Chemkin

A SOFTWARE PACKAGE FOR THE ANALYSIS OF GAS-PHASE CHEMICAL AND PLASMA KINETICS.

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Introduction

- CHEMKIN is...

  is a powerful software system for solving complex chemical kinetics problems.

- CHEMKIN includes...

  a choice of Application programs that treat industry-specific reacting-flow conditions, a set of Core Utilities (on which the Applications are built), an Application User Interface for easy set-up and solution of problems, and a Graphical Post-processor for quick visualization of results.

- CHEMKIN provides...

  solutions for combustion, catalysis, chemical vapor deposition, and plasma etching and is packaged to align with the needs of specific industries.

Structure

- Core utilities
  - Gas-phase kinetics
  - Surface kinetics
  - Transport
  - Thermodynamic data
  - Twopnt

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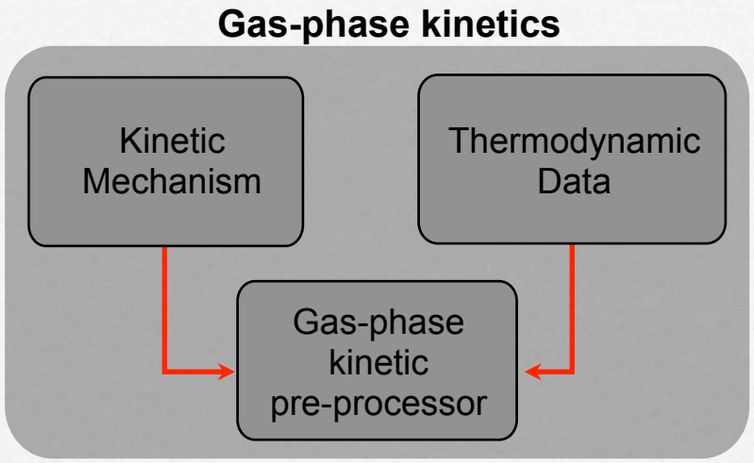

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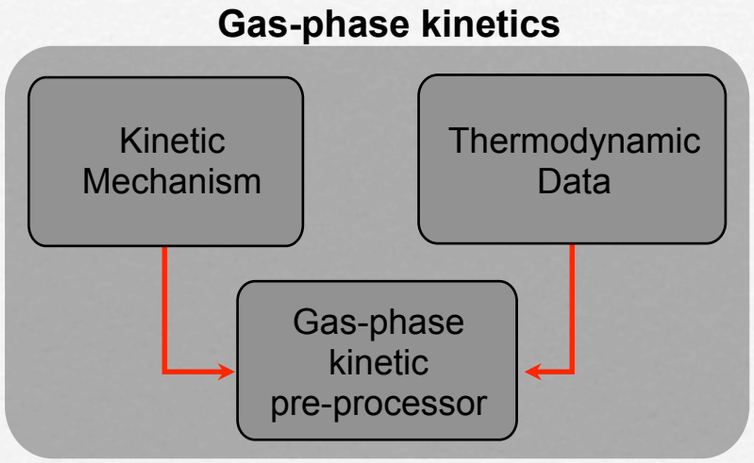

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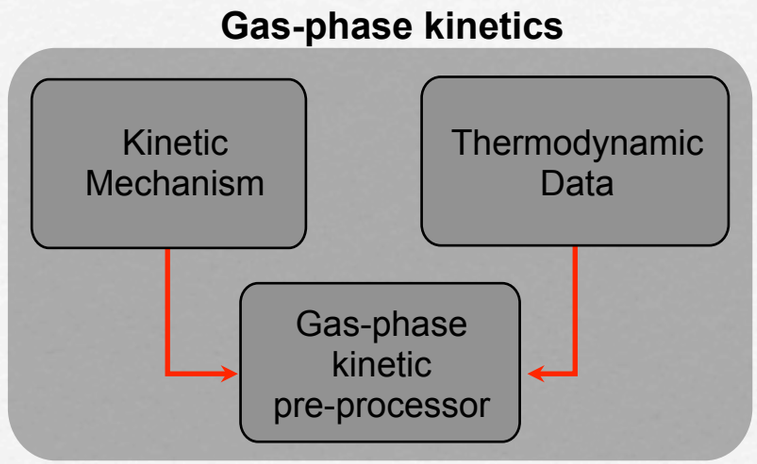

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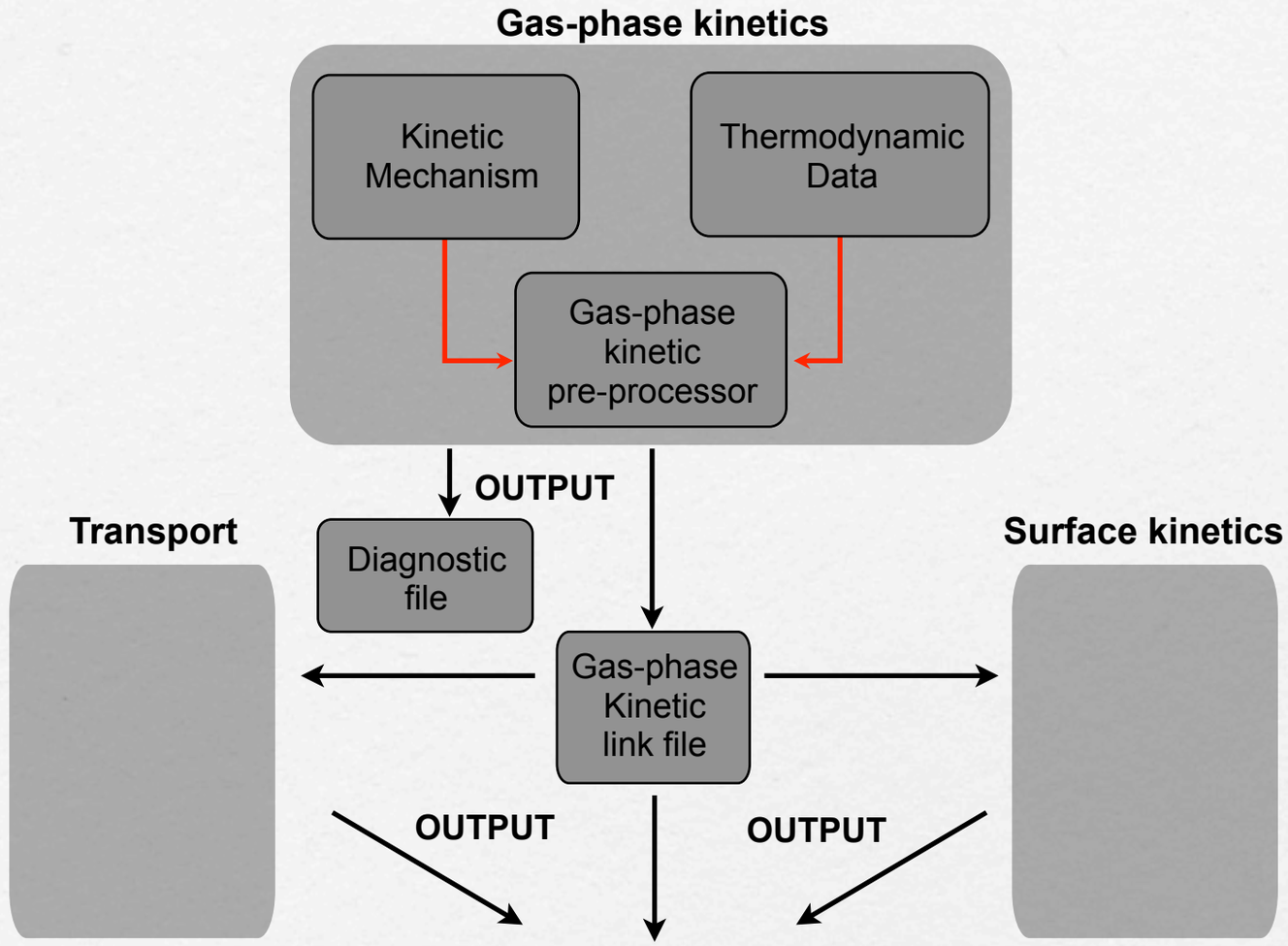

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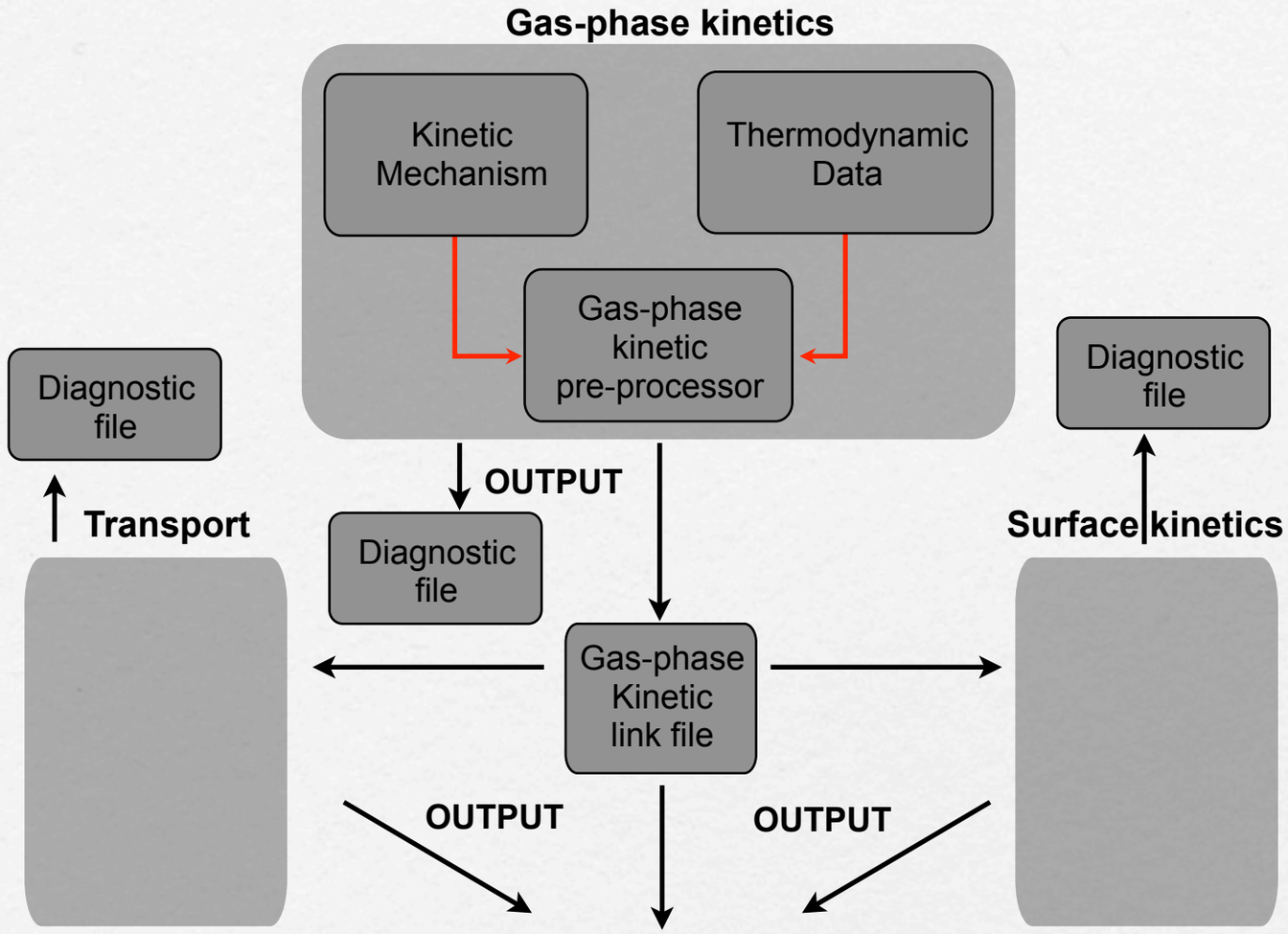

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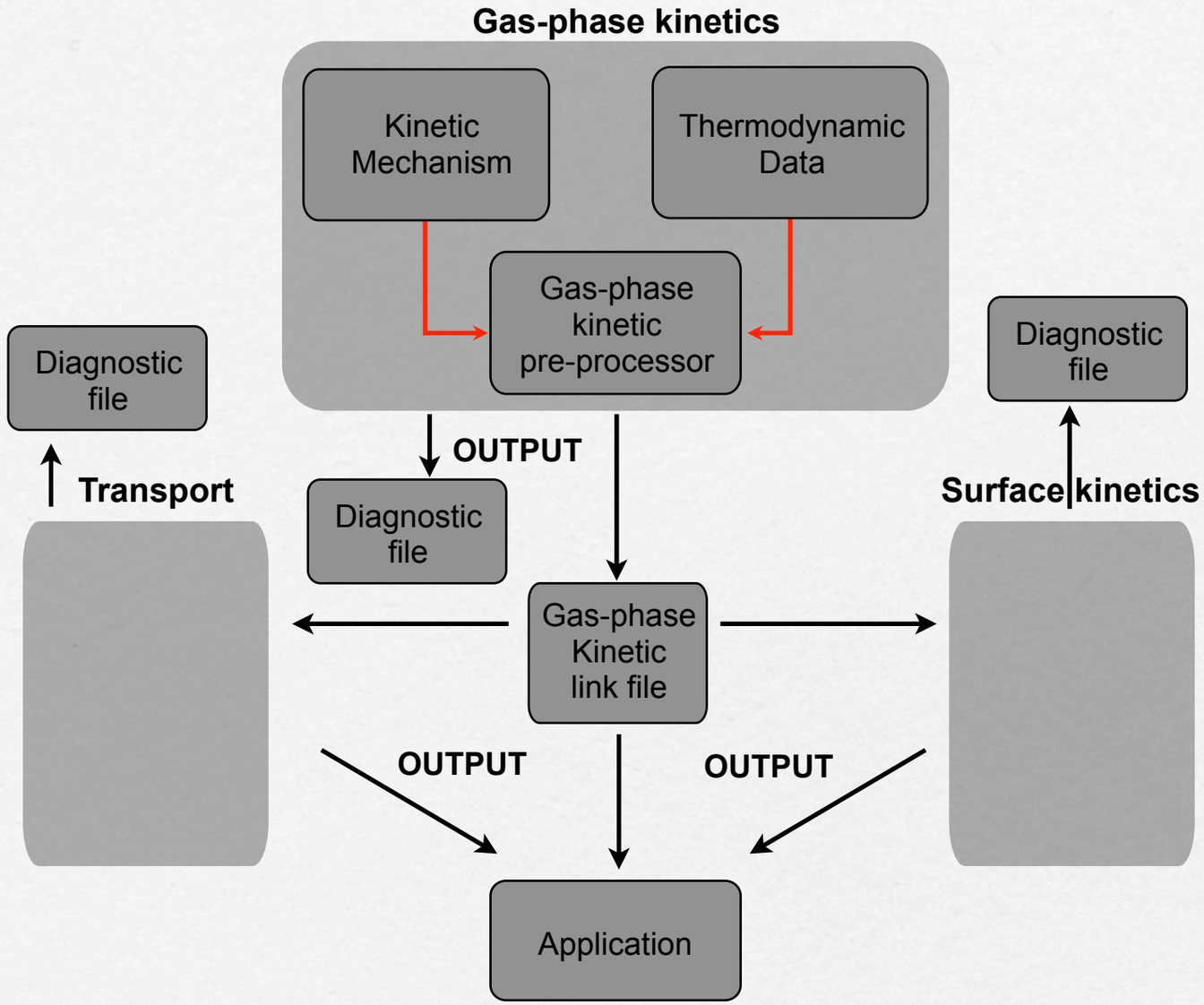

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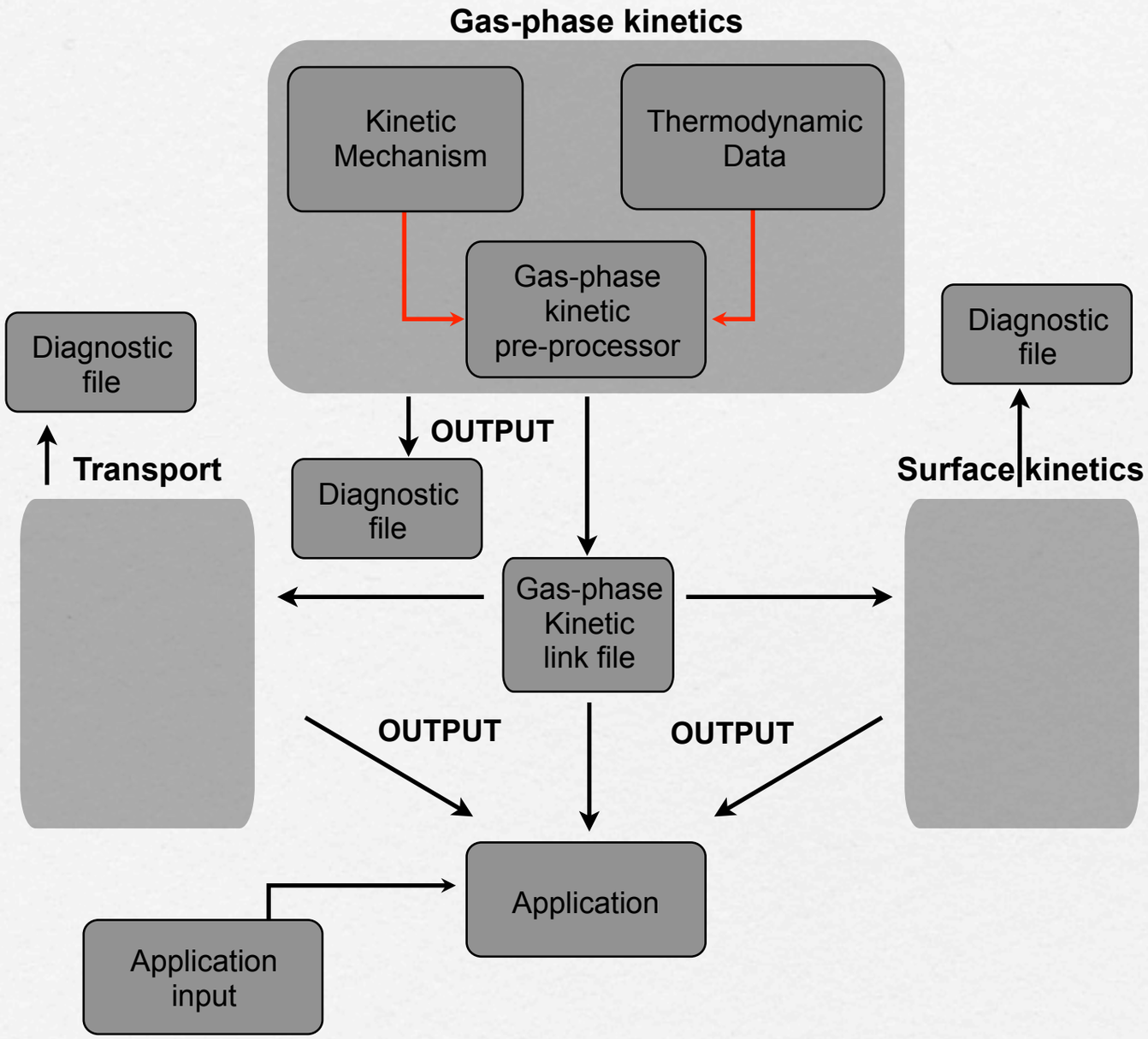

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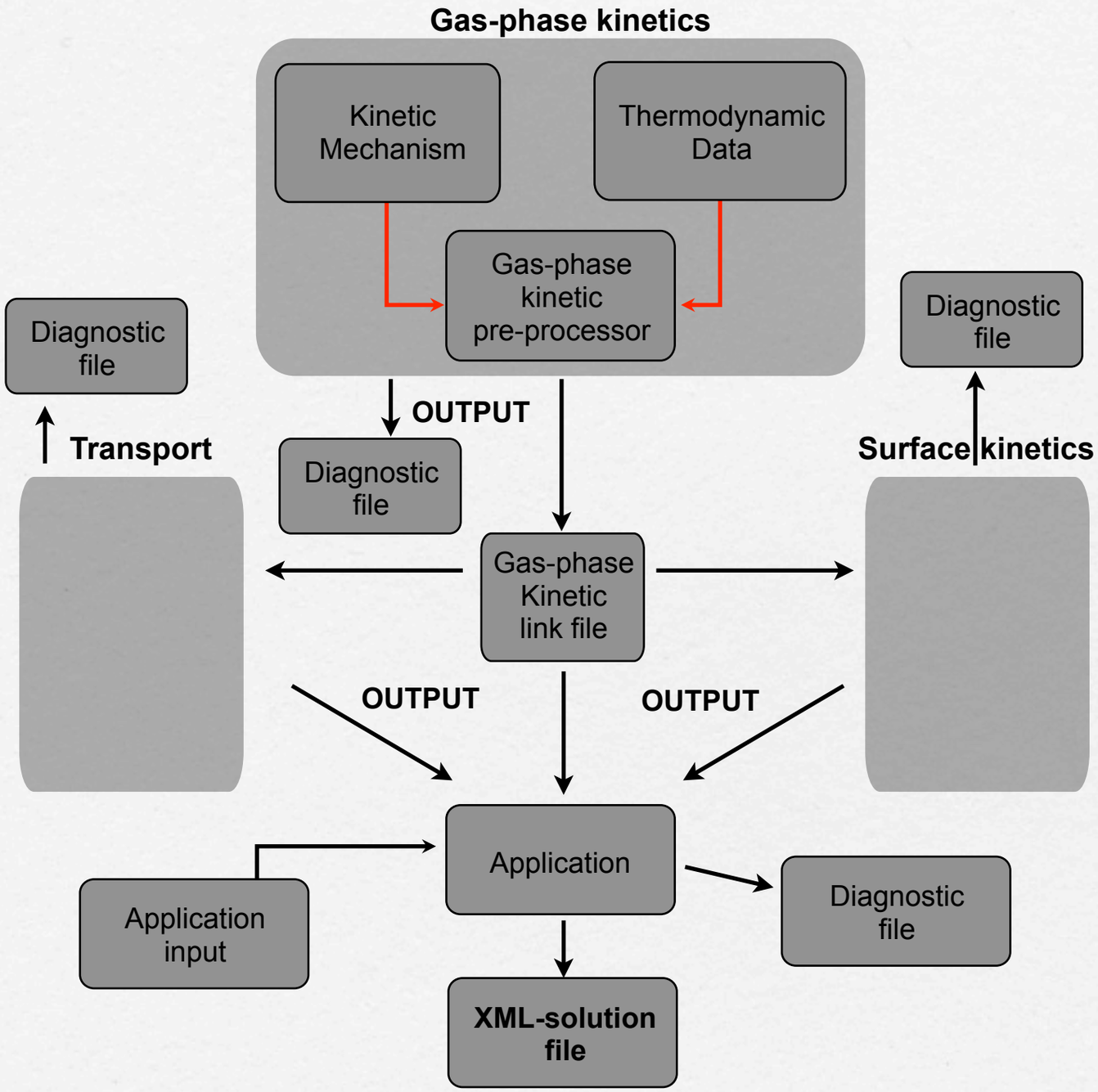

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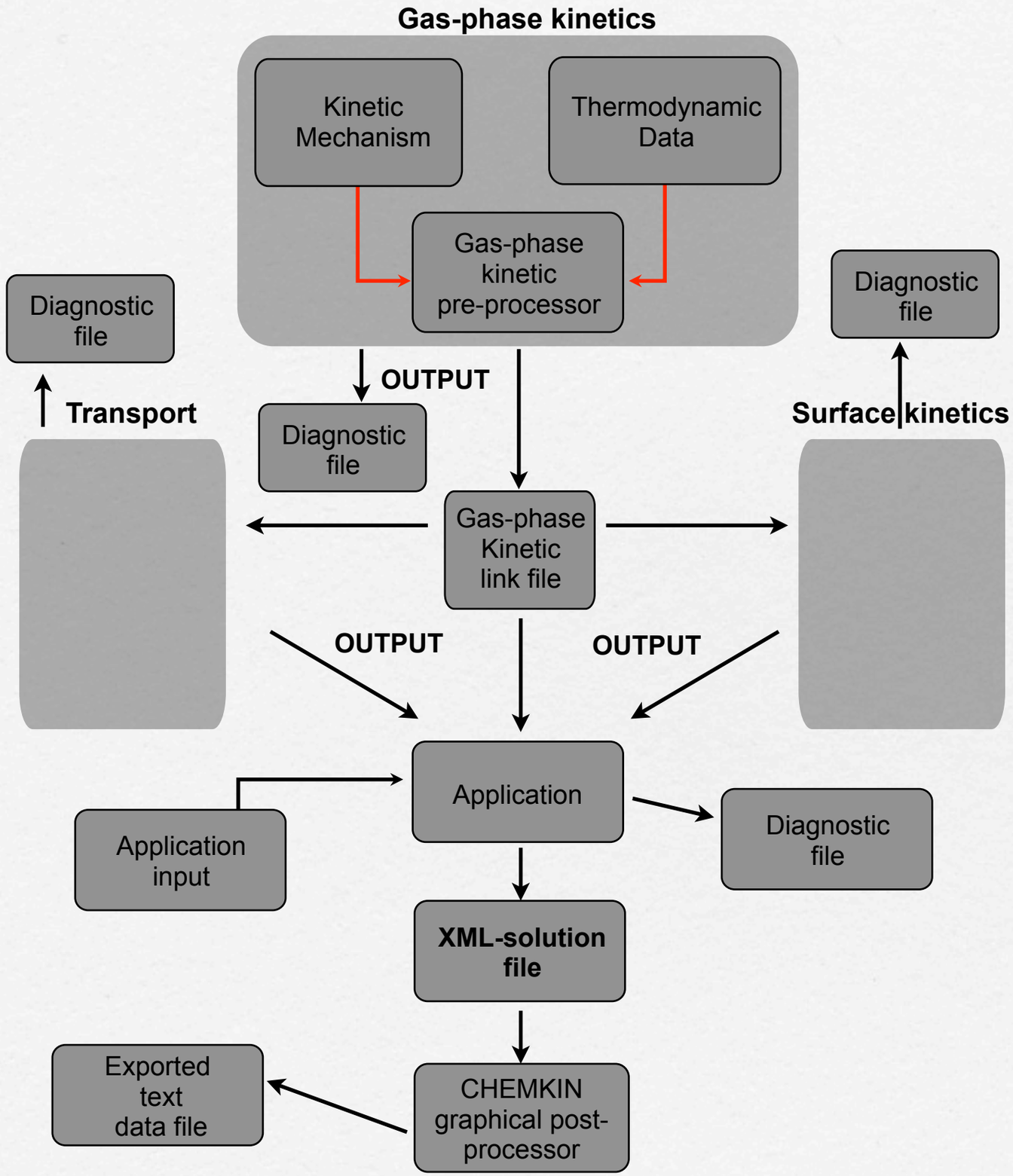
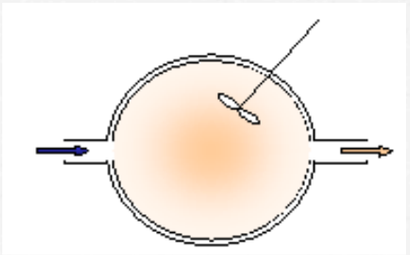
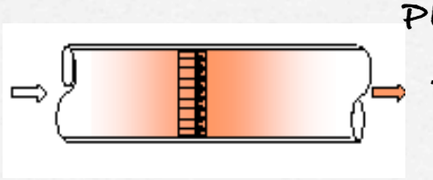


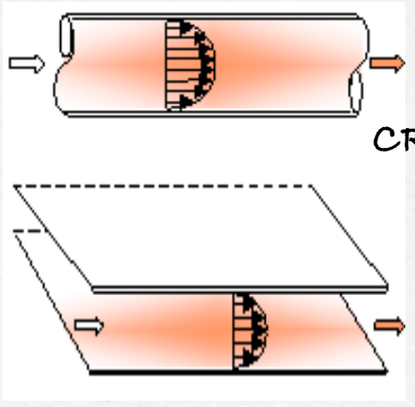
Applications...1



Continuously stirred tank (CSTR) or perfectly stirred reactor (PSR) models have been in use for many years in the study of chemistry within a unit process for a variety of applications.

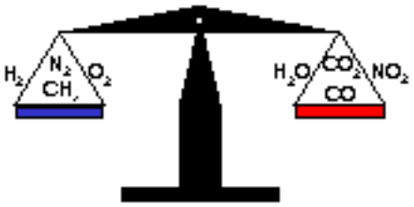


PLUG simulates the behavior of plug-flow chemical reactors. More specifically, the Application is designed to model the non-dispersive, one-dimensional flow of a chemically reacting, ideal-gas mixture in a conduit of essentially arbitrary geometry.

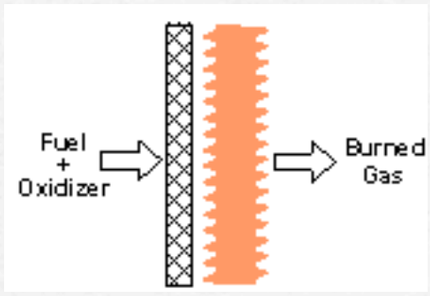


CRESLAF predicts the velocity, temperature, and species profiles in two-dimensional (planar or axisymmetric) channels. Applications of CRESLAF include chemical vapor deposition (CVD) reactors, heterogeneous catalysis on reactor walls, and corrosion processes.

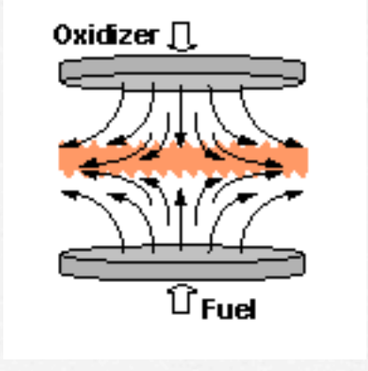
Applications...2



EQUIL is a application that computes the chemical equilibrium state of an ideal gas or solution mixture.

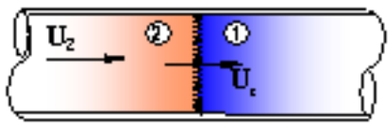


PREMIX computes species and temperature profiles in steady-state burnerstabilized and freely propagating premixed laminar flames. PREMIX can be used to determine laminar flame speeds of combustive gas mixtures that are important for flammability studies.

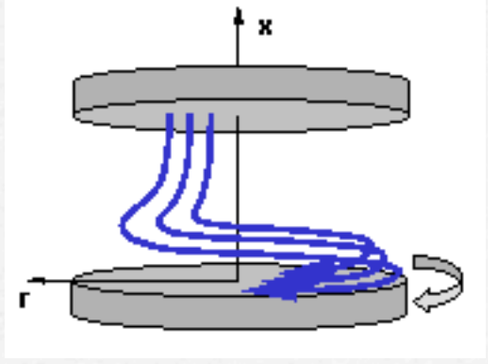


OPPDIF computes the diffusion flame between two opposing nozzles.

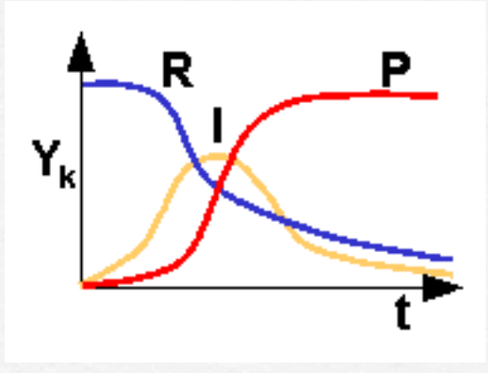
Applications...3



SHOCK is a CHEMKIN Application that predicts the chemical changes that occur after the shock heating of reactive gas mixtures.



The SPIN Application computes species, temperature and velocity profiles, as well as deposition rates in a steady-state, one-dimensional rotating disk or stagnationpoint flow chemical vapor deposition (CVD) reactor.



Analisis of reaction sensitivity

Kinetic Mechanism

$$k_{f,i} = A_i T^{n_i} \exp\left(\frac{-E_i}{RT}\right)$$

Definitions of elements

Definitions of species

Definitions of reactions

```
ELEMENTS O H N END
SPECIES  O  O2  H  H2  OH  HO2  H2O  H2O2 N2 END
REACTIONS
  H+O2 = O+OH                1.1E16   -0.82  16510 !MILLER 81
  H2+O = H+OH                1.8E10    1.0    8830 !MILLER 77
  H2+OH = H2O+H              1.2E09    1.3    3630 !DIXON-LEWIS 77
  OH+OH = H2O+O              6.0E08    1.3     0.0 !COHEN 79
  H+OH+M = H2O+M             7.5E23   -2.6     0.0 !MILLER 77
    H2O /20.0/
  O2+M = O+O+M               1.9E11    0.5   95560 !MILLER 81
  H2+M = H+H+M               2.2E12    0.5   92600 !MILLER 77
    H2O /6.0/
    H   /2.0/
    H2  /3.0/
  H2+O2 = OH+OH              1.7E13    0.0   47780 !MILLER 77
  H+O2+M = HO2+M             2.1E18   -1.0     0.0 !SLACK 77
    H2O /21.0/
    H2  /3.3/
    O2  /0.0/
    N2  /0.0/
  H+O2+O2 = HO2+O2           6.7E19   -1.42    0.0 !SLACK 77
  H+O2+N2 = HO2+N2           6.7E19   -1.42    0.0 !SLACK 77
  HO2+H = H2+O2              2.5E13    0.0     700 !LLOYD 74
  HO2+H = OH+OH              2.5E14    0.0    1900 !LLOYD 74
  HO2+O = OH+O2              4.8E13    0.0    1000 !LLOYD 74
  HO2+OH = H2O+O2            5.0E13    0.0    1000 !LLOYD 74
  HO2+HO2 = H2O2+O2          2.0E12    0.0     0.0 !TROE 69
  H2O2+M = OH+OH+M           1.2E17    0.0   45500 !BAULCH 72
  H2O2+H = HO2 + H2          1.7E12    0.0    3750 !BAULCH 72
  H2O2+OH = H2O+HO2          1.0E13    0.0    1800 !BAULCH 72
END
```

Kinetic Mechanism is written in a text file

Definitions of reactions

Kinetic Mechanism

Third body efficiency

```
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
```

Pressure dependence

Thermodynamic Data

THERMODYNAMIC DATA contains polynomial fits to specific heats, standard state enthalpies, and standard state entropies.

Table 3. Summary of the Rules for Thermodynamic Data

Line Number	Contents	Format	Column
1	THERMO (or THERMO ALL*)	Free	Any
2**	Temperature ranges for 2 sets of coefficients: lowest T, common T, and highest T	3F10.0	1 to 30
3	Species name (must start in Column 1)	18A1	1 to 18
	Date (not used)	6A1	19 to 24
	Atomic symbols and formula	4(2A1,I3)	25 to 44
	Phase of species (S, L, or G for solid, liquid, or gas, respectively)	A1	45
	Low temperature	E10.0	46 to 55
	High temperature	E10.0	56 to 65
	Common temperature (if needed, else blank)	E8.0	66 to 73
	Atomic symbols and formula (if needed, else blank)	2A1,I3	74 to 78
	The integer 1	I1	80
	Atomic symbols and formula (if needed, else blank)	4(2A1,I3)	81 to 100
4	Coefficients a_1 - a_5 in Eqs. (19) - (21), for upper temperature interval	5(E15.8)	1 to 75
	The integer 2	I1	80
5	Coefficients a_6, a_7 for upper temperature interval, and a_1, a_2, and a_3 for lower	5(E15.8)	1 to 75
	The integer 3	I1	80
6	Coefficients a_4, a_5, a_6, a_7 for lower temperature interval	4(E15.8)	1 to 60
	The integer 4	I1	80
...	Repeat lines 3 - 6 for each species.		
last	END (Optional, end of thermodynamic data.)	Free	Any

Thermodynamic Properties

Specific heats

$$\frac{c_p}{R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

Standard State enthalpies

$$\frac{H^0}{RT} = a_1 + \frac{a_2}{2} T + \frac{a_3}{3} T^2 + \frac{a_4}{4} T^3 + \frac{a_5}{5} T^4 + \frac{a_6}{T}$$

Standard State entropies

$$\frac{S^0}{R} = a_1 \ln T + a_2 T + \frac{a_3}{2} T^2 + \frac{a_4}{3} T^3 + \frac{a_5}{4} T^4 + a_7$$

Thermodynamic Data

Species

Coefficients

Comment

Elements

Phase

Range of temperatures

```
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
```

Diagnostic file

Elements

Species

Reactions

Note

Commments

```
                                ELEMENTS      ATOMIC
                                CONSIDERED    WEIGHT
                                ----------------------
                                 1. O         15.9994
                                 2. H         1.00797
                                 3. N         14.0067
                                ----------------------
------------------------------------------------------------------------------------------

                                C
                              P H
                              H A
                              A R
SPECIES                       S G MOLECULAR TEMPERATURE    ELEMENT COUNT
CONSIDERED                    E E WEIGHT    LOW     HIGH   O   H   N
------------------------------------------------------------------------------------------
  1. O                        G 0  15.99940   300.0 5000.0  1   0   0
  2. O2                       G 0  31.99880   300.0 5000.0  2   0   0
  3. H                        G 0   1.00797   300.0 5000.0  0   1   0
  4. H2                       G 0   2.01594   300.0 5000.0  0   2   0
  5. OH                       G 0  17.00737   300.0 5000.0  1   1   0
  6. HO2                      G 0  33.00677   300.0 5000.0  2   1   0
  7. H2O                      G 0  18.01534   300.0 5000.0  1   2   0
  8. H2O2                     G 0  34.01474   300.0 5000.0  2   2   0
  9. N2                       G 0  28.01340   300.0 5000.0  0   0   2
------------------------------------------------------------------------------------------
```

```
                                                                (k = A T**b exp(-E/RT))
   REACTIONS CONSIDERED                                           A          b          E

  1.  H+O2=O+OH                                                 5.10E+16     -.8     16510.0
  2.  H2+O=H+OH                                                 1.80E+10     1.0      8830.0
  3.  H2+OH=H2O+H                                               1.20E+09     1.3      3630.0
  4.  OH+OH=H2O+O                                               6.00E+08     1.3         .0
  5.  H+OH+M=H2O+M                                              7.50E+23    -2.6         .0
        H2O                     Enhanced by     2.000E+01
  6.  O2+M=O+O+M                                                1.90E+11      .5     95560.0
  7.  H2+M=H+H+M                                                2.20E+12      .5     92600.0
        H2O                     Enhanced by     6.000E+00
        H                       Enhanced by     2.000E+00
        H2                      Enhanced by     3.000E+00
  8.  H2+O2=OH+OH                                               1.70E+13      .0     47780.0
  9.  H+O2+M=HO2+M                                              2.10E+18    -1.0         .0
        H2O                     Enhanced by     2.100E+01
        H2                      Enhanced by     3.300E+00
        O2                      Enhanced by     0.000E+00
        N2                      Enhanced by     0.000E+00
 10.  H+O2+O2=HO2+O2                                            6.70E+19    -1.4         .0
 11.  H+O2+N2=HO2+N2                                            6.70E+19    -1.4         .0
 12.  HO2+H=H2+O2                                               2.50E+13      .0      700.0
 13.  HO2+H=OH+OH                                               2.50E+14      .0     1900.0
 14.  HO2+O=OH+O2                                               4.80E+13      .0     1000.0
 15.  HO2+OH=H2O+O2                                             5.00E+13      .0     1000.0
 16.  HO2+HO2=H2O2+O2                                           2.00E+12      .0         .0
 17.  H2O2+M=OH+OH+M                                            1.20E+17      .0     45500.0
 18.  H2O2+H=HO2+H2                                             1.70E+12      .0      3750.0
 19.  H2O2+OH=H2O+HO2                                           1.00E+13      .0      1800.0

 NOTE:  A units mole-cm-sec-K, E units cal/mole
```

```
NO ERRORS FOUND ON INPUT...CHEMKIN LINKING FILE WRITTEN.

WORKING SPACE REQUIREMENTS ARE
   INTEGER:       457
   REAL:          444
   CHARACTER:      12
```

Six basic steps...

There are six basic steps involved in using the CHEMKIN Collection to solve a typical chemical process modeling problem. Depending on the particular CHEMKIN Application, some of the input discussed here will not be require for a particular problem; these are indicated in parentheses.

1. Decide on your modeling approach For some problems the choice of CHEMKIN Application will be obvious. In other cases, users have a range of options, where the reacting-flow region may be modeled as a network of zones, or as a single, well mixed zone, for example. For network models, there may be recirculation between zones and multiple inlets that need to be defined. Other options include using a zero-dimensional descript 2- dimensional description. For complex systems, we recommen proaches, progressing from simpler models (e.g. a well-mixed or pl ulations (e.g. networks or 2-D boundary-layer flow) as the system and model behavior.

2. Prepare GAS-PHASE KINETICS Input (SURFACE KINETICS Input)

3. Acquire t ta for all species in the chemical system Gas-phase species thermoc odynamic data) (Gas-phase species transport data)

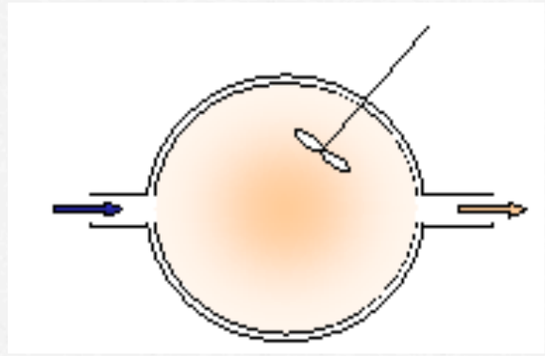
4. Prepare the Application-specific input file (Geometry) Process Conditions (Solution method options)

5. Run the Pre-processors and the Application from the Application User Interface

6. Post-process the results using the Graphical Post-processor

Aurora Application

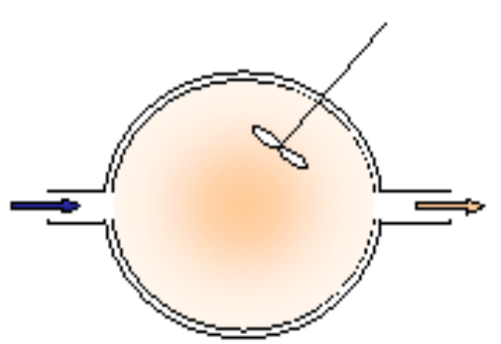
1. The first four characters of the line are reserved for the keyword, and it must begin at the first column.
2. Any further input associated with the keyword can appear anywhere in columns 5 through 80. The specific starting column is unimportant.
3. When more than one piece of information is required, 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. AURORA 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 CHEMKIN and SURFACE CHEMKIN Interpreter input files.
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, AURORA 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 can be inserted by placing either an exclamation point (!), or a slash (/) in the first column. The program ignores such lines, but will echo them back in the printed output. In addition, on any keyword line, any input that follows the required input and is enclosed in parentheses is taken to be a comment.
9. The keyword END must be the last input card. END keywords are required between sets of parameters for continuations.



Continuously stirred tank (CSTR) or perfectly stirred reactor (PSR) models have been in use for many years in the study of chemistry within a unit process for a variety of applications.

The AURORA model allows simulation of both dynamic and steady-state reactor systems. For dynamic systems, the user may specify controlling conditions that vary as a function of time. For steady-state systems, AURORA can compute a series of steady-state conditions varying one or more parameters, such as heat-loss or pressure, between simulations.The AURORA Application also includes an option to represent multiple PSRs that are connected in reactor network.

File di input Aurora: Keywords



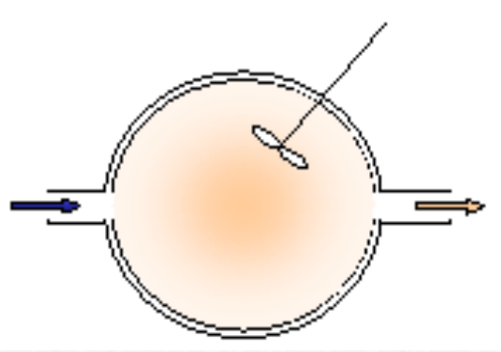
TGIV— Inclusion of this keyword means that AURORA will not solve the gas energy equation, but will instead use a fixed user-supplied temperature (see TEMP).

ENRG— Inclusion of this keyword means that AURORA will solve the gas-energy equation.

TINL— The inlet temperature.
Units—K
Default— none; required input for all problems where ENRG and is specified and the system is not closed.
Example: TINL 400.

REAC— Mole fraction of the reagent gases entering the reactor. One of these REAC inputs must appear for each species in the inlet gas stream. For example, REAC C2H2 0.5, would indicate that acetylene has a mole fraction of 0.5 in the inlet gas. The sum of all the reactant mole fractions should equal to one. However, if they do not, AURORA will proceed to normalize the mole fractions so that they do sum to one, and print a warning message in the output file.
Units—none
Default—none; at least one REAC keyword is required, unless the EQUI /FUEL /OXID /PROD option is used.
Example: REAC C2H2 0.5

File di input Aurora: Keywords



3.4.1 REACTOR CONDITIONS

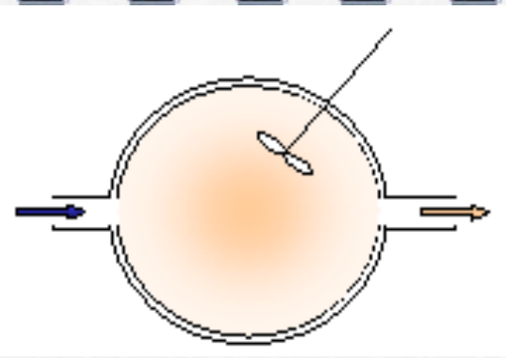
TEMP – The reactor gas temperature. Depending on the problem this is either the user supplied temperature (TGIV), an initial estimate of the temperature (ENRG), or the initial reactor temperature (for transient cases). An optional second number on the keyword line specifies the PSR number. If no number is given, the first value is assumed to apply to all PSRs in series.

Units – K
Default – required input for all PSRs.
Example: TEMP 1000.

PRES – The reactor pressure in atmospheres. Depending on the problem, this is either the user supplied pressure (for steady-state problems), or the initial reactor pressure (for transient cases). An optional second number on the keyword line specifies the PSR number. If no number is given, the first value is assumed to apply to all PSRs in series.

Units – atm
Default – required input for all PSRs.
Example: PRES 1.0

File di input Aurora: Keywords



TAU — The nominal residence time of the gas in the reactor when flow is present, for steady-state problems only. TAU will be ignored for transient cases. If none of TAU, FLRT, or SCCM are specified, the reactor is assumed to be a closed system. An optional number on the keyword line specifies the PSR number. If no number is given, the keyword is assumed to apply to all PSRs in series.

Units — sec

Default — if none of TAU, FLRT, or SCCM is specified or are nonzero, then a closed-system is assumed. For series PSRs, one of these keywords must be present for the first PSR. For all subsequent PSRs in series, the flow rate of the preceding PSR is assumed to be the flow rate into the next PSR.

Example: TAU 1.E-3 1

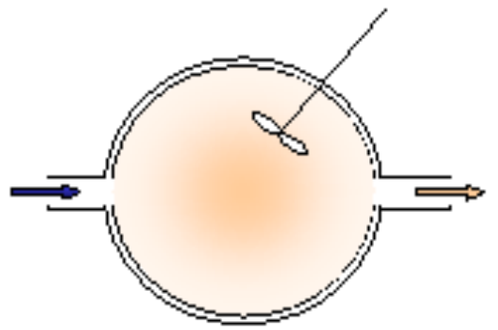
FLRT — The mass flow rate into the reactor. If FLRT is set to zero, then a closed-system is assumed.

Units — g/sec

Default — if none of TAU, FLRT, or SCCM is specified or are nonzero, then a closed-system is assumed. For series PSRs, one of these keywords must be present for the first PSR. For all subsequent PSRs in series, the flow rate of the preceding PSR is assumed to be the flow rate into the next PSR.

Example: FLRT 0.013

File di input Aurora: Keywords



VOL – The volume of the reactor. An optional second number on the keyword line specifies the PSR number. If no number is given, the first value is assumed to apply to all PSRs in series.

Units – cm^3

Default – none; required input for all PSRs, unless both TAU and FLRT or both TAU and SCCM are specified and nonzero.

Example: VOL 1200

QLOS – The heat loss of the reactor at an optionally specified surface material. This keyword is only significant when the ENRG keyword is used. An optional second number on the keyword line specifies the PSR number. If no number is given, the first value is assumed to apply to all PSRs in series.

Units – cal/sec

Default – 0.0; The QLOS and HTRN keywords are mutually exclusive for each PSR. If neither keyword is supplied for a PSR, then QLOS is assumed to have a value of 0.0. . If the material name is not specified, then the same value will be used for all materials.

Example: QLOS MATERIAL1 50 1

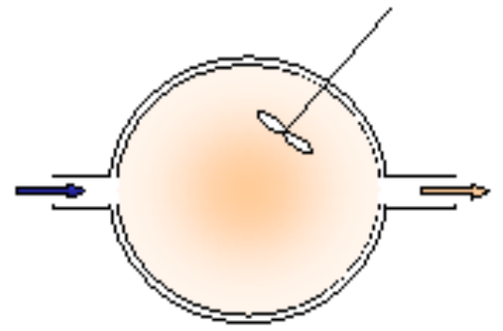
HTRN – The heat transfer coefficient and ambient temperature for specification of the heat loss from the reactor at an optionally specified surface material. This keyword is only significant when the ENRG keyword is used. An optional third number on the keyword line specifies the PSR number. If no number is given, the first value is assumed to apply to all PSRs in series.

Units – h_t has units of cal/(cm^2-K-sec); T_o is in units of K.

Default – 0.0; The QLOS and HTRN keywords are mutually exclusive for each PSR. If neither keyword is supplied for a PSR, then QLOS is assumed to have a value of 0.0. . If the material name is not specified, then the same value will be used for all materials.

Example: HTRN MATERIAL1 1.E-4 298 1.

File di input Aurora: Keywords



TRAN— The solution will be obtained using a transient calculation (with the solver DASPK) instead of a steady-state calculation (using the solver TWOPNT).

Default—a steady-state calculation will be performed.

STST— The solution will be obtained using a steady-state calculation (with the solver TWOPNT) instead of a transient calculation (using the solver DASPK).

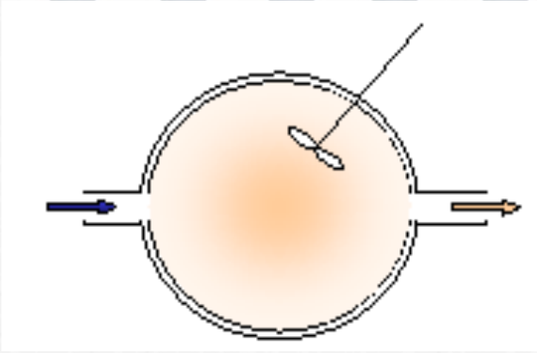
Default—a steady-state calculation will be performed.

NPSR— Number of PSRs in series. Currently the maximum number of PSRs in series that the program can consider is 10. This number can be changed, however, but modifying a parameter statement in AURORA.

Default—1

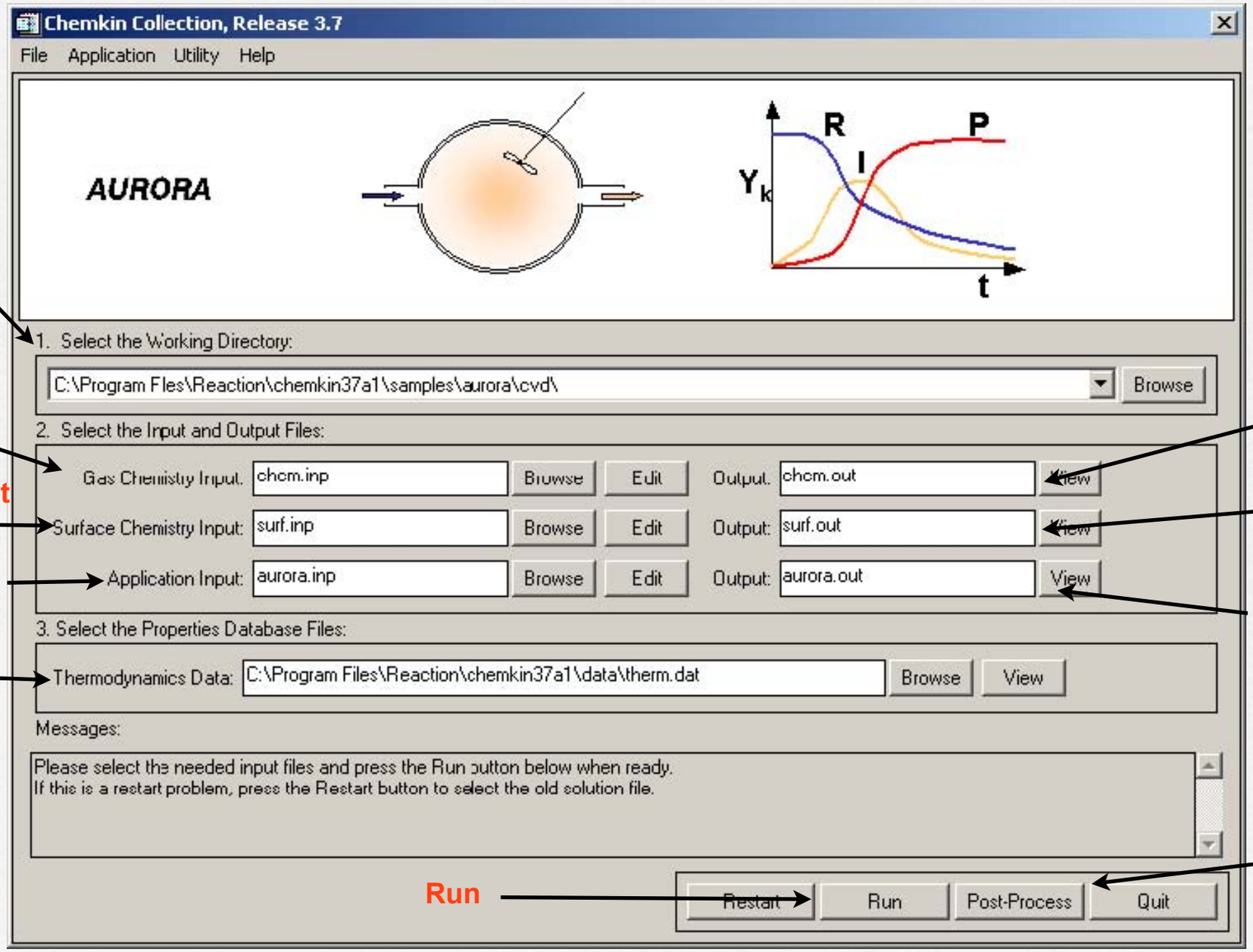
Example: NPSR 5

File di input Aurora: Keywords



```
! This is a steady-state combustion problem
! The conditions are for an adiabatic PSR with H2/O2/N2|
! steady-state
!
STST
!           solve the energy equation
ENRG
!           fix the equivalence ratio of the fuel/oxidizer
!           for the inlet
REAC  H2    0.2
REAC  N2    0.7
REAC  O2    0.1
!           pressure in atmospheres
PRES  1.0
!           volume in cm3
VOL   70
!           residence time in seconds
TAU   3.0E-05
!           temperature of the inlet gases
TINL  600
!           rate of heat loss to the environment in cal/mole
QLOS  0.0
!           printing level (higher is more printing)
PRNT  0
!           initial estimate of the gas temperature in the reactor
TEMP  1700
!           lower bounds for the species fractions during iterations
SFLR  -1.E-10
END
```

Interface Aurora Application



Working Directory

Gas Chemistry input

Surface Chemistry input

File input application

Thermodynamic data

Run

Diagnostic file Gas chemistry

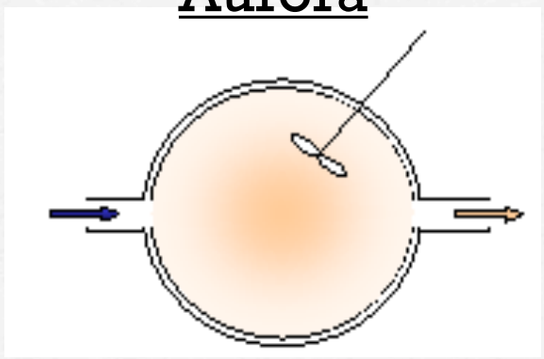
Diagnostic file Surface Chemistry

Diagnostic File Application

Graphical Post-Precessor

Example

Aurora



Conditions

1. Adiabatic PSR
2. Volume = 2000 cm3
3. Temperature 1000 K
4. C/O feed ratio = 0,25
5. Pressure = 1 atm
6. Integration time = 10 sec
7. Criterion adopted = 10 K

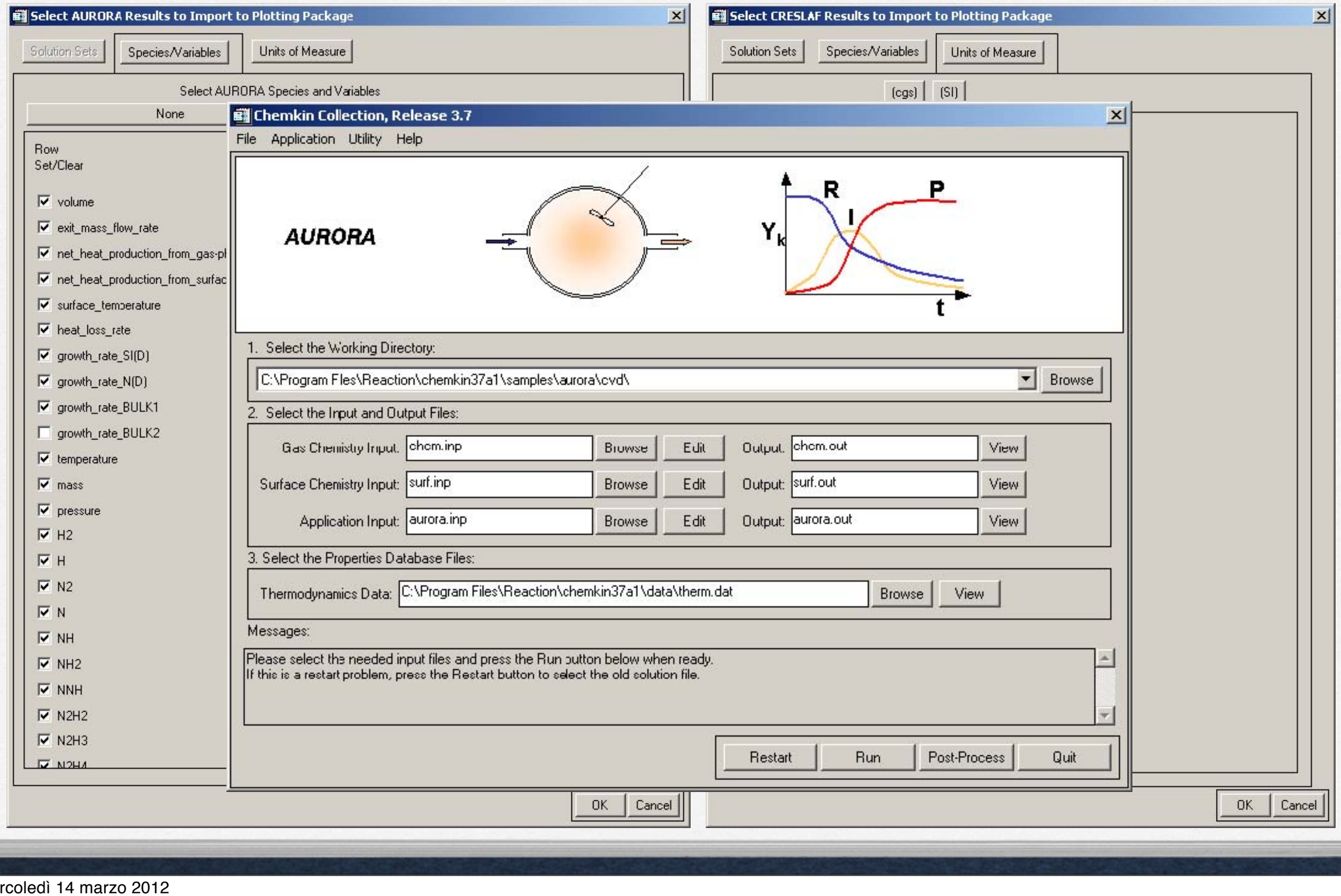
File di input

```
TRAN
TIME 10
QLOS 0.0
!SENT
!
CONP
PRES 1
!ATOL 1.E-1
!
VOL 2000
!
TEMP 1000
TINL 1000
TLIM 1010
!
REAC CH4 0.05
REAC O2 0.1
REAC N2 0.85
!
END
```

Results

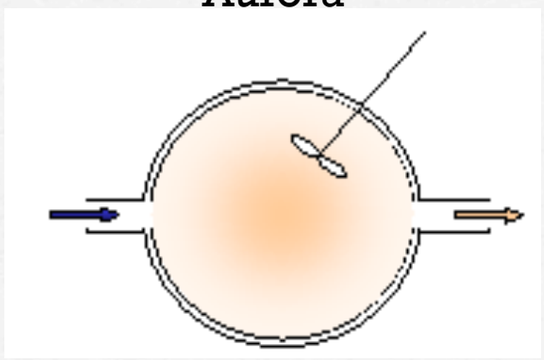
1. Temperature profile by changing initial temperature
2. Temperature profile by changing C/O feed ratio
3. Species Profile

Graphical Post-process



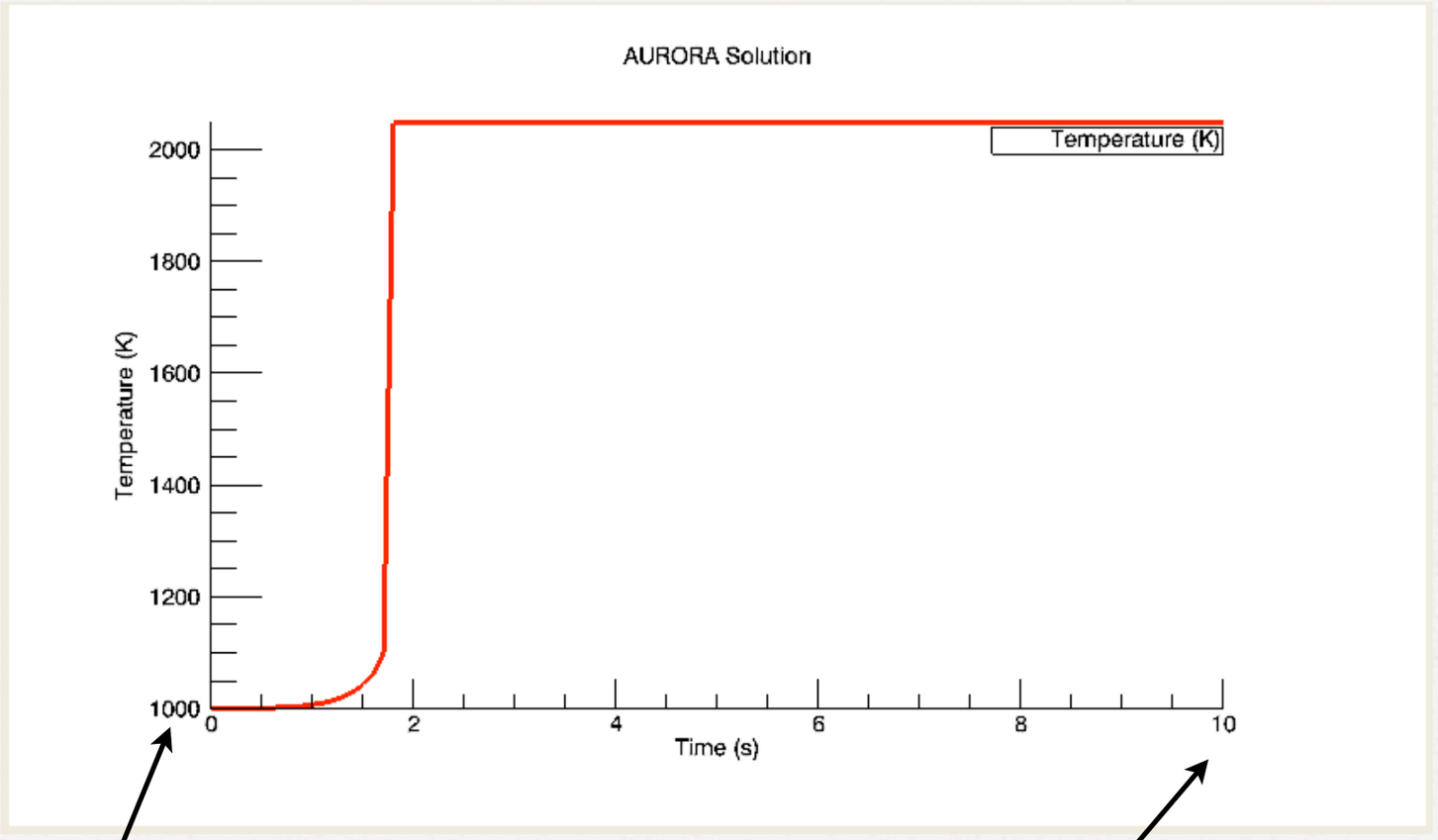
Results....

Aurora



Temperature profile by changing initial temperature

1000 K C/O 0.25

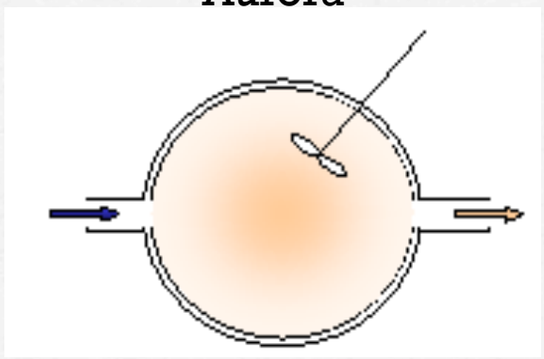


Initial Temperature

Integration time

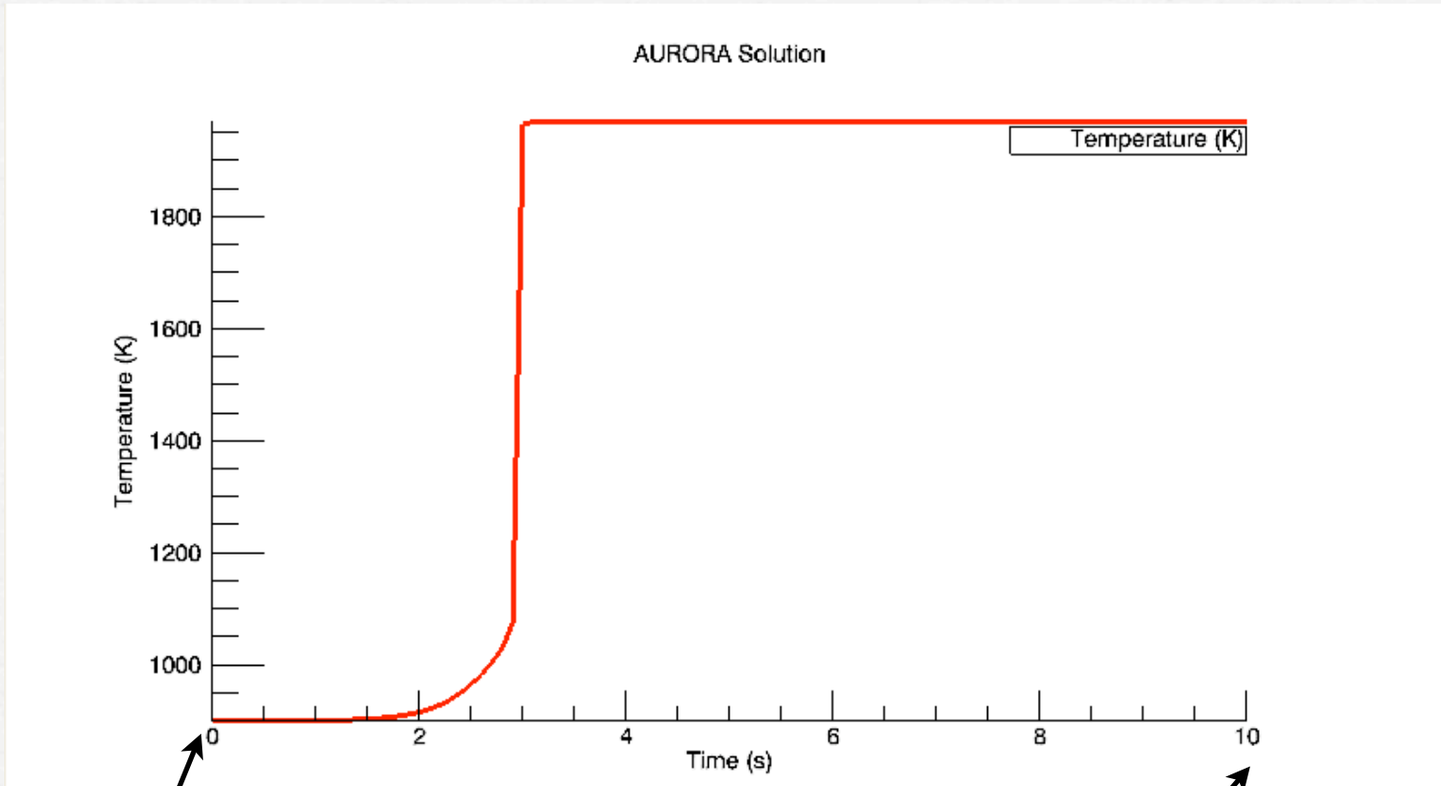
Results....

Aurora



Temperature profile by changing initial temperature

900 K C/O 0.25

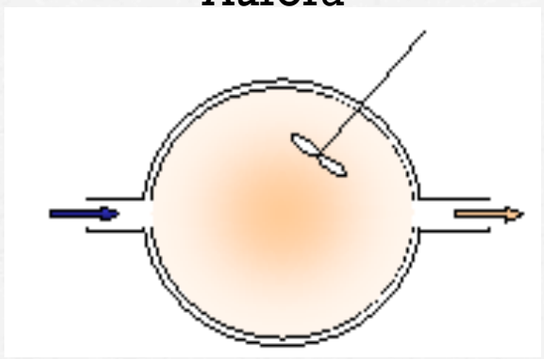


Initial Temperature

Integration time

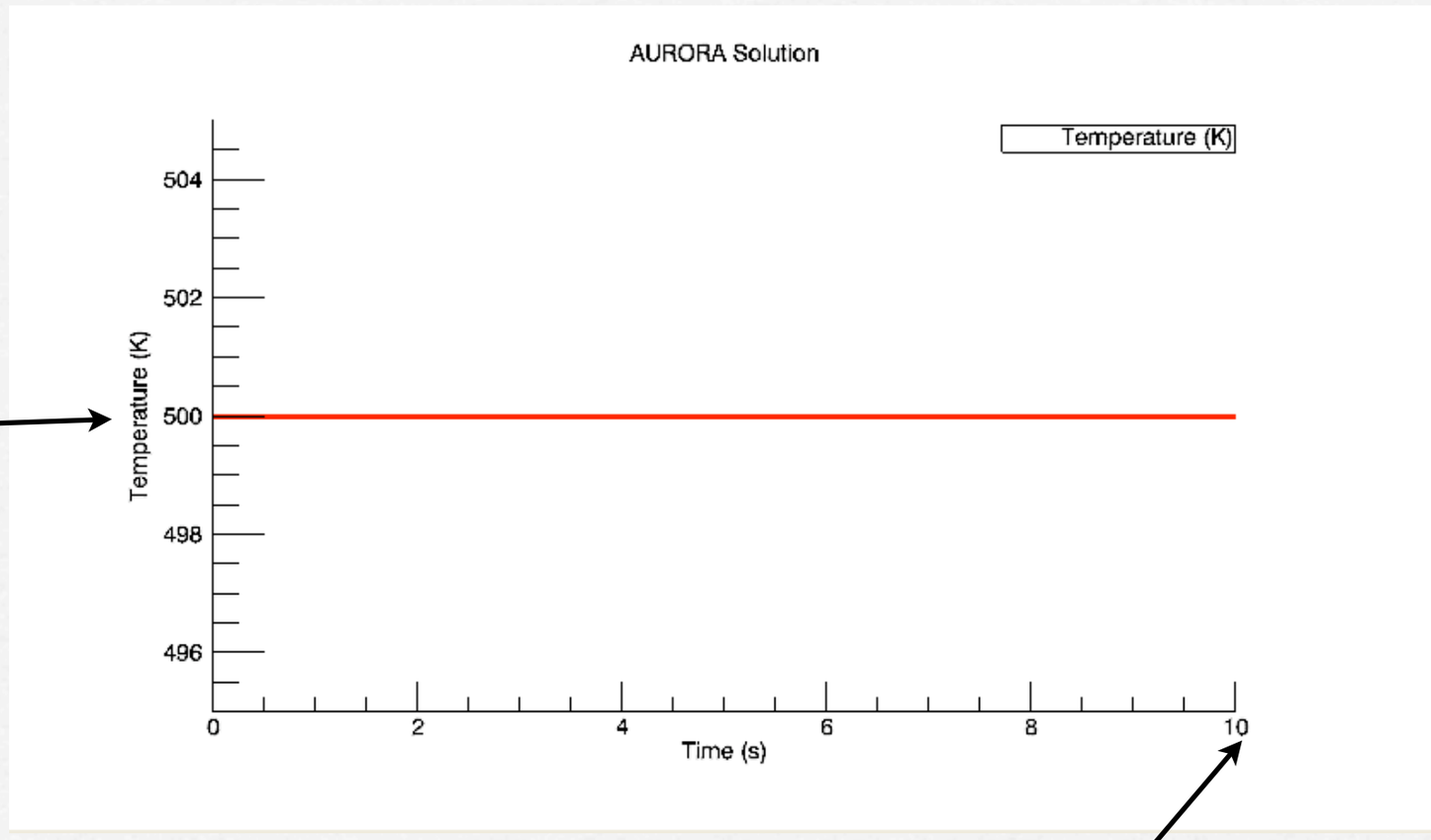
Results....

Aurora



Temperature profile by changing initial temperature

500 K C/O 0.25

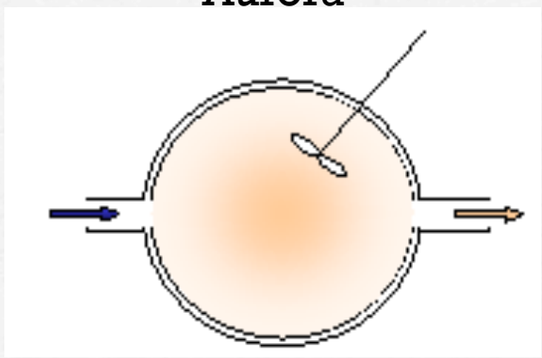


Initial Temperature

Integration time

Results....

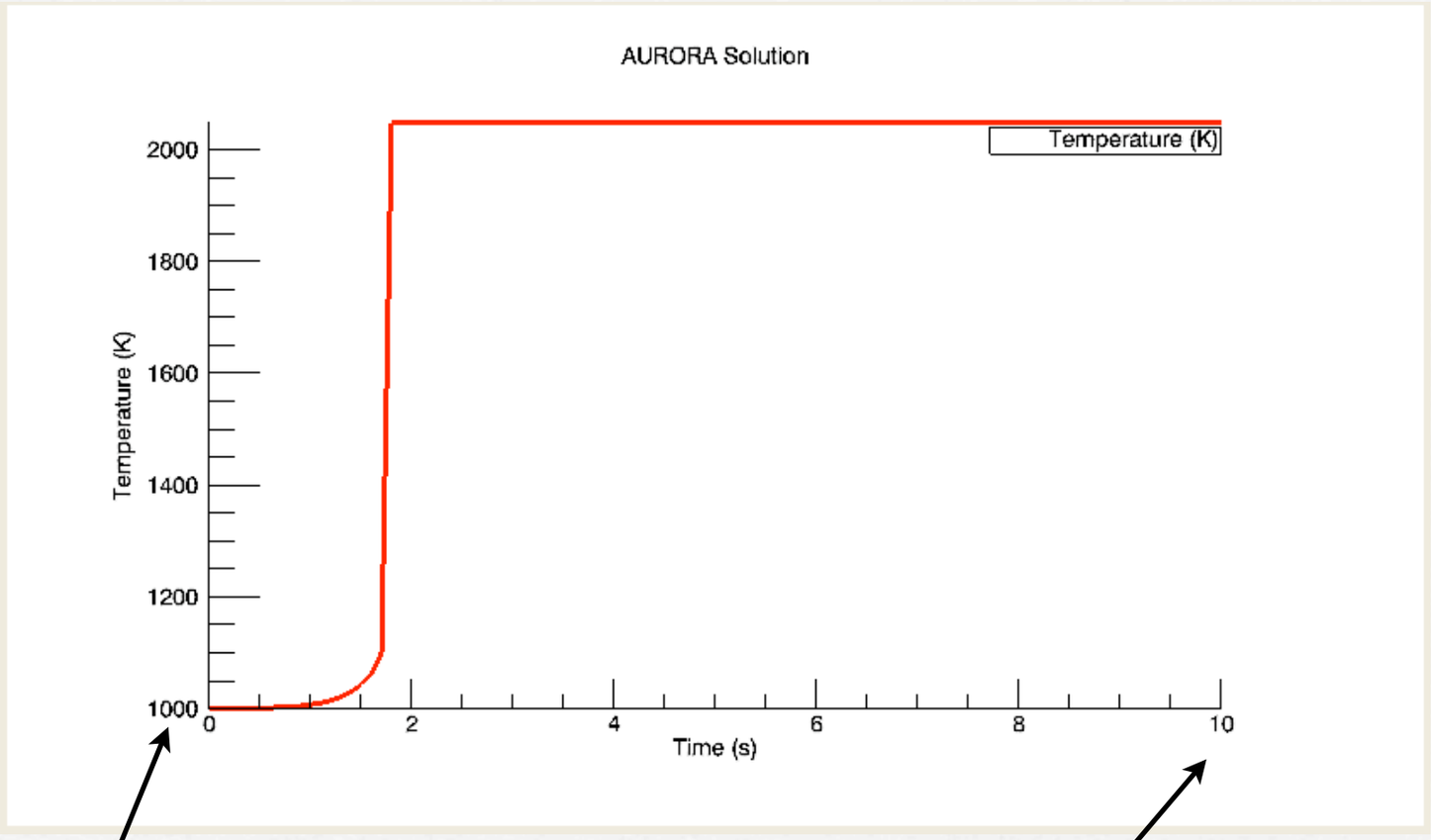
Aurora



Temperature profile by changing C/O feed ratio

1000 K

C/O 0.25

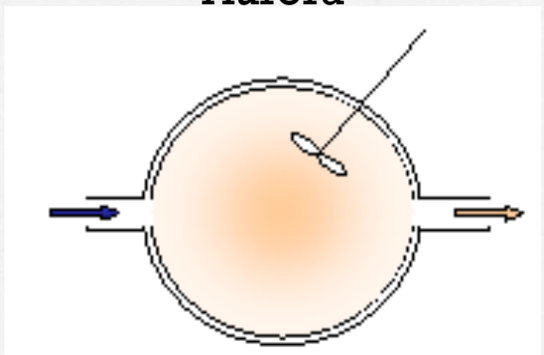


Initial Temperature

Integration time

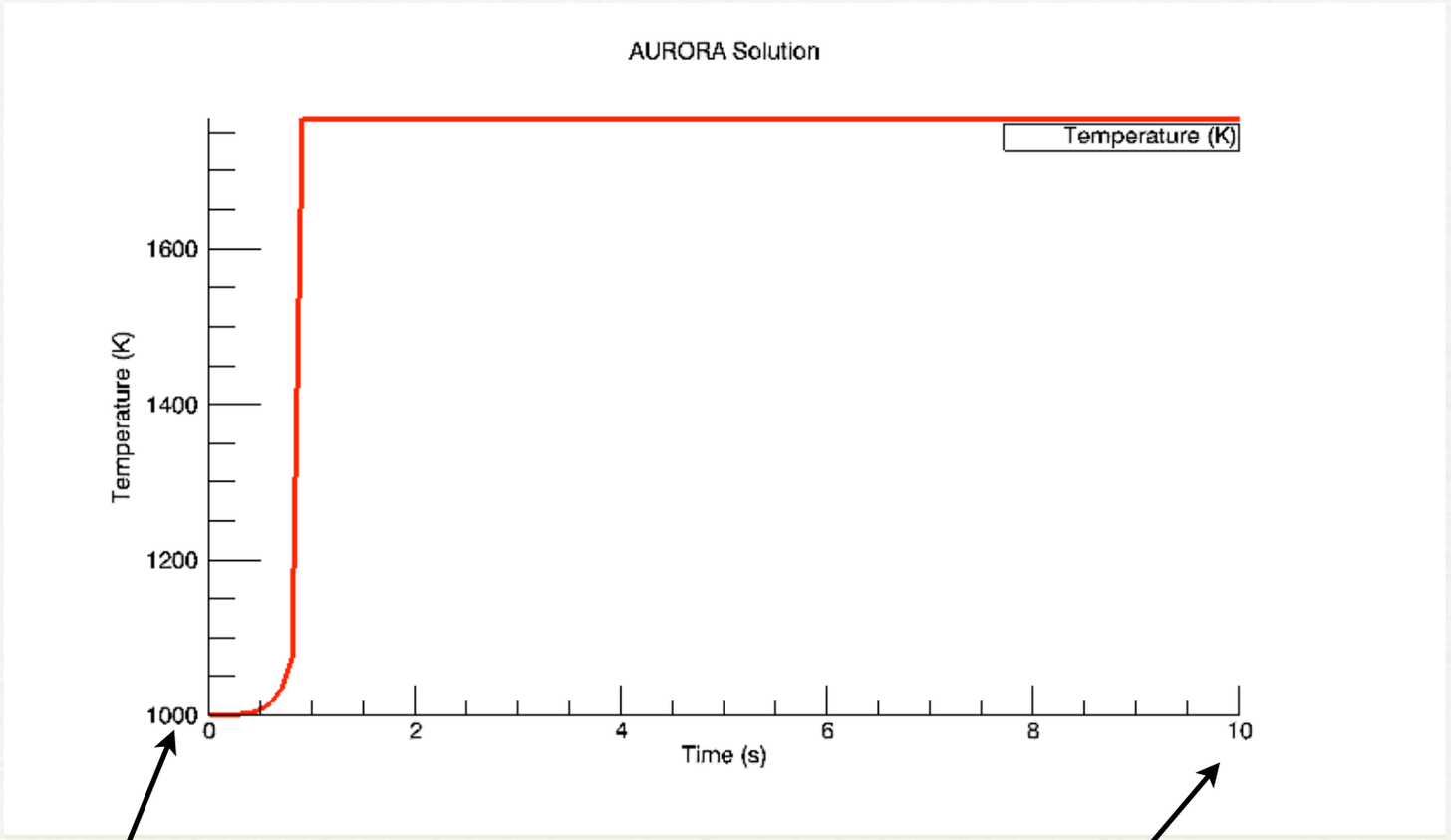
Results....

Aurora



Temperature profile by changing C/O feed ratio

1000 K C/O 0.15

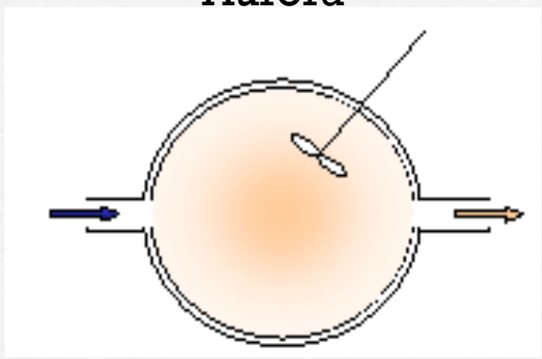


Initial Temperature

Integration time

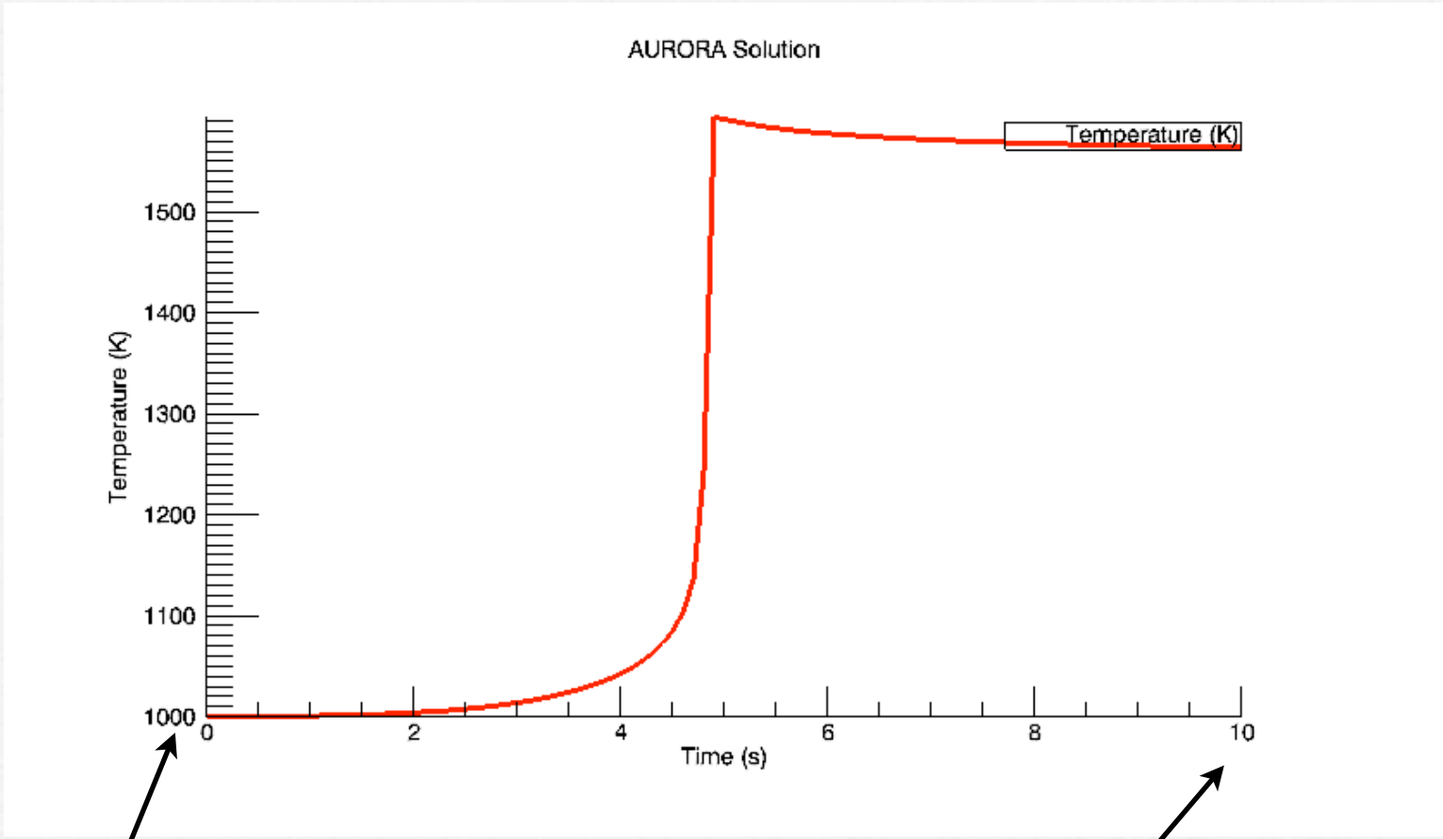
Results....

Aurora



Temperature profile by changing C/O feed ratio

1000 K C/O 0.5

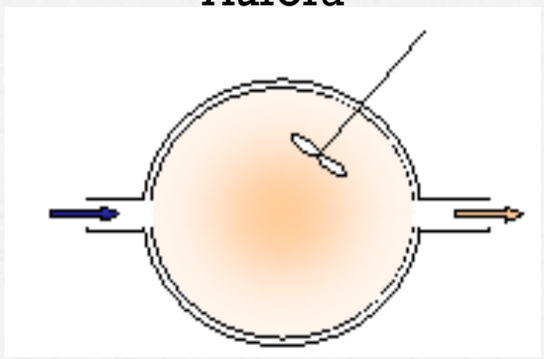


Initial Temperature

Integration time

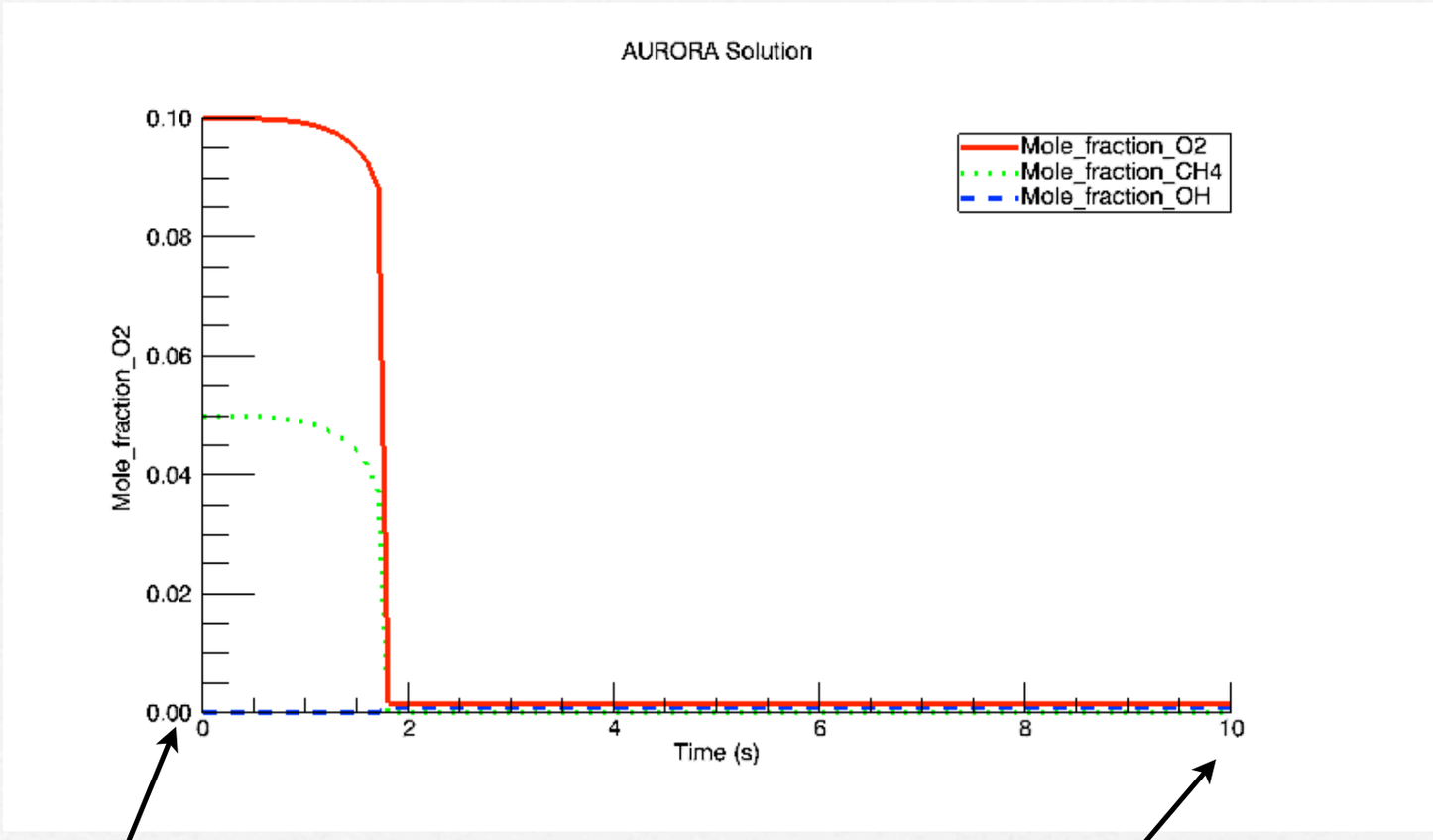
Results....

Aurora



Species Profile

1000 K C/O 0.25



Molar fraction

Integration time

References

1. http://www.reactiondesign.com/lobby/open/index.html (sito di riferimento CHEMKIN)
2. http://maeweb.ucsd.edu/~combustion/cermech/ (SANDIEGO mechanism)
3. http://www.me.berkeley.edu/gri-mech/ (GRI mechanism)
4. http://creckmodeling.chem.polimi.it/kinetic.html (Ranzi mechanism)