KINTECUS

"From thence all things flow; and there is besides necessity, and that which is for the advantage of the whole universe, of which thou art a part. But that is good for every part of nature which the nature of the whole brings, and what serves to maintain this nature. Now the universe is preserved, as by the changes of the elements so by the changes of things compounded of the elements." - Marcus Aurelius / "The Meditations"

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1. Introduction

Kintecus is a compiler to model the reactions of chemical, biological, nuclear and atmospheric processes using three input spreadsheet files: a reaction spreadsheet, a species description spreadsheet and a parameter description spreadsheet. For thermodynamics, an optional thermodynamics description spreadsheet can be supplied. In addition, one can fit/optimize almost any numerical value (rate constants, initial concentrations, Troe factors, third body enhancements, energy of activation, starting temperature, etc.) against an experimental or "fabricated" dataset. Kintecus has been designed with ease of use in mind. Absolutely no programming, compiling or linking required.

A quick overview of the main features:

- The ability to convert Chemkin-II/Chemkin-III/Senkin models to Kintecus format. Kintecus can run almost any converted Chemkin model. Once converted, you may apply **any Kintecus feature** to the system. Do not be surprised to see the converted system run much faster! In addition, Kintecus can use multiple Chemkin thermodynamic databases at the same time and provides a way to use "reserve" species to a respective thermodynamic database. One can also convert the databases to a "freeform" format, which can be loaded into Excel or Lotus 1-2-3. The "freeform" database is much easier to maintain and update. In addition, the converted model is not limited to several elements, in fact, your model can contain the entire Periodic Table.

- The ability to model thousands and thousands of reactions in a relatively short time. Kintecus has been used with models as large as **120,000+ chemical reactions**. You will not find anything faster than Kintecus.

- Fit/Optimize rate constants, initial concentrations, Lindemann/Troe/SRI/LT parameters, enhanced third body factors, initial temperature, residence time, energy of activation and many other parameters against your dataset(s). Note that Kintecus will actually fit the parameters at EXACTLY the time your data was measured. Unlike other programs, Kintecus DOES NOT interpolate a function against your data and then fit the values against this interpolation. There is absolutely no need to "clean" your data, suggest interpolation methods nor specify timing meshes against your experimental data since Kintecus calculates values at exactly the times you specify in your experimental datafile.

- Full output of normalized sensitivity coefficients selectable at any specified time or times. Normalized sensitivity coefficients are used in accurate mechanism reduction, determining which reactions are the main sources and sinks (network analysis) and which also shows which reactions require accurate rate constants and which ones can have essentially guessed rate constants.

- The ability to use **profiles or perturbations** of any wave pattern for any species, temperature, volume or hv. Using profiles/perturbations can also be used for studying very realistic systems, such as quenching affects, dissolution of various gases into a system over time, induction of current into a system, heat flow into a system, a piston compressing the reaction chamber and so on.

- A powerful parser with mass & charge balance checker for those reactions that the graduate student "supposedly" entered in correctly but the model is yielding incorrect results or is divergent. Do you know a kinetics program that can completely parse and check for mass/charge balance on a reaction like this:

  Rate Constants , (m and Ea), REACTIONS:
  1.234e-20, 1.2, 3000,$CH_3(((NO_2)_3(CO)_{93})_3\ (CH_2)_9)$+23.30$H_2O^+ + Co_2 = A^{---} + B^{++++}$
  +C+C+C+C+C

  Or how about this:

  Rate Constants , REACTIONS:
  5.043e+20 , 3.43234 $(CH_4(N(PO_{342})_{43}(CH_3)_3)_{34})(Os(S_7)_8)_{34}{}^{++++}$ + 199.432
  X++++ $5CH_5^+ ==>$5.434 Some_Really_Funky_Long_Enzyme_Name+ 8 HCl + HCO_3^-

  Kintecus is able to accurately check the above reaction for mass and charge balance because you can create an optional name file containing common names for species and then their mass representation. This smart mass balance can be used for biological and nuclear reactions! Kintecus also provides duplicate reaction and species checking.

- As you can see in the above reaction, fractional coefficients for species! Now you can finally model that last step in the Oregonator or crunch 100 elementary reaction steps in one reaction step!

- Quickly and easily, hold one or more concentrations of any species at a constant level just by typing the value in the field of the species.

- Built in support for special reactions such as: reactions involving third-bodies (M), fall-off reactions (Troe, Lindemann, SRI, etc.) , enhanced third bodies, exclusive **multiple** enhanced third bodies, vibrational transfer reactions (Landau-Teller) and many others.

- **Heterogeneous chemistry** can be modeled. For example, a species in the aqueous phase will not contribute to the overall pressure in the system or be involved in third-body reactions or fall-off reactions. Gaseous species can “enter” other phases through out a simulation and vice-versa.

- Model reactions from femtoseconds to years! A special switch in Kintecus allows it to output the concentration of the species that are displayed only if its concentration has changed significantly from its past values. This may seem like no big deal, but if you model reactions that last from days to years, you can easily generate files that are dozens of megabytes in size or more. Such a file is nearly impossible or extremely time consuming to plot or print, but in Kintecus a special option turns a 100-multimeg file into a 100 kilobyte file without almost any loss in data!

- Automatic generation of the species spreadsheet file using the reaction spreadsheet file. Why waste time finding, entering and initializing all the different species in your kinetic scheme?

- The ability to do reactions in a continuous stirred tank reactor (CSTR) with multiple inlets and outlets.

- The ability to compute all internal Jacobians analytically. This is very useful for simulating very large kinetic mechanisms (more than 50,000). Finite difference methods can cause underflow or overflow errors in approximately such large Jacobians during the simulation.

- Support for Excel and Lotus spreadsheet programs.

2. The Program

Running Kintecus for Windows-95 or Higher

On the Windows Start button select RUN, type “command” and press the <ENTER> key. You will be in a command prompt. Change to the directory where you uncompressed the Kintecus files (ie. cd c:\kintecus). You can see what is in the directory by typing, “dir /p”. You can run Kintecus as:
“**Kintecus (any switches you may want to use)**”, or if you wish to capture the on-screen information type:
“**Kintecus (any switches you may want to use) > view.txt**”.
This will output any errors, warnings and information to the file view.txt, which can be viewed with any text editor or word processor. The output file, CONC.TXT, will contain the species’ concentrations and temperature (if the model is in thermodynamics mode). If you are fitting data to your model, the final optimized parameters are stored in OPTOUT.TXT.

If you have Microsoft's Excel or SUN Microsystems's **free** Star-Office you can load and edit one of the following xls worksheets that contain **Visual Basic code for easy running, editing and plotting** of Kintecus runs: Kintecus_workbook.xls, Enzyme_Regression_Fitting.xls, Ethanol_Combustion.xls, GRI_MECH_30.xls, Oregonator_in_CSTR.xls, Combustion_Workbook_OH.xls and Wolfrum_with_Temp_Program.xls. Please note if **you do not** have a **Kintecus key**, after clicking the RUN button, you will have **to press the <ENTER> key three times** to continue the run.

Entering Simple Models

For your reactions, you must first create a model spreadsheet file. If you have Microsoft's Excel or SUN Microsystems's **free** Star-Office you can open the Kintecus_workbook.xls or any one of the sample xls workbooks and edit the model, species or parm data worksheets. Afterwards, you can run/plot your model by clicking on one of the buttons located on the CONTROL worksheet. If you are not going to use a spreadsheet, it's recommended to use a text editor (such as MS-DOS's "EDIT" or OS/2's "qbasic /EDITOR" or UNIX's vi or emacs) and use a comma to separate the fields. In the first column enter the reaction constants, and in the second column enter the reaction. If you start a line with, "#', or double quotes, ' " ', the line will be taken as a comment. End the reaction sheet with END + RETURN on one line. Use "==>' to represent

yields and "=" to represent a reaction that can go forward and backward (with the backward step having a reverse rate constant, k_b , of one (1.0) if thermodynamic mode is NOT specified). An example :

#		
# My first reaction		
#		
1.75E-05	CH3C00H + H2O = H3O+ + CH3COO-	Optional comments
END		

Figure 1

When entering reactions do not use the following characters: | , the comma, TAB in the spreadsheet cell unless you are using a text editor in which case you can use the comma or colon to separate the various fields. Just be sure to pick one separator, do not randomly switch from the comma to the colon on the same line. You can name the reaction file anything you want and Kintecus will read it, but for now save the spreadsheet file as a Text (or plain text) file. If you are using Excel select, under the File menu select “Save As”, enter model.dat as the filename, and select the type as “Text (Tab delimited)”. Kintecus looks for this model.dat as the default reaction filename (you can override this option). As a side note, anything after the END is ignored, so you can have equations entered below the "END" as you modify your model or place a # to comment one whole reaction line out of the model.

Make sure the reaction text file (MODEL.DAT) and a parameter description file (PARM.DAT) are now in the same directory as Kintecus and run it with the following line: KINTECUS -c . This will automatically create the species spreadsheet file, ADDSPEC.TXT with all values and switches set to 0.0 and "No" respectively.

Go back in your favorite spreadsheet program and load this file. In Excel, under the File menu select “Open” and in the file request prompt, select “All files” for “Files of type”. You should see the ADDSPEC.TXT file. If not, make sure you are in the correct directory. Now, double click on the ADDSPEC.TXT file. The Text Import Wizard will automatically open, just click the Finish button. If you originally created the model.dat file with Excel, then the ADDSPEC.TXT file should load easily into Excel. If it does not load easily, make sure Excel’s Text Import Wizard is installed and Delimited is selected under “Original data type”. Under Step 2 for the Text Import Wizard, make sure that “Tab” is selected under “Delimiters”. Click Finish. As a note, whatever character was used to separate the fields in the model.dat file, Kintecus will used that same character for all its output files. This means that if you are using another spreadsheet program (like Lotus) and you save the model.dat spreadsheet as a text file for Kintecus to load, the ADDSPEC.TXT file will have commas in it too. For Excel, you should see something like this:

# Species	Residence	Initial	Display Outpu	External	SSA ?	Constant File?	
#	Time in CSTR(s)	Conc.	(Y/N) ?	Conc.	(Y/N)	(Filename/#/No)	
CH3COOH	0	0	No	0	No	No	Optional comment
H2O	0	0	No	0	No	No	water
H3O+	0	0	No	0	No	No	hydronium
CH3COO-	0	0	No	0	No	No	Acetate
END							

Figure 2

Enter 1.0 and 55.56 in the initial concentration fields (Initial Conc.) for CH3COOH and H2O respectively. Also, enter "Y" in all the display output fields. This allows you to view the concentration of the species at selected time intervals as the simulation runs. You can name the species description file anything you want and Kintecus will read it, but for now save the spreadsheet file as an ASCII (or plan text) file under the name, "SPECIES.DAT". Also, be sure to save it in the same directory as Kintecus. That's it! Now run Kintecus. An output file containing the concentration profile of all the species that are being displayed are saved in this file. You can now view the concentration profile of all the displayed species by loading this file in your favorite spreadsheet program and plotting it!

If you wish to alter the time of the simulation, you can load in the PARM.DAT file. Once this file is loaded, you can see the line "Simulation Length", there are five fields: DAYS, HOURS, MINUTES, SECONDS, and PICOSECONDS under that.

# Parameter	Description	SpreadSheet		
# See the	documentation file	for an	explanation	of each field
#				
# Minimum	Maximum	Ea Units	Concentration	
# Integration Time(s)	Integration Time(s)		Units	X0
1.00E-06	1.00E-01	CAL	MOLES/L	0
# Temperature	Pressure-Constant ?	Volume Profile ?		
# (K)	(Yes/No)	(Filename/"NO")	X0	X0
1000	No	No	0	0
# Simulation	Length:			
# DAYS	Hours	Minutes	Seconds	PicoSeconds
0	0	0	1.00E+00	0
#				
#hv(filename)	Sampling Interval	Percent(%)	Accuracy	X9
None1	1	0	1.00E-08	0
#				
# X10	X0	X0	X0	X0
0	0	0	0	0
#				
END				

Figure 3

If you want the simulation to run for one hour, just enter "1" below the Hours field and make sure there are zeroes in the other fields. For now, do not worry about the other fields.

Intermediate Models

The Parameter Spreadsheet File

This section will describe some intermediate modeling techniques Kintecus can do, but first a more detail explanation of the parameter file (PARM.DAT) will be needed. The parameter file is shown below:

# Parameter	Description	SpreadSheet		
# See the	documentation file	for an	explanation	of each field
#				
# Minimum	Maximum	Ea Units	Concentration	
# Integration Time(s)	Integration Time(s)		Units	X0
1.00E-06	1.00E-01	CAL	MOLES/L	0
# Temperature (K)	Pressure-Constant ?	Volume Profile ?		
# or Filename	(Yes/No)	(Filename/"NO")	X0	X0
1000	No	No	0	0
# Simulation	Length:			
# DAYS	Hours	Minutes	Seconds	PicoSeconds
0	0	0	1.00E+00	0
#				
#hv(filename)	Sampling Interval	Percent(%)	Accuracy	X9
None1	1	0	1.00E-08	0
#				
# X10	X0	X0	X0	X0
0	0	0	0	0
#				
END				

Figure 4

As one can see, there are a number of fields. The field name is located directly above the spreadsheet cell. The 'X0' field names are for future use. For example, the Temperature field has 1000 degrees set in it. Most of the settings in the parameter description spreadsheet usually do not have to be changed, but it is a good idea to know what exactly each field is.

It is obvious what should be entered in the Temperature field, just be sure the units for that field is in Kelvins. If your model is not using the Arrhenius expression, special reactions or thermodynamics then this field is not used. You can also enter a filename here containing a temperature program. If you do wish to use a program temperature then please skip to applying perturbations under the Constant File Field in the Species Description Spreadsheet. Kintecus treats temperature programs exactly like perturbations to species concentrations.

The "Pressure Constant ?" field excepts two values: "Yes" or any entry other than "Yes" (which translates to Kintecus, ignore this field). If you specify "Yes", then the volume of the system will change to keep all gaseous products at the same exact pressure the simulation started. Kintecus calculates the starting pressure from summing all gaseous species' concentrations, and then multiplying that by the gas constant, R, and temperature.

The volume profile fields allows one to enter a perturbation file (see the species spreadsheet file section for a full explanation on the types of perturbations allowed) containing the volume profile of the system through a simulation run. This allows one to model piston compressions. Kintecus treats the numbers in the perturbation file as divisors into the gaseous species concentrations. For example, a value of one does nothing to the system, while a value of 0.5 tells Kintecus to cut the volume in the system by half, so the concentrations of all gaseous species are doubled. A value of two, 2, directs Kintecus to double the volume, so the concentrations of all gaseous species are halved. A gaseous species has no phase information attached to the end of the species name or will have a **{g}** appended to the end of the species name. Look below in the Species Description Spreadsheet for a description of species phase information.

The DAYS, Hours, Minutes, Seconds and PicoSecond fields control the length of the simulation. This easily allows one to set the total time of the simulation during a run from yearly events to femtosecond laser experiments.

The Ea Units field allows you to specify the units associated with the energy of activation used in the exponent of the expanded Arrhenius equation (the $\exp(-E_a/\mathbf{R}T)$). If you are not using the expanded Arrhenius equation then you do not have to worry about this field. Possible values (values are case insensitive) and their respective concentration units in this field are:

Energy Type	Other Synonyms allowed
Joule	J
Calorie	CAL
Kelvin	Kelv
KiloCalorie	KCAL
KiloJoule	KJ
KiloKelvin	KKelv

Table 1

The Units field allows you to use different concentration units during a run. Possible values (values are case insensitive) and their respective concentration units in this field are:

Concentration Type	Other Synonyms allowed	Other Synonyms allowed	Other Synonyms allowed	Other Synonyms allowed
Moles/Liter	Moles/L	Mol/L	Mol/liter	
Molecules/cm^3	Molecules/cc	Molec/cc	Molec/cm^3	1/cc or 1/cm^3
ppm	Parts per million			
Moles/cm^3	Moles/cc			

Table 2

It is recommended to use moles/cm^3 if you wish to use the thermodynamic databases associated with Chemkin models.

The hv(filename) and Sampling Interval(s) are used together and are mainly for the simple use of hv in your equations (i.e. M + hv ==> M+ + e-). The hv(filename) can be one of three things: if None1 is entered then hv=0 always, if None2 then hv=1 always, if anything else then the field will hold the name of a file containing data that represents a profile for hv. The Sampling Interval holds the spacing in time (in seconds) between each data point. The number of data points in the filename and the sampling interval determine the total length of the hv profile. If the time of your run goes beyond the total computed time of the hv profile, then the data will repeat itself from the beginning of the profile (time 0). See the example profiles given under the "Constant File Field" below.

The Percent (%) field is used to limit the size of the output concentration file (whose default name is CONC.TXT) without causing distortion. Kintecus will only output the concentration of all the species only when one or more Displayed species (see below in the Species Description Sheet) has changed more than Percent*Previously_Outputted_Value. Through the author's personal experience, using 1% as default does not distort the outputted concentration profile too much and keeps an okay file size. There is slight distortion at 20% but can drastically reduced the size of the concentration file. This field is extremely useful for cutting the size of models that run for simulated years. A value of 7% is good for knowing how high certain peaks in concentrations you might be interested in. A value of 0% will output all values. Since most computers are now quite fast in plotting abilities, **it is recommended to use 0%.**

The Minimum Integration Time, Maximum Integration Time and Accuracy fields determine how fast Kintecus can integrate your model and the error in the final concentrations. These fields are very important.

Accuracy determines how far out in the decimal place to keep the concentration accurately computed. Therefore, a value of 1.0E-9 will keep the first nine digits of the integrated concentration accurately computed. The smaller you make the accuracy field the slower Kintecus runs your model. If you have a huge model, you may want to increase this to 1.0E-5 or larger. Of course, if you have stiff reactions and Kintecus can't seem to integrate your model, you should decrease this field to 1.0e-10 or so. See the Overflows, Underflows, Division by Zero, Singularities, Domain Errors section for a further description.

The Minimum Integration Time (in seconds) determines the starting time step to integrate your model. After the first integration, this will change and grow larger if your accuracy is large and/or the stiffness of your model is low (meaning a decrease in execution -time of the program) , or grow smaller if your accuracy is very small and/or the stiffness of your model is high (meaning an increase in execution time of the program). You should not have to change this in most cases. A special note for combustion modelers: since most combustion reactions happen in the first few tenths of a microsecond, you might wish to decrease this to 1.0e-7 or 1.0e-8 if you are having troubling near the very beginning of the simulation run.

The Maximum Integration Time has a few uses in Kintecus. If you are not using a concentration profile on any species (see below in the Species Description Sheet), then this field is only used to determine the minimum timing threshold which has to be exceeded before outputting the concentration of displayed species. In this case a value of 1 to 10 seconds is fine for simulations lasting from 10 minutes to a few days respectively, but if you are doing simulation which only last a few nanoseconds, then a value of a few femtoseconds (1 x 10(-15)) should suffice. If you only have, some species loaded as a concentration profile (see below in the Species Description Sheet) then this will determine how often the data is retrieved from the concentration profile files. Reducing the maximum integration time will output more

concentration values. If you have a final model and you wish to have a nice plot full of points that looks good for publication, you can trying reducing this field by 10/100/1000 and so on. Although, be warned, the simulation time will increase.

Kintecus will look for the Parameter Description SpreadSheet under PARM.DAT as the default filename. This can be overridden see KINTECUS Switches Section setting below.

The Species Description Spreadsheet

Here is a detailed description of how exactly each field in the species description spreadsheet is used by Kintecus.

The fields in the Species Description Spreadsheet are:

# Species	Residence	Initial	Display Output	External	SSA ?	Constant File?	
#	Time in CSTR(s)	Conc.	(Y/N) ?	Conc.	(Y/N)	(Filename/#/No)	
CH3COOH	0	1	YES	0	No	No	Optional comment
H2O	0	55	No	0	No	No	water
H3O+	0	0	Yes	0	No	No	hydronium
CH3COO-	0	0	No	0	No	No	Acetate
END							

Figure 5

The Species, Initial Concentration and Display Output fields are obvious in what they represent. The Species field holds the name of a species that will show up in a chemical reaction and can be up to 240 characters long. An important note is that the charge of the species is only computed for species name if a "+" or "-" is appended at the end of the name, but before the phase descriptor, {}.

By default, the phase of any species is in the gas phase if the species name has no phase information at the end. Overriding the default gas phase can be accomplished by appending the species name with the phase name surrounded by braces, for example, {aq} to represent aqueous phase (i.e. CH_3COO^-{aq}), or {l} (i.e. Br_2{l}), to represent the liquid phase. Again, no phase information present at the end of a species name can also represent a species in the gas phase, such as Ar or N_2. It should be **very important** to note that if all your species are in one phase (such as gas or aqueous) then **you do not have to append each species name with a phase descriptor**. It is just a waste of time to append every species name with {g} or {aq} if they are all in the same phase. Kintecus V2.0 only really "understands" gas phase, {g}, and any other phase that is not in the gas phase. Kintecus uses the gas phase information mainly for third-body reactions involving [M], pressure fall-off reactions and enhanced third body reactions used in [M]. Future versions will incorporate other phases. The phase descriptor must **always** appear at the **end** of the species name. The species Cl^{++}{g} is the chlorine molecule with a +2 charge in the gas phase, **but** Cl{g}++ is some species name of Cl{g} with a +2 charge.

The Initial Concentration field holds the starting concentration of each species in the reaction.

The Display Output field can hold either a Yes or No ("Y" and "N" also work). If yes the respective species' concentration will be stored in the default output file, "CONC.TXT", if no then the species' concentration will not be stored.

The Constant File Field can hold one of three things: “No” (“N” works too), a number such as 4.234E-4 (in which case that species will always have that concentration of 4.23E-4) or the name of a file that contains values in a special format. The format is that the very first line that contains the time spacing (in seconds) between each data point. The lines that follow contain the data. Please make sure the very last data point has a carriage return or enter! Kintecus will place the respective data point at the respective time of the simulation from the constant file into the species’ concentration. If the time in the simulation goes beyond the time of the very last data point in the constant file, Kintecus will start over in the constant file using the very first data point and continue onward. If the very first line (the time spacing) has a minus sign in front of it, Kintecus will go through the entire data series once then automatically place the very last value in the datafile for the rest of the simulation time. Confused? Okay, here’s some examples:

Examples:

In the Profile_A.TXT file contains these values:
43200
2
1

For a species that has the filename Profile_A.TXT in it’s “CONSTANT FILE ?” field, Kintecus will load this concentration pulse step profile. Assuming Molar units, Kintecus will force the species to have a concentration of 2 Molar until at 43201 seconds where then the species concentration will drop to 1 Molar, at 86401 seconds the species will go back up to 2 Molar and this will repeat. Now, if the 43200 were -43200, then at time 86401 the concentration of the species will goto 1 and stay there for the entire simulation. If “-ADD” was appended to the file name (in this example “Profile_A.TXT-ADD”), the species will **NOT be a constant**, but a variable with perturbations added to it during the simulation:

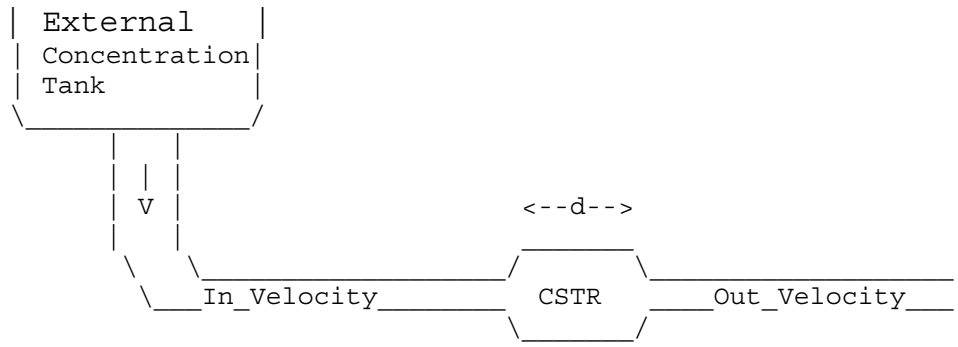
In the Profile_A.TXT file contains these values:
-500
0
0
1

When the simulation is running, the instant the time goes over 1000 seconds, 1 Molar will be added to the species containing the “Profile_A.TXT-ADD” in the “Constant File ?” field, Kintecus will not perform any more perturbations to the respective species. Another example: Suppose one wished to add 2 Molar after 1000 seconds, then add 4 Molar after 1030 seconds, then **REMOVE** -3 Molar after 1034 seconds the Profile_A.txt file would look like this:

-1
(999 zeroes)
2
(29 zeroes)
4
0
0
0
-3

As one can see, this is indeed a **very powerful technique** to study various perturbation methods to kinetic systems with the slightest of ease! Of course, you can have very long perturbation files (upto 25,000 points for any species and 32,000 points for the hv file)!
The above description on using perturbation files can also be used the same exact way for programmed temperature and volume runs.

The Residence Time in CSTR and the External Concentration fields are used together for the modeling of Continuous Stirred Tank Reactors (CSTR) or any other process that contains well mixed, isothermal reactions with external flux in and flux out:



Naturally the External Concentration field does not contain the actual concentration of the external tank but the concentration that it will become once it is diluted in the CSTR before any reactions take place. A rough approximation of the residence time in a CSTR can be calculated as follows:2 x d (the distance across the CSTR parallel to the in/out flow) / (In_Velocity+Out_Velocity). You can have different residence times for different species.

The SSA field stands for Steady-State Approximation and it is not used in this version. You should never use SSA's. It has been shown repeatedly [2,3] that doing SSA's without knowing the actual output can result in disastrous results.

At the end of the species description spreadsheet make sure there is an END + carriage return.

Kintecus will look for SPECIES.DAT at the default filename. This can be overridden see KINTECUS Switches Section setting below.

The Species Name Spreadsheet

This spreadsheet is optional. The main reason for this spreadsheet is to keep Kintecus checking for mass balance without typing long molecular, empirical or mass formulae in the reaction spreadsheet. The fields in this spreadsheet are:

#"Nickname"	Molecular/Empirical/Mass formula
# or Common Name	
#	
E-	C0-
Decane	CH3(CH2)8CH3
END	

Figure 6

Common Name can contain any name up to 240 characters long. The Molecular/Empirical/Mass formula field must contain any valid molecular, empirical or mass formula such as $CH_3CH_2CH_3$ or $CH_3(CH_2CH_2O_2)_{90000}CH_3$ or $Pu_2U_3Pr_{43}$ or $C_{100000}H_{200002}$. The following characters are ignored if they are contained in the molecular, empirical or mass formula: ".", "=", "_", "*", "^", "&", "/", "\", "-", "+". An important note is that the charge of the species is only computed for the common name if a "+" or "-" is appended at the end. The charges are completely ignored if they appear in the molecular, empirical or mass formula.
An example:

The reaction:
Enzyme_B + $5H_2O$ ==> Enzyme_hydrate.

The SpecName.dat file:

#	
# My nicknames for my own kinetics simulation	
#	
Enzyme_B	C43H70N10S2
Enzyme_hydrate	C43H70N10S2(H2O)5
END	

Figure 7

Kintecus will look for SPECNAME.DAT as the default filename. This can be overridden see KINTECUS Switches Section setting below.

The Model Description Spreadsheet

Here is a detailed description of how exactly each field in the model description spreadsheet is used by Kintecus.

The fields in the Model Description Spreadsheet and some possible reactions listed are:

# Sample				
# Reactions				
#				Optional
# A	T^m	Ea	REACTION	Comments
1.75E-05	0.3	3000	CH3C00H + H2O = H3O+ + CH3COO-	Sample Reaction 1
5.00E+17	-1	0	O+H+M[H2(2);H2O(6);CH4(2);CO(1.5);CO2(2);C2H6(3);AR(.7)]=OH+M	Sample Reaction 2
5.00E+17	-1	0	O+H+M=OH+M	Sample Reaction 3
5.00E+17	-1	0	O+H+M[-H2(2);-H2+(3.5)]=OH+M	Sample Reaction 4
1.00E+17	-1	0	H+C2H+M[TROE;3.750E+33;-4.8;1900;.6464;132;1315;5566]=C2H2	Sample Reaction 5
4.30E+07	1.5	79600	H2+CO+M[TROE;5.07E+27;-3.42;84350;.932;197;1540;10300;CO(1.5);CO2(2);C2H6(3);AR(.7)]=CH2O	Sample Reaction 6
4.30E+07	1.5	79600	H2+CO+M[TROE;5.07E+27;-3.42;84350;.932;197;1540;10300;-N2(1);-N2+(2)]=CH2O	Sample Reaction 7
7.91E+01	0	56020	N2O+M[LIN;6.37E+14;0.3;56640]=N2+O	Sample Reaction 8
1.80E+01	0	2385	O+CO+M[LIN;6.020E+14;0.3;3000;H2(2);O2(6);AR(.5)]=CO2	Sample Reaction 9
5.00E+01	0.3	4433	N2O+M[SRI;6.37E+14;0.3;56640;6.370E+14;0.3;56640]=N2+O	Sample Reaction 10
5.00E+01	0.3	4433	N2O+M[SRI;6.37E+14;0.3;56640;6.370E+14;0.3;56640;H2(2);O2(6);AR(.5)]=N2+O	Sample Reaction 11
2.00E+00	0	6555	O2+O+S[LT;-63;68.8]=O3	Sample Reaction 12
END				

Figure 8. Some sample reaction types Kintecus can read.

Irreversible Reactions

The reaction field holds either a reversible (represented by a single "=") or an irreversible (represented by "==>") reaction, for irreversible reactions:

k_f, A+B+C ==> D+E+F, Optional Comment

OR

A, m, E_a, A+B+C==>D+E+F, Optional Comment

Although it is not recommended, it is possible to mix the above two formats throughout a model. The commas used to delimit the A, m and E_a can also be TABS, colons, "|" or "!". If you are using Excel as a means to enter the reactions, then by default the delimiter will be TABs.

You can have only three unique reactants and three unique products per reaction line. The multiplicity of a species is represented by using numerical coefficients such as 5A to represent A+A+A+A+A or 98H_2O or possibly 4.2343E-23H_2O. Signs can be postfixed to a species such as $Cl^{-------}$ or H_3O^+ and even ylides and zwitterions such as $C_8H_{15}P^{+-}$ (which will have no overall charge.). All reactions are checked for mass and charge balance (which can be turned off). At the end of the model description spreadsheet, make sure there is an END plus a carriage return. It is very important to note that enhanced body, fall-off reactions and special

reactions represented by +M[….] or +S[…] DO NOT COUNT AS REACTANTS! A reaction such as the one shown below is **perfectly fine**.

A+B+C+M[-O2(1);-N2(1) ;H2(1);-Ar(1); -HO2(1);-CO2(1)]==>D+E+F

Reversible Reactions

For reversible reactions (represented by a single "=") the reverse rate will always be one, "1", **but** if you are using the Thermodynamics mode, then the reverse rate constant, k_b , will be calculated through the equilibrium constant, K_c, and the forward rate constant, k_f: $k_b=k_f/K_c$. For a detailed description on the complete calculation of K_p , K_c and k_b turn to the Incorporation of Thermodynamics section. An example of a reversible reaction is shown above in Figure 8 as Sample Reaction 1.

Enhanced Third Bodies

Enhanced third bodies can be represented using the following form:

Reactants + M[SPECIES (enhancement); SPECIES (enhancement);…] ==> Products

as shown in Sample Reaction 2. The difference between "regular" M (Sample Reaction 3) and M[..] is shown by the following two equations:

$$[M]=\sum_{n=1}^{N}[Species]_n \qquad \text{Eqn 1.}$$

$$[M]=\sum_{n=1}^{N}\alpha_n[Species]_n \qquad \text{Eqn 2.}$$

The α character in the above equation represents the enhancement value of the third body species, and the N represents all species in the gas phase. It should be noted that the summation shown in the above equation is only for gaseous species. As you might recall, gaseous species have **no phase information** attached to the end of the species name or have a **{g}** appended to the end of the species name, i.e. Ar{g}. Again, it should be **very important** to note that if all your species are in one phase (such as gas or aqueous) then **you do not have to append each species name with a phase descriptor**. Once M is calculated, k_f, is multiplied by it. It is possible to combine the enhanced third bodies with fall-off reactions as described in the fall-off reactions section below.

Kintecus also supports exclusive third-body enhancements through the prefixing the enhanced body by a dash, "-". More then one species can become an exclusive third body (rate constants/parameters not shown below):

Reactants+M[-SPECIES(enhancement); -SPECIES(enhancement);…] ==> Products

The difference between exclusive third bodies and non-exclusive third bodies is that exclusive third bodies (the species names designated by the user between the M[and]) are the ***only*** species the are summed in Equations 1 and 2 above. An example is shown in Sample Reaction 4.

Fall-Off Reactions

➢ *Lindemann Reactions*

Kintecus provides several methods to represent fall-off reactions. The classical Lindemann low-pressure reaction can be represented as follows:

Reactants + M[LIN:A_0;m_0;E_{a0}] ==> Products

OR

Reactants + M[LIN:A_0;m_0;E_{a0};(Enhanced bodies if present)] ==> Products

The A_0, m_o, E_{a0} are values used in the Arrhenius rate expression at the low pressure limit:

$$k_0 = A_0 T^{m_0} \ell^{\left(-E_0/RT\right)} \qquad \text{Eqn 3.}$$

The A, m, and E_a values present before the reaction (not shown) are used in the Arrhenius rate expression at the high pressure limit. An overall rate constant, k_f, is then computed:

$$k_f = k_\infty \left(\frac{\frac{k_0[M]}{k_\infty}}{1+\frac{k_0[M]}{k_\infty}} \right) F \qquad \text{Eqn 4.}$$

The F parameter shown above is always one for Lindemann reactions. Sample Reaction 8 in Figure 8 shows a Lindemann reaction with no enhanced third bodies. Sample Reaction 9 shows a Lindemann reaction with enhanced third bodies.

➢ *Troe Reactions*

The TROE fall-off reaction can be represented as follows:

Reactants + M[TROE:A_0;m_0;E_{a0};P_1;P_2;P_3; (P_4)] ==> Products

OR

Reactants + M[TROE:A_0;m_0;E_{a0};P_1;P_2;P_3;(P_4;)(Enhanced bodies if present)] ==> Products

The A_0, m_o, E_{a0} are values used in the Arrhenius rate expression at the low-pressure limit. The A, m, and E_a values present before the reaction (not shown) are used in the Arrhenius rate expression at the high-pressure limit. The Troe parameters **P_1, P_2** and **P_3** (**P_4** is optional) allow Kintecus to compute the Troe Factor, F:

$$\log F = \left[1 + \left[\frac{\log\left(\frac{k_0[M]}{k_\infty}\right) + c}{n - 0.14\left(\log\frac{k_0[M]}{k_\infty} + c\right)}\right]^2\right]^{-1} \log F_{cent} \qquad \text{Eqn 5.}$$

$$c = -0.4 - 0.67 \log F_{cent} \qquad \text{Eqn 6.}$$

$$n = 0.75 - 1.27 \log F_{cent} \qquad \text{Eqn 7.}$$

$$F_{cent} = (1 - P_1)\ell^{\left(-T/-P_2\right)} + P_1\ell^{\left(-T/P_3\right)} + \ell^{\left(-P_4/T\right)} \qquad \text{Eqn 8.}$$

Once F is computed, it is inserted into equation 4. In some references **P_1=a, P_2=T***, P_3=T* and P_4=T**.** Examples of the Troe reaction (with and without enhanced third bodies) in Kintecus are shown as Sample Reactions 5,6 and 7 in Figure 8.

- ***SRI Reactions***

The SRI fall-off reaction can be represented as follows:

Reactants + M[SRI;A_0;m_0;E_{a0};P_1;P_2;P_3 (;P_4(;P_5))] ==> Products

OR

Reactants + M[SRI;A_0;m_0;E_{a0};P_1;P_2;P_3(;P_4(;P_5)) (Enhanced bodies if present)] ==> Products

The A_0, m_o, E_{a0} are values used in the Arrhenius rate expression at the low-pressure limit. The A, m, and E_a values present before the reaction (not shown) are used in the Arrhenius rate expression at the high-pressure limit. The SRI parameters **P_1, P_2** and **P_3** (**P_4** is optional, and if **P_4** is supplied **P_5** is optional) allow Kintecus to compute the SRI Factor, F:

$$F = \left[P_1 \ell^{\left(-P_2/T\right)} + \ell^{\left(-T/P_3\right)} \right]^X P_4 T^{P_5} \qquad \text{Eqn 9.}$$

$$X = \frac{1}{1 + \left(\log \frac{k_0[M]}{k_\infty} \right)^2} \qquad \text{Eqn 10.}$$

In some references **P_1=a, P_2=b, P_3=c, P_4=d and P_5=e.** Examples of the SRI reaction (with and without enhanced third bodies) in Kintecus are shown as Sample Reactions 10 and 11.

Special Reactions

Special reactions are reactions that usually do not follow the standard Arrhenius form, or simply belong in their own category. Additional parameters are supplied to special reactions through +S[….] appearing on the reactant's side.

➢ *Landau-Teller Reactions*

Landau-Teller reactions are essentially vibrational energy transfer reactions and they are represented in Kintecus as:

A , m , E_a, Reactants + S[LT; P_1;P_2] ==> Products

The parameters A, m, E_a, P_1 and P_2 are used to compute the forward rate constant:

$$k_f = A T^M \ell^{\left(\frac{-E_a}{RT} + \frac{P_1}{\sqrt[3]{T}} + \frac{P_2}{\sqrt[3]{T^2}} \right)} \qquad \text{Eqn 11.}$$

In some references m= β, E_a=E, P_1=B and P_2=C. An example of a Landau-Teller reaction is shown in Figure 8 as Sample Reaction 12.

Kintecus will look for MODEL.DAT as the default filename. This can be overridden see KINTECUS Switches Section setting below.

Periodic Table SpreadSheet

This is another optional spreadsheet, which is invoked through the "-P" or "-p" Kintecus command line option. Once either "-P" or "-p" is specified on the command line, Kintecus will look for a spreadsheet file named PERIOD.DAT. The Periodic Table Spreadsheet (PTS) allows you to redefine or add new elements/isotopes to the periodic table. Kintecus has the molecular weight of the elements internally stored. The PTS PERIODDF.DAT contains a copy of those elements stored internally in Kintecus. If you wish to modify or add new elements/isotopes copy the PERIODDF.DAT file to PERIOD.DAT and modify that file. Kintecus will report an error if elements appear more than once in the PTS if the "-P" switch is used, **but** if the "-p" switch is used, only the first instance of an element will be used. The duplicate element appearing further down the list will simply be ignored. You can insert comments in this file or comment out lines by placing a "#" or a quote ' " ' as the first character on a line.

Advanced Modeling

Incorporation of Thermodynamics

Kintecus provides a powerful means to control various thermodynamic aspects in a model. Isothermal, non-isothermal, constant pressure, constant volume, programmed temperature runs/perturbations, programmed volume runs/perturbations, multiple thermodynamic databases can be used and much more.

The Thermodynamic Description SpreadSheet

Specifying the "–THERM" switch on the Kintecus command line directs Kintecus to go into thermodynamic mode. Thermodynamic mode forces Kintecus to compute enthalpies, heat capacities and reverse rate constants (for any reversible reactions present) for all the reactions. The computed enthalpy and heat capacity of the system allows Kintecus to compute the temperature of the system at any time:

$$\frac{dT}{dt} = -\left(\frac{1}{C_p(T)}\right)\sum_{r=1}^{N_R}\left(\frac{d[n]}{dt}\right)\Delta\dot{H}(T)_r \qquad \text{Eqn 12.}$$

The above equation requires enthalpies and heat capacities to be calculated:

$$\left.\begin{aligned} H_{sp}(T) &= RT\left(la_{1,sp} + \frac{la_{2,sp}}{2}T + \frac{la_{3,sp}}{3}T^2 + \frac{la_{4,sp}}{4}T^3 + \frac{la_{5,sp}}{5}T^4 + \frac{la_{6,sp}}{T}\right) \quad ,if\ Low \le T < Common \\ H_{sp}(T) &= RT\left(ha_{1,sp} + \frac{ha_{2,sp}}{2}T + \frac{ha_{3,sp}}{3}T^2 + \frac{ha_{4,sp}}{4}T^3 + \frac{ha_{5,sp}}{5}T^4 + \frac{ha_{6,sp}}{T}\right) \quad ,if\ Common \le T \le High \end{aligned}\right\} \qquad \text{Eqn 13.}$$

$$\Delta\dot{H}(T)_r = \sum_{n=1}^{N_p}\frac{d[n]_n}{dt}H_n(T) - \sum_{n=1}^{N_r}\frac{d[n]_n}{dt}H_n(T) \qquad \text{Eqn 14.}$$

$$\left.\begin{aligned} C_{p,sp} &= R\left(la_{1,sp} + la_{2,sp}T + la_{3,sp}T^2 + la_{4,sp}T^3 + la_{5,sp}T^4\right) \quad ,if\ Low \le T < Common \\ C_{p,sp} &= R\left(ha_{1,sp} + ha_{2,sp}T + ha_{3,sp}T^2 + ha_{4,sp}T^3 + ha_{5,sp}T^4\right) \quad ,if\ Common \le T \le High \end{aligned}\right\} \qquad \text{Eqn 15.}$$

$$C_p = \sum_{n=1}^{N_p}[n]_n C_{p,n} \qquad \text{Eqn 16.}$$

where the H_{sp} is the enthalpy of a species, C_{sp} is the heat capacity of a species, $\Delta H(T)_r$ represents the enthalpy of a reaction, r, C_p the heat capacity of the entire gas phase system and $[n]_n$ is the concentration of species n. The thermodynamic coefficients la_1-la_6 and ha_1-ha_6 are only used if

the current thermodynamic temperature falls within the low, common and high temperature range for that species.

The thermodynamic coefficients shown above are obtained from the thermodynamic database(s) which are the user names in the Thermodynamic Description SpreadSheet. In addition to enthalpies and heat capacities calculations, Kintecus will also compute reverse rates for reversible equations:

$$\left.\begin{aligned} S_{sp}(T) &= R\left(la_{1,sp}\ln(T) + la_{2,sp}T + \frac{la_{3,sp}}{2}T^2 + \frac{la_{4,sp}}{3}T^3 + \frac{la_{5,sp}}{4}T^4 + la_{7,sp} \right) \quad ,if\ \ Low \le T < Common \\ S_{sp}(T) &= R\left(ha_{1,sp}\ln(T) + ha_{2,sp}T + \frac{ha_{3,sp}}{2}T^2 + \frac{ha_{4,sp}}{3}T^3 + \frac{ha_{5,sp}}{4}T^4 + ha_{7,sp} \right) \quad ,if\ \ Common \le T \le High \end{aligned}\right\} \qquad \text{Eqn 17.}$$

$$\Delta S(T)_r = \sum_{n=1}^{N_p} [stoi.coef.]_n S_n(T) - \sum_{n=1}^{N_r} [stoi.coef.]_n S_n(T) \qquad \text{Eqn 18.}$$

$$\Delta G(T)_r = \Delta H(T)_r - T\Delta S(T)_r \qquad \text{Eqn 19.}$$

$$K_{p,r} = \ell^{\left(-\frac{\Delta G(T)_r}{RT}\right)} \qquad \text{Eqn 20.}$$

$$K_{c,r} = \left(\frac{1}{RT}\right)^{\Delta n} K_{p,r} \qquad \text{Eqn 21.}$$

where S_{sp} is the entropy of species, sp, $\Delta S(T)_r$ is the entropy of reaction, r, $\Delta G(T)_r$ is the Gibbs free energy of reaction, r, $K_{p,r}$, is the equilibrium gas constant for reaction, r, and $K_{c,r}$, is the equilibrium constant in concentration units and [stoi.coef.] is the stoichiometric coefficient from the reaction for the respective species. The thermodynamic coefficients la_1-la_7 and ha_1-ha_7 are only used if the current thermodynamic temperature falls within the low, common and high temperature range for that species. Again, the thermodynamic coefficients shown above are obtained from the thermodynamic database(s) which are provided in the Thermodynamic Description SpreadSheet.

As noted above, once Kintecus is in the thermodynamic mode, it will look for the Thermodynamic Description SpreadSheet. The default name of this sheet is **THERM.DAT**. You can override this name. The thermodynamic description spreadsheet contains a listing of all related thermodynamic databases that can be used with your model. The thermodynamic databases contain information describing the heat capacities and entropies for wide range of temperatures. For a complete description on how the range of heat capacities and entropies are calculated for each species refer to the Chemkin-II reference [11]. There are many public thermodynamic databases out there in the Internet. Some starting search links are given: www.sandia.gov , www.llg.gov or http://wwwcms.llnl.gov/combustion/combustion2.html .

If you cannot find a thermodynamic database containing information for your species', you can try to obtain a heat capacity listing from NIST-JANAF tables at http://www.nist.gov/srd/thermo.htm , Burcat & Mcbride Data [22] or roughly estimate them using group additivity [21]. You can also calculate the thermodynamic values using the technique described in Chemkin-II reference[11]. There are programs already available to

produce thermodynamic coefficients that fit a user provided range of heat capacities. One such program is THERM [20]. If you still cannot find either a thermodynamic database containing information on your species' or NIST heat capacities to compute the thermodynamic coefficients then you will have to either perform experiments to obtain the heat capacities or compute the heat capacities. Methods to compute heat capacities are provided in manuals for Gaussian, GAMMES, DISCOVER, COLUMBUS, CHARM, Jaguar, Mopac and many other quantum programs. Be warned! It is highly recommended to use high level *ab initio* (such as MP2/MP4theory) using large basis sets for accurate heat capacities or combination methods such as the G2/G3 theory, or at the very least DFT theory (such as B3LYP using large basis sets). Blindly using semi-empirical techniques (such as AM1, PM3, MINDO and many others) can provide disastrous results.

A sample Thermodynamic Description Spreadsheet is show below:

# Database			Database	Species
# FileName	INPUT	MAP	Special Switches	Reservation List
1995_NASA_data	F18:IG26:F1:F10:F10:F10:NL	SP:PH:LT:HT:MW:HA1:HA2:HA3:	U1234:UPPL:CHF:FLUFF:PHS:SET(CT=1000):SYN	
1994_thermo.dat	F18:IG26:F1:F10:F10:F10:NL	SP:PH:LT:HT:CT:HA1:HA2:HA3:H	U1234:UPPL:CHF:PHS:UPC	O2:O3:C2H4
freeoh1.dat	FREE	SP:LT:CT:HT:LA1:LA2:LA3:LA4:L	UPPL	CH4
#1995_Burcat_data	F18:IG26:F1:F10:F10:F10:NL	SP:PH:LT:HT:MW:HA1:HA2:HA3:	U1234:UPPL:CHF:FLUFF:PHS:SET(CT=1000):SYN	
END				

Figure 9

There are five columns for the thermodynamic description spreadsheet. The first column, Database Filename, contains the filename for the thermodynamic database. As one might recall, the thermodynamic database contains the thermodynamic coefficients for the species in your model. Kintecus provides a mean to provide multiple thermodynamic database by allowing one to enter additional Database Filenames in column one. It should be noted that Kintecus uses the thermodynamic coefficients for a species from the first match in a thermodynamic database. This can be overridden by using Species Reservation List explained below.

The INPUT and MAP columns direct Kintecus on how exactly to read in the thermodynamic database**. YOU SHOULD NOT HAVE TO DERIVE INPUT AND MAP FIELDS!** It **is highly recommended** that you copy the sample thermodynamic description spreadsheet, THERMCK.DAT as THERM.DAT and follow the quick instructions in CK2KIN.EXE (CHEMKIN-II/III ➔ KINTECUS MODEL CONVERTER).

Of the many thermodynamic example simulations that come with Kintecus, copying and pasting the entire INPUT, MAP and Database Special Switches from a preexisting thermodynamic description spreadsheet should allow you to read most thermodynamic databases. Sometimes the removal or addition of a Database Special Switch might also be needed to finally read in that stubborn database.

There are only four keywords in the INPUT field:**F**(characters to read), **IG**(characters to skip) , **NL** (new line or carriage return) and the exclusive **FREE**. All keywords must be delimited by a **colon, ":".** A full sample INPUT field is shown below:

F18:IG26:F1:F10:F10:F10:NL:F15:F15:F15:F15:F15:NL:F15:F15:F15:F15:F15:NL:F15:F15:F15:F15

The F() keywords directs Kintecus that here is an important field of length () characters. The IG() keyword directs Kintecus to "ignore" or skip () characters. The NL keyword directs Kintecus to go to the next line. The F() keyword and the fields in the MAP column must have a

perfect one-to-one mapping. The FREE keyword directs Kintecus that this thermodynamic database is in a FreeForm. FreeForm allows each field to be separated by a delimiter (spaces are ignored). The delimiter is a TAB by default, but this can be overridden by entering in the ASCII value of the delimiter after the FREE keyword, i.e. FREE(44) directs Kintecus to use commas to delimit each field in the thermodynamic database. The oh2f.bat model and its related files show an example use of this feature.

The MAP fields converts the value each F() field into a MAP keyword. A listing of all MAP keywords and their respective thermodynamic value are shown below:

Map Keyword(s)	Thermodynamic Value
SP	Species Name
LT	Low Temperature for Low Range
CT(optional)	Common Temperature Separating Low/High
HT	High Temperature for High Range
LA1, LA2,LA3,LA4,LA5,LA6,LA7	Thermodynamic Coefficients for the Low Range
HA1,HA2,HA3,HA4,HA5,HA6,HA7	Thermodynamic Coefficients for the High Range
PH (optional)	Phase of Species
CH(optional)	Numeric charge of species (usually not needed). Charge can be retrieved from end of species name
MW (optional)	Molecular Weight of Species. This will override Kintecus' internally calculated Mw for that species.
CMW (optional)	Convert Chemkin empirical molecular weight (usually in columns 25-44 on first row) to Mw. Note, some thermo. databases have more than 4 elements defined for a species, you can specify a larger field to encompass it. Specifying the CMW Map Keyword will override Kintecus' internally calculated Mw for that species.

Table 3. Possible Map keywords available to read physical properties from a thermodynamic database.

A sample MAP field is shown below:

SP:PH:LT:HT:MW:HA1:HA2:HA3:HA4:HA5:HA6:HA7:LA1:LA2:LA3:LA4:LA5:LA6:LA7

Using the sample INPUT field given above here are exactly how the values from F() to MAP keywords are converted:SP=F18, PH=F1, LT=F10, HT=F10, MW=F10, HA1=F15, HA2=F15, HA3=F15, HA4=F15, HA5=F15, HA6=F15, HA7=F15, LA1=F15, LA2=F15, LA3=F15, LA4=F15, LA5=F15, LA6=F15, LA7=F15. Obtaining the following RUN-TIME error is a good indication that your INPUT field is not correctly defined.

Run-time error F6103 : READ(internal)
-invalid REAL

Your INPUT field is probably "capturing" non-numeric characters and that you should go over the "F" and "IG" field lengths to be sure they are of the right length.

The Database Special Switches Field has an assortment of Text Filtering and Value Setting for those databases which do not exactly conform to Chemkin/NASA format. A listing of all the Database Special Switches keywords and a short explanation of what they do are shown below:

Database Special Switch Keyword	Action
UPC	Convert all database species' names to UPPERCASE
FLUFF	Any extra characters after the first space in a database species name is erased.ie. SP="C3CH8 #Hanson et a," is converted to SP=C3CH8
SET(Any Map Keyword = default value)	You can set ANY MAP keyword to any default value. Mainly useful for setting the Common Temperature to some value. Ie. SET(CT=1000) .
SYN	Some databases have two species name in one field. Ie, C4H8,butene. SYN allows Kintecus to match either C4H8 or butene to a species in your model. Without this keyword, Kintecus will literally interpret C4H8,butene as the full species name!
U1234	Directs Kintecus that this thermodynamic database is using the Chemkin/NASA standard format of using the numerals 1,2,3,4 in column 80 to continue species thermodynamic values onto multiple lines.
UPPL	Convert any uppercase "L" present in a database species name to a lowercase "l". ie. If SP="CL" then SP="Cl"
CHF	Ignore charge field CH
PHS	Interpret possible phase information at the end of the database species name. Ie. Ga(IV) is converted to Ga{IV}.

Table 4. Special switches available for the parsing of thermodynamic databases.

The Species Reservation List field specifically allows one to direct Kintecus to use the thermodynamic values for a species from a specific database. It allows one to switch values from one thermodynamic database to another without the need of deleting and re-inserting rows of data, which could lead, to a big mess. This allows one to test various thermodynamic values created by different authors or groups. As with all values in the thermodynamic description spreadsheet, the list in the Species Reservation List field must be delimited by a colon, ":".

Creating Freeform Thermodynamic Databases

A NASA/Chemkin thermodynamic database can be converted to Freeform simply by providing the –OF switch on the Kintecus command line. This switch will direct Kintecus to

output a spreadsheet file in freeform containing all the thermodynamic values in columns delimited by whatever delimiter is used in the MODEL.DAT file. It is important to note that ONLY the species used in your model.dat will be stored in the freeform spreadsheet. The name of the freeform spreadsheet will always be “FREETHRM.TXT”. A sample is shown below in which the model modoh.dat using the NASA thermodynamic databases was run with the “–OF” switch. The converted database (freeoh1.dat) containing the species used in the modoh.dat file is shown on the next page.

# Species	LOW	Common	Hi	Thermodynamic coeffic. (LOW then HIGH)														
#	TEMP.	TEMP.	TEMP.	LA1	LA2	LA3	LA4	LA5	LA6	LA7	HA1	HA2	HA3	HA4	HA5	HA6	HA7	MW
H2	200	1000	6000	2.344331	7.98E-03	-1.95E-05	2.02E-08	-7.38E-12	-917.935	0.683	2.9329	8.27E-04	-1.46E-07	1.54E-11	-6.89E-16	-813.07	-1.0243	2.01588
O2	200	1000	6000	3.782456	-3.00E-03	9.85E-06	-9.68E-09	3.24E-12	-1063.94	3.6577	3.661	6.56E-04	-1.41E-07	2.06E-11	-1.30E-15	-1216	3.41536	31.9988
OH	200	1000	6000	3.992015	-2.40E-03	4.62E-06	-3.88E-09	1.36E-12	3615.081	-0.104	2.8386	1.11E-03	-2.94E-07	4.21E-11	-2.42E-15	3943.96	5.84453	17.00734
H2O	200	1000	6000	4.198641	-2.04E-03	6.52E-06	-5.49E-09	1.77E-12	-30293.7	-0.849	2.677	2.97E-03	-7.74E-07	9.44E-11	-4.27E-15	-29886	6.88256	18.01528
H	200	1000	6000	2.5	0	0	0	0	25473.66	-0.447	2.5	-5.65E-09	3.63E-12	-9.20E-16	7.95E-20	25473.7	-0.4467	1.00794
O	200	1000	6000	3.168267	-3.28E-03	6.64E-06	-6.13E-09	2.11E-12	29122.26	2.0519	2.5436	-2.73E-05	-4.19E-09	4.95E-12	-4.80E-16	29226	4.92229	15.9994
HO2	200	1000	6000	4.301798	-4.75E-03	2.12E-05	-2.43E-08	9.29E-12	294.808	3.7167	4.1723	1.88E-03	-3.46E-07	1.95E-11	1.76E-16	61.8103	2.95768	33.00674
H2O2	200	1000	6000	4.276113	-5.43E-04	1.67E-05	-2.16E-08	8.62E-12	-17754.3	3.4351	4.5733	4.05E-03	-1.29E-06	1.97E-10	-1.13E-14	-18055	0.70428	34.01468
N2	200	1000	6000	3.531005	-1.24E-04	-5.03E-07	2.44E-09	-1.41E-12	-1046.98	2.9675	2.9526	1.40E-03	-4.93E-07	7.86E-11	-4.61E-15	-923.95	5.87189	28.01348
NO	200	1000	6000	4.218599	-4.64E-03	1.10E-05	-9.34E-09	2.81E-12	9845.1	2.2806	3.2607	1.19E-03	-4.29E-07	6.94E-11	-4.03E-15	9921.43	6.36901	30.00614
N	200	1000	6000	2.5	0	0	0	0	56104.64	4.1939	2.4159	1.75E-04	-1.19E-07	3.02E-11	-2.04E-15	56133.8	4.64961	14.00674
END																		

Figure 10

Kintecus Switches

Kintecus provides a large number of various switches/options to control the program's behavior, input files, outputs files and even screen messages. The switches are always provided on the command line for Kintecus right after the program name:

> Kintecus (switches, if any)

Here is the current listing of all the switches available for Kintecus:

```
-ah See advanced Kintecus settings.
-QUIET Don't diplay output or warnings.
-PARM:filename (Parameter Description Input File)
-SPNAME:filename (Species Common_Name/Mass Input File)
-SPEC:filename (Species Description Input File)
-MOD:filename (Model Description Input File)
-OUT:filename (Concentration Output File)
-THERM:filename (Enter thermodynamics mode and use
filename as the thermodynamic database spreasheet)
-c Create SPECIES.DAT file from model, then stop.
-show Display to screen the concentration of species,
      time and dt's.
-ig:mass Ignore Mass Balance.
-ig:charge Ignore Charge Balance.
-ig:warn Ignore all warnings.

-SENSIT:  Output Sensitivity Analysis Output File
 -SENSIT:1(:n1 (:n2) ) Use sensitivity analysis #1 with
 the following optional numeric entries:
 n1 :perform analysis at various parts in the simulation
 (default is three: beginning, middle and the end)
 -OR- n1=TIMES,t1,t2,tn... where t1,t2 and tn are
 times(in sec.) to perform the sensitivity analysis.
 n2 = percent difference in k's used (5% default)
 just typing -SENSIT:1 is equal to -SENSIT:1:3:5
-KINSTAT Output statistics on the kinetic system
         into the file KINSTAT.TXT .
-SEEMW Output all species and their corresponding
 molecular weight into the file MW.TXT.
-P Load a user provided periodic table from the text
   file PERIOD.DAT
-o:Y/N:Y/N:Y/N:Y/N Output files based on various
   physical properties/rates on the system as it runs.
-h/? You get this list.
```

```
-FIT:a:b:c:d:e:f[:g:h:i] Fit/Optimize your model against
    experimental/fabricated data.
a=Fitting Algorithm=1, 2, 3
b=Comparison Operator=1, 2, 3
c=User Dataset Filename=Any allowed text filename
d=Tolerance=1 to 10(-14)
e=Maximum Iterations Allowed=1-32767
f=Starting Vectors=1x10(-99) to 1x10(10)
g=Starting Temperature=1x10(-100) to 1x10(10)
h=Number of Cycles to Stay At Current Temperature
Before Reducing Temperature=1-32767
i=Percent Temperature Reduction=0 - 0.99999

-FIT sets default values to, a=1, b=1,
c=FITDATA.TXT, d=1x10(-6),e=9000
f=1x10(-35)
```

Advanced Kintecus Switches:

```
-anjac Use analytically calculated jacobians.
-d### Where ### is the ASCII code of the data
       delimiter used in the input files.
-INT:n1 Where n1 is the type of integrator
        n1 = 1 Modified Bader-Deuflhard (default)
        n1 = 2 Cash-Karp Runge-Kutta integrator
-OF Output a freeform thermodynamic database spreadsheet
-y Set the lower threshold for the concentration.
-i Run in interactive mode
-f:F:F Alter format settings for the numbers in CONC.TXT
  where F's represent FORTRAN format descriptors.
```

3. Advanced Analysis

This section will describe the various numerical techniques provided with Kintecus to significantly enhance one's modeling capabilities. In addition, Kintecus can output various physical properties on the system which can help one's analysis.

Numerical Techniques

Sensitivity Analysis

Kintecus can generate normalized sensitivity coefficients at any time or times during a simulation run. What are normalized sensitivity coefficients (NSC) and why should I care? Well, first of all, normalized sensitivity coefficients are the partial derivatives of each species with respect to each reaction constant normalized by multiplying by Rate_Constant/Concentration_of_Species:

$$NSC = \left(\frac{\frac{\partial k}{k}}{\frac{\partial [Species]}{[Species]}} \right)_k = \left(\frac{\partial \ln k}{\partial \ln [Species]} \right)_k \qquad \text{Eqn 22.}$$

It is a matrix with signed numbers, which indicate the reactions that have the biggest influence on what species. By examining the matrix and sorting the largest NSC's by reactions for each species one can see that the large positive NSC's are the major sources and the large negative NSC's are the major sinks[10]. A reaction that has a very small NSC for a species indicates that reaction has almost no influence on the species no matter what the rate constant or the reaction's concentration of reactant species. The method to make Kintecus actually output the NSC matrix, S, is by using the **-SENSIT:1** switch on the command line. Currently there is one NSC matrix producing method and to use it just enter **-SENSIT:1** on the command line. This will output three NSC matrices at three times:the beginning of the simulation, the middle and the end. If you wish to produce more S matrices then simply append the number you want at the end of the SENSIT switch. For example, if I want 25 S matrices calculated over an evenly spaced time period during my simulation, just place -SENSIT:1:25 on the command line. Kintecus will output 25 files with the names SENSIT01.TXT to SENSIT25.TXT. Please note that Kintecus

actually outputs the transpose of the NSC matrix ($\mathbf{S}^T$). If you wish for unevenly spaced timed periods to output S matrices, you must use this form of the SENSIT switch: **-SENSIT:1:TIMES,n1,n2,n3.....nn** with **TIMES** in UPPERCASE and commas to delimit the **exact** times you wish to output time periods.

One might think that, "Hey, if I just sum up the squares of the NSC's for each reaction then I'll know what reaction to drop because the reactions with very small NSC's should have no affect on any of the species". This might be true for most kinetic mechanisms, but in some cases this is not the case. NSC only tests for direct routes of influence of species X, it does not directly show strongly interacting reactions. A very simple method to see which reactions can actually be "thrown out the window" is a method of principal component analysis used by Turanyi, Vajda and Valko[9] applied to the normalized sensitivity analysis matrix, **S**. The steps described by this paper can easily be done in MATLAB or Lotus 1-2-3.It involves finding NSC matrices**,** $\mathbf{S_1, S_2 ,S_3...S_n}$, at various times in the simulation, for example at ten evenly spaced periods (use -SENSIT:1:10 switch). By using a spreadsheet program or MATLAB, you must concatenate all the **S**'s at each calculated time into one big matrix, **BS**. Again, do not forget to transpose each **S** before concatenating all of them into **BS**. Now multiply **BS** by it's transpose, $\mathbf{BS^T * BS = D}$. Determine the eigenvalues, e, and eigenvectors, v, of **D**. Now, calculate the lower threshold for the eigenvalues by multiplying the number of NSC matrices calculated by the number of species (which are NOT constants in your simulation) by 1 x 10^(-4), call this **L**. Note all the eigenvalues that are equal or under **L**, call these **LL**. Now the last step, for all the elements of each eigenvector of each respective **LL** that are greater than 0.2 mark those. Those elements of the eigenvectors correspond to reactions that have no overall affect on the kinetics scheme and can be safely "thrown out the window". The author has tried this with the formaldehyde oxidation mechanism and obtained similar results that the paper[9] has computed.

Jacobians

The default integration method used in Kintecus [1] requires the calculation of Jacobians. By default, the Jacobians are calculated by a finite difference method. The earlier versions of Kintecus calculated the Jacobian analytically, that is, exactly. It was found that the analytical method was 2-5% slower than the finite difference method for kinetic mechanisms of less than 20,000 reactions so the finite difference method was selected to be used as the default method for calculating Jacobians. If you happen to experience underflow or overflow errors during the integration process (especially for large stiff systems composed of more than 25,000 reactions), switching to analytically calculated Jacobians might alleviate this problem. To switch to analytically calculated Jacobians use the -anjac switch on the command line (i.e. > kintecus -anjac).. It is important to note that analytically computed Jacobians **are NOT supported** for systems containing Arrhenious expressions, thermodynamics, special/fall-off/[M] reactions or constant pressure settings.

Additional Output

If you supply the –KINSTAT keyword on the Kintecus command line, Kintecus will output a spreadsheet containing some statistics on your kinetic system. An example is shown below in Figure 11.

A new feature in Kintecus V2.3 is the ability to output various kinetic and thermodynamic results. By using the "-o" switch, these various system properties can be outputted in four separate files. The "-o" switch has four fields and **all four** must be included on the command line to output these properties: -o:**1:2:3:4** . The Table below shows the name of file created when a user specifies a "Y" as a field. An example, -o:Y:N:N:Y will create two files: one named RATESOUT.TXT and the other SYSTEMOUT.TXT.

Field	Possible Values	File Created	What the File Contains
1	"Y" or "N"	RATESOUT.TXT	Each Reaction Rate: d[reaction]/dt ***for each reaction*** ! (can be a lot of data)
2	"Y" or "N"	SPECRATE.TXT	Overall Species, Formation and Destruction Rates: d[species]/dt
3	"Y" or "N"	THERMOUT.TXT	Overall System Enthalpy, Entropy, Heat Capacity, Gas Molar Volume, Gas Density
4	"Y" or "N"	SYSTEMOUT.TXT	Enthalpies, Entropies, Gibbs Energy, K_p, K_c, k_f, k_b for ***each reaction!*** (can be a lot of data)

The frequency of the data stored in each of the above four files is directly related to the frequency at which the species/temperature data is stored in the concentration file: CONC.TXT . To refresh your memory, to increase the amount of points in any of the above files, you can decrease the Maximum Integration Time in the Parameter Description Spreadsheet. This can be a lot of data if you have a lot of reactions and trying to output a RATESOUT.TXT or a SYSTEMOUT.TXT file. Conversely, to decrease the amount of points in any of the above files, you can increase the Maximum Integration Time in the Parameter Description Spreadsheet.

There are sample RATESOUT.TXT, SPECRATE.TXT, THERMOUT.TXT and SYSTEMOUT.TXT files created by specifying the additional Kintecus command line option –o:Y:Y:Y:Y for the adiabatic, constant pressure O_2 combustion model OH2.BAT .

If you supply the –SEEMW keyword on the Kintecus command line, Kintecus will output a spreadsheet named MW.TXT containing the molecular weight of each species in your Species Description Spreadsheet.

Species	Sources	Sinks	Total Terms	% Total Terms
NO2	18	15	33	11.4
NO	4	18	22	7.6
O	1	7	8	2.8
O2	8	14	22	7.6
O3	1	6	7	2.4
NO3	7	3	10	3.5
N2O5	1	2	3	1
H2O	4	0	4	1.4
HNO3	2	0	2	0.7
HNO2	3	1	4	1.4
OH	9	9	18	6.2
CO	2	1	3	1
CO2	2	0	2	0.7
HO2	9	3	12	4.2
H2O2	1	0	1	0.3
C3H6	0	8	8	2.8
CH3CH2	1	1	2	0.7
CHO	8	2	10	3.5
CH3	3	1	4	1.4
CH3CO	5	1	6	2.1
C2H4O2	2	3	5	1.7
HCHO	10	4	14	4.8
CH3CHO	9	4	13	4.5
CH2O2	1	3	4	1.4
CH3O2	1	2	3	1
CH3O	4	4	8	2.8
CH3NO3	1	0	1	0.3
CH3CH2O2	1	2	3	1
CH3CH2O	3	4	7	2.4
CH3CH2NO3	1	0	1	0.3
CH3C(O2)HCH2(	1	2	3	1
CH3CH2CHO	1	0	1	0.3
CH3C(O)HCH2O	1	1	2	0.7
HOCH2O2	1	2	3	1
HOCH2O	1	1	2	0.7
CH3C(OH)HCH2	1	2	3	1
(CH3)2CO	1	0	1	0.3
CH3C(OH)HCH2	1	1	2	0.7
CH3C(OH)HO2	1	2	3	1
CH3C(OH)HO	1	2	3	1
CH3COOH	3	0	3	1
CH2CHCH2	1	0	1	0.3
CH3(CO)O2	1	2	3	1
CH3(CO)O	3	4	7	2.4
CH3(CO)O2NO2	1	2	3	1
CH3O2NO2	1	2	3	1
CH3CH2O2NO2	1	2	3	1
H	1	0	1	0.3
CH3OH	1	0	1	0.3
CH3CH2OH	1	0	1	0.3
Average:	Sources	Sinks	Terms	
	2.9	2.9	5.8	

Figure 11

Miscellaneous

A smaller version of Kintecus is provided and it is named **Kintecus_small**. The smaller version requires **much less memory** than the regular version. The smaller version is provided if one wished to include Kintecus in a mass/fluid flow **1D/2D/3D-grid** calculations. However, because of the memory constraints, the Kintecus_small version can only handle about 800 reactions.

An interactive mode has been implemented for users who wish to create a separate "control" program or graphical interface that runs Kintecus remotely. The interactive mode is turned on by including the **"-i**" or **"-I**" switch on the command line. Once this switch is specified, Kintecus will output various small files during its execution. The table below shows all the files outputted during the Kintecus run in interactive mode:

File	When It Appears	What It Contains
KRUN.TMP	Kintecus starts up and is running. This file is deleted by Kintecus once the program is finished running through Successful or Fatal completion.	Usually nothing
KDONE.OUT	Once Kintecus is finished.	Successful or Fatal Error
KERR.OUT	Kintecus has experienced a FATAL error and has halted	Fatal Error #. View the output to see a more detailed description.
KWARN.OUT	Kintecus has come across one or more warnings.	Warning Error #'s, could be more than one. View the output to see a more detailed description.

Table 5

It is very important to note that if Kintecus experiences an error it cannot trap, such as an Overflow error or Domain error the files KDONE.OUT or KERR.OUT may never appear. The user is directed to look at the Visual Basic scripts in the Kintecus_workbooks.xls files for examples on how to monitor these error exceptions.

A switch has been provided to add or remove the amount of decimal places for the "Time(s)" column and concentrations/temperature columns that appear in the CONC.TXT ouput file. The switch and its arguments are **-f:F:F**. Where the "F" stands for a FORTRAN Format Descriptor. The default FORTRAN Format Descriptor used is "**E14.6:E14.6**" . An example, if you need four more decimals places for the Time(s) column you would place the switch **-f:E18.10:E14.6**. If you needed five more decimal places for the Time(s) and four more for the concentrations you would add the switch: **-f:E19.11:E18.10** . Other FORTRAN Format Descriptors can be used such as F, I or G, ie **-f:G14.6:G14.6** . This will display numbers that fit with the field size of 14 with no exponent, numbers that cannot fit in the 14 field size will be displayed with exponents.

4. Examples!

This section contains numerous example models that have been tested against refereed published models obtained through extensive custom modeling, programming and experimentation. The example models range from the very simple, stiff.bat, to the more complex, ethanol1.bat. The .bat files simply contain a one line Kintecus command with the required switches.

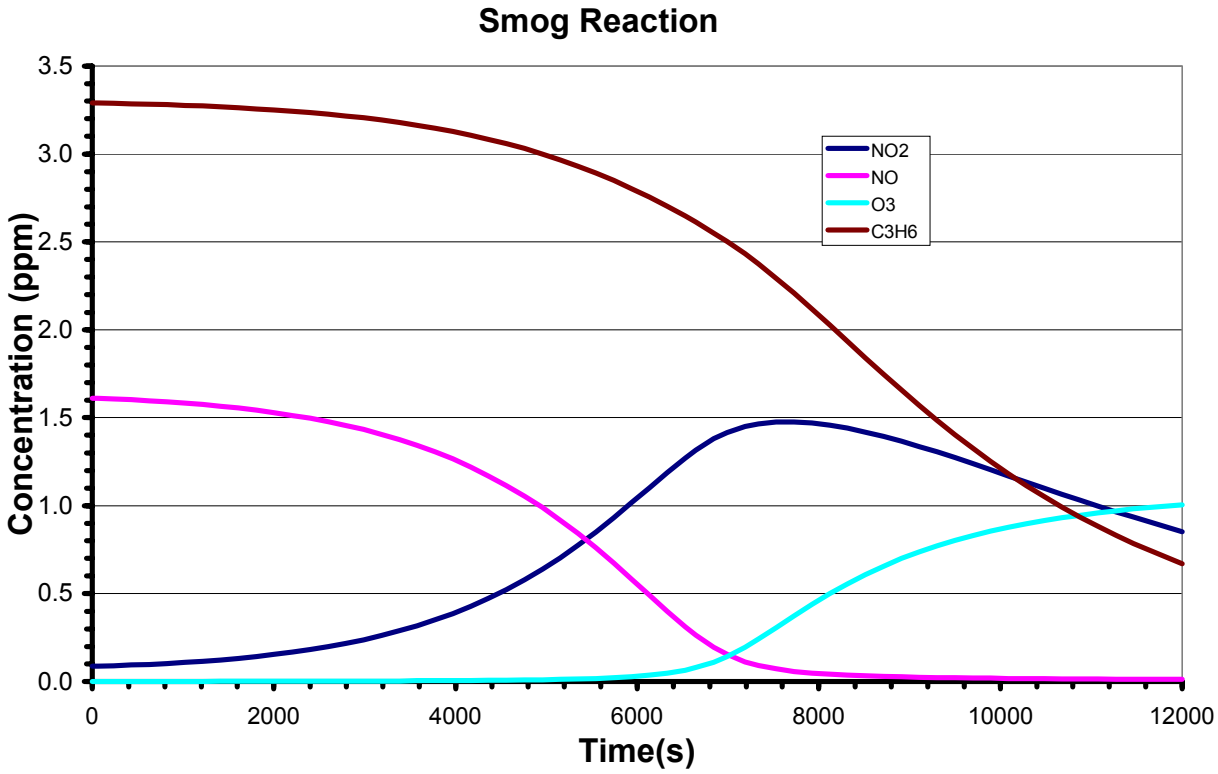
Simple Sample Model Runs

The following sample models below involve non-Arrhenius expressions, no fall-off reactions, no enhanced bodies, no special reactions, no thermodynamics, no perturbations and no volume changes. Also, some of the following examples have been transferred to Excel workbooks containing specialized Visual Basic code to run the models with a click of the RUN button. Here is the current listing of models completely transferred into Excel/Star-Office workbooks: Enzyme_Regression_Fitting.xls, Ethanol_Combustion.xls, GRI_MECH_30.xls, Oregonator_in_CSTR.xls, Combustion_Workbook_OH.xls and Wolfrum_with_Temp_Program.xls.

The Smog Reaction Model

The output concentration file, CONCSMOG.TXT, matches Figure 1 in the paper[3].

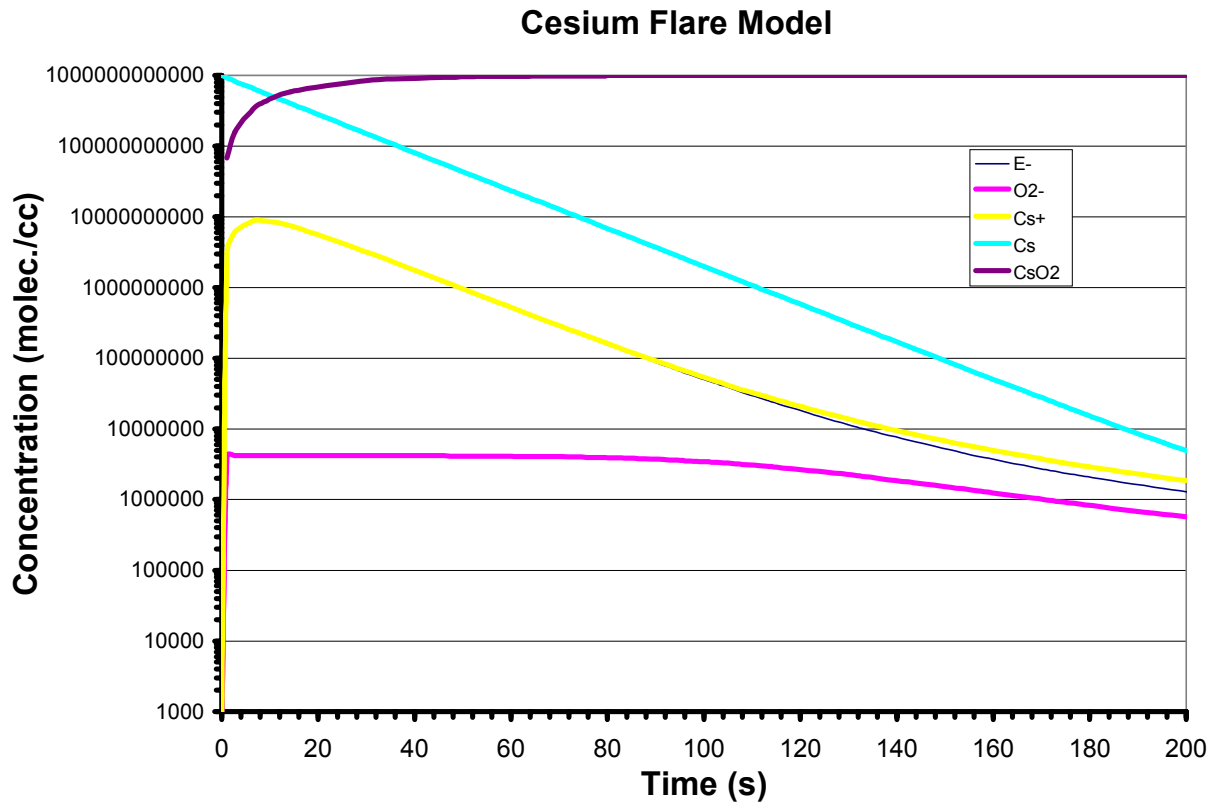
MODSMOG.TX2 - The kinetics reactions
SPECSMOG.TX2 - The species involved
PARMSMOG.TX2 - The parameters used
CONCSMOG.TXT - A simulation run.
SMOG.BAT - A very simple one line batch file that will run the above model producing the concentration profile equal to CONCSMOG.TXT.



The Cesium Flare Model

The output concentration file, CONCCES.TXT, matches Table II in the paper[4].

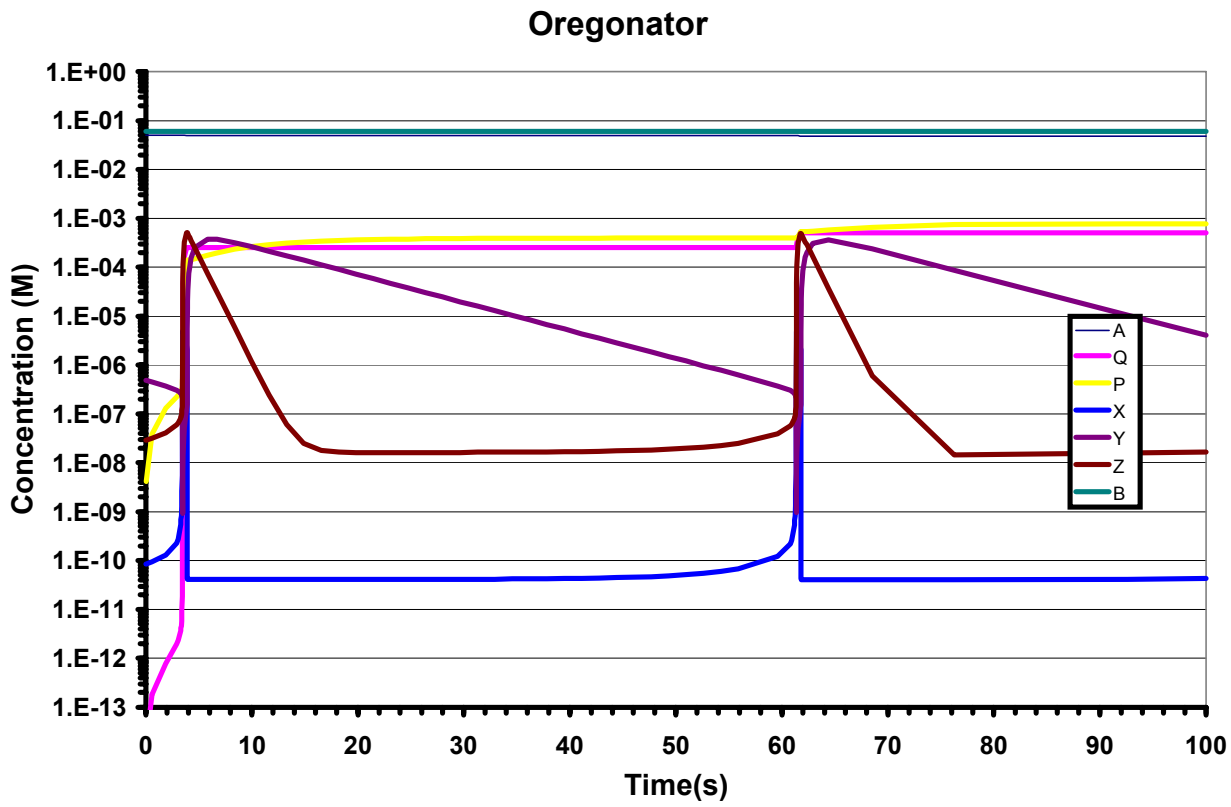
NAMECES.TX2 - A species name file containing common names and their MW.
MODCES.TX2 - The kinetics reactions
SPECCES.TX2 - The species involved
PARMCES.TX2 - The parameters used
CONCCES.TXT - A simulation run.
CES.BAT - A very simple one line batch file that will run the above model producing the concentration profile equal to CONCCES.TXT.



The Oscillating Oregonator

The output concentration file, CONCOREG.TXT,matches Figure 1 in the paper[5].

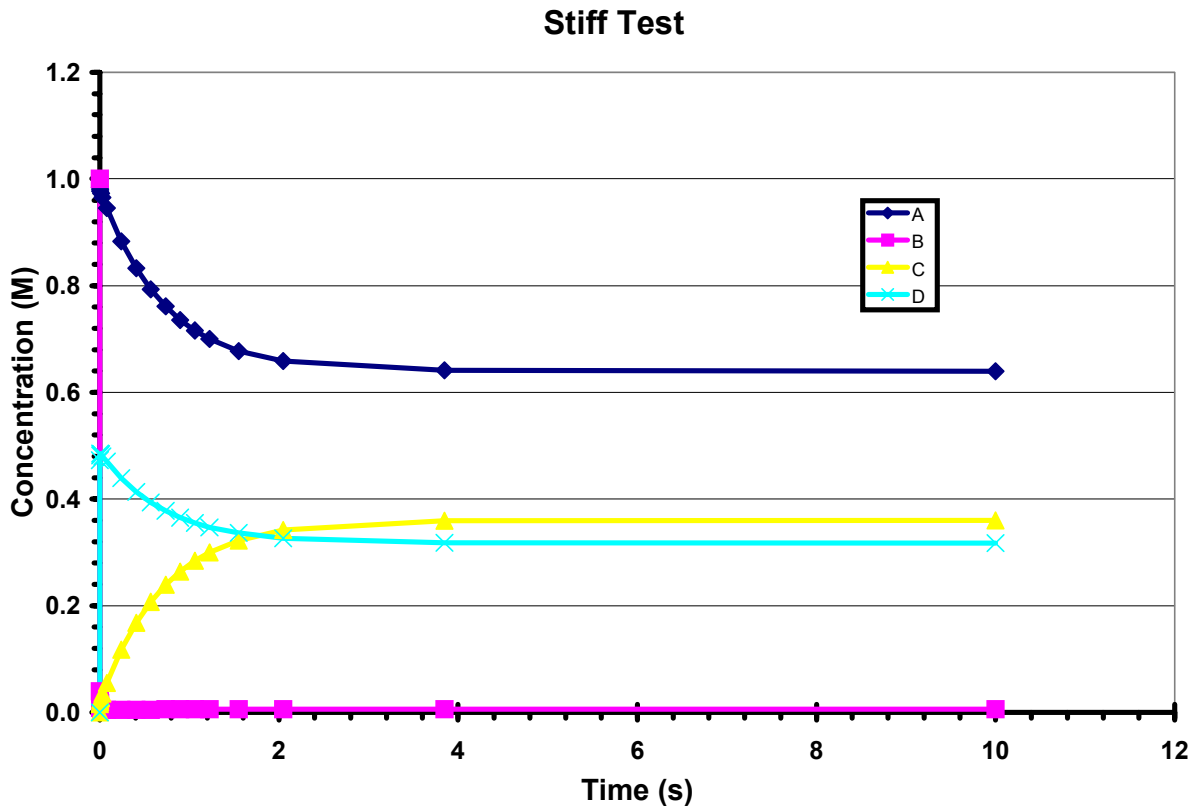
MODOREG.TX2 - The kinetics reactions
SPECOREG.TX2 - The species involved
PARMOREG.TX2 - The parameters used
CONCOREG.TXT - A simulation run.
OREG.BAT - A very simple one line batch file that will run the above model producing the concentration profile equal to CONCOREG.TXT.



The Stiff Test

The output concentration file, CONCSTIF.TXT, matches the results on page 89[6].

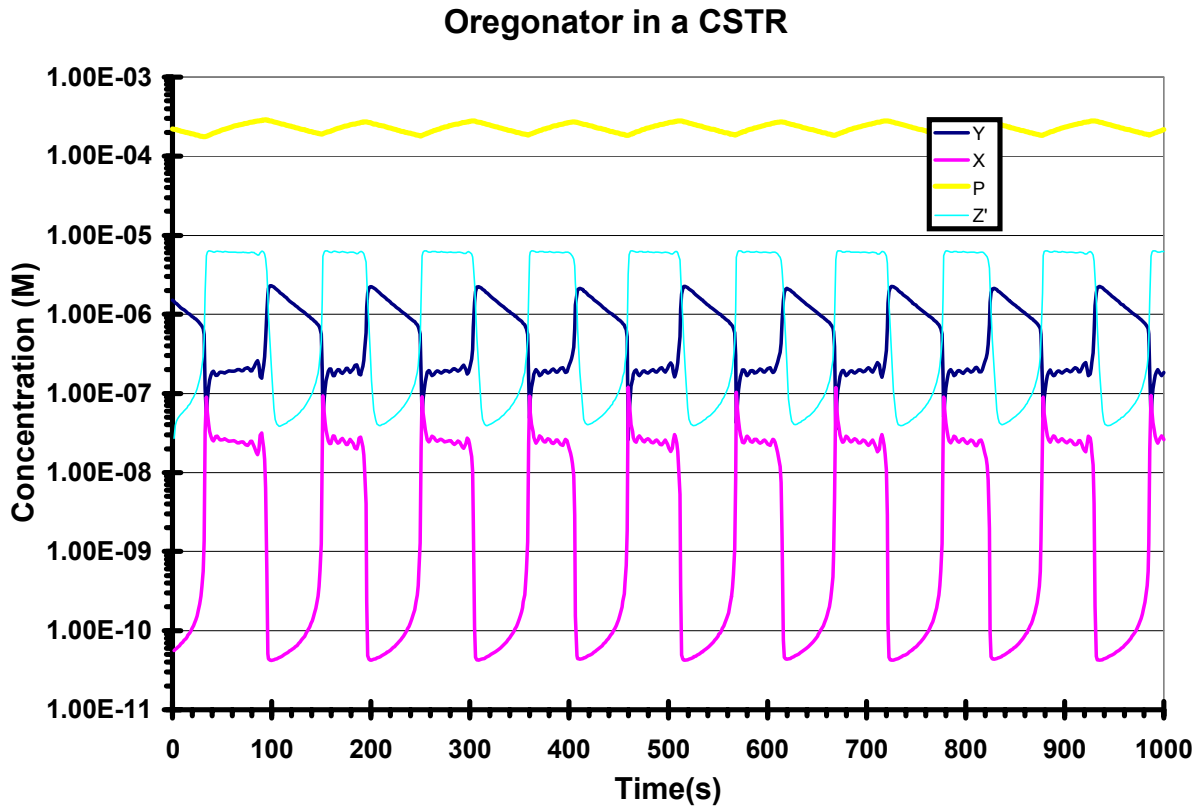
MODSTIF.TX2 - The kinetics reactions
SPECSTIF.TX2 - The species involved
PARMSTIF.TX2 - The parameters used
- A simulation run.
STIFF.BAT - A very simple one line batch file that will run the above model producing the concentration profile equal to CONCSTIF.TXT.



The Oregonator in a CSTR

The output concentration file, CONCFORG.TXT, matches figures 5 and 6[7]. This model can also be executed by loading the Excel or Star-Office workbook: Oregonator_in_CSTR.xls and then clicking the **RUN** button located on the CONTROL worksheet.

MODFORG.TX2 - The kinetics reactions
SPECFORG.TX2 - The species involved
PARMFORG.TX2 - The parameters used
CONCFORG.TXT - A simulation run.
OREGFLOW.BAT - A very simple one line batch file that will run the above model producing the concentration profile equal to CONCFORG.TXT.



Advanced Sample Model Runs

The following sample models below now involve any combination of Arrhenius expressions, fall-off reactions, enhanced bodies, special reactions, thermodynamics, perturbations and volume changes.

Combustion of H_2 and O_2 at constant pressure

The output concentration file, CONCOH2.TXT, matches the results (after converting the concentrations to mole fractions) on page 110 of the Chemkin-II/III manual example [11]. This model can also be executed by loading the Excel or Star-Office workbook: Combustion_Workbook_OH.xls and then clicking the **RUN** button located on the CONTROL worksheet.

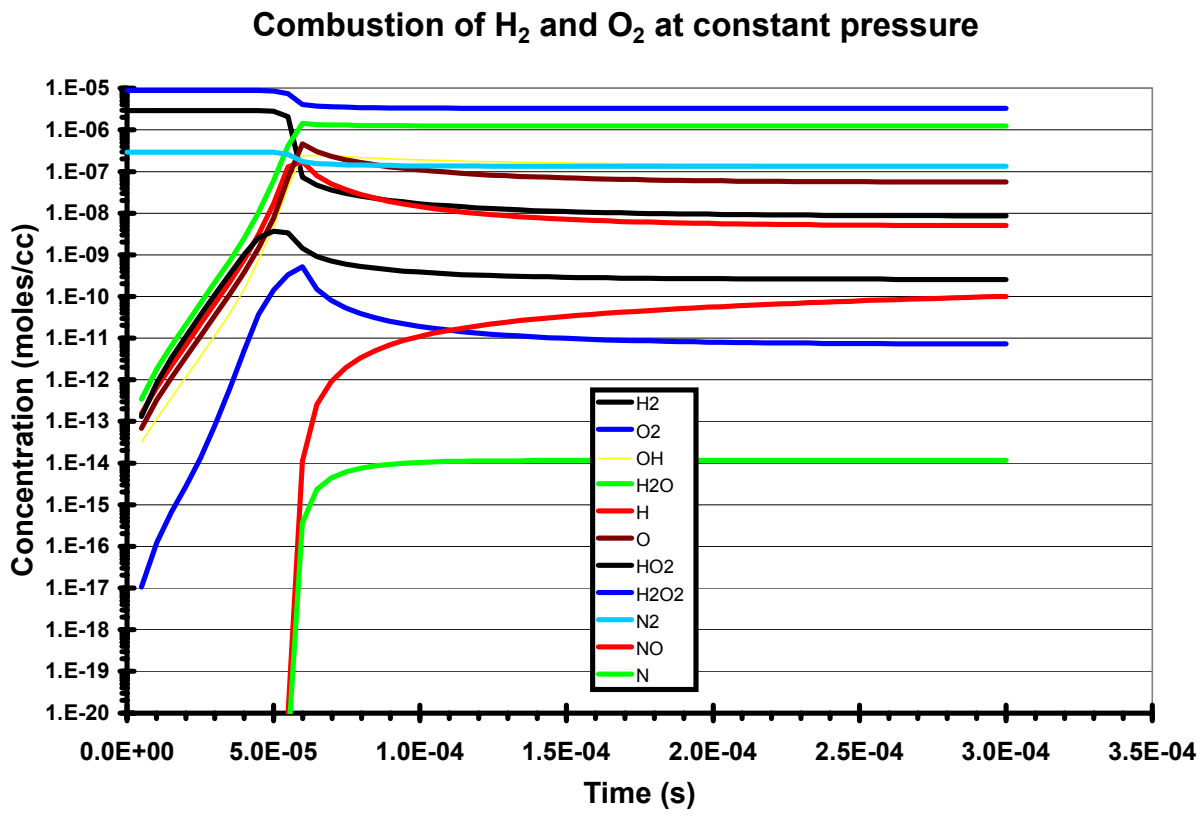
MODOH.DAT - The kinetics reactions (Converted from the Chemkin-II/III manual example)
SPECOH.DAT - The species involved
PARMOH2.DAT - The parameters used
THERMOH.DAT – The thermodynamic description spreadsheet
CONCOH2.TXT - A simulation run.

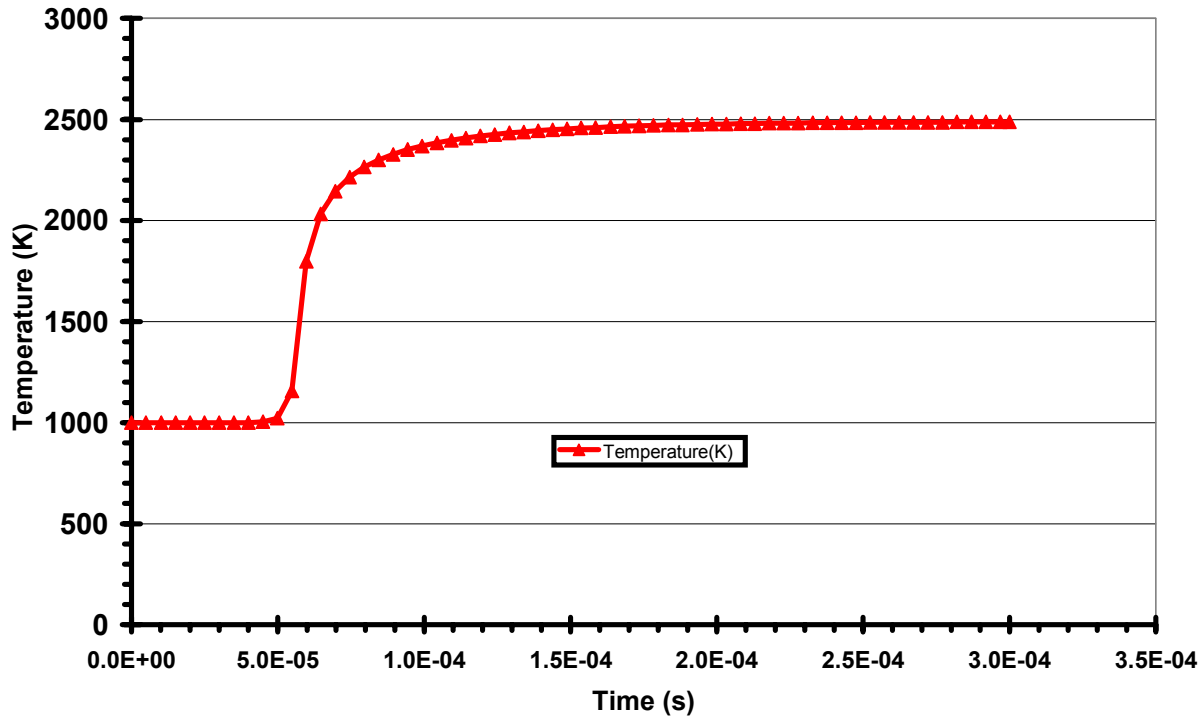
OH2.BAT - A very simple one line batch file that will run the above model producing the concentration profile equal to CONCOH2.TXT.

Note: OH.BAT runs the same exact model BUT at constant volume (variable pressure, the default in most models). Compare the two!

In addition, oh2f.bat uses the Chemkin thermodynamic database converted into **FREEFORM**! Examine the THERMFOH.DAT thermodynamic description spreadsheet.

Combustion of H_2 and O_2 at constant pressure Comparison of results at 3x 10^{-4} seconds						
	H_2	O_2	OH	H_2O	H	O
KINTECUS	1.80E-03	6.72E-01	3.02E-02	2.56E-01	1.04E-03	1.15E-02
CHEMKIN-II	1.79E-03	6.72E-01	3.07E-02	2.56E-01	1.03E-03	1.14E-02
Percent Difference	0.6%	0.0%	-1.5%	0.1%	0.9%	0.9%
	HO_2	H_2O_2	N_2	NO	N	Temp.(K)
KINTECUS	5.36E-05	1.50E-06	2.74E-02	2.10E-05	2.41E-09	2.49E+03
CHEMKIN-II	6.00E-05	1.52E-06	2.73E-02	2.17E-05	2.41E-09	2.49E+03
Percent Difference	-10.7%	-1.4%	0.2%	-3.2%	0.1%	0.0%


Combustion of H2 and O2 at constant pressure
Concentration (moles/cc)
1.E-05
1.E-06
1.E-07
1.E-08
1.E-09
1.E-10
1.E-11
1.E-12
1.E-13
1.E-14
1.E-15
1.E-16
1.E-17
1.E-18
1.E-19
1.E-20
0.0E+00
5.0E-05
1.0E-04
1.5E-04
2.0E-04
2.5E-04
3.0E-04
3.5E-04
Time (s)
H2
O2
OH
H2O
H
O
HO2
H2O2
N2
NO
N


Combustion of H2 and O2 at constant pressure
Temperature (K)
3000
2500
2000
1500
1000
500
0
0.0E+00
5.0E-05
1.0E-04
1.5E-04
2.0E-04
2.5E-04
3.0E-04
3.5E-04
Time (s)
Temperature(K)

GRI-Mech-3.0 Sample Runs

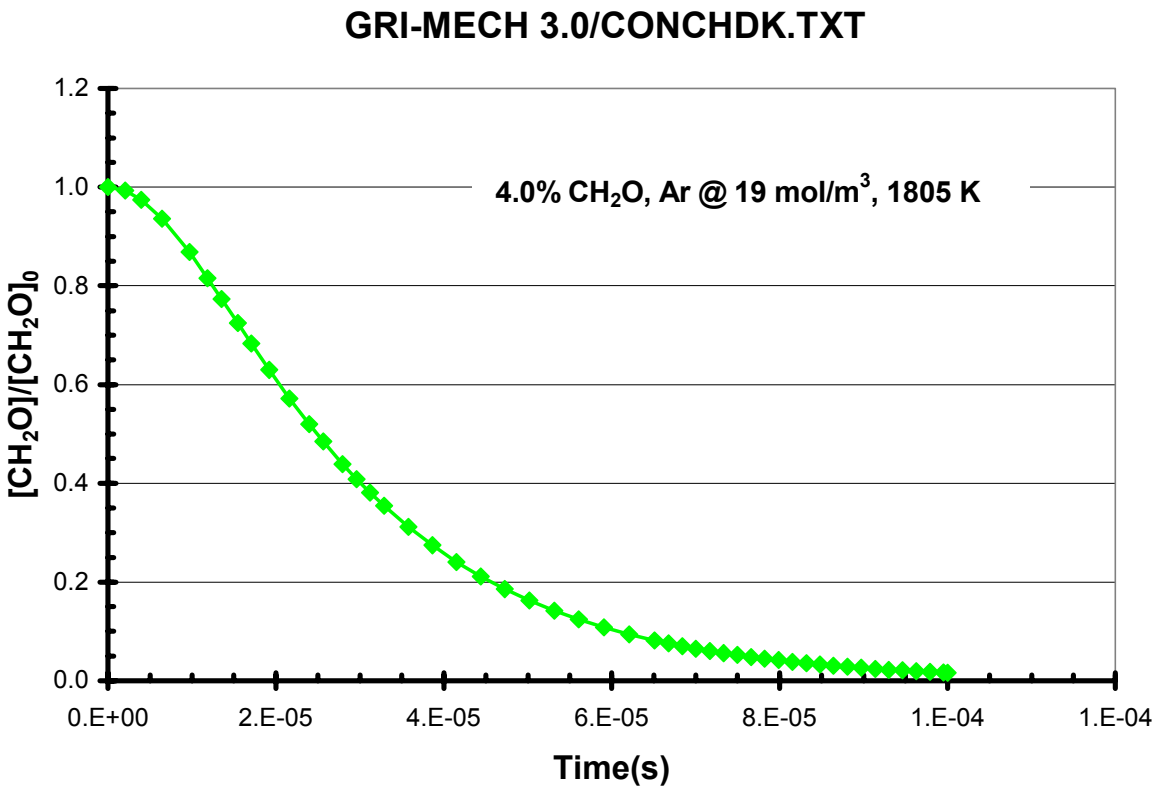
The GRI (Gas Research Institute)-Mech 3.0 mechanism is used by many research groups around the world for various combustion models. The chemical model MODGRI.DAT is a direct conversion from the Chemkin-II model. No alterations were made to the MODGRI.DAT once the CK2KIN program converted it. You can get more information on this fabulous model at http://www.me.berkeley.edu/gri_mech [19]. There have been many publish papers on experiments that have verified their chemical combustion mechanism using GRI-Mech. Examining the home page of GRI-Mech will show many, many references in journals (refereed and non-refereed), conferences and posters. You may wish to examine the following sample runs using GRI-Mech very closely. These models can also be executed by loading the Excel or Star-Office workbook: GRI_MECH_30.xls and then clicking the **RUN** button located on the CONTROL worksheet.

GRI-MECH RUN 4.0% CH_2O

The output concentration file, CONCHDK.TXT, matches the results by Hidka, et al [12] under the same conditions (4.0% CH_2O in Ar at 19.0 mole/m^3 and T = 1805 K). These models can also be executed by loading the Excel or Star-Office workbook: GRI_MECH_30.xls and then clicking the **RUN** button located on the CONTROL worksheet.

MODGRI.DAT - The kinetics reactions (Converted from the Chemkin-II/III GRI model using the CK2KIN.EXE program)
SPECHDK.DAT - The species involved
PARMHDK.DAT - The parameters used
THERMGRI.DAT – The thermodynamic description spreadsheet
CONCHDK.TXT - A simulation run.

grihdk.BAT - A very simple one line batch file that will run the above model producing the concentration profile equal to CONCHDK.TXT.

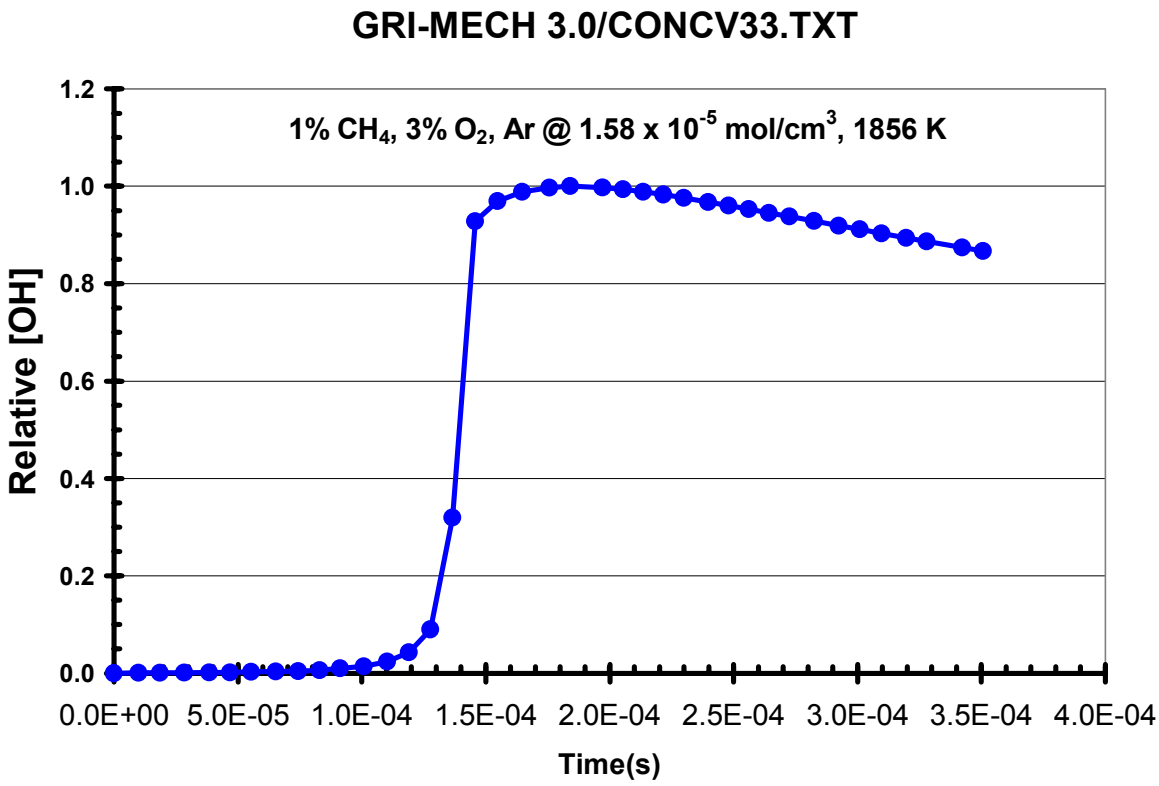


GRI-MECH RUN 1% CH_4 3% O_2

The output concentration file, CONCV33.TXT, matches the results by Yu, et al [13] under the same conditions (1% CH_4, 3% O_2 in Ar at 1.58 x 10^{-5} mole/cm^3 and T = 1856 K). These models can also be executed by loading the Excel or Star-Office workbook: GRI_MECH_30.xls and then clicking the **RUN** button located on the CONTROL worksheet.

MODGRI.DAT - The kinetics reactions (Converted from the Chemkin-II/III GRI model using the CK2KIN.EXE program)
SPECV33.DAT - The species involved
PARMV33.DAT - The parameters used
THERMGRI.DAT – The thermodynamic description spreadsheet
CONCV33.TXT - A simulation run.

griv33.BAT - A very simple one line batch file that will run the above model producing the concentration profile equal to CONCV33.TXT.

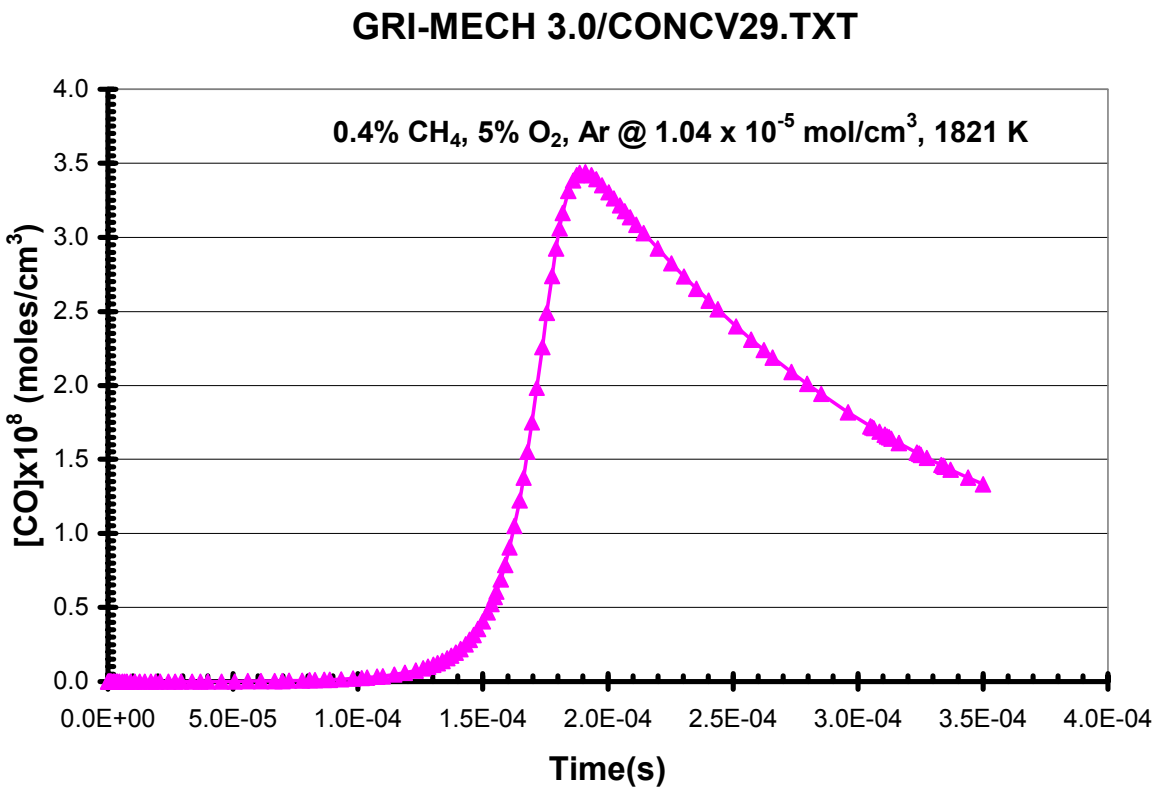


GRI-MECH RUN 0.4% CH_4 5% O_2

The output concentration file, CONCV29.TXT, matches the results by Yu, et al [13] under the same conditions (0.4% CH4, 5% O2 in Ar at 1.04 x 10^{-5} mole/cm3 and T = 1821 K). These models can also be executed by loading the Excel or Star-Office workbook: GRI_MECH_30.xls and then clicking the **RUN** button located on the CONTROL worksheet.

MODGRI.DAT - The kinetics reactions (Converted from the Chemkin-II/III GRI model using the CK2KIN.EXE program)
SPECV29.DAT - The species involved
PARMV29.DAT - The parameters used
THERMGRI.DAT – The thermodynamic description spreadsheet
CONCV29.TXT - A simulation run.

griv29.BAT - A very simple one line batch file that will run the above model producing the concentration profile equal to CONCV29.TXT.

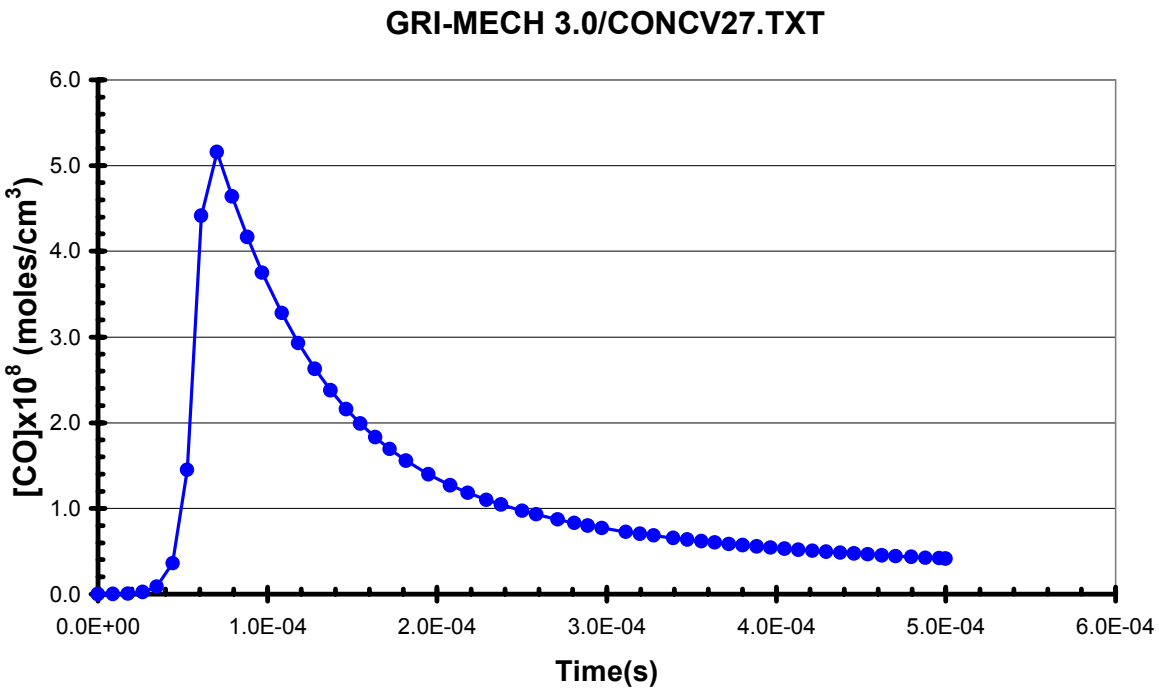


GRI-MECH RUN 0.4% CH_4 5% O_2

The output concentration file, CONCV27.TXT, matches the results by Yu, et al [13] under the same conditions (0.4% CH4, 5% O2 in Ar at 1.58 x 10^{-5} mole/cm3 and T = 1941 K). These models can also be executed by loading the Excel or Star-Office workbook: GRI_MECH_30.xls and then clicking the **RUN** button located on the CONTROL worksheet.

MODGRI.DAT - The kinetics reactions (Converted from the Chemkin-II/III GRI model using the CK2KIN.EXE program)
SPECV27.DAT - The species involved
PARMV27.DAT - The parameters used
THERMGRI.DAT – The thermodynamic description spreadsheet
CONCV27.TXT - A simulation run.

griv27.BAT - A very simple one line batch file that will run the above model producing the concentration profile equal to CONCV27.TXT.

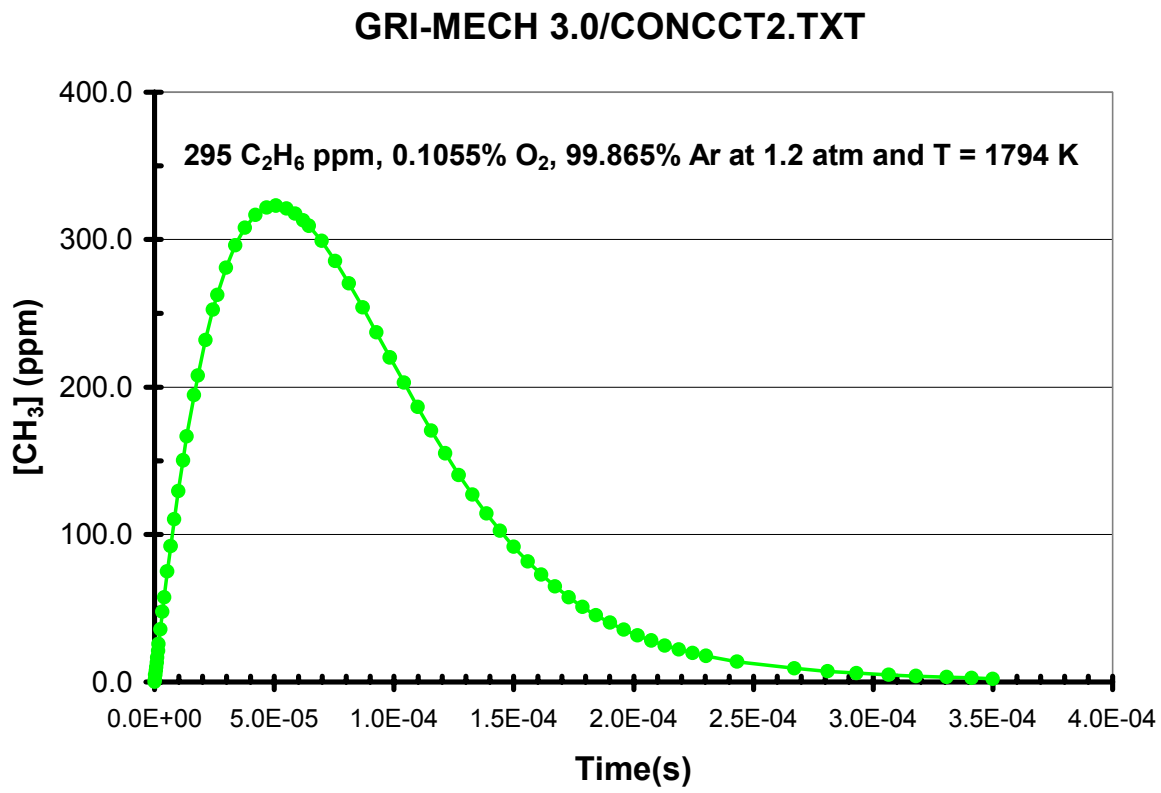


GRI-MECH RUN 295 C_2H_6 ppm, 0.1055% O_2, 99.865% Ar

The output concentration file, CONCCT2.TXT, matches the results by Chang, et al [25] under the same conditions (295 C_2H_6 ppm, 0.1055% O_2, 99.865% Ar at 1.2 atm and T = 1794 K). These models can also be executed by loading the Excel or Star-Office workbook: GRI_MECH_30.xls and then clicking the **RUN** button located on the CONTROL worksheet.

MODGRI.DAT - The kinetics reactions (Converted from the Chemkin-II/III GRI model using the CK2KIN.EXE program)
SPECCT2.DAT - The species involved
PARMCT2.DAT - The parameters used
THERMGRI.DAT – The thermodynamic description spreadsheet
CONCCT2.TXT - A simulation run.

grict2.BAT - A very simple one line batch file that will run the above model producing the concentration profile equal to CONCCT2.TXT.

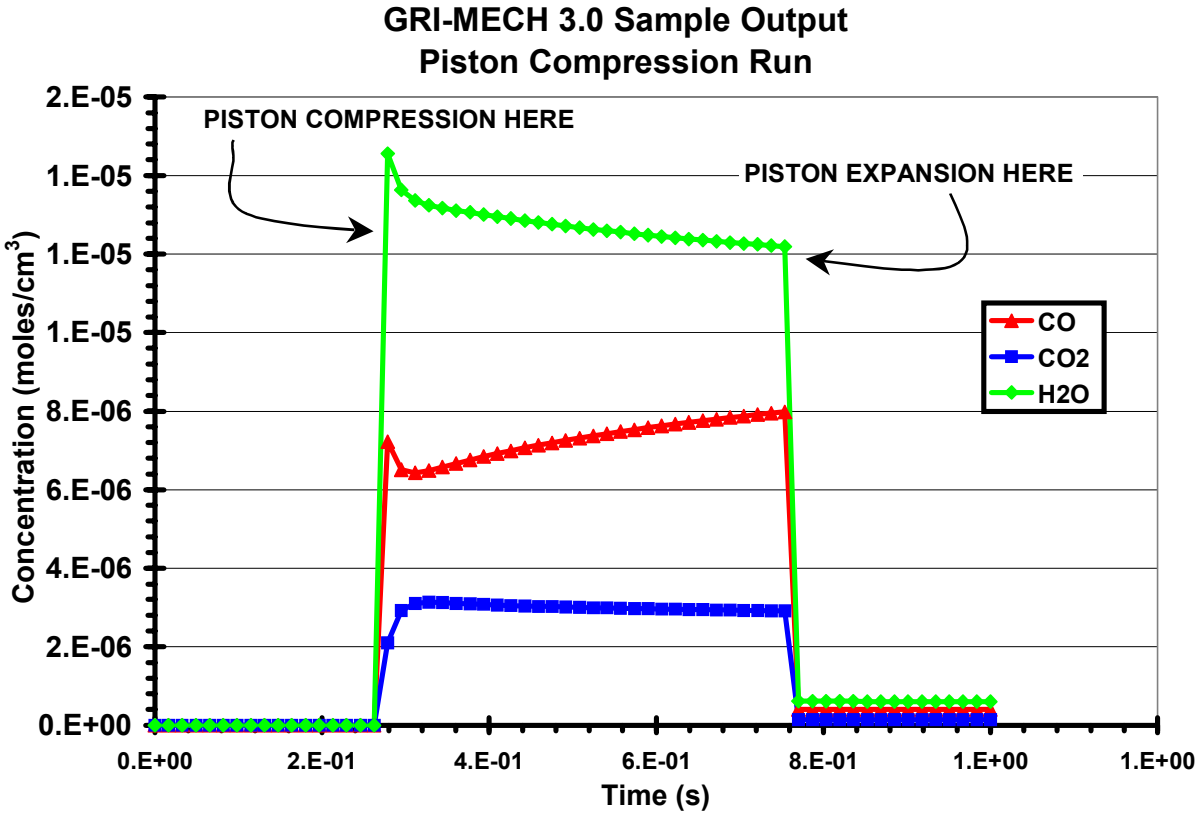


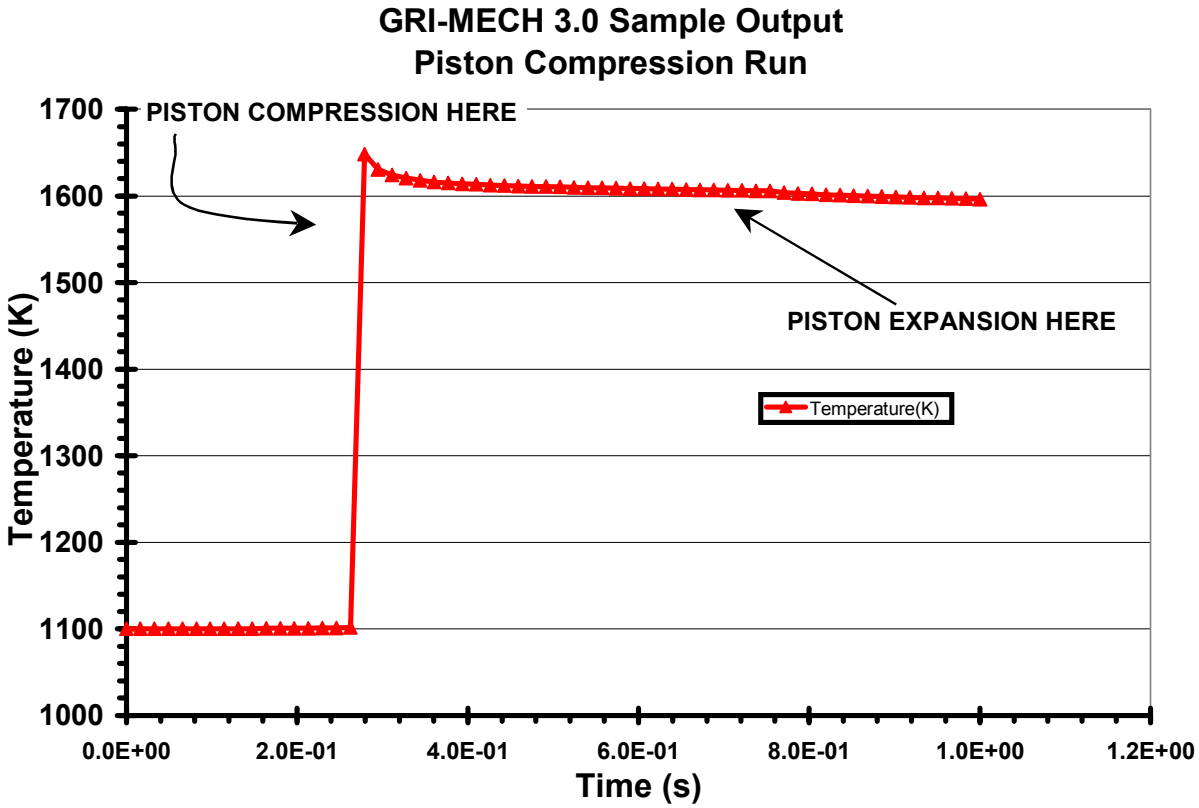
GRI-MECH PISTON COMPRESSION RUN

This sample run shows one how to use a volume profile to simulate piston compress on a chamber.

MODGRI.DAT - The kinetics reactions (Converted from the Chemkin-II/III GRI model using the CK2KIN.EXE program)
SPECPIST.DAT - The species involved
PARMPIST.DAT - The parameters used
THERMGRI.DAT – The thermodynamic description spreadsheet
CONCPIST.TXT - A simulation run.

gripist.BAT - A very simple one line batch file that will run the above model producing the concentration profile equal to CONCPIST.TXT.




GRI-MECH 3.0 Sample Output
Piston Compression Run
PISTON COMPRESSION HERE
PISTON EXPANSION HERE
Temperature(K)
Temperature (K)
1700
1600
1500
1400
1300
1200
1100
1000
0.0E+00
2.0E-01
4.0E-01
6.0E-01
8.0E-01
1.0E+00
1.2E+00
Time (s)

Ethanol Combustion Runs

The following three sample runs involve the combustion of ethanol at different starting conditions. The chemical model is a direct conversion of the Chemkin-II model. No alterations were made to the MODETH.DAT once the CK2KIN program converted it. These models can also be executed by loading the Excel or Star-Office workbook: Ethanol_Combustion.xls and then clicking the **RUN** button located on the CONTROL worksheet.

Ethanol Combustion Run 1

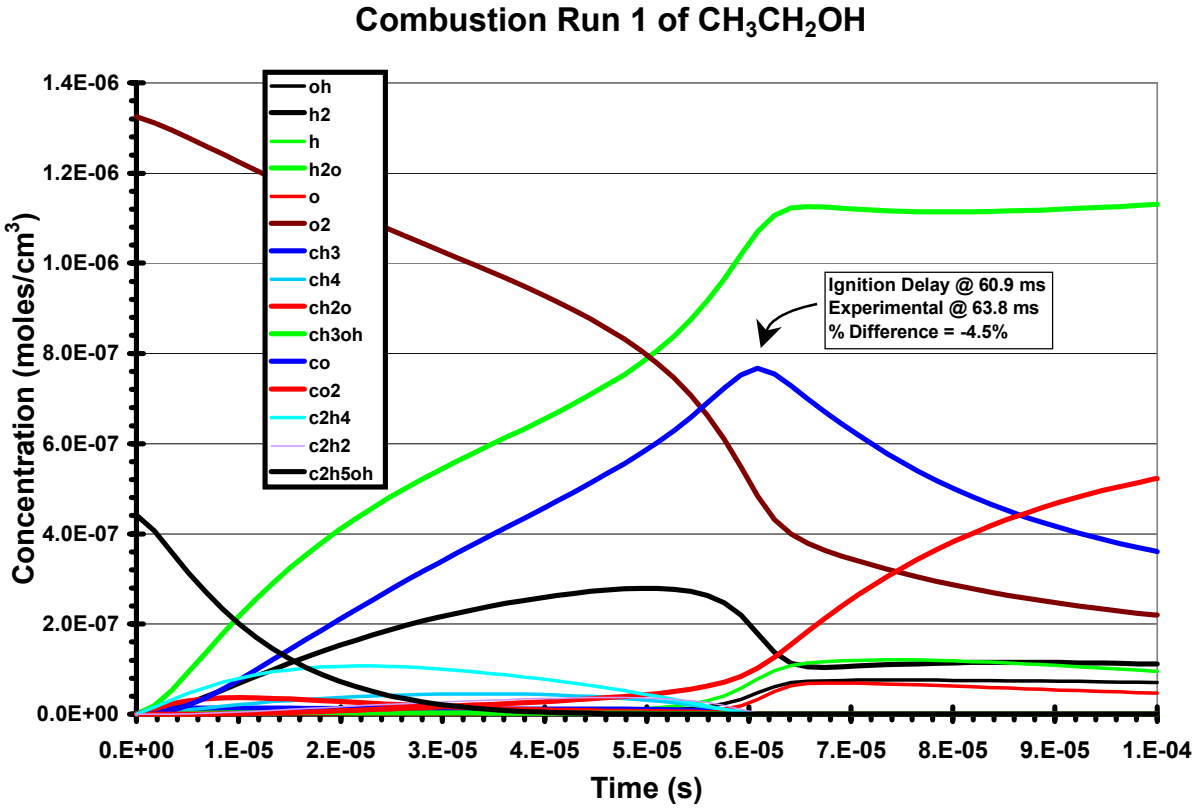
The ignition delay obtained from the output concentration file, CONCETH1.TXT, matches the experimental results given by Dunphy and Simmie [15]. Dunphy and Simmie correlated their experimental ignition times with the expression:

$$\text{ignition_delay(sec)}=1.0 \times 10(-14)\ \exp(15500\ K/T)\ [C_2H_5OH]^{-0.315}[O_2]^{-0.78}[Ar]^{0.259}$$

where the temperature is in Kelvin and all the initial concentrations are in moles/cm^3.

MODETH.DAT - The kinetics reactions (Converted from the Chemkin-II/III ethanol combustion model of Marinov [14] using the CK2KIN.EXE program)
SPECETH1.DAT - The species involved / PARMETH1.DAT - The parameters used
THERMETH.DAT – The thermodynamic description spreadsheet
CONCETH1.TXT - A simulation run.

ETHANOL1.BAT - A very simple one line batch file that will run the above model producing the concentration profile equal to CONCETH1.TXT. These models can also be executed by loading the Excel or Star-Office workbook: Ethanol_Combustion.xls and then clicking the **RUN** button located on the CONTROL worksheet.



Ethanol Combustion Run 2

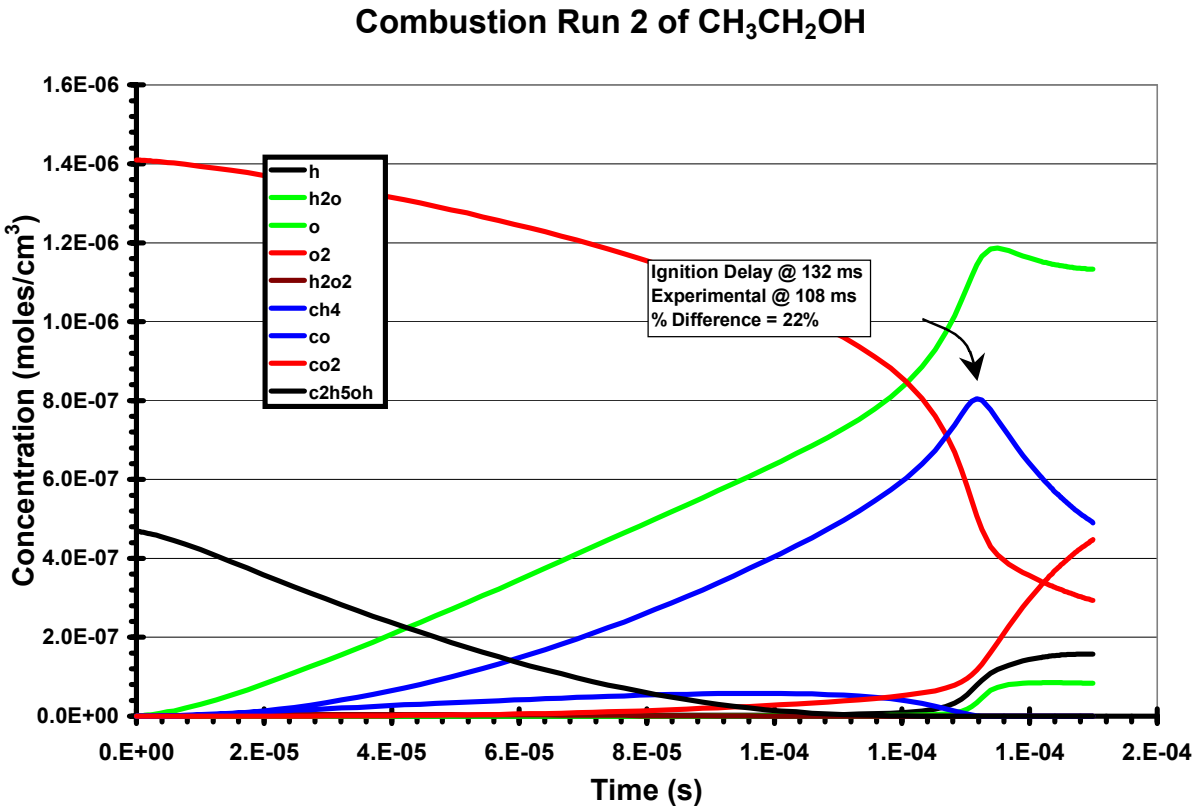
The ignition delay obtained from the output concentration file, CONCETH2.TXT, matches the experimental results given by Dunphy and Simmie [15]. Dunphy and Simmie correlated their experimental ignition times with the expression:

$$\text{ignition_delay(sec)}=1.0 \times 10(-14)\ \exp(15500\ K/T\ )\ [C_2H_5OH]^{-0.315}[O_2]^{-0.78}[Ar]^{0.259}$$

where the temperature is in Kelvin and all the initial concentrations are in moles/cm^3.

MODETH.DAT - The kinetics reactions (Converted from the Chemkin-II/III ethanol combustion model of Marinov [14] using the CK2KIN.EXE program)
SPECETH2.DAT - The species involved / PARMETH2.DAT - The parameters used
THERMETH.DAT – The thermodynamic description spreadsheet
CONCETH1.TXT - A simulation run.

ETHANOL2.BAT - A very simple one line batch file that will run the above model producing the concentration profile equal to CONCETH2.TXT. These models can also be executed by loading the Excel or Star-Office workbook: Ethanol_Combustion.xls and then clicking the **RUN** button located on the CONTROL worksheet.



Ethanol Combustion Run 3

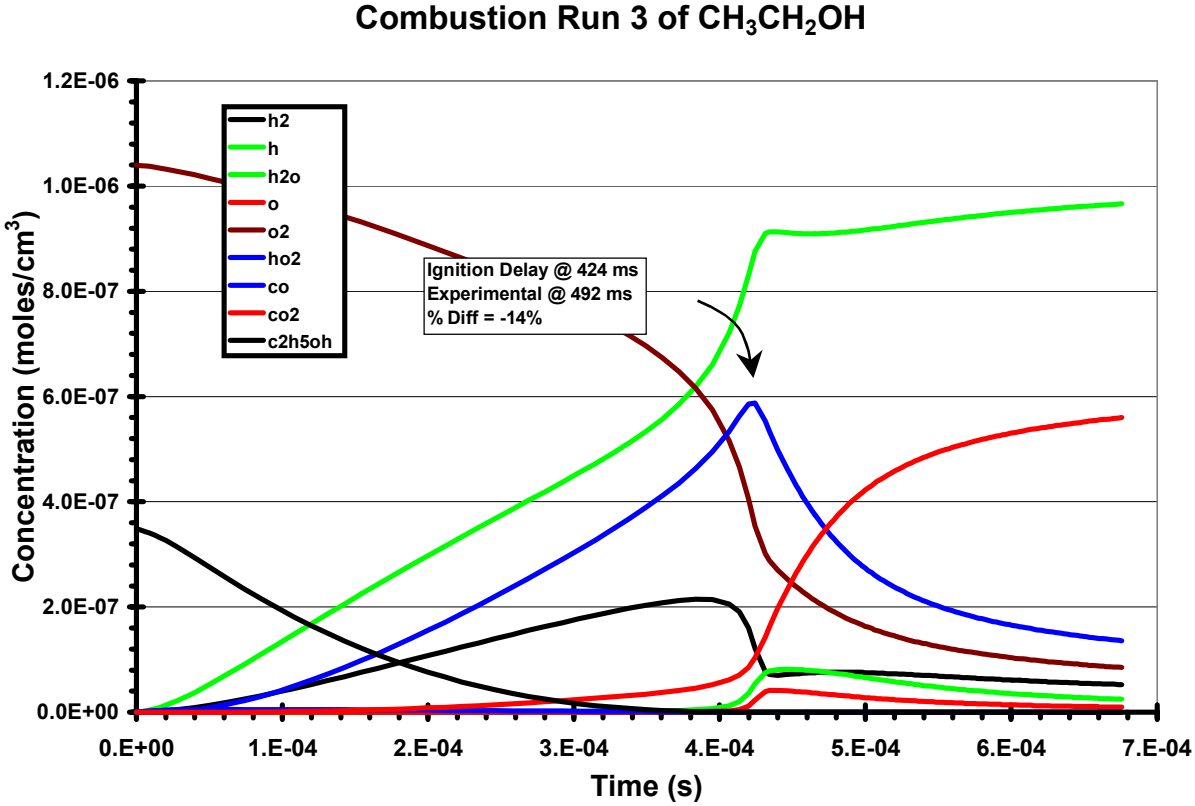
The ignition delay obtained from the output concentration file, CONCETH1.TXT, matches the experimental results given by Dunphy and Simmie [15]. Dunphy and Simmie correlated their experimental ignition times with the expression:

$$\text{ignition_delay(sec)}=1.0 \times 10(-14)\ \exp(15500\ K/T\ )\ [C_2H_5OH]^{-0.315}[O_2]^{-0.78}[Ar]^{0.259}$$

where the temperature is in Kelvin and all the initial concentrations are in moles/cm^3.

MODETH.DAT - The kinetics reactions (Converted from the Chemkin-II/III ethanol combustion model of Marinov [14] using the CK2KIN.EXE program)
SPECETH3.DAT - The species involved / PARMETH3.DAT - The parameters used
THERMETH.DAT – The thermodynamic description spreadsheet
CONCETH3.TXT - A simulation run.

ETHANOL3.BAT - A very simple one line batch file that will run the above model producing the concentration profile equal to CONCETH3.TXT. These models can also be executed by loading the Excel or Star-Office workbook: Ethanol_Combustion.xls and then clicking the **RUN** button located on the CONTROL worksheet.

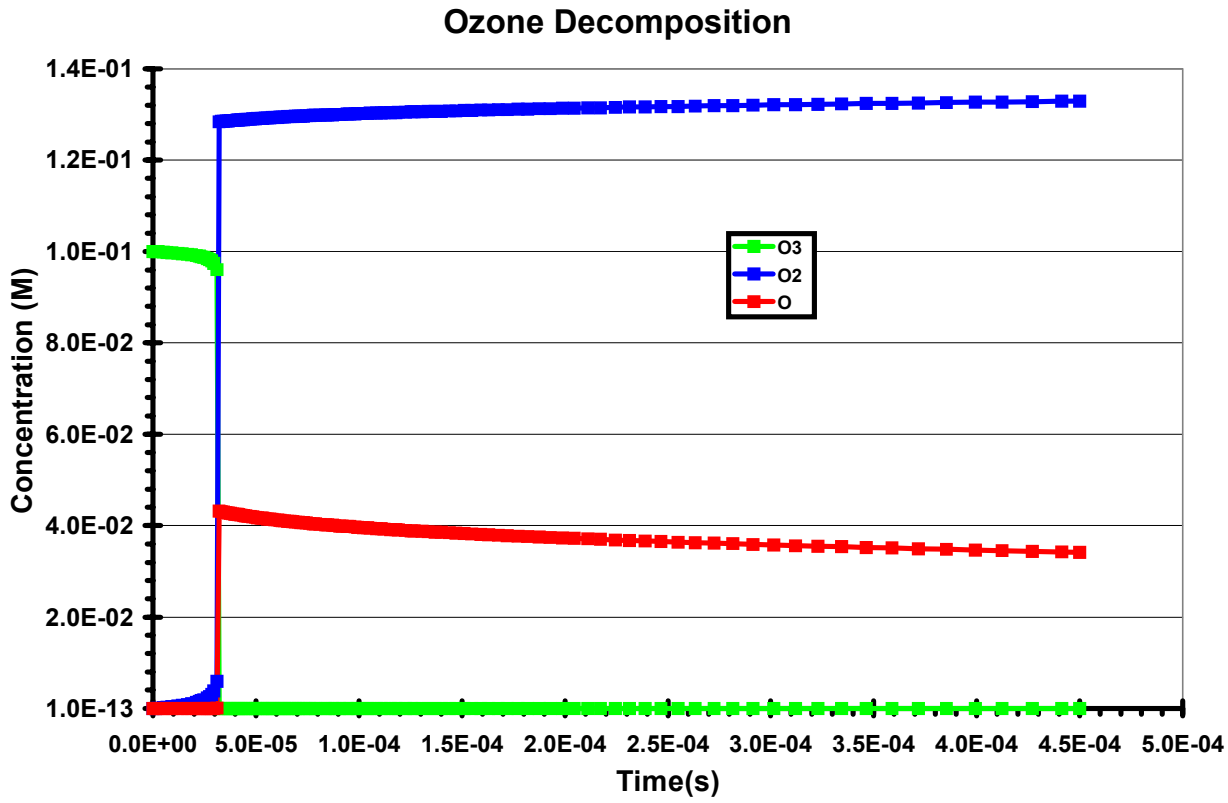


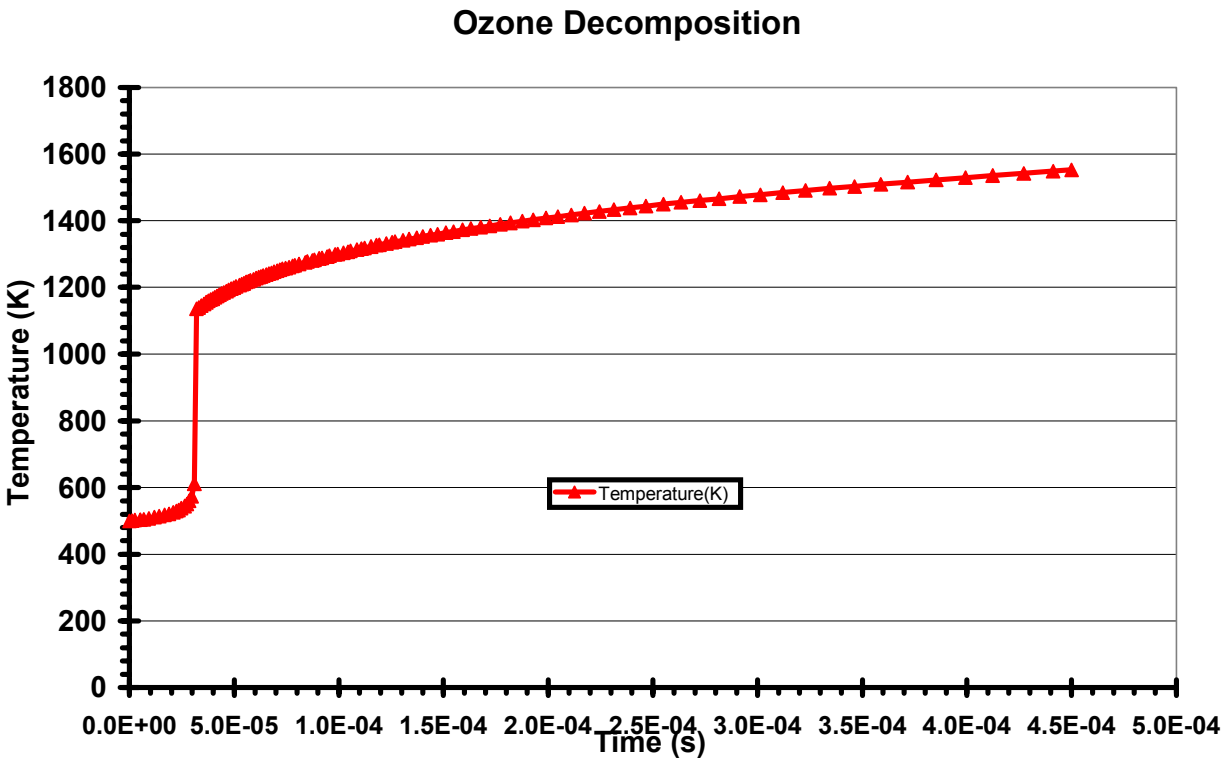
Ozone Decomposition

The concentration output file, CONCOZON.TXT, matches the sample ozone decomposition model in the CKS software[17].

MODOZO.DAT - The kinetics reactions
SPECOZO.DAT - The species involved
PARMOZO.DAT - The parameters used
THRMOZON.DAT – The thermodynamic description spreadsheet
CONCOZO.TXT - A simulation run.

OZONE.BAT - A very simple one line batch file that will run the above model producing the concentration profile equal to CONCOZON.TXT.



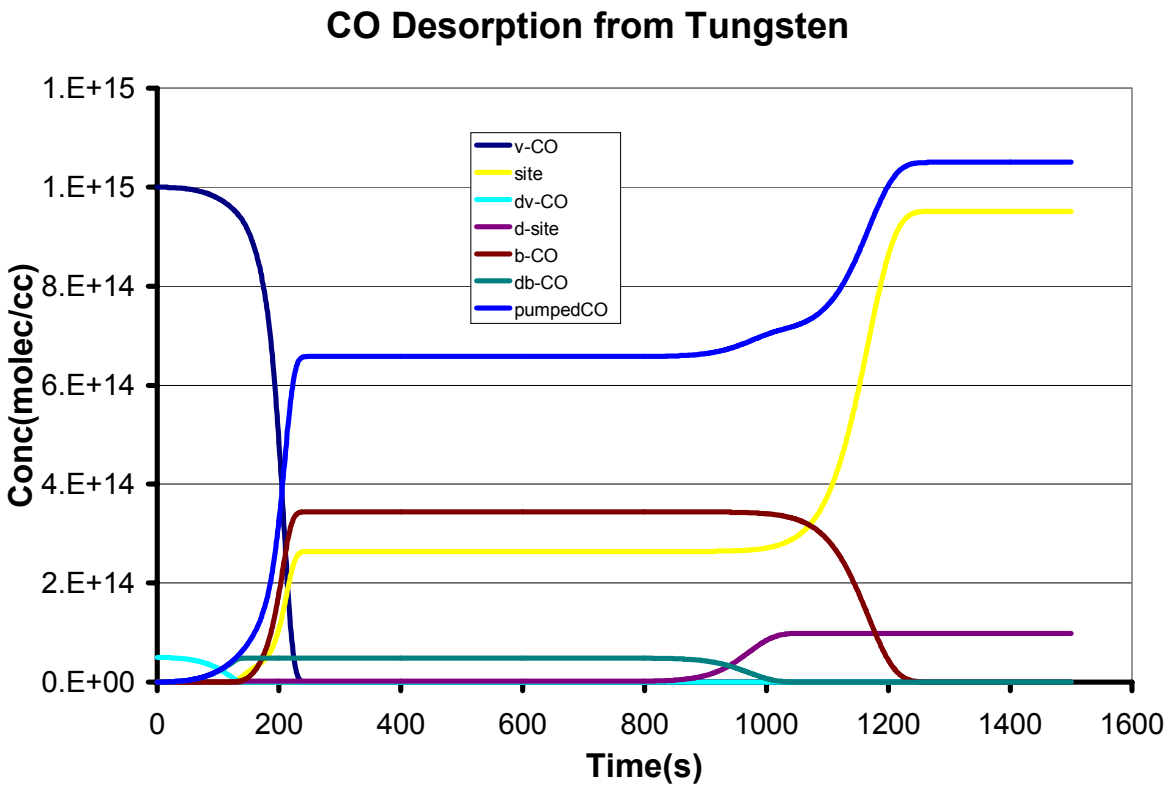

Ozone Decomposition
1800
1600
1400
1200
1000
800
600
400
200
0
Temperature (K)
Temperature(K)
0.0E+00
5.0E-05
1.0E-04
1.5E-04
2.0E-04
2.5E-04
3.0E-04
3.5E-04
4.0E-04
4.5E-04
5.0E-04
Time (s)

CO Desorption from Tungsten

The concentration output file, CONCWOLF.TXT, matches the plots in Houle and Hinsberg [16]. These models can also be executed by loading the Excel or Star-Office workbook: Wolfrum_with_Temp_Program.xls and then clicking the **RUN** button located on the CONTROL worksheet.

MODWOLF.TX2 - The kinetics reactions
SPECWOLF.TX2 - The species involved
PARMWOLF.TX2 - The parameters used
CONCWOLF.TXT - A simulation run.
TEMPPROF.TXT – A temperature program

WOLFRUM.BAT - A very simple one line batch file that will run the above model producing the concentration profile equal to CONCWOLF.TXT.



Isothermal 1-butene = cis-2-butene Isomerization

The results match with those calculated by hand using the values from the CRC Handbook of Chemistry & Physics[18]. **This one line model also shows the use of quotes surrounding species names that begin with a number, i.e. "1-butene". Do not surround the species name in quotes in the species description file!**

MODT1.TX2 - The kinetics reactions
SPECT1.TX2 - The species involved
PARMT1.TX2 - The parameters used
THERMT1.DAT – The thermodynamic description spreadsheet
CONCT1.TXT - A simulation run.

ISOBUT.BAT - A very simple one line batch file that will run the above model producing the concentration profile equal to CONCT1.TXT.

Isothermal 2 butene = cis-2-butene + t-butene

The results match with those calculated by hand using the values from the CRC Handbook of Chemistry & Physics[18].

MODBUT.DAT - The kinetics reactions
SPECBUT.DAT- The species involved
PARMBUT.DAT - The parameters used
THERMT1.DAT – The thermodynamic description spreadsheet
CONCBUT.TXT - A simulation run.

BUTENE.BAT - A very simple one line batch file that will run the above model producing the concentration profile equal to CONCBUT.TXT.

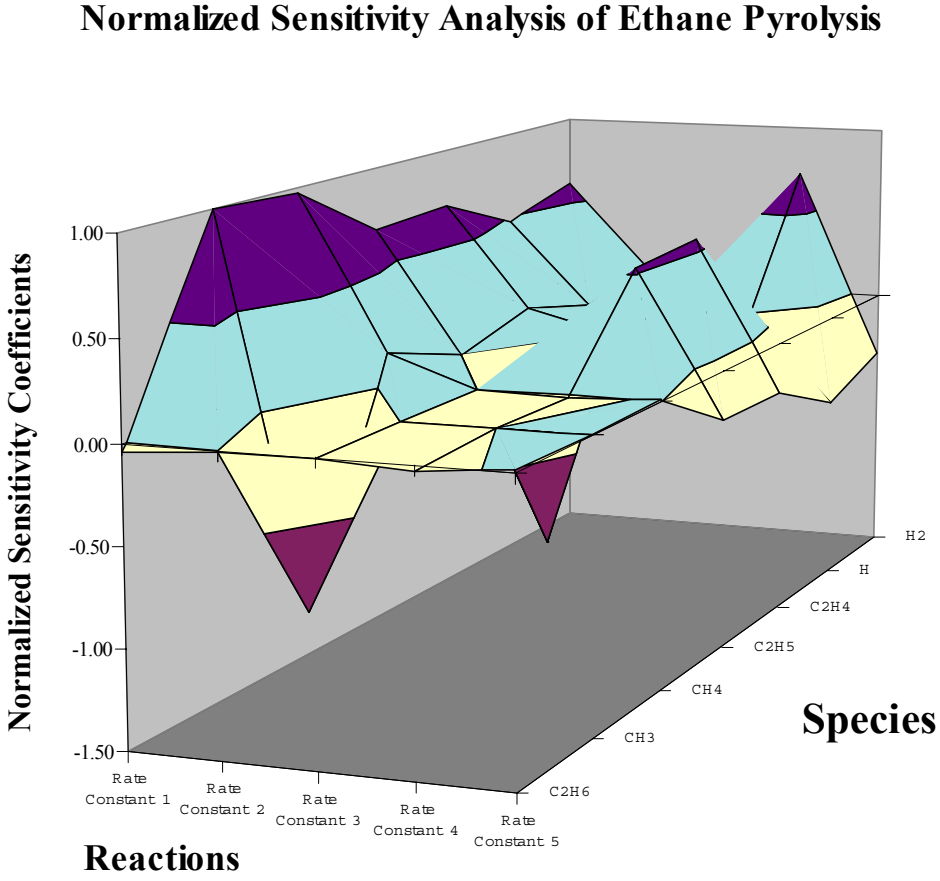
Sensitivity Analysis Sample Runs

Sensitivity Analysis of Ethane Pyrolysis

Output sensitivity analysis files 1SENSIT1.TXT and 1SENSIT2.TXT match TABLES I & II in the paper[8].

MODSEN1.TX2 - The kinetics reactions
SPECSEN1.TX2 - The species involved
PARMSEN1.TX2- The parameters used

SENSIT1.BAT - A very simple one line batch file that will run the above model producing the normalized sensitivity coefficient files equal to 1SENSIT1.TXT and 1SENSIT2.TXT.

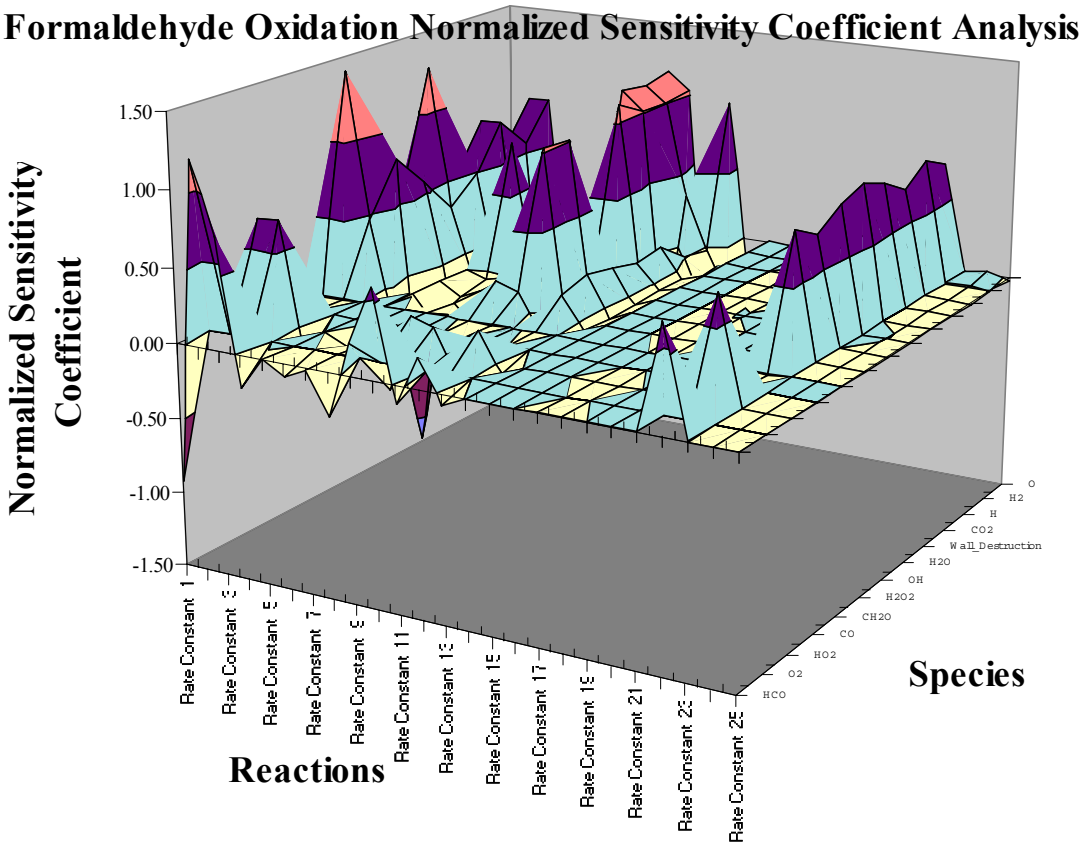


Sensitivity Analysis of the Oxidation of Formaldehyde Mechanism

Output the sensitivity analysis file 2SENSIT1.TXT, which will match TABLE IV in the paper [8].

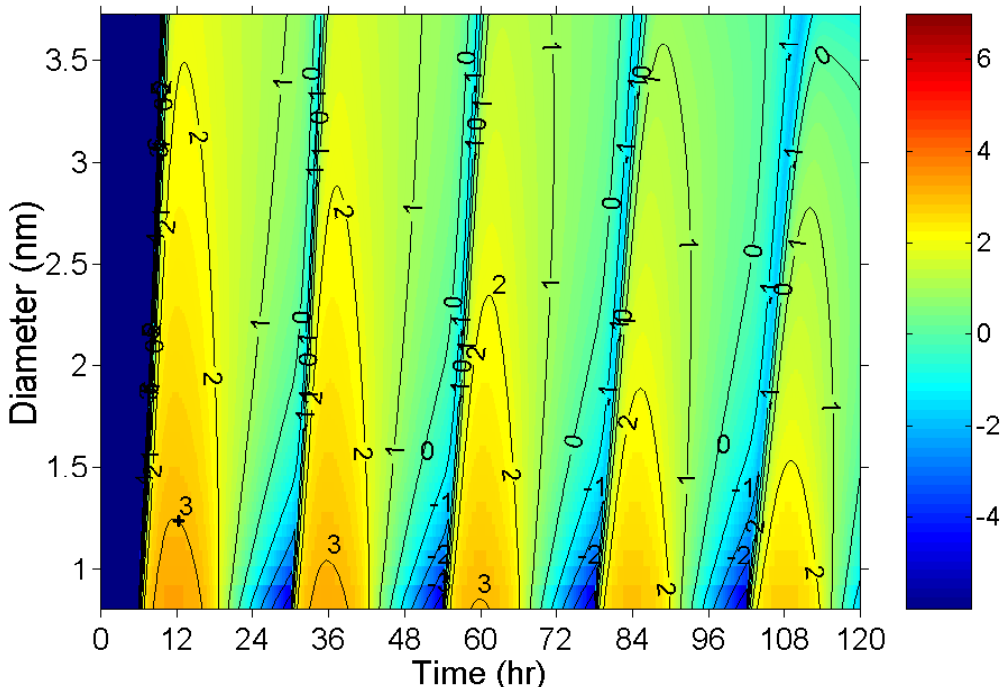
MODSEN2.TX2 - The kinetics reactions
SPECSEN2.TX2 - The species involved
PARMSEN2.TX2- The parameters used

SENSIT2.BAT - A very simple one line batch file that will run the above model producing the normalized sensitivity coefficient file equal to 2SENSIT1.TXT



Large Models

Kintecus can handle well over hundreds of thousands of reactions. The color contour plot below shows a kinetics run of over **120,000+** chemical reactions running for **several days (that is simulation time, NOT REAL-TIME)!** The model and concentration files were not included because of their extremely large size. The author can provide these reactions upon request. The thesis chapter 8 explaining the contour plot below and their experimental comparisons is included with Kintecus. The chapter also contains many other large example Kintecus simulation runs.



5. Fitting/Optimization

This section will explain how one can fit almost any numerical value (rate constants, initial concentrations, Troe factors, third body enhancements, energy of activation, starting temperature, etc.) against an experimental or "fabricated" dataset. One might wish to use fabricated datasets to optimize numerical values such as initial concentrations of species to values which would minimize the presence of some harmful intermediate species, maximize certain products, reduce/increase temperature and so on. Note that Kintecus will actually fit the parameters at EXACTLY the time your data was measured. Unlike other programs, Kintecus DOES NOT interpolate a function against your data and then fit the values against this interpolation. There is absolutely no need to "clean" your data, suggest interpolation methods nor specify timing meshes against your experimental data since Kintecus calculates values at exactly the times you specify in your experimental datafile.

The Fitting Procedure

Fitting Options

The fitting procedure in Kintecus can be specified with the inclusion of the –FIT switch on the command line. The –FIT switch has many options:

-FIT:a:b:c:d:e:f [:g:h:i]

FIT Switch Option	Description	Possible Values	Default Value
a	Fitting Algorithm	1, 2, 3	1
b	Comparison Operator	1, 2, 3	1
c	User Dataset Filename	Any allowed text filename	FITDATA.TXT
d	Tolerance	$1 - 10^{-14}$	1×10^{-7} for Fitting Algorithms 1 and 3 1×10^{-5} for Fitting Algorithm 2
e	Maximum Iterations Allowed	1 - 32767	9000
f	Starting Vectors	$1 \times 10^{-100} - 1 \times 10^{10}$	1×10^{-35}
g	Starting "Temperature"	$1 \times 10^{-100} - 1 \times 10^{10}$	1×10^{6}
h	Number of Cycles to Stay At Current Temperature Before Reducing Temperature	1 - 32767	25
i	Percent Temperature Reduction	0 - 0.99999	0.20 (20%)

Table 6. Options for the –FIT switch. Specifying a "D" on any option field will force Kintecus to use the Default Value.

The first three options (fitting algorithm, comparison operator, dataset filename) are the most important. Options d, e, and f can be used with all three optimization algorithms. Options g, h, and i are only for the Simulated Annealing fitting algorithm method 3. Specifying a "D" on any option field will force Kintecus to use the Default Value.

There are three fitting/optimization algorithms: 1=Mead & Nelder [23], 2=Powell [1] and 3=Simulated Annealing [24]. With each optimization algorithm, a user can choose from three comparison operators: 1=relative least squares, 2=standard least squares and 3=a proprietary function the author has devised. The comparison operators compare the experimental/fabricated data and the simulated data and respond back to the optimizer with a number showing this difference. Once the user chooses a fitting/optimization algorithm and comparison operator, he must then supply the experimental or fabricated data in a text file named FITDATA.TXT. The default filename, FITDATA.TXT, can be change to a user-defined filename. The only

requirements for the datafile is that “Time(s)” must be in the first column, first row, “END” must be in the first column last row, the measured/fabricated species names/Temperature(K) must be in the first row. The species names/Temperature(K) can be in any order on the first row. You can insert comments in this file or comment out lines by placing a “#” or a quote ‘ ” ’ as the first character on a line. If there is missing data point(s) for a species then the cell must have an UPPERCASE “N” as the first letter, so “NaN” or “None” or “Nothing” or just “N” are all allowed to represent no data at that time point. An example datafile (created in Excel, then saved as a TAB delimited text file) is shown below (this datafile is used in enzyme fitting test #4, FITTEST4.BAT) :

Time(s)	E	S	ES	EIS
3.55E+00	1.52E-09	5.90E-02	2.48E-09	1.38E-13
2.38E+01	1.62E-09	5.34E-02	2.38E-09	1.33E-13
5.33E+01	1.77E-09	4.56E-02	2.23E-09	1.24E-13
8.28E+01	1.94E-09	3.84E-02	2.06E-09	1.14E-13
1.12E+02	2.13E-09	N	1.87E-09	1.04E-13
1.42E+02	2.33E-09	N	1.67E-09	9.24E-14
1.71E+02	2.55E-09	N	1.45E-09	8.05E-14
2.01E+02	N	N	1.23E-09	6.83E-14
2.30E+02	N	N	1.01E-09	N
2.60E+02	N	N	8.13E-10	N
2.89E+02	N	N	6.33E-10	N
.	.	.	.	.
.	.	.	.	.
.	.	.	.	.
1.65E+03	4.00E-09	N	4.39E-14	N
1.68E+03	4.00E-09	N	4.39E-14	N
1.71E+03	4.00E-09	N	4.39E-14	N
1.74E+03	4.00E-09	N	4.39E-14	7.31E-16
1.76E+03	4.00E-09	N	4.39E-14	7.31E-16
1.80E+03	4.00E-09	N	4.39E-14	7.31E-16
END				

Table 7. Sample user supplied spreadsheet containing experimentally obtained data ready for fitting.

The Fit Switch Option d is the optimization tolerance. This tolerance sets the minimum value between successive fits that must be met before the data is considered optimized. Decreasing this value will cause more optimizations (longer execution time but numbers that are more accurate) to be performed. Conversely, increasing this value will cause less optimizations (shorter execution time but numbers that are less accurate) to be performed. It is very important to note that the tolerance is a minimum threshold needed to stop optimization when successive fits (compares between the data and simulated data) falls at or below this value. If the data and simulated data falls at or below the tolerance, the optimization will halt even if the data-simulated comparison is **terrible** (very large difference). In other words, just because Kintecus states that optimization is finished, there is a good chance it has not. Kintecus had to stop the optimization because the program was going in circles (trapped in a local minimum) and

that the user should try another optimization method, comparison operator or a different starting guess(es). For more help, see the Optimizing Tips section below.

Optimization algorithm #2 (Powell method) is fairly sensitive to the tolerance. It is suggested that you do not set a value above 1 x 10(-5). Setting smaller values (under 1 x 10(-8)) can result in a substantial longer optimization run in some cases. Optimization algorithms #1 and #3 are more insensitive to the tolerance than the Powel method.

The Fit Switch Option **e** set the maximum iterations allowed. If the number of optimizations reaches this value, the program will quit. Please note that the average amount of optimization iterations for just two values is between 400-1200 optimizations at a tolerance of 1 x 10(-6).

The Fit Switch Option f sets the starting vectors. The optimization of values, N, is actually an optimization of starting vectors of size, N, in vector space N (or N+1 for the fitting algorithms #1 and #3). Consult references for a full explanation.

The Fit Switch Options g, h and i are for the Simulated Annealing Optimization method #3. The g option is the starting "Temperature", this is NOT the physical, real thermodynamic temperature of the system, but an analogy to a starting data "cooking" temperature. Refer to references for a full explanation. Option h is the actual "annealing" or "cooking" time in cycles. It is also the number of simulations to be performed before the data "temperature" is reduced by a percent represent by Fit Switch Option i.

There are many examples (examine the various Kintecus command line options in the .BAT files) in the FITTESTS sub-directory demonstrating various parameters and models that Kintecus can fit data to.

What and How Can I Fit/Optimize ?

Selection of numeric parameters for fitting/optimization can easily be done simply by appending the number (actually your guess) with a question mark, "?". The sample model spreadsheet below (See **Enzyme_sheet.xls** in the **FITTESTS** sub-directory, this model is actually run with FITTEST4.BAT) shows three rate constants that have been selected for fitting. These models can also be executed by loading the Excel or Star-Office workbook: Enzyme_Regression_Fitting.xls and then clicking the **RUN** button located on the CONTROL worksheet. (note the **extremely poor guesses**! But Kintecus actually obtains the exact answer that is **orders of magnitude away**!):

# Non-competitive Inhibition # of an enzymatic reaction	
# Example spreahsheet. You can see comments by moving pointer above the red triangles # *Note, if you wish to use this model with KINTECUS, be sure to save # it as a Text Tab Delimited sheet, and don't forget to also save it # as a regular Excel spreadsheet or you lose all your formatting and notes!!	**Equilibrium Constants**
1? E+S==>ES **1?** ES ==> E+S	75
1? E+I==>EI 112687259.7 EI==>E+I	0.07543
9.57E+06 ES+I==>EIS 3782608.696 EIS==>ES+I	2.53
5.53E+07 EI+S==>EIS 3.09E+06 EIS==>EI+S	17.87
7.13E+06 EI+P==>EIS 2.01E+05 EIS==>EI+P	35.5
1.14E+05 ES==>E+P	

END

One can fit initial temperature, initial concentration, external concentration, flux, rate constant, Arrhenius factor, energy of activation, and any parameters for Troe, Lindemann, SRI, Landau-Teller and third body enhancement factors. There are sample batch files, **FITTESTx.BAT**, located in the **FITTESTS** subdirectory. These sample batch files when run will fit various parameters to various data. Some use different –FIT options, such as larger tolerance settings (-FIT switch option 'd' in Table 5 above) which cause the optimization to finish much quicker. You can examine the one line Kintecus call in those files and modify them.

Once Kintecus is finished optimizing your parameters, it will write a file name **optout.txt** in the current directory. This file will contain the final optimized results, the final data to simulation difference and the total amount of iterations. These values are also duplicated to the screen. In addition the output concentration file, CONC.TXT will contain the concentrations/temperature for the final optimized model. You should plot this file, CONC.TXT against your experimental data and compare them. Note that the heading for CONC.TXT is not present, but it is stored in the file HEADINGS.TXT, which can be inserted at the top of the CONC.TXT file. Since most, if not, all the time series in CONC.TXT should line up with your experimental values, you should be able to easily plot the residuals (your data minus the simulated data) and see if the residuals are small and "noisy", this indicates a good fit.

Some Tips To Quickly Start Optimizing

Once you have saved your data in a text file named FITDATA.TXT (this is the default name for your datafile Kintecus looks for, you can name it to another filename by using the –FIT switch). You can quickly get started by using the –FIT:2:3:FITDATA.TXT switch on the Kintecus Command line. **ALSO** try –FIT:1:3:FITDATA.TXT on the Kintecus Command line and compare the results. In addition you should also re-run with the –FIT:1:1:FITDATA.TXT and also the –FIT:2:1:FITDATA.TXT and compare all four sets. Be prepared, optimizing more than one value can take some time.

Optimizing stiff reactions such as a combustion model can be quite challenging. You will most likely get OVERFLOW ERRORS. This is due to the optimizer picking values that are making the system stiffer than where it started. A quick solution is to reduce the accuracy in the parameter spreadsheet to 1/100, 1/1000 or even 1/10,000 of the current accuracy value. You should end up with an accuracy in the range of 1 x 10(-8) to 1 x 10(-12). Another problem with optimizing combustion models is that the optimizer might put the system where the temperature is too high (or low) for one or more species' thermodynamic coefficients' range. An additional option has been provided for the –THERM switch: **FORCE**, ie. -THERM:THERM.DAT:FORCE or –THERM:D:FORCE . This will "force" the optimizer **AND** the integrator to use temperature values that are within all the species' thermodynamic coefficients' range and should alleviate your OVERFLOW problems.

Be Careful!

Just because you managed to get a great fit to your data and it passes every statistical test you can throw at it, the fitted values can be COMPLETELY WRONG! This can be especially true when you are fitting more than one value. For example, if a user tried to optimize all three expanded Arrhenius options at the same time at one temperature. Depending on your starting guess, one user might get A=9.20E+16, m=-0.6 and an E_a=1.1841 KJ, but another user might get A=1.10E+15, m=0.588, E_a=2.57 KJ and at 298 K both sets yield the overall rate constant 4.08 x 10(14)! Who's right? That depends on further molecular detail on the system. Can E_a be estimated and frozen in the optimization ? Maybe the Arrhenius factor can be calculated or referenced from literature and frozen during the optimization? Maybe you should just optimize k, and forget about the three expanded Arrhenius parameters? Other examples can be shown! Be careful!

FASTSTART

This section is for people who do not read or even scan the main documentation. If you still cannot run your model after following the below short procedure then you should read the tutorial in the first section of the documentation.

1) Go into command mode (on the Windows start button select RUN, type "command" and press the <ENTER> key) and create a file named MODEL.DAT. If you have Excel97/2000/XP or Sun Microsystem's FREE Star-Office you can use the *blank* **Kintecus_workbook.xls** or **Enzyme_Regression_Fitting.xls** or **GRI_MECH_30.xls** EXCEL Visual Basic graphical interface modules and click the **MODEL tab** located at the bottom. If you use a text editor than enter your reactions like so:

```
1.323e-4, A- + Widget-- + C==>G+++ + F---+H20
3.2     , E+F ==> G + DNA_A_Replicated
54.34   , G = A
END  ( <==-- Make sure this END is here)
```

If you have Arrhenius expressions, then do your reactions like this (make sure you specify the correct Energy of Activation units in the parm.dat spreadsheet, look for the Ea Units field and type either Calories, Cal, Joules, J, KJ, KCAL or Kelvin:

```
1.323e-4, -1.2, 3000, A- +Widget-- + C==>G+++ + F---+H20
3.2     ,  0.3, 2000, E+F == > G + DNA_A_Replicated
54.34   , 2.1,5430, G = A
END  ( <==-- Make sure this END is here)
```

2) Run Kintecus with the following switch: >Kintecus –c
(**EXCEL**: click the **"Make Species Worksheet from Model" button** located on the **CONTROL** worksheet)

3) Now copy the created ADDSPEC.TXT file as a SPECIES.DAT file
(ie. >COPY ADDSPEC.TXT SPECIES.DAT)

4) Edit the Initial concentration fields in species.dat for your model and type "Y" in the DISPLAY field for species' concentrations you want to save. (**EXCEL:** click the **species tab** located near the bottom and then edit the same fields in the species worksheet)

5) Run kintecus: >KINTECUS -ig:mass -show. (**EXCEL:** click the **CONTROL tab** located near the bottom and then click the **RUN button** to start your model!)

6) If you are using the EXCEL modules, on the **CONTROL** worksheet, click the **Plot Results** button to plot your results!

7) ***OPTIONAL:*** If you wish to do include thermodynamics (temperature and reverse rate autocalculations), just use the –THERM switch on the command line.
8) ***OPTIONAL:*** If you wish to do sensitivity analysis just use the –SENSIT:1 on the command line.
9) ***OPTIONAL:*** If you wish to FIT experimental data to a model, have your data in a text file named, FITDATA.TXT with Time(s) as the first column, first row. The species names should follow the Time(s) heading on the same row. Place your species/temperature data under the appropriate species column (if a species is missing data for a time point, place an "N" in the cell). Append a question mark, "?", to the end of ***any number*** you wish for Kintecus to regress/fit. Run Kintecus with –FIT:2:3:FITDATA.TXT. You can also try –FIT:1:3:FITDATA.TXT , -FIT:1:1:FITDATA.TXT and –FIT:2:1:FITDATA.TXT .

Errors, Warnings and Convergence Problems

This file explains each Fatal and Warning message you may receive when running a simulation. In addition, it is quite possible to obtain errors in which Kintecus cannot catch.

Some errors list the line to screen and the source line. The source line is the actual line number in the original file that is giving Kintecus trouble. If you have many warnings/errors that scroll by on the computer screen too fast you can pause the listing by pressing the Pause/Break key and resuming by pressing the Enter key, or you can output everything that normally goes to the screen to a file by using redirection such as: Kintecus -show -PARM:C/FL/P1.TXT > View.txt .All screen output can be seen in the file view.txt using a text editor.

Errors That Can Not Be Caught by Kintecus

These are mainly math processor errors that are displayed by the operating system.

Hanging

Windows 95 and higher users should not have any 'Hanging' problems. Windows 3.11 or MS-DOS users using the PHAR-LAP 32-bit version of Kintecus might have these hanging problems. What is 'Hanging'? Kintecus just stops and does nothing, you can't quit the program.

To eliminate most of them, IT IS VERY IMPORTANT THAT THE VERY LAST LINE OF ALL THE INPUT FILES HAVE A CARRIAGE RETURN (Press the ENTER key)! The Model Spreadsheet, the Species Description Spreadsheet, the Parameter Spreadsheet and the Species Name Spreadsheet should all end with END + Carriage Return. It is possible for Kintecus to detect the end of a file has been reached without the explicit END at the end, but strangely there are a few occasions when it won't 'see' it and the program hangs. Also make sure if you have any concentration profile files that the last line that has a number on it has a Carriage Return and only one carriage return. You should be able to see what file is causing Kintecus to hang by following the screen output on where Kintecus is in reading and parsing files.

Overflows, Underflows, Division by Zero, Singularities, Domain Errors

Kintecus quits and reports some error with one of the above following words.

To eliminate these errors:

1) ***Make sure you entered in the initial concentrations for relevant reactants. If all the reactants have an initial concentration of zero then this will cause problems.***

2) ***If you are sure you've done that than it's very likely you have a very stiff system of reactions so you must first make sure the value in the Minimum Integration Field has a value of 1 x 10(-7) or smaller then decrease the number in the Accuracy field in the Parameter Spreadsheet file. Decrease it by ten and try again, keep trying until the Accuracy is around 1 x 10(-13). If you still get errors, it's likely that your system of reactions is not mass or charge balance.***

3) ***Try to eliminate any mass or charge balance warnings.***

4) ***If you did and you still have these errors, make sure your equations make sense, i.e. A==> A is a meaningless reaction.***

5) ***If your reaction scheme consists of thousands of reactions you could be experiencing large round-off error, try using the analytically calculated Jacobians by using the -anjac program switch. The -anjac switch used on the command line will force Kintecus to calculate Jacobians analytically instead of trying to approximate it by finite difference.***

6) ***Try a different integrator through the –INT switch i.e. Kintecus –INT:2.***

For **combustion reactions or systems using thermodynamics** you can try this additional recommendations:

7) *****NEW: If you are using the "-THERM" switch, ie, you are doing a combustion reaction, append :FORCE to the end of the –THERM switch like so –THERM:THERMO.DAT:FORCE . This will force the integrator to stay within the temperature limits of the thermodynamic coefficients of all the species.***

8) ***If the thermodynamic coefficients in the thermodynamic database have a very narrow temperature range (the low temperature and high temperatures) for a species can cause possible problems. Can the simulation be started with a different temperature, starting concentration? Can you get new coefficient values that have a broader range for that species?***

Common Fatal Error Messages

These severe errors when encountered will not allow the simulation to run. These errors must be corrected.

Fatal Error #1

```
No data fields in (filename).
Make sure data delimiters (comma, TAB, etc.) are'
in (filename)  and/or the correct data delimiter is'
set. If you haven't set it, then by default a TAB'
is used to separate fields.
Use the -d option to change this (Type Kintecus ?).
```

Explanation:
Kintecus will try to figure out what data delimiter you are using. It will try TABS, commas, semi-colons, colons and '|'. If you are not using any of those characters to delimit your data please do so. Do not use a space to
delimit your data!

Fatal Error #2

```
'ERROR!, MORE THAN (number) COLUMNS OF DATA IN '
  (filename)
```

Explanation:
You are using a data delimiter, which is part of the field data. You can not use TABS, commas, colons and '|' as part of a field, these characters are only used for data delimiters. Do not use a space to delimit your data! Spaces are ignored by Kintecus in all data spreadsheets!

Fatal Error #3

```
NO DATA DELIMITERS FOUND IN (filename)
Make sure data delimiters (comma, TAB, etc.) are'
in (filename) and/or the correct data delimiter is'
set. If you haven't set it, then by default a TAB'
is used to separate fields. '
Use the -d option to change this (Type Kintecus ?).'
```

Explanation:
Make sure you are using either a TABS, commas, colons and '|' as a data delimiter. You can not use a space as a data delimiter. Spaces are ignored by Kintecus in all data spreadsheets!

Fatal Error #5

```
The hv energy output file (filename)
does not exist. Please correct.'
```

Fatal Error #6

```
Too many data items in (filename)
on a line. Make sure the Data Separator in your '
file is a valid ASCII Separator.'
```

Explanation:
Make sure you are using either a TABS, commas, semi-colons, colons and '|' as a data delimiter. You can not use a space as a data delimiter. All spaces are ignored by Kintecus. There may be extra data delimiters accidentally put at the end of the line.

Fatal Error #10

```
Duplicate species found in (filename)
has duplicate! Please correct.'
```

Explanation:
Remove one of the duplicates you entered.

Fatal Error #11

```
Concentration profile file:(filename)
 can not be loaded. Please correct.'
```

Fatal Error #14

```
Ill-formed reaction line in the model description'
file :(filename)
Remember to use ''==>'' to represent ''produces''
on a reaction line. Check for other possible errors.'
```

Fatal Error #15

```
Missing Reactant/Product on reaction line'
in (filename) Please correct.'
```

Fatal Error #21

```
You have exceeded the maximum number of species'
```

```
allowed in this version of Kintecus.'
(Number)
```

Explanation:
If you need this to be larger, email the author. For the disabled shareware version, buy the registered version (see Registration) which allows a very large amount.

Fatal Error #22

```
You have exceeded the maximum number of reactions'
allowed in this version of Kintecus.'
```

Explanation:
If you need this to be larger, email the author. For the disabled shareware version, buy the registered version (see Registration) which allows a very large amount.

Fatal Error #23

```
You have exceeded the maximum number of times a'
species can appear as a reactant/product in each'
reaction in this version of Kintecus.'
```

Explanation:
If you need this to be larger, email the author. For the disabled shareware version, buy the registered version which (see Registration) allows a very large amount.

Fatal Error #24

```
An illformed reaction line has been found '
in (filename) !!'
Remember to place charges on species on the'
right-hand side, i.e. Cl+++ .'
Remember to use ''==>'' to represent ''produces'' '
on a reaction line. Check for other possible errors.'
```

Fatal Error #28, 29

```
Not a valid species name in (filename)
(invalid species name)
```

Explanation
You can not use TABS, commas, semi-colons, colons and '|' as characters in your species names, nor can you use the characters

Fatal Errors #30, 31, 32

```
Species description file (filename),  or parameter description
file (filename)
Model description file (filename)
CAN NOT BE FOUND !!!!'
Make sure the file exists and/or is in the correct'
directory. (Usually the same directory as KINTECUS.)'
```

Fatal Error #33

```
Thermodynamic description file (filename)
CANNOT BE FOUND !!!!
Make sure the file exists and/or is in the correct
directory. (Usually the same directory as KINTECUS.)
```

Explanation:
The –THERM switch was provided on the command line, so now Kintecus is looking for a Thermodynamic description file THERM.DAT which must now be provided.

Fatal Error#34

```
Thermodynamic database file (filename)
CANNOT BE FOUND !!!!
Make sure the file exists and/or is in the correct
directory. (Usually the same directory as KINTECUS.)
```

Explanation:
The thermodynamic description spreadsheet that must be provided when thermodynamics being invoked (through the –THERM switch) contains thermodynamic database filenames in the first column. Kintecus cannot find the thermodynamic database (filename) in the current directory.

Fatal Error #35

```
A duplicate reaction has been found!'
'Reaction #'s (Number1) and (Number2)
 ( Source line numbers (Number3) & (Number4)
 in (filename)
 are duplicates! Please correct or delete.'
```

Explanation:
Get rid of one of the duplicate reaction lines. Go to the line (Number3) or (Number4) and correct the reaction line or delete it.

Fatal Error #36

Obsolete. You should not get this error.

Fatal Errors #39, 40

```
You have exceeded the number of reactants
that can appear in one reaction.
Try to split the global reaction
into two global reactions. You can do this
with ANY global reaction.
 -OR-
Contact company for an upgrade.
LINE READS:
```

Explanation:
Currently, you can only have a total of three unique reactants and three unique products in one reaction. This restriction DOES NOT include +M[…] or +S[…] appearing as a reactant, so the following reaction is allowed:

A+B+C+M[-O2(1);-N2(1) ;H2(1);-Ar(1); -HO2(1);-CO2(1)]==>D+E+F

Fatal Errors #70, 71, 72, 73, 75, 77, 78

All these errors have to do with the thermodynamic database descriptor fields used in the Thermodynamic Description SpreadSheet .

Fatal Error #74

```
The species (species name)
has NOT been located in any of the thermodynamic
database(s) specified in the thermodyamic description
file:THERM.DAT
```

Explanation:
If you wish to use thermodynamics in your model, then you must provide thermodynamic coefficients for ALL species. If you are sure you did do this, then make sure that if you are using the Species Reservation field in the Thermodynamic Database Description Spreadsheet correctly. If you reserve a species for a database that does not contain the reserved species, you will get this error.

Fatal Error #76

```
To compute reverse rates using the thermodynamic
database, please use UNITS of mol./liter, mol./cc or
```

```
molecules/cm^3.
```

Fatal Errors #79-85,87,89,91

Please refer to The Model Description Spreadsheet for full explanations on handling these types of reactions.

Fatal Error #90

```
There are NO reactions to compute!!!'
```

Explanation:
Did you accidentally put in an END before all the reaction lines? Remember, a '#' or a double quote as the very first non-space character on a line will comment the whole line out.

Warning Messages

Warnings will not halt a simulation run, but it may lead Kintecus to crashing, or to yield incorrect results. They can also just waste computer time for Kintecus to correct automatically. They should be eliminated.

Warning #1

```
'You can not define ''hv'' and ''M'' as species.'
'These are internal species that have special'
'definitions in Kintecus. Remove ',
(hv or M) from your species file: (Filename)
'You DO NOT have to define these species.'
'(Ignoring line...)'
```

Warning #3

```
'THE SPECIES: (Species Name)
' DOES NOT EXIST (spelling? or watch your letter 'O' '
' from the numeral zero, '0', or the lowercase'
'letter ,''l'',and the numeral one, ''1'')'
'in the species containing file: ',
'Adding in the species and initializing all values as 0.'
```

Explanation:
You have entered in a reaction, which has an undefined species. Kintecus cannot locate the species in the Species Description Spreadsheet. You should halt the simulation, append the

created species file (ADDSPEC.TXT) to the end of your The Species Description Spreadsheet , and initialize any fields. Re-run.

Warning #6

```
'???? Possible error ????:'
'A negative concentration was detected!!!'
'Halt program and re-RUN with MIN.-Interg.=Min. Interg./10
and/or'
'Accuracy=Accuracy/10.'
'Also CHECK YOUR EQUATIONS!!! Do they make sense? '
```

Explanation:
See "Overflows, Underflows, Division by Zero, Singularities" under the above section "[Errors That Can Not Be Caught by Kintecus]".

Warning #8

```
'You are not displaying the output of ANY SPECIES!'
'You will not be able to see the concentration of any'
 'species!!!'
```

Explanation:
You have not entered a single "yes" or "y" on the "Display Output ?" field of any of the species in the The Species Description Spreadsheet .

Warning #9

```
'One or more left parenthesis are missing for species:'
(Species Name) in your species file: (Filename)
'any equations containing this species can not be'
'checked for mass balance.'
```

Explanation:
You have entered an invalid species name such as CN2)2. Correct by placing in a left parenthesis, i.e. C(N2)2.

Warning #10

```
'You have reached the maximum amount of parenthesis'
'nesting in the species , (Species Name)
'in your species file: , (Filename)
'Expand the inner most parenthesis.'
'Any equations containing this species can not be'
'checked for mass balance.'
```

Warning #11

```
'One or more right parenthesis are missing for species:'
(Species Name),in your species file: , (filename)
'Any equations containing this species can not be'
'checked for mass balance.'
```

Explanation:
You have entered an invalid species name such as C(N22. Correct by placing in a right parenthesis, i.e. C(N2)2.

Warning #12

```
'The species (SpeciesName)
 can not be mass determined nor does it exist as'
 an entry in your names file:(filename)
 Any equations containing this species can not be'
 checked for mass balance.'
```

Explanation:
You have entered an invalid Species Name such as OPL or DNA. If you wish to use such names and still check for mass balance you must create a The Species Name Spreadsheet file containing the name and it's mass.

Warning #13

```
'One or more left parenthesis are missing for '
 mass formula ,(Mass Formula Shown)
of the name: (Species Common Name)
in your name file: (File Name)
 any equations containing this species can not be'
 checked for mass balance.
```

Explanation:
You have entered an invalid species name such as CN2)2. Correct by placing in a left parenthesis, i.e. C(N2)2.

Warning #15

```
One or more right parenthesis are missing for '
mass formula,(Mass Formula Shown)
of the name:,(Species Common Name)
in your name file: (File Name)
Any equations containing this species can not be'
```

```
checked for mass balance.'
```

Explanation:
You have entered an invalid species name such as C(N22. Correct by placing in a right parenthesis, i.e. C(N2)2.

Warning #16

```
The mass formula (Mass Formula Shown) of the name: (Common Name
Shown) can
not be mass determined in your names file: (File Name)
Any equations containing this species can not be'
checked for mass balance.
```

Explanation:
Kintecus can not determine the mass of the (Mass Formula Shown). Please make sure it's a valid molecular weight or mass.

Warning #17

```
Charge conservation is *NOT CONSERVED*'
in reaction # (Number)
( Source line number (Number) )
This can possibly lead to divergence in the solution!'
'Please correct.'
```

Warning #18

```
'Mass conservation is *NOT CONSERVED*'
' in reaction # (Number)
'( Source line number (Number) )'
'This can possibly lead to divergence in the solution!!'
'Please correct.'
```

Warning #19

```
Mass conservation for reaction # (line)
( Source line number (Source Line) )
can not be determined because one of the species in'
the reaction has either an illegal molecular weight'
or it's name is not located in the name file or'
'a name file has not been created. A name file'
'contains the common name of the species and it's
'molecular weight such as: Methanol , CH3OH .'
'This can possibly lead to divergence in the solution!!'
'Please correct.'
```

Warning #20

```
Parameter description file (filename),
CAN NOT BE FOUND !!!!'
Make sure the file exists and/or is in the correct'
directory. (Usually the same directory as KINTECUS.)'
Using default values:
```

Explanation:
The The Parameter Spreadsheet File contains fields that tell Kintecus how long to run the simulation, the accuracy of the simulation and many other very important fields (see the Kintecus.doc file for a full description). If Kintecus can't find this file it will assume values for all the fields. Those values are equivalent to the supplied parameter spreadsheet file:PARMDEF.DAT which you should copy as PARM.DAT and go over any relevant fields to your simulation.

Support Programs

Most of these programs listed below are designed to help you transfer your experimental data into concentration profiles or convert text files from another platform (such as the Mac, UNIX or Amiga) to MS-DOS or the other way around. For the programs ending in .bas to run these, just type at the Command prompt >qbasic /run program.bas.

CK2KIN.EXE (CHEMKIN-II/III → KINTECUS MODEL CONVERTER)

Running this program from the Windows command prompt (click START→RUN, type command, use command cd to change directories) will start this program. CK2KIN will ask you for the Chemkin model file. Make sure the Chemkin model file is a valid Windows/MS-DOS text file. If the Chemkin model (a text file) was downloaded from a UNIX site, the text file will be in UNIX format and will NOT be readable by this program. Use the CRADD program below to add carriage returns to the text file or before downloading the Chemkin model from the UNIX site, run a unix2dos program on the Chemkin Text file. The Chemkin→Kintecus converted model file will always be named: MODEL.DAT. Also, please be sure to download the thermodynamic database that came with the Chemkin Model. Sometimes the thermodynamic database is inside the Chemkin file and you will have to cut and paste this into a text file. Last step, copy the **parmck.dat** to **parm.dat** and the **THERMCK.DAT** to **THERM.DAT**. Make sure the thermodynamic database name in the first column matches the filename to the extracted Chemkin thermodynamic database. Note, not all Chemkin thermodynamic databases are a like, and you might have to try different ways of reading in the database. You can do this by simply uncommenting out the other lines in the THERM.DAT file. Naturally, be sure to comment out the line in the THERM.DAT that was not set correctly. Example:

ORIGINAL THERM.DAT

#Database			Database	Species
#FileName	INPUT	MAP	Special Switches	Reservation List
NAME_OF_MY_DATABASE	F18:IG26:F1:	SP:PH:LT:HT	U1234:FLUFF:CHF:PHS	
#(insert THERM database name)	F18:IG26:F1:	SP:PH:LT:HT	U1234:CHF:PHS	
#(insert THERM database name)	F18:IG26:F1:	SP:PH:LT:HT	U1234:UPPL:CHF:PHS:UPC	
#(insert THERM database name)	F18:IG26:F1:	SP:PH:LT:HT	U1234:UPPL:CHF:FLUFF:PHS:SET(CT=1000):SYN	
#(insert THERM database name)	FREE	SP:LT:CT:HT	UPPL	
END				

CHANGED TO

#Database			Database	Species
#FileName	INPUT	MAP	Special Switches	Reservation List
## NAME_OF_MY_DATABASE	F18:IG26:F1:	SP:PH:LT:HT	U1234:FLUFF:CHF:PHS	
NAME_OF_MY_DATABASE	F18:IG26:F1:	SP:PH:LT:HT	U1234:CHF:PHS	
#(insert THERM database name)	F18:IG26:F1:	SP:PH:LT:HT	U1234:UPPL:CHF:PHS:UPC	
#(insert THERM database name)	F18:IG26:F1:	SP:PH:LT:HT	U1234:UPPL:CHF:FLUFF:PHS:SET(CT=1000):SYN	
#(insert THERM database name)	FREE	SP:LT:CT:HT	UPPL	
END				

If you still cannot read in your thermodynamic database then comment out the current line (note the "#" at the beginning of the line) and enter the database name on the next line and so on:

#Database			Database	Species
#FileName	INPUT	MAP	Special Switches	Reservation List
## NAME_OF_MY_DATABASE	F18:IG26:F1:	SP:PH:LT:HT	U1234:FLUFF:CHF:PHS	
## NAME_OF_MY_DATABASE	F18:IG26:F1:	SP:PH:LT:HT	U1234:CHF:PHS	
NAME_OF_MY_DATABASE	F18:IG26:F1:	SP:PH:LT:HT	U1234:UPPL:CHF:PHS:UPC	
#(insert THERM database name)	F18:IG26:F1:	SP:PH:LT:HT	U1234:UPPL:CHF:FLUFF:PHS:SET(CT=1000):SYN	
#(insert THERM database name)	FREE	SP:LT:CT:HT	UPPL	
END				

INTERPOL.BAS

"Program to convert scattered data file of time,data to"
"a sequential list of data spaced exactly at an "
"entered timing interval."
"(Values in-between are linearly interpolated...)"

CRADD.BAS

This program converts text files from another platform (such as the Mac, Unix or Amiga) to Windows/MS-DOS.

LOOK.BAS

A program to look at the ASCII values in a file.

FILTER.BAS

This will convert MS-DOS text files to Mac/Unix text files.

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Kintecus Version 2 Registration

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