optional/Reqd.</th><th>Units</th><th>Examples</th></tr>
<tr><td>Temperature</td><td>Option-al.</td><td>K</td><td>TFIX 500.</td></tr>
<tr><td>Keyword Usage</td><td colspan="3">Optional keyword. With TPROF, default is the average of unburned gas temperature (TUNBURNT) and mixture equilibrium temperature. With TPRO, the default is the average of the first and last Temperature profile values.</td></tr>
<tr><td>Reactor Models</td><td colspan="3">• Premixed Laminar Flame-speed Calculation</td></tr>
<tr><td>Notes</td><td colspan="3">• This keyword can be changed for a restart run.</td></tr>
</table></td></tr>
<tr><td>TGIV

Problem Type</td><td>Do not solve the gas energy equation, but will instead use a fixed user-supplied temperature (see TEMP).
<table>
<tr><th>Parameters</th><th>Optional/Reqd.</th><th>Units</th><th>Examples</th></tr>
<tr><td>Reactor number (PSR clusters only)</td><td>Optional If no number is given, the keyword is assumed to apply to all reactors in a cluster.</td><td>--</td><td>TGIV 2</td></tr>
<tr><td>Keyword Usage</td><td colspan="3">Optional keyword. Either TGIV or ENRG must be specified, unless CONP, CONV, or COTV problem-types are specified for a closed system.</td></tr>
<tr><td>Reactor Models</td><td colspan="3">• Closed Homogeneous Batch Reactor
• Closed Plasma Reactor
• Diffusion or Premixed Opposed-flow Flame
• Non-reactive Gas Mixer
• Honeycomb Reactor
• Perfectly Stirred Reactor (PSR)
• Plasma Plug Flow Reactor
• Plasma PSR
• Plug Flow Reactor</td></tr>
</table></td></tr>
</table>

<table>
<tr><th>Keyword</th><th colspan="4">Definition</th></tr>
<tr><td></td><td></td><td colspan="3">• Premixed Laminar Burner-stabilized Flame
• Rotating Disk CVD Reactor
• Stagnation Flow CVD Reactor</td></tr>
<tr><td></td><td>Notes</td><td colspan="3">• This keyword can be removed or added for a restart run.</td></tr>
<tr><td>THIG
Reactor Property</td><td colspan="4">Set the upper limit of the temperature range (K) in all tables where the temperature is varied. The default is 1500 K.</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td></td><td>Temperature</td><td>Required</td><td>K</td><td>THIG 298.15</td></tr>
<tr><td></td><td>Keyword Usage</td><td colspan="3">Optional keyword. By default, the high temperature is 1500.</td></tr>
<tr><td></td><td>Reactor Models</td><td colspan="3">• Mechanism Analyzer</td></tr>
<tr><td>THRM
Output</td><td colspan="4">Prints out individual thermodynamics tables for the species in the mechanism. The default is ALL, which generates the tables for all species in the mechanism. The GAS, SUR, and BULK options will cause thermodynamic tables for only species in the specified phase to be printed. Listing individual species by their name or by their number (as listed in the Gas-phase Kinetics or Surface Kinetics Pre-processor output files) will generate thermodynamic tables for the specified species. The keyword NONE will suppress all of the species thermodynamic tables.</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td></td><td>ALL option</td><td>Optional</td><td>--</td><td>THRM ALL</td></tr>
<tr><td></td><td>NONE option</td><td>Optional</td><td>--</td><td>THRM NONE</td></tr>
<tr><td></td><td>GAS option</td><td>Optional</td><td>--</td><td>THRM GAS</td></tr>
<tr><td></td><td>SUR option</td><td>Optional</td><td>--</td><td>THRM SUR</td></tr>
<tr><td></td><td>BULK option</td><td>Optional</td><td>--</td><td>THRM BULK</td></tr>
<tr><td></td><td>Species name</td><td>Optional</td><td>--</td><td>THRM CH4</td></tr>
<tr><td></td><td>Species number</td><td>Optional</td><td>--</td><td>THRM 3</td></tr>
<tr><td></td><td>Keyword Usage</td><td colspan="3">Optional keyword. By default, the table output is determined by the ALL or NONE keyword.</td></tr>
<tr><td></td><td>Reactor Models</td><td colspan="3">• Mechanism Analyzer</td></tr>
<tr><td>TIFP
Output</td><td colspan="4">Calculate the ignition delay as the time when the slope of the temperature profile reaches its maximum value. You need to use sufficient number of time points to obtain an accurate temperature profile. Only applicable when you are solving the energy equation with the transient solver.</td></tr>
<tr><td></td><td>Keyword Usage</td><td colspan="3">Optional keyword. See also TLIM and DTIGN .</td></tr>
<tr><td></td><td>Reactor Models</td><td colspan="3">• Closed Homogeneous Batch Reactor
• Closed Plasma Reactor
• Honeycomb Monolith Reactor</td></tr>
</table>

<table>
<tr><th>Keyword</th><th colspan="4">Definition</th></tr>
<tr><td></td><td colspan="4">-IC HCCI Engine
Perfectly Stirred Reactor (PSR)
Plasma PSR
Plasma Plug Flow Reactor
Plug Flow Reactor
SI Engine Zonal Simulator</td></tr>
<tr><td>TIM1

Solver</td><td colspan="4">For the steady-state solver, Twopnt, if the Newton method fails to converge, then the application takes some pseudo time steps in order to bring the current iterate within the domain of convergence of Newton's method. This input specifies how many time steps to take and the initial size of the time step, for the initial fixed-temperature calculation.</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td></td><td>Number of time steps</td><td>Required</td><td>--</td><td>TIM1 50 3.E-7</td></tr>
<tr><td></td><td>Initial size of time step</td><td>Required</td><td>sec</td><td>TIM1 50 3.E-7</td></tr>
<tr><td></td><td>Keyword Usage</td><td colspan="3">Optional keyword. By default, the number of time steps is 100 and the initial size of the time step is 1.E-6. See also TIM2 .</td></tr>
<tr><td></td><td>Reactor Models</td><td colspan="3">Diffusion or Premixed Opposed-flow Flame
Non-reactive Gas Mixer
Perfectly Stirred Reactor (PSR)
Plasma PSR
Premixed Laminar Burner-stabilized Flame
Premixed Laminar Flame-speed Calculation
Rotating Disk CVD Reactor
Stagnation Flow CVD Reactor</td></tr>
<tr><td></td><td>Notes</td><td colspan="3">In previous versions, TIME keyword was used.</td></tr>
<tr><td>TIM2

Solver</td><td colspan="4">For the steady-state solver, Twopnt, if the Newton method fails to converge, then the application takes some pseudo time steps in order to bring the current iterate within the domain of convergence of Newton's method. This input specifies how many time steps to take and the initial size of the time step, when the energy equation is being solved.</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
</table>

Keyword	Definition			
	Number of time steps	Required	--	TIM2 **50** 3.E-7
	Initial size of time step	Required	sec	TIM2 50 **3.E-7**
	Keyword Usage	Optional keyword. By default, the number of time steps is 100 and the initial size of the time step is 1.E-6. See also TIM1 .		
	Reactor Models	• Diffusion or Premixed Opposed-flow Flame • Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Plasma PSR • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
	Notes	• This input is only used when ENRG or ENGE is included.		
TIME Solver	The total integration time for the transient simulation. If the job is a continuation run and the keyword CNTT is specified, the final time value will be the starting time plus the value of TIME.			
	Parameters	Optional/Reqd.	Units	Examples
	Total integration time	Required	sec	TIME **1.0E-2**
	Keyword Usage	Required keyword, except in case of IC HCCI Engine, where NREV can be specified instead.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Partially Stirred Reactor (PaSR) • Closed Plasma Reactor • IC HCCI Engine • Non-reactive Gas Mixer • Normal Incident Shock • Normal Reflected Shock • Partially Stirred Reactor (PaSR) • Perfectly Stirred Reactor (PSR)		

<table>
<tr><th>Keyword</th><th colspan="4">Definition</th></tr>
<tr><td></td><td></td><td colspan="3">• Plasma PSR
• Rotating Disk CVD Reactor
• SI Engine Zonal Simulator
• Stagnation Flow CVD Reactor</td></tr>
<tr><td></td><td>Notes</td><td colspan="3">• See also CNTT keyword.</td></tr>
<tr><td>TINF

Reactor Property</td><td colspan="4">Ambient temperature of the external environment, used for certain heat-transfer options.</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td></td><td>ambient temperature</td><td>Required</td><td>K</td><td>TINF 500</td></tr>
<tr><td></td><td>Keyword Usage</td><td colspan="3">Shear Flow Reactors: Optional keyword. Only used if HTRN option is included. By default, the inlet gas temperature is used for the ambient temperature (TINL). Premixed and Diffusion Flames: Optional keyword. Only used if the user subroutine QFUN is enabled.</td></tr>
<tr><td></td><td>Reactor Models</td><td colspan="3">• Cylindrical Shear Flow Reactor
• Diffusion or Premixed Opposed-flow Flame
• Planar Shear Flow Reactor
• Premixed Laminar Burner-stabilized Flame
• Premixed Laminar Flame-speed Calculation</td></tr>
<tr><td>TINL

Inlet Property</td><td colspan="4">The inlet temperature for an inlet stream.</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td></td><td>Inlet stream name (for PSRs and CVD Reactors only)</td><td>Optional
If there is no stream name than the inlet temperature applies to all streams.</td><td>--</td><td>TINL secondary_air
400</td></tr>
<tr><td></td><td>Inlet temperature</td><td>Required</td><td>K</td><td>TINL 400</td></tr>
<tr><td></td><td>Keyword Usage</td><td colspan="3">Required for each inlet stream when then energy equation will be solved.</td></tr>
<tr><td></td><td>Reactor Models</td><td colspan="3">• Cylindrical Shear Flow Reactor</td></tr>
</table>

Keyword	Definition			
		• Diffusion or Premixed Opposed-flow Flame • Non-reactive Gas Mixer • Partially Stirred Reactor (PaSR) • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma PSR • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
	Notes	• In previous versions, **TFUE**, **TOXI**, **TINF**, and **GTMP** keywords were used.		
TINL Reactor Property	The temperature of the stagnation plane.			
	Parameters	Optional/Reqd.	Units	Examples
	Stagnation plane name	Optional If there is no stream name than the inlet temperature applies to all streams.	--	TINL **StagPlane** 600
	Stagnation plane temperature	Required	K	TINL **600**
	Keyword Usage	Required for each stagnation plane when then energy equation will be solved.		
	Reactor Models	• Burner-stabilized Stagnation Flow Reactor		
TION Reactor Property	Specified temperature of ions. In this version of the software, there is no separate energy balance that accounts for ion energy gain above the gas temperature. The ions may, however, be much hotter than the neutral species, and this is accounted here as an additional energy loss from the deposited power required to heat the ions to the assumed temperature.			
	Parameters	Optional/Reqd.	Units	Examples
	Specified temperature of ions	Required	K	TION **11500.**
	Reactor number (PSR clusters only)	Optional	--	TION 11500. **1**

Keyword	Definition			
		If no number is given, the value is assumed to apply to all reactors in a cluster.		
	Keyword Usage	Optional keyword. By default, the ions have the same temperature as the neutral gas.		
	Reactor Models	• Closed Plasma Reactor • Plasma Plug Flow Reactor • Plasma PSR		
TJAC Solver	For the steady-state solver *Twopnt*, specifies the maximum number of Newton steps that can be taken in performing the pseudo time-stepping before a new Jacobian is evaluated. If TJAC=1, then a full Newton method will result.			
	Parameters	Optional/Reqd.	Units	Examples
	Retirement age	Required	--	TJAC **15**
	Keyword Usage	Optional keyword. By default, the retirement age is set at 20.		
	Reactor Models	• Cylindrical Shear Flow Reactor • Diffusion or Premixed Opposed-flow Flame • Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Plasma PSR • Planar Shear Flow Reactor • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
TLIM Output	For all transient problems in which the temperature is allowed to vary, an "ignition time" is computed, which is defined as the time or distance when the temperature first reaches a value equal to TLIM.			
	Parameters	Optional/Reqd.	Units	Examples

Keyword	Definition			
	Ignition temperature	Required	K	TLIM **500**
	Keyword Usage	Optional keyword. See also DTIGN .		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Honeycomb Monolith Reactor • IC HCCI Engine • Perfectly Stirred Reactor (PSR) • Plasma PSR • Plasma Plug Flow Reactor • Plug Flow Reactor • SI Engine Zonal Simulator		
TLOW Reactor Property	Set the lower limit of the temperature range (K) in all tables where the temperature is varied. The default is 300 K.			
	Parameters	Optional/Reqd.	Units	Examples
	Temperature	Required	K	TLOW **100.**
	Keyword Usage	Optional keyword. By default, the low temperature is 300 K.		
	Reactor Models	• Mechanism Analyzer		
TMAX Reactor Property	Maximum temperature for use with profiles defined by the LINE or PLAT options.			
	Parameters	Optional/Reqd.	Units	Examples
	Maximum temperature	Required	K	TMAX **2500.**
	Keyword Usage	Optional keyword. By default, the maximum temperature is set at 2200 K.		
	Reactor Models	• Diffusion or Premixed Opposed-flow Flame		
TOFF Reactor Property	This keyword is used to tell the *Twopnt* solver to ignore the temperature when adapting the grid. This can be useful for strained flames, since the temperature gradients can be very steep and, without this option, too many points will be placed in the same place without improving the solution. The flame can be well resolved by basing adaptation only on the species and velocity profiles.			
	Keyword Usage	Optional keyword. By default, the temperature is considered during adaptation.		
	Reactor Models	• Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		

Note: PDF user guides no longer in Chemkin-Pro install after release 19.0

<table>
<tr><th>Keyword</th><th colspan="4">Definition</th></tr>
<tr><td>TP

Problem Type</td><td colspan="4">Constant pressure and temperature constraint.</td></tr>
<tr><td></td><td>Keyword Usage</td><td colspan="3">Optional keyword. Exactly one problem-type keyword must be included.</td></tr>
<tr><td></td><td>Reactor Models</td><td colspan="3">• Chemical and Phase Equilibrium Calculations</td></tr>
<tr><td></td><td>Notes</td><td colspan="3">• PT keyword is equivalent.</td></tr>
<tr><td>TPRO

Reactor Property Profiles</td><td colspan="4">Reactor gas temperature profile specified as a function of time for transient 0-D homogeneous systems or as a function of distance for channel-flow reactors or reactors where there is a constrained temperature. For 1-D steady-state Reactor Models where the energy equation is being solved, TPRO is used to specify an initial temperature profile estimate.</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td></td><td>Time or Distance value, depending on Reactor Model</td><td>Required</td><td>sec or cm</td><td>TPRO 1.0E-4 1000</td></tr>
<tr><td></td><td>Gas Temperature</td><td>Required</td><td>K</td><td>TPRO 1.0E-4 1000</td></tr>
<tr><td></td><td>Reactor number (PSR clusters only)</td><td>Optional

If no number is given, the profile described by the first two values is assumed to apply to all reactors in a cluster.</td><td>--</td><td>TPRO 1.0E-4 1000 1</td></tr>
<tr><td></td><td>Keyword Usage</td><td colspan="3">Optional keyword. By default, no profile is provided.</td></tr>
<tr><td></td><td>Reactor Models</td><td colspan="3">• Closed Homogeneous Batch Reactor

• Closed Plasma Reactor

• Cylindrical Shear Flow Reactor

• Diffusion or Premixed Opposed-flow Flame

• Honeycomb Reactor

• Non-reactive Gas Mixer

• Perfectly Stirred Reactor (PSR)</td></tr>
</table>

Keyword	Definition	
		• Planar Shear Flow Reactor • Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor
TPROF Reactor Property	Reactor gas temperature profile estimated as a function of distance for flame speed simulator and pre-mixed burner simulator with the energy equation being solved. It uses unburned gas temperature and mixture equilibrium temperature as corresponding upper and lower bounds. When TPROF is used, user-specified values of estimated center position (XCEN), estimated zone width (WMIX), and optional temperature constraint (TFIX) are ignored and pre-defined values are used. When TPROF is used with no NPTS, a default non-linear12-point grid is initialized, while TPROF with NPTS initializes a linear NPTS-point grid.	
	Keyword Usage	Optional keyword.
	Reactor Models	• Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation
TPRO-FILE_n Reactor Property	Choice for the initial temperature profile. Integer n can be 1 or 2. Option 1 means a dumped energy profile (that is, all internal grid-points at specified maximum temperature) and option 2 means a linear profile from the boundary to grid-point where mixture fraction value is stoichiometric.	
	Keyword Usage	Required keyword. The default value is TPROFILE_1.
	Reactor Models	• Diffusion Flamelet Generator
TRAD Reactor Property	Temperature of a radiating disk located above and parallel to the substrate, used in calculating a surface radiation balance. A hot radiating disk may be included in addition to a cool "wall" (TWAL), to represent, for example, a burner inlet. The geometry and location of the radiating disk are controlled by keywords RDSK and RRAD. TRAD is used only if the disk temperature is being calculated by including keyword RADB . See Equation 14.18 of the Chemkin-Pro Theory Manual .	
	Parameters	Optional/Reqd. / Units / Examples
	Temperature of a radiating disk	Required / K / TRAD **2500.**
	Keyword Usage	Optional keyword. By default, the temperature of a radiating disk is 1000 K.
	Reactor Models	• Rotating Disk CVD Reactor

Keyword	Definition	
		• Stagnation Flow CVD Reactor
TRAN Solver	Perform a transient calculation instead of a steady-state calculation. Forflame simulators, this input also specifies how many time steps to take and the initial size of the time step. Perform a transient calculation (with the solver DASPK) instead of a steady-state calculation (using the solver *Twopnt*).	
	Keyword Usage	Required keyword for Closed Homogeneous Batch Reactor, Closed Plasma Reactor, and the IC HCCI Engine. Otherwise, a steady-state calculation is performed by default.
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • IC HCCI Engine • Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Plasma PSR • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor • Diffusion or Premixed Opposed-flow Flame • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • SI Engine Zonal Simulator
	Notes	• See also STST.
TRAN Output	Prints out the transport database properties (intermolecular potential parameters) for each gas-phase species in the mechanism. This feature also expands the thermo table to create a table of transport properties as a function of temperature. The NONE option turns off printing of this table. The *Transport* Pre-processor must have been run successfully, unless the NONE option is used.	
	Parameters / Optional/Reqd. / Units / Examples	
	ALL option / Optional / -- / TRAN **ALL**	
	NONE option / Optional / -- / TRAN **NONE**	
	Keyword Usage	Optional keyword. By default, the table output is determined by the ALL or NONE keyword.
	Reactor Models	• Mechanism Analyzer
TRCE	Including this keyword causes the calculation to be run by setting the mass fraction of the last-named *Gas-phase Kinetics* gas-phase species (or when REOR	

Keyword	Definition			
Reactor Property	is used, the species with the largest concentration) to be one minus the sum of the mass fractions of the other species. A conservation equation is not solved for the last (or largest-concentration) species.			
	Keyword Usage	Optional keyword. By default, correction velocity formalism is used.		
	Reactor Models	• Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
	Notes	• This keyword can be removed or added for a restart run.		
TRES Restart	Assigns a new initial time for a calculation that starts using the solution read from an XML Solution File.			
	Parameters	Optional/Reqd.	Units	Examples
	Initial time	Required	sec	TRES **0.0**
	Keyword Usage	Optional keyword. By default, the value of time found on the XML Solution File will be used.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Partially Stirred Reactor (PaSR) • Closed Plasma Reactor • IC HCCI Engine • Partially Stirred Reactor (PaSR) • Perfectly Stirred Reactor (PSR) • Plasma PSR • SI Engine Zonal Simulator		
TRMAX-ITER Solver	The maximum number of iterations time step in TWOPNT's time stepping algorithm. If TWOPNT exceeds this maximum, then it will cut its time step and try again. You may occasionally need to use this option is the time stepping algorithm is having difficulty solving your problem.			
	Parameters	Optional/Reqd.	Units	Examples
	Maximum iterations per time step	Optional	--	TRMAXITER **50**
	Keyword Usage	Optional keyword. By default, the maximum number of iterations is 25.		
	Reactor Models	• Cylindrical Shear Flow Reactor • Diffusion or Premixed Opposed-flow Flame		

<table>
<tr><th>Keyword</th><th colspan="4">Definition</th></tr>
<tr><td></td><td></td><td colspan="3">• Non-reactive Gas Mixer
• Perfectly Stirred Reactor (PSR)
• Planar Shear Flow Reactor
• Plasma PSR
• Premixed Laminar Burner-stabilized Flame
• Premixed Laminar Flame-speed Calculation
• Rotating Disk CVD Reactor
• Stagnation Flow CVD Reactor</td></tr>
<tr><td></td><td>Notes</td><td colspan="3">• TRMAXITER must be >=1.</td></tr>
<tr><td>TRST

Restart</td><td colspan="4">Tells the application which time value in an XML Solution File to use for the initial conditions of the current calculation.</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td></td><td>Time value</td><td>Required</td><td>sec</td><td>TRST 1.0E-5</td></tr>
<tr><td></td><td>Keyword Usage</td><td colspan="3">Optional keyword. By default, the last time value found on the XML Solution File will be used.</td></tr>
<tr><td></td><td>Reactor Models</td><td colspan="3">• Closed Homogeneous Batch Reactor
• Closed Plasma Reactor
• Honeycomb Reactor
• IC HCCI Engine
• Perfectly Stirred Reactor (PSR)
• Plasma Plug Flow Reactor
• Plasma PSR
• Plug Flow Reactor
• SI Engine Zonal Simulator</td></tr>
<tr><td>TS

Problem Type</td><td colspan="4">Constant entropy and temperature constraints.</td></tr>
<tr><td></td><td>Keyword Usage</td><td colspan="3">Optional keyword. Exactly one problem-type keyword must be included.</td></tr>
<tr><td></td><td>Reactor Models</td><td colspan="3">• Chemical and Phase Equilibrium Calculations</td></tr>
<tr><td></td><td>Notes</td><td colspan="3">• ST keyword is equivalent.</td></tr>
</table>

<table>
<tr><th>Keyword</th><th>Definition</th></tr>
<tr><td>TSCCM

Inlet Property</td><td>Sets the standard reference temperature used to define the flow rate when it is input in standard cubic centimeters per minute (sccm), i.e., when SCCM or SCCMPRO keywords are used.
<table>
<tr><th>Parameters</th><th>Optional/Reqd.</th><th>Units</th><th>Examples</th></tr>
<tr><td>Standard temperature</td><td>Required</td><td>K</td><td>TSCCM 300</td></tr>
<tr><td>Keyword Usage</td><td colspan="3">Optional keyword. By default, the reference temperature is set to 298.15 K.</td></tr>
<tr><td>Reactor Models</td><td colspan="3">• Non-reactive Gas Mixer
• Perfectly Stirred Reactor (PSR)
• Plasma PSR
• Rotating Disk CVD Reactor
• Stagnation Flow CVD Reactor</td></tr>
</table></td></tr>
<tr><td>TS-PL

Reactor Property Profiles</td><td>This keyword allows an optional specification of a spline-fit surface temperature profile of the lower wall for planar non-symmetric cases or otherwise the surface temperature profile of the upper wall. The data point describing the surface temperature profile is formatted as an (x,T) pair. There is a TSPL keyword line for each desired (x,T) pair. The x coordinates of each TSPL line must be given in ascending order. A spline fit is used to interpolate between points.
<table>
<tr><th>Parameters</th><th>Optional/Reqd.</th><th>Units</th><th>Examples</th></tr>
<tr><td>x coordinate</td><td>Required</td><td>cm</td><td>TSPL 0.1 973</td></tr>
<tr><td>T coordinate</td><td>Required</td><td>K</td><td>TSPL 0.1 973</td></tr>
<tr><td>Keyword Usage</td><td colspan="3">Optional keyword. By default, for symmetric cases default is specified constant temperature; for non-symmetric cases the wall is adiabatic.</td></tr>
<tr><td>Reactor Models</td><td colspan="3">• Cylindrical Shear Flow Reactor
• Planar Shear Flow Reactor</td></tr>
<tr><td>Notes</td><td colspan="3">• See also: TPRO.</td></tr>
</table></td></tr>
<tr><td>TS-RF

Reactor Property</td><td>The temperature of the surfaces in the reactor. Use only if you want the surface temperature, which controls the surface chemistry rates, to be different than the gas temperature.
<table>
<tr><th>Parameters</th><th>Optional/Reqd.</th><th>Units</th><th>Examples</th></tr>
<tr><td>Material (for 0-D homogeneous and plug-flow reactors only)</td><td>Optional
If not specified, then the temperature is the same for</td><td>--</td><td>TSRF WAFER 1200.</td></tr>
</table></td></tr>
</table>

Keyword	Definition			
		all materials.		
	Surface temperature	Required	K	TSRF 1200.
	Reactor number (PSR clusters only)	Optional If no number is given, the value is assumed to apply to all reactors in a cluster.	--	TSRF 1200. **1**
	Keyword Usage	Closed Homogeneous, PSRs, and Plug Flow Reactors: Optional keyword. If not specified, the surface temperature is assumed to be the same as the gas temperature. Shear Flow Reactors: Required keyword.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Cylindrical Shear Flow Reactor • Diffusion or Premixed Opposed-flow Flame • Honeycomb Reactor • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor		
	Notes	• In previous versions, **STMP** keyword was used.		
TSTP Solver	Initial time step used for integration of the fictitious transient equations used to determine an initial set of surface site fractions for the plug-flow simulation. Steady-state is assumed to be reached when there is no significant change in the surface site fractions over the course of one time step (see RCHG).			
	Parameters	Optional/Reqd.	Units	Examples
	Initial time step	Required	cm	TSTP **0.1**
	Keyword Usage	Optional keyword. By default, the initial time step is 1.		

<table>
<tr><th>Keyword</th><th colspan="4">Definition</th></tr>
<tr><td></td><td>Reactor Models</td><td colspan="3">• Honeycomb Reactor
• Plasma Plug Flow Reactor
• Plug Flow Reactor</td></tr>
<tr><td>TSTR

Cluster Property</td><td colspan="4">This keyword is valid when using the XMLI, XMLS or RSTR option, when the XML Solution File used for initialization or restart contains transient data. In this case, select the values to use in initialization or restart as those corresponding to the time that is closest to (greater than or equal to) the specified time.</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td></td><td>Time</td><td>Required</td><td>sec</td><td>TSTR 0.01</td></tr>
<tr><td></td><td>Keyword Usage</td><td colspan="3">Optional keyword. By default, uses the data from the last time-step found in the XML Solution File.</td></tr>
<tr><td></td><td>Reactor Models</td><td colspan="3">• Chemical and Phase Equilibrium Calculations
• Closed Homogeneous Batch Reactor
• Closed Plasma Reactor
• Cylindrical Shear Flow Reactor
• Diffusion or Premixed Opposed-flow Flame
• Honeycomb Reactor
• IC HCCI Engine
• Mechanism Analyzer
• Non-reactive Gas Mixer
• Normal Incident Shock
• Normal Reflected Shock
• Perfectly Stirred Reactor (PSR)
• Planar Shear Flow Reactor
• Plasma Plug Flow Reactor
• Plasma PSR
• Plug Flow Reactor
• Premixed Laminar Burner-stabilized Flame
• Premixed Laminar Flame-speed Calculation
• Rotating Disk CVD Reactor
• SI Engine Zonal Simulator</td></tr>
</table>

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Keyword	Definition			
		• Stagnation Flow CVD Reactor		
TSTR Solver	Starting time for the simulation.			
	Parameters	Optional/Reqd.	Units	Examples
	Time	Required	sec	TSTR **0.01**
	Keyword Usage	Optional keyword. By default, the starting time is 0.0		
	Reactor Models	• Normal Incident Shock • Normal Reflected Shock		
TSUM Output	Controls the printing of summary tables for the thermodynamic functions at the bath gas conditions (see TBTH, PRES, and XBTH). There are three sets of thermodynamic tables: one for the species, one for the gas reactions, and one for the surface reactions. The last three options turn on each table individually. The default is ALL, which will print all three thermodynamic tables. They may all be suppressed with NONE.			
	Parameters	Optional/Reqd.	Units	Examples
	ALL option	Optional	--	TSUM **ALL**
	NONE option	Optional	--	TSUM **NONE**
	SPECIES option	Optional	--	TSUM **SPECIES**
	GAS option	Optional	--	TSUM **GAS**
	SUR option	Optional	--	TSUM **SUR**
	Keyword Usage	Optional keyword. By default, the table output is determined by the ALL or NONE keyword.		
	Reactor Models	• Mechanism Analyzer		
TSWH Reactor Property	Defines when the calculation will be switched from TGIV to ENRG with Woschni correlation as the heat transfer model. The default value is 0 sec (always use energy equation).			
	Parameters	Optional/Reqd.	Units	Examples
	Time in seconds	Required	sec	TSWH 0.001
	Keyword Usage	Optional keyword.		
	Reactor Models	• Multi-Zone HCCI Engine Simulation		
TTIM Reactor Property	The solution will be obtained with pressure and temperature given as specified functions of time through a user-programmed subroutine. The SUBROUTINE PSTEMPT (TIME, LOUT, TEMP, PA) must be provided to specify the temperature and linked to the application program. See the Application Programming Interface Manual for information on how to work with user subroutines.			
	Keyword Usage	Optional keyword. By default, temperature and pressure will be specified by keyword. See also TPRO and PPRO.		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor		

Keyword	Definition			
		• IC HCCI Engine • Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Plasma PSR • SI Engine Zonal Simulator		
	Notes	• See also TPRO and PPRO as alternative ways to specify temperature and pressure as functions of time.		
TUN-BURNT Reactor Property	Unburned gas temperature.			
	Parameters	Optional/Reqd.	Units	Examples
	Unburned gas temperature	Required	K	TUNBURNT **300.0**
	Keyword Usage	Required keyword.		
	Reactor Models	• Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation		
TV Problem Type	Constant volume and temperature constraints.			
	Keyword Usage	Optional keyword. Exactly one problem-type keyword must be included.		
	Reactor Models	• Chemical and Phase Equilibrium Calculations		
	Notes	• **VT** keyword is equivalent.		
TWAB Solver	Absolute error tolerance used by the steady-state *Twopnt* solver in the initial calculation at the inlet boundary.			
	Parameters	Optional/Reqd.	Units	Examples
	Absolute error tolerance	Required	--	TWAB **1.0E-5**
	Keyword Usage	Optional keyword. By default, the absolute error tolerance is 1.0E-13.		
	Reactor Models	• Cylindrical Shear Flow Reactor • Planar Shear Flow Reactor		
TW-AL Reactor Property	Temperature of a neighboring “wall” used in calculating a surface radiation balance. This value is used only if the disk temperature is being calculated by including keyword RADB . See Equation 14.18 of the Chemkin-Pro Theory Manual .			
	Parameters	Optional/Reqd.	Units	Examples
	Wall temperature	Required	K	TWAL **850.0**

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Keyword	Definition			
	Keyword Usage	Optional keyword. By default, the wall temperature is 500 K.		
	Reactor Models	• Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
TW-PR Output	Specifies print level for the initial steady-state solution of the inlet boundary by the *Twopnt* solver.			
	Parameters	Optional/Reqd.	Units	Examples
	Print level	Required	--	TWPR **0**
	Keyword Usage	Optional keyword. By default, the print level is set at 22.		
	Reactor Models	• Cylindrical Shear Flow Reactor • Planar Shear Flow Reactor		
TWRE Solver	Relative error tolerance used by the steady-state *Twopnt* solver in the initial calculation at the inlet boundary.			
	Parameters	Optional/Reqd.	Units	Examples
	Relative error tolerance	Required	--	TWRE **1.0E-10**
	Keyword Usage	Optional keyword. By default, the relative error tolerance is 1.0E-4.		
	Reactor Models	• Cylindrical Shear Flow Reactor • Planar Shear Flow Reactor		
TWST Solver	Number of time steps before trying another Newton step, used by the steady-state *Twopnt* solver in the initial calculation at the inlet boundary.			
	Parameters	Optional/Reqd.	Units	Examples
	Number of time steps	Required	--	TWST **50**
	Keyword Usage	Optional keyword. By default, the number of time steps is set at 100.		
	Reactor Models	• Cylindrical Shear Flow Reactor • Planar Shear Flow Reactor		
UFAC Solver	Factor by which to multiply the time step in the steady-state *Twopnt* 's pseudo time stepping procedure when the number of time steps at the current step size reaches the number specified by IRET.			
	Parameters	Optional/Reqd.	Units	Examples
	Multiply factor	Required	--	UFAC **2.2**
	Keyword Usage	Optional keyword. By default, the multiplication factor is set to 2.0.		

<table>
<tr><th>Keyword</th><th colspan="4">Definition</th></tr>
<tr><td></td><td>Reactor Models</td><td colspan="3">• Diffusion or Premixed Opposed-flow Flame
• Non-reactive Gas Mixer
• Perfectly Stirred Reactor (PSR)
• Plasma PSR
• Rotating Disk CVD Reactor
• Stagnation Flow CVD Reactor</td></tr>
<tr><td>UIGN

Output, User Subroutine</td><td colspan="4">Use the ignition delay time definition given in the user routine PSIGNT. Only applicable when you are solving the energy equation with transient solver. See the Application Programming Interface Manual for details on how to work with user subroutines.</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td></td><td>Keyword Usage</td><td colspan="3">Optional keyword.</td></tr>
<tr><td></td><td>Reactor Models</td><td colspan="3">• Closed Homogeneous Batch Reactor
• Closed Plasma Reactor
• Honeycomb Monolith Reactor
• IC HCCI Engine
• Perfectly Stirred Reactor (PSR)
• Plasma PSR
• Plasma Plug Flow Reactor
• Plug Flow Reactor
• SI Engine Zonal Simulator</td></tr>
<tr><td>UINL

Reactor Property</td><td colspan="4">The axial velocity at the inlet boundary. If the rotations rate OMEG is zero, or if the STAG option is used, then UINL is no longer optional, but must be given to specify the problem.</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td></td><td>Axial inlet velocity</td><td>Required</td><td>cm/sec</td><td>UINL 23.6</td></tr>
<tr><td></td><td>Keyword Usage</td><td colspan="3">Diffusion or Premixed Opposed-flow Flames: Required keyword for each inlet stream. Rotating Disk CVD Reactor: Optional keyword. The velocity at the outer domain is calculated as a part of the solution. However, using the keyword UINL, one may impose this velocity upon the solution. By default, the axial inlet velocity is 0. Stagnation Flow CVD Reactor: Required keyword.</td></tr>
<tr><td></td><td>Reactor Models</td><td colspan="3">• Diffusion or Premixed Opposed-flow Flame</td></tr>
</table>

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Keyword	Definition	
		• Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor
	Notes	• In previous versions: **UINF**, **VFUE**, or **VOXI** keywords were used.
UP-ROF Reactor Property, User Subroutine	Reactor inlet profiles will be given by a user-programmed subroutine. SUBROUTINE CRUPROF must be provided to specify the inlet profiles of all variables and linked to the application program. See the Application Programming Interface Manual for details on how to work with user subroutines.	
	Keyword Usage	Optional keyword. By default, a uniform inlet profile is used for all variables except axial velocity. The axial velocity profile is uniform in the Planar Shear Flow Reactor model and is parabolic (or fully developed) in the Cylindrical Shear Flow Reactor model.
	Reactor Models	• Cylindrical Shear Flow Reactor • Planar Shear Flow Reactor
UREF Reactor Property	For the IC HCCI Engine (ICEN), the heat transfer model (ICHT) evaluates viscosity and thermal conductivity using the instantaneous temperature and pressure inside the cylinder. The UREF keyword is a flag that instructs the heat transfer model to use transport properties evaluated at the initial condition instead. UREF is turned off by default therefore it must be added to old input files in which keyword ICHT is used to reproduce the old results.	
	Keyword Usage	Optional keyword. By default, properties are evaluated using local conditions.
	Reactor Models	• IC HCCI Engine • SI Engine Zonal Simulator
USE _TPRO_GRID Reactor Property	Uses an initial non-uniform grid based on points specified in the estimated temperature profile (TPRO or TPROF).	
	Keyword Usage	Optional keyword.
	Reactor Models	• Premixed Laminar Burner-Stabilized Flame • Premixed Laminar Flame-Speed Calculation
USEP Cluster Property	For use with XMLI, XMLS, or RSTR, to override the values of pressure found on the XML Solution File used for restart or initialization with those specified in the user input file.	
	Keyword Usage	Optional keyword. By default, the program uses the pressure from the XML Solution File.
	Reactor Models	• Chemical and Phase Equilibrium Calculations • Closed Homogeneous Batch Reactor

Keyword	Definition	
		• Closed Plasma Reactor • Cylindrical Shear Flow Reactor • Diffusion or Premixed Opposed-flow Flame • Honeycomb Reactor • IC HCCI Engine • Mechanism Analyzer • Non-reactive Gas Mixer • Normal Incident Shock • Normal Reflected Shock • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor
USET Cluster Property	For use with XMLI, XMLS, or RSTR, override the values of temperature found on the XML Solution File used for restart or initialization with those specified in the user input file.	
	Keyword Usage	Optional keyword. By default, the program uses the temperature from the XML Solution File.
	Reactor Models	• Chemical and Phase Equilibrium Calculations • Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Cylindrical Shear Flow Reactor • Diffusion or Premixed Opposed-flow Flame • Honeycomb Reactor • IC HCCI Engine

Keyword	Definition	
		• Mechanism Analyzer • Non-reactive Gas Mixer • Normal Incident Shock • Normal Reflected Shock • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor • SI Engine Zonal Simulator • Stagnation Flow CVD Reactor
	Notes	• In previous versions, **USTG** keyword was used.
USEV Restart	This keyword is valid when using XMLI or the RSTR options. When this keyword is included, it overrides the values of velocity or flow-rate found on the XML Solution File used for restart or initialization with those specified in the user input file.	
	Keyword Usage	Optional keyword. By default, the program uses the velocity or flow-rate from the XML Solution File.
	Reactor Models	• Honeycomb Reactor • Perfectly Stirred Reactor (PSR) • Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor

Keyword	Definition	
USEV XMLI	When using XMLI, XMLS, or RSTR, overrides the values of velocity or flow-rate found on the XML Solution File used for restart or initialization with those specified in the user input file.	
	Keyword Usage	Optional keyword. By default, the program uses the velocity or flow-rate from the XML Solution File.
	Reactor Models	• Cylindrical Shear Flow Reactor • Honeycomb Reactor • Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor
USRIN Inlet Property	Specification of a reactor inlet stream using a user-programmed subroutine. Use of USRIN requires that a user routine SUBROUTINEUSRINLET (LIUIN, IINWRK, LRUIN, RINWRK, INAME, KNAMES, FLRT, TINL, TEIN, XIN) is written and linked to the application program. Calls to this routine will be used to obtain the corresponding flow rate (FLRT), inlet temperature (TINL), engine-out electron temperature (TEIN), and composition (REAC). See the Application Programming Interface Manual for more information on how to work with user subroutines.	
	Parameters	Optional/Reqd. / Units / Examples
	Stream	Required / -- / USRIN **engineout** 2
	Reactor number (PSR clusters only)	**Optional, if not defined, then reactor #1 is assumed.** / -- / USRIN engineout **2**
	Keyword Usage	Optional keyword. By default, streams are defined using the INLET and related keyword.
	Reactor Models	• Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR)

Keyword	Definition			
		• Plasma PSR		
	Notes	• See User Supplemental Programming of the Application Programming Interface Manual for details.		
UTRN Reactor Property, User Subroutine	Use the mixture average transport properties defined in user-programmed routine CRUTRANS (for Shear Flow reactors), 0PUTRANS (for Opposed-flow Flame Simulator) or PRUTRANS (for Premixed Laminar Flame or Flame-speed Calculation). See the Application Programming Interface Manual for details on how to work with user subroutines.			
	Keyword Usage	Optional keyword. By default, transport properties will be calculated based on the fundamental transport properties provided in the chemistry set.		
	Reactor Models	• Cylindrical Shear Flow Reactor • Opposed-flow Flame Simulator • Planar Shear Flow Reactor • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation		
VCOR Reactor Property	Including this keyword causes the calculation to be run using a correction velocity to ensure mass conservation, i.e., the sum of the diffusion fluxes is zero. See Equation 14.11 of the Chemkin-Pro Theory Manual . If VCOR is not used, then TRCE is in effect.			
	Keyword Usage	Optional keyword. By default, correction velocity is not used.		
	Reactor Models	• Cylindrical Shear Flow Reactor • Planar Shear Flow Reactor • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
VDOT Inlet Property	Inlet volumetric flow rate.			
	Parameters	Optional/Reqd.	Units	Examples
	Inlet volumetric flow rate	Required	cm^3 /sec	VDOT **100.**
	Keyword Usage	Optional keyword. Either VDOT or VEL must be specified, unless this is a restart run. **PFRs and Monolith Reactors:** Flow specification via one of VEL, VDOT, VDOTPRO SCCM SCCMPRO FLRT, or FPRO is required.		

<table>
<tr><th>Keyword</th><th colspan="4">Definition</th></tr>
<tr><td></td><td>Reactor Models</td><td colspan="3">• Honeycomb Reactor
• Plasma Plug Flow Reactor
• Plug Flow Reactor</td></tr>
<tr><td>VDOTPRO

Inlet PropertyProfiles</td><td colspan="4">Specifies a transient profile or function of mass flow rate vs. independent variable (time or position) for an inlet stream, in cubic centimeters per minute. The profile specified will be interpolated linearly from the VD0TPR0 points provided.</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td></td><td>Inlet stream name</td><td>Optional
If no stream name is given, the profile described is assumed to apply to all reactors in a cluster.</td><td>-</td><td>VDOTPRO purge 0.19
300</td></tr>
<tr><td></td><td>Time (Distance for flow reactor)</td><td>Required</td><td>sec
(cm for flow reactor)</td><td>VDOTPRO purge 0.19
300</td></tr>
<tr><td></td><td>Equivalent volumetric flow rate</td><td>Required</td><td>cm ^{3} /min</td><td>VDOTPRO purge 0.19
300</td></tr>
<tr><td></td><td>Keyword Usage</td><td colspan="3">PFRs and Monolith Reactors: Flow specification via one of VEL, VDOT, VD0TPR0 SCCM SCCMPRO FLRT, or FPRO is required. PSRs and PaSRs: Optional keyword. If none of TAU, FLRT/FPRO, SCCM/SCCMPRO, or VDOT/VD0TPR0 are specified or are nonzero, then a closed-system is assumed. FLRT/FPRO, SCCM/SCCMPRO, or VDOT/VD0TPR0 is required for each INLET stream defined. Stagnation Flow CVD Reactors: FLRT/FPRO, SCCM/SCCMPRO or UINL is required for each inlet stream defined. Rotating Disk CVD Reactors: Optional keyword.</td></tr>
</table>

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Keyword	Definition			
			Reactor Models	• Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Plasma PSR • Plug Flow Reactor (PFR) • Plasma PFR • Honeycomb Monolith Reactor • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor
VEL Inlet Property	The gas-phase velocity at the inlet (for plug-flow reactors) or the maximum gas velocity at the inlet (for shear-flow reactors).			
	Parameters	Optional/Reqd.	Units	Examples
	Velocity	Required	cm/sec	VEL **15**
	Keyword Usage	Plug Flow Reactors: Optional keyword. Either VDOT or VEL must be specified, unless this is a restart run. Shear Flow Reactors: If the problem is in cartesian coordinates, then the average velocity equals two-thirds of the maximum velocity of the parabolic velocity profile. In cylindrical coordinates, the average velocity is half of the maximum velocity. If the keyword BLTK is given, a flat velocity profile will be used, i.e., everywhere the velocity will be set equal to VEL except within a distance BLTK of the wall		
	Reactor Models	• Cylindrical Shear Flow Reactor • Honeycomb Reactor • Planar Shear Flow Reactor • Plasma Plug Flow Reactor • Plug Flow Reactor		
VELPRO Reactor Property	flow velocity along the distance of a plug reactor.			
	Parameters	Optional/Reqd.	Units	Examples
	Distance value	Required	cm	VELPRO 1.0 10.0
	Velocity	Required	cm/sec	VELPRO 1.0 10.0
	Keyword Usage	Optional keyword. By default, no profile is provided.		
	Reactor Models	• Plug Flow Reactor		

Keyword	Definition			
VH Problem Type	Constant volume and enthalpy constraints.			
	Keyword Usage	Optional keyword. Exactly one problem-type keyword must be included.		
	Reactor Models	• Chemical and Phase Equilibrium Calculations		
VIS Inlet Property	Viscosity of the inlet gas mixture.			
	Parameters	Optional/Reqd.	Units	Examples
	Viscosity	Required	g/(cm · sec)	VIS **0.01**
	Keyword Usage	Optional keyword. By default, the viscosity is 0, i.e., viscous drag is neglected.		
	Reactor Models	• Honeycomb Reactor • Plasma Plug Flow Reactor • Plug Flow Reactor		
	Notes	• A poise is equivalent to g/(cm · sec).		
VISC Reactor Property	Viscosity of the mixture at 300 K. Required input for boundary layer corrections.			
	Parameters	Optional/Reqd.	Units	Examples
	Viscosity at 300 K	Required	g/(cm · sec)	VISC 2.65E-4
	Keyword Usage	Optional keyword. By default, the viscosity is not set. This keyword is required for boundary layer corrections.		
	Reactor Models	• Normal Incident Shock		
VOL Reactor Property	The volume of the reactor. In multi-zone models, users can enter zone volume fractions rather than exact zone volumes. The software will calculate the initial cylinder volume, normalize the volume fractions, and compute the exact zone volumes at the start of simulation. VOL is used to give Zone volumes and Zone volume fractions.			
	Parameters	Optional/Reqd.	Units	Examples
	Volume	Required	cm^3	VOL 1200

Keyword	Definition			
	Reactor number (PSR clusters only)	Optional If no number is given, the keyword is assumed to apply to all reactors in a cluster.	--	VOL 1200 **1**
	Keyword Usage	Optional keyword. By default, volume is required input for all PSRs unless		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Partially Stirred Reactor (PaSR) • Closed Plasma Reactor • Non-reactive Gas Mixer • Partially Stirred Reactor (PaSR) • Perfectly Stirred Reactor (PSR) • Plasma PSR		
VOL Reactor Property	The fraction of the total volume inside the cylinder for each zone in a Multi-Zone HCCI Engine model.			
	Parameters	Optional/Reqd.	Units	Examples
	Zone volume fraction	Required	--	VOL 0.15 4
	Zone number	Required	--	VOL 0.15 4
	Keyword Usage	Optional keyword.		
	Reactor Models	• Multi-Zone HCCI Engine Simulator • SI Engine Zonal Simulator		
VOL Reactor Property	The initial specific volume of the gas mixture.			
	Parameters	Optional/Reqd.	Units	Examples
	Specific volume of the gas mixture	Required	cm^{3}/g	VOL 1200
	Keyword Usage	Optional keyword. The user must specify two state variables and the composition to define the initial mixture.		
	Reactor Models	• Chemical and Phase Equilibrium Calculations		

Keyword	Definition			
VOLC Reactor Property	Engine cylinder clearance volume.			
	Parameters	Optional/Reqd.	Units	Examples
	Engine cylinder clearance volume	Required	cm^3	VOLC **2.0**
	Keyword Usage	Optional keyword. Any two of VOLC, VOLD, or CMPR must be specified.		
	Reactor Models	• IC HCCI Engine • SI Engine Zonal Simulator		
VOLD Reactor Property	Engine displacement volume, or the volume swept by the piston during compression.			
	Parameters	Optional/Reqd.	Units	Examples
	Displacement volume	Required	cm^3	VOLD **2.0**
	Keyword Usage	Optional keyword. Any two of VOLC, VOLD, or CMPR must be specified		
	Reactor Models	• IC HCCI Engine • SI Engine Zonal Simulator		
VPRO Reactor Property Profiles	Reactor volume profile specified as a function of time.			
	Parameters	Optional/Reqd.	Units	Examples
	Time value	Required	sec	VPRO **1.0E-4** 1.0
	Volume	Required	cm^3	VPRO 1.0E-4 **1.0**
	Reactor number (PSR clusters only)	Optional If no number is given, the profile described by the first two values is assumed to apply to all reactors in a cluster.	--	VPRO 1.0E-4 1.0 **1**
	Keyword Usage	For constrained-volume problems, VOL or VPRO must be specified. Otherwise, a default value of 1.0 is used for the initial reactor volume.		

Keyword	Definition			
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Partially Stirred Reactor (PaSR) • Closed Plasma Reactor • Non-reactive Gas Mixer • Partially Stirred Reactor (PaSR) • Perfectly Stirred Reactor (PSR) • Plasma PSR		
VRS Reactor Property	Reflected shock velocity. If specified, it is used to determine the state of the gas after the shock. The reflected shock velocity is never used unless the incident shock velocity is also given.			
	Parameters	Optional/Reqd.	Units	Examples
	Reflected shock velocity	Required	cm/sec	VRS **100**
	Keyword Usage	Optional keyword. By default, no shock velocities are computed, but U_5=0.		
	Reactor Models	• Normal Reflected Shock		
VS Problem Type	Constant volume and entropy constraints.			
	Keyword Usage	Optional keyword. Exactly one problem-type keyword must be included.		
	Reactor Models	• Chemical and Phase Equilibrium Calculations		
	Notes	• **SV** keyword.is equivalent.		
VSHK Reactor Property	Incident shock velocity.			
	Parameters	Optional/Reqd.	Units	Examples
	Velocity	Required	cm/sec	VSHK **3000.**
	Keyword Usage	This input is required for all incident shock problems, and may be used for some reflected shock problems.		
	Reactor Models	• Normal Incident Shock • Normal Reflected Shock		
VTIM Reactor Property	The solution will be obtained with the volume as a function of time specified through a user programmed subroutine. SUBROUTINE PSVOLT(TIME, LOUT, VOL, DVDT) must be provided to specify the volume, and linked to the application program.			
	Keyword Usage	Optional keyword. By default, volume is specified through VOL or VPRO.		

Keyword	Definition			
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Plasma PSR		
	Notes	• See also VPRO as an alternative way to specify volume as a function of time. • See the Application Programming Interface Manual for more information on how to work with user subroutines.		
VU Problem Type	Constant volume and energy constraints.			
	Keyword Usage	Optional keyword. Exactly one problem-type keyword must be included.		
	Reactor Models	• Chemical and Phase Equilibrium Calculations		
	Notes	• **UV** keyword is equivalent.		
VWALL Reactor Property	Specify a constant axial slip velocity at the walls.			
	Parameters	Optional/Reqd.	Units	Examples
	Axial slip velocity	Required	cm/sec	VWALL **1.1**
	Keyword Usage	Optional keyword. See also SLIP .		
	Reactor Models	• Cylindrical Shear Flow Reactor • Planar Shear Flow Reactor		
WBFB Solver	Specifies the *b* parameter of the Wiebe function. *b* must be greater than 0 and is set to 5.0 by default.			
	Parameters	Optional/Reqd.	Units	Examples
	Value of the b parameter	Required	--	WBFB 9.0
	Keyword Usage	Optional keyword.		
	Reactor Models	• SI Engine Zonal Simulator		
WBFN Solver	Specifies the *n* parameter of the Wiebe function. *n* must be greater than 0 and is set to 2.0 by default.			
	Parameters	Optional/Reqd.	Units	Examples
	Value of the n parameter	Required	--	WBFN 4.0
	Keyword Usage	Optional keyword.		
	Reactor Models	• SI Engine Zonal Simulator		

Keyword	Definition			
WDIF Solver	Use windward differencing on convective terms in the equations.			
	Keyword Usage	Optional keyword. By default, windward differencing is used.		
	Reactor Models	• Diffusion or Premixed Opposed-flow Flame • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation		
WELL Reactor Property	Flag indicating that a well mixed model will be used to simulate the molecular mixing within the computational particle.			
	Keyword Usage	Optional keyword. By default, a well mixed model is assumed.		
	Reactor Models	• Closed Partially Stirred Reactor (PaSR) • Partially Stirred Reactor (PaSR)		
WENG Reactor Property	The reactor wall temperature will be obtained by solving energy conservation equations for the reactor wall. When WENG is used, all the external heat fluxes, i.e., heat loss to the environment and heat exchange between the reactors in a network, are applied to the wall energy equation instead of the gas phase energy equation. Also, the heat generated by surface reactions will be included in the wall energy equation. If a surface has more than one material, the wall temperature is always assigned to the first material.			
	Parameters	Optional/Reqd.	Units	Examples
	Thermal mass	Required	cal/K	WENG **0.1** 500 1
	Heat transfer coefficient	Required	cal/(cm^2 · sec · K)	WENG 0.1 **500** 1
	Reactor number (PSR clusters only)	Optional If no number is given, the keyword is assumed to apply to all reactors in a cluster.	--	WENG **0.1** 500 **1**

Keyword	Definition			
	Keyword Usage	Optional keyword. By default the surface temperature is fixed. The two required numbers on the keyword line specify the thermal mass of the reactor wall and the heat transfer coefficient between the inner wall surface and the gas mixture inside the reactor. The initial wall temperature can be specified by the keyword TSRF otherwise the gas temperature will be used. For Plug Flow Reactors the **thermal mass parameter** is described in units of cal/(cm · K).		
	Reactor Models	• Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Honeycomb Reactor • IC HCCI Engine • Non-reactive Gas Mixer • Perfectly Stirred Reactor (PSR) • Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor • SI Engine Zonal Simulator		
WMIX Reactor Property	Width of the mixing region; used in defining the initial profile for the LINE or PLAT options.			
	Parameters	Optional/Reqd.	Units	Examples
	Width of mixing region	Required	cm	WMIX **2.0**
	Keyword Usage	Optional keyword. By default the width of the mixing region is XEND * 0.5.		
	Reactor Models	• Diffusion or Premixed Opposed-flow Flame • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
WOSP1 Reactor Property	Specify parameters of the Woschni heat transfer correlation for the compression period.			
	Parameters	Optional/Reqd.	Units	Examples

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Keyword	Definition			
	C11 in the average gas velocity correlation.	Required	--	WOSP1 2.28 0.318 0.0 1.57
	C12 in the Woschni correlation.	Required	cm/(sec - K)	WOSP1 2.28 0.318 0.0 1.57
	C2 in the Woschni correlation.	Required	--	WOSP1 2.28 0.318 0.0 1.57
	Ratio of swirl velocity to mean piston speed.	Required	--	WOSP1 2.28 0.318 0.0 1.57
	Keyword Usage	Optional keyword.		
	Reactor Models	• Multi-Zone HCCI Simulator • IC HCCI Engine • SI Engine Zonal Simulator		
WOSP2 Reactor Property	Specify parameters of the Woschni heat transfer correlation for the combustion period.			
	Parameters	Optional/Reqd.	Units	Examples
	C11 in the average gas velocity correlation.	Required	--	WOSP2 2.28 0.318 0.0 1.57
	C12 in the Woschni correlation.	Required	cm/(sec - K)	WOSP2 2.28 0.318 0.0 1.57
	C2 in the Woschni correlation.	Required	--	WOSP2 2.28 0.318 0.0 1.57
	Ratio of swirl velocity to mean piston speed.	Required	--	WOSP2 2.28 0.318 0.0 1.57
	Keyword Usage	Optional keyword.		
	Reactor Models	• Multi-Zone HCCI Simulator • IC HCCI Engine • SI Engine Zonal Simulator		
WOSP3 Reactor Property	Specify parameters of the Woschni heat transfer correlation for the expansion period.			
	Parameters	Optional/Reqd.	Units	Examples
	C11 in the average gas velocity correlation.	Required	--	WOSP3 2.28 0.318 0.0 1.57
	C12 in the Woschni correlation.	Required	cm/(sec - K)	WOSP3 2.28 0.318 0.0 1.57

Keyword	Definition			
	C2 in the Woschni correlation.	Required	--	WOSP3 2.28 0.318 0.0 1.57
	Ratio of swirl velocity to mean piston speed.	Required	--	WOSP3 2.28 0.318 0.0 1.57
	Keyword Usage	Optional keyword.		
	Reactor Models	• Multi-Zone HCCI Simulator • IC HCCI Engine • SI Engine Zonal Simulator		
WPRO Reactor Property Profiles	Plasma power deposition profile specified as a function of time.			
	Parameters	Optional/Reqd.	Units	Examples
	Time value	Required	sec	WPRO **1.0E-4** 500
	Plasma power deposition	Required	watts	WPRO 1.0E-4 **500**
	Reactor number (PSR clusters only)	Optional If no number is given, the profile described by the first two values is assumed to apply to all reactors in a cluster.	--	WPRO 1.0E-4 500 **1**
	Keyword Usage	Optional keyword. By default, no profile is provided.		
	Reactor Models	• Closed Plasma Reactor • Plasma Plug Flow Reactor • Plasma PSR		
WS-RC Reactor Property	Half-width of the Gaussian source term if the gas is being heated by an optional heat source. See Equation 14.12 of the Chemkin-Pro Theory Manual .			
	Parameters	Optional/Reqd.	Units	Examples
	Half-width	Required	cm	WSRC **0.07**
	Keyword Usage	Optional keyword. By default, the half-width is 0.0. This is a required keyword when QDOT is not 0.0.		

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Keyword	Definition			
	Reactor Models	• Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
XBTH Reactor Property	Specifies the bath gas composition. The [**Species name**] (or number as it appears in the Pre-processor output) and desired mole fraction are required parameters. If at least one species in a phase has been set with the XBTH keyword, then all of the specified mole fractions for that phase are summed and normalized so that they add up to one. If no XBTH parameters have been specified for any species in the phase, then mole fractions for all species in that phase are set equal to one another.			
	Parameters	Optional/Reqd.	Units	Examples
	Species name	Optional	--	XBTH **H2** 1.0
	Species number value	Optional	mole fractions	XBTH CH(S) **0.5**
	Keyword Usage	Optional keyword. By default, the table output is determined by the ALL or NONE keyword.		
	Reactor Models	• Mechanism Analyzer		
XCEN Reactor Property	Center of the mixing region; used in defining the initial profile for the LINE or PLAT options. Note that the fuel inlet is assumed to be located at x=0.			
	Parameters	Optional/Reqd.	Units	Examples
	Center of mixing region	Required	cm	XCEN **3.0**
	Keyword Usage	Optional keyword. By default the center of the mixing region is XEND * 0.35.		
	Reactor Models	• Diffusion or Premixed Opposed-flow Flame • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
XEND Reactor Property	Physical length of the computational domain, or value of x at the end of the domain. Depending on the reactor, the beginning of the domain is either 0.0 or the value of XSTR.			
	Parameters	Optional/Reqd.	Units	Examples
	Channel length	Required	cm	XEND **25**
	Keyword Usage	Required keyword.		

<table>
<tr><th>Keyword</th><th colspan="4">Definition</th></tr>
<tr><td></td><td>Reactor Models</td><td colspan="3">• Cylindrical Shear Flow Reactor
• Diffusion or Premixed Opposed-flow Flame
• Honeycomb Reactor
• Planar Shear Flow Reactor
• Plasma Plug Flow Reactor
• Plug Flow Reactor
• Premixed Laminar Burner-stabilized Flame
• Premixed Laminar Flame-speed Calculation
• Rotating Disk CVD Reactor
• Stagnation Flow CVD Reactor</td></tr>
<tr><td>XEST

Reactor Property</td><td colspan="4">For steady-state calculations, these are the estimated gas-phase mole fractions to begin the iteration. For transient problems, this keyword provides the initial values for the gas-phase mole fractions in the reactor. For example, XEST H2O 0.5 assigns an initial mole fraction of 0.5 to water vapor in the reactor.</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
<tr><td></td><td>Species name</td><td>Required</td><td>--</td><td>XEST H2O 0.5</td></tr>
<tr><td></td><td>Initial fraction</td><td>Required</td><td>mole fractions</td><td>XEST H2O 0.5</td></tr>
<tr><td></td><td>Keyword Usage</td><td colspan="3">Transient cases: Required keyword; Steady-state cases: Optional keyword. By default, the initial or estimated gas-phase mole fractions are 0.0. For steady-state cases, if no XEST keywords are given, then an equilibrium calculation is performed to determine the initial estimates for the reactor composition.</td></tr>
<tr><td></td><td>Reactor Models</td><td colspan="3">• Perfectly Stirred Reactor (PSR)
• Plasma PSR
• SI Engine Zonal Simulator</td></tr>
<tr><td></td><td>Notes</td><td colspan="3">• The sum of all the estimated mole fractions should equal one. If they do not sum to one, they will be normalized and a warning message will be printed to the output file.</td></tr>
<tr><td>XIMN

Reactor Property</td><td colspan="4">Minimum mass or mole fraction value applied to intermediate species estimates, when the (default) equilibrium is used to determine product estimates. Ignored in the case that INTM keywords are present. In this case, the intermediate species fraction is initialized to be the average of its PROD2 and REAC values; or XIMN, if XIMN is greater than this average.</td></tr>
<tr><td></td><td>Parameters</td><td>Optional/Reqd.</td><td>Units</td><td>Examples</td></tr>
</table>

Keyword	Definition			
	Intermediate fractions	Required	mole fractions	XIMN **1.0E-10**
	Keyword Usage	Optional keyword. By default, the intermediate fraction is set to 0.		
	Reactor Models	• Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation		
XMLI Cluster Property	Read a solution from the XML Solution File used for initialization (*XMLdata.zip*), which may be a solution from any other Reactor Model (see also RSTR). When initialization (XMLI) is used from an XML Solution File with spatial profiles (i.e., 1-D or channel-flow models), the initial values are actually averages of the profiles stored in the XML Solution File. The integral averages are calculated using trapezoidal integration rules.			
	Keyword Usage	Optional keyword. By default, the program does not look for an XML Solution File used for restart or initialization.		

Keyword	Definition		
	Reactor Models	• Chemical and Phase Equilibrium Calculations • Closed Homogeneous Batch Reactor • Closed Plasma Reactor • Cylindrical Shear Flow Reactor • Diffusion or Premixed Opposed-flow Flame • Honeycomb Reactor • IC HCCI Engine • Mechanism Analyzer • Non-reactive Gas Mixer • Normal Incident Shock • Normal Reflected Shock • Partially Stirred Reactor (PaSR) • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor • SI Engine Zonal Simulator • Stagnation Flow CVD Reactor	
	Notes	• For shear-layer flow solutions, we use the value integrated over the height (or radius) and divided by the cross-sectional area for the specified axial-distance location. • For Opposed-flow Flames and CVD Reactors, we use the value integrated over the spatial domain, divided by the total axial distance.	

Keyword	Definition			
XMLS Cluster Property	Use a previously stored XML Solution File or the XML Solution File from an upstream reactor to initialize the inlet conditions of this inlet.			
	Keyword Usage	Optional keyword. By default, the program does not look for an XML Solution File used restart or initialization.		
	Reactor Models	• Cylindrical Shear Flow Reactor • Diffusion or Premixed Opposed-flow Flame • Honeycomb Reactor • Non-reactive Gas Mixer • Partially Stirred Reactor (PaSR) • Perfectly Stirred Reactor (PSR) • Planar Shear Flow Reactor • Plasma Plug Flow Reactor • Plasma PSR • Plug Flow Reactor • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
XRES Restart	Force the starting distance for the new solution to be this value and ignore the value of distance from the XML Solution File used for restart or initialization.			
	Parameters	Optional/Reqd.	Units	Examples
	Initial distance	Required	cm	XRES **10**
	Keyword Usage	Optional keyword. By default, the value of the XML Solution File is used during a continuation or restart run.		
	Reactor Models	• Honeycomb Reactor • Plasma Plug Flow Reactor • Plug Flow Reactor		
XRST Restart	This keyword is valid when using RSTR option. In this case, select the values to use in restart as those corresponding to the distance that is closest to (greater than or equal to) the specified distance.			
	Parameters	Optional/Reqd.	Units	Examples

Keyword	Definition			
	Distance	Required	cm	XRST **5.0**
	Keyword Usage	Optional keyword. By default, the point where the previous solution ended is used.		
	Reactor Models	• Cylindrical Shear Flow Reactor • Planar Shear Flow Reactor		
XSDF Reactor Property	Default value for a momentum-transfer cross-section between electrons and each species. This value is used for all species not specified with the XSEK keyword.			
	Parameters	Optional/Reqd.	Units	Examples
	Momentum-transfer cross-section	Required	cm^2	XSDF **1.0E-16**
	Keyword Usage	Optional keyword. By default, the cross-section value is 0. In a plasma problem the user must either specify XSDF or include an XSEK keyword for all species except electrons.		
	Reactor Models	• Closed Plasma Reactor • Plasma Plug Flow Reactor • Plasma PSR		
XSEK Reactor Property	Momentum-transfer collision cross-section between electrons and a specified species. For example, "XSEK AR 1.0E-16" would indicate a momentum-transfer cross-section of 10^{-16} cm^2 between electrons and argon atoms. For any species not specified by the XSEK keyword, a user-specified default value will be used.			
	Parameters	Optional/Reqd.	Units	Examples
	Species	Required	--	XSEK **AR** 1.0E-16
	Momentum-transfer cross-section	Required	cm^2	XSEK AR **1.0E-16**
	Keyword Usage	Optional keyword. By default, the cross-section value is 0. In a plasma problem the value for every species is specified by the XSDF keyword.		
	Reactor Models	• Closed Plasma Reactor • Plasma Plug Flow Reactor • Plasma PSR		
XSRC Reactor Property	Height above the disk which is the center of a Gaussian-shaped power source. See Equation 14.12 of the Chemkin-Pro Theory Manual .			
	Parameters	Optional/Reqd.	Units	Examples
	Height	Required	cm	XSRC **0.6**
	Keyword Usage	Optional keyword. By default, the height is 0.0.		

Keyword	Definition			
	Reactor Models	• Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
XSTR Reactor Property	The beginning of the computational domain. For burner-stabilized flames, this is the burner location.			
	Parameters	Optional/Reqd.	Units	Examples
	Inlet axial position	Required	cm	XSTR **1.5**
	Keyword Usage	Optional keyword. By default, the starting or inlet axial position is 0.		
	Reactor Models	• Honeycomb Reactor • Plasma Plug Flow Reactor • Plug Flow Reactor • Premixed Laminar Burner-stabilized Flame • Premixed Laminar Flame-speed Calculation • Rotating Disk CVD Reactor • Stagnation Flow CVD Reactor		
XTMP Reactor Property	If TSRF is used to specify the surface temperature, the application will set the surface temperature to TINL at $x=0$ and smoothly ramp the temperature up to TSRF at a distance of XTMP.			
	Parameters	Optional/Reqd.	Units	Examples
	distance between TINL point and TSRF point	Required	cm	XTMP **0.25**
	Keyword Usage	Optional keyword. By default, the distance is set to 0.5.		
	Reactor Models	• Cylindrical Shear Flow Reactor • Planar Shear Flow Reactor		
ZONEAVG Output	Flag to store only the zone-average solution data in the Multi-Zone HCCI Engine Simulator.			
	Keyword Usage	Optional keyword. By default, all solution data is stored in the Multi-Zone HCCI Engine Simulator output.		
	Reactor Models	• Multi-Zone HCCI Engine Simulator • SI Engine Zonal Simulator		

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