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.

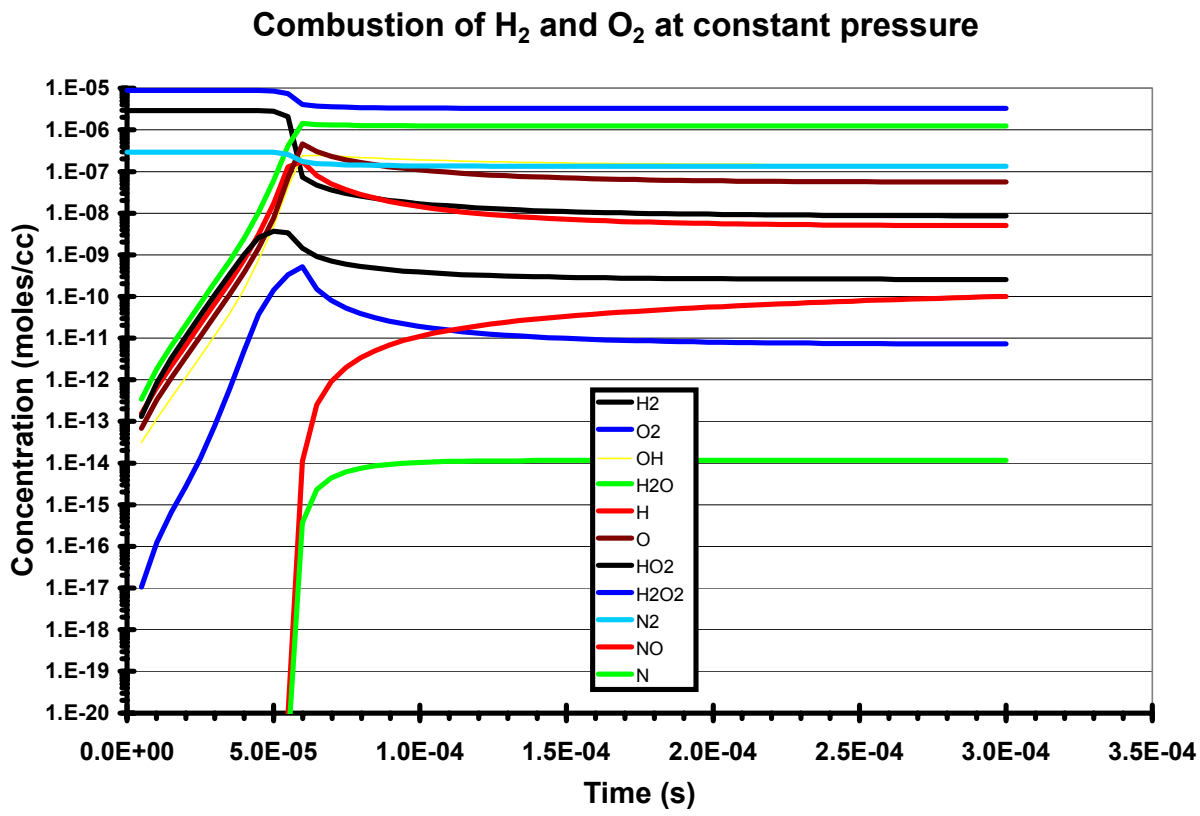
MODOH.DAT - The kinetics reactions (Converted from the Chemkin-II/III manual example)
SPECOH.DAT - The species involved
PARMOH2.DAT - The parameters used
THERMOH.DAT – The thermodynamic description spreadsheet
CONCOH2.TXT - A simulation run.

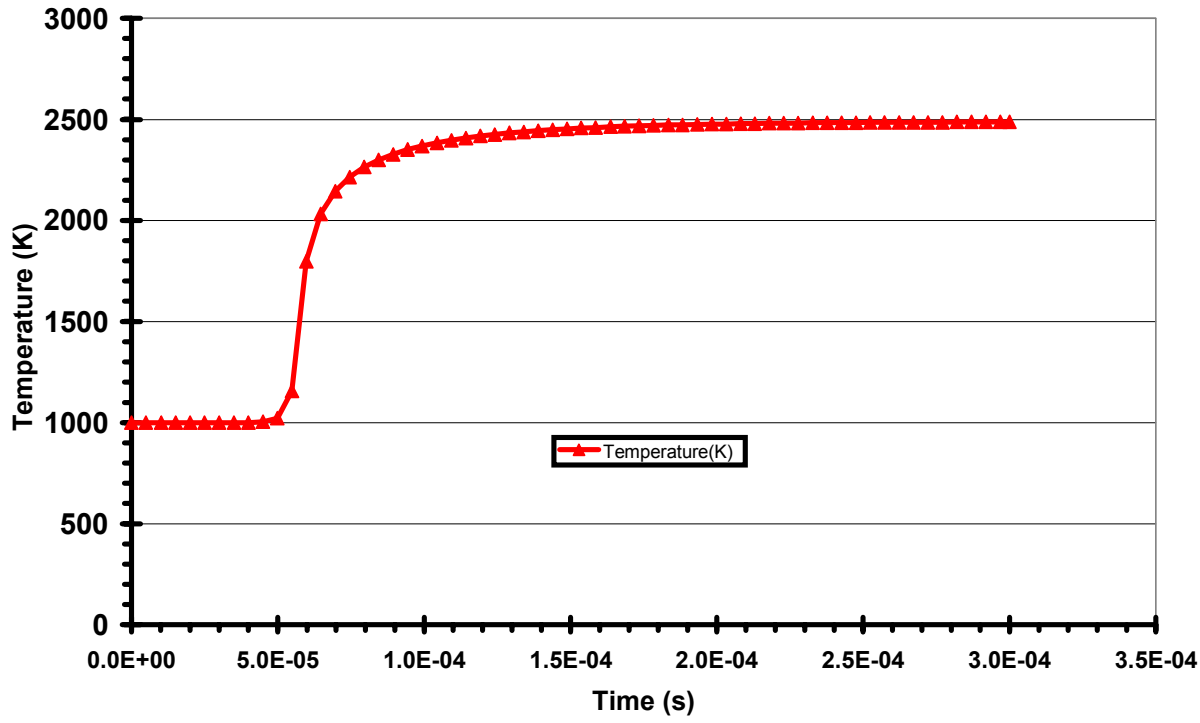
OH2.BAT - A very simple one line batch file that will run the above model producing the concentration profile equal to CONCOH2.TXT.

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	1.82E-03	6.72E-01	3.04E-02	2.56E-01	1.05E-03	1.16E-02
CHEMKIN-II	1.79E-03	6.72E-01	3.07E-02	2.56E-01	1.03E-03	1.14E-02
Percent Difference	1.6%	0.0%	-0.9%	0.0%	2.3%	1.9%
	HO_2	H_2O_2	N_2	NO	N	Temp.(K)
KINTECUS	5.39E-05	1.51E-06	2.73E-02	2.15E-05	2.47E-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	-10.2%	-1.0%	0.2%	-0.8%	2.4%	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

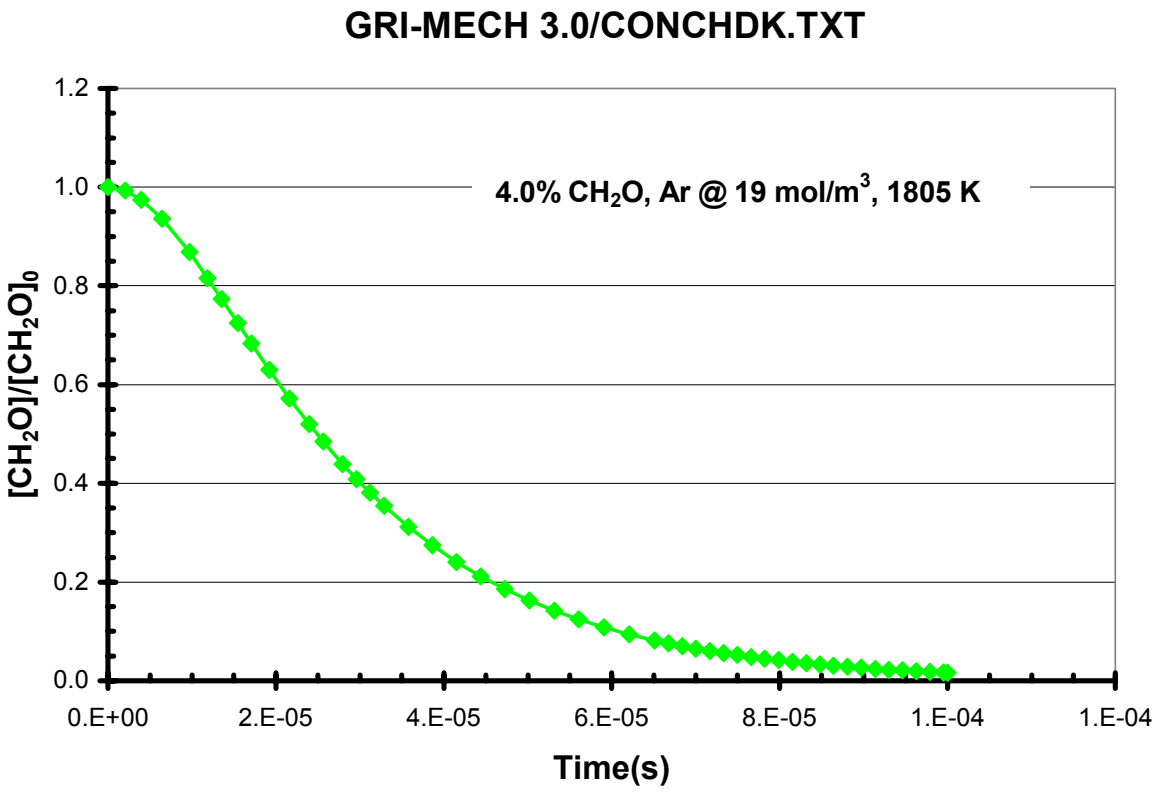
The GRI (Gas Research Institute)-Mech 3.0 mechanism is used by many research groups around the world for various combustion models. The chemical model MODGRI.DAT is a direct conversion from the Chemkin-II model. No alterations were made to the MODGRI.DAT once the CK2KIN program converted it. You can 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.

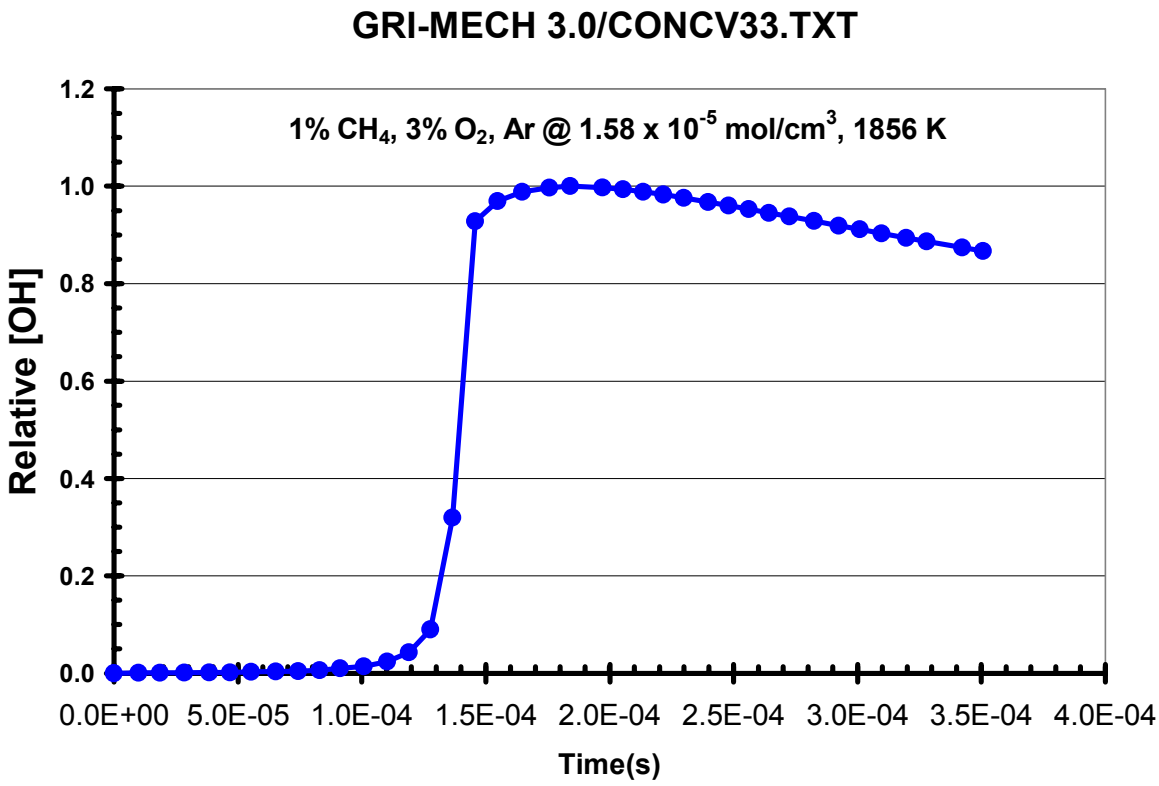


GRI-MECH RUN 1% CH_4 3% O_2

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.

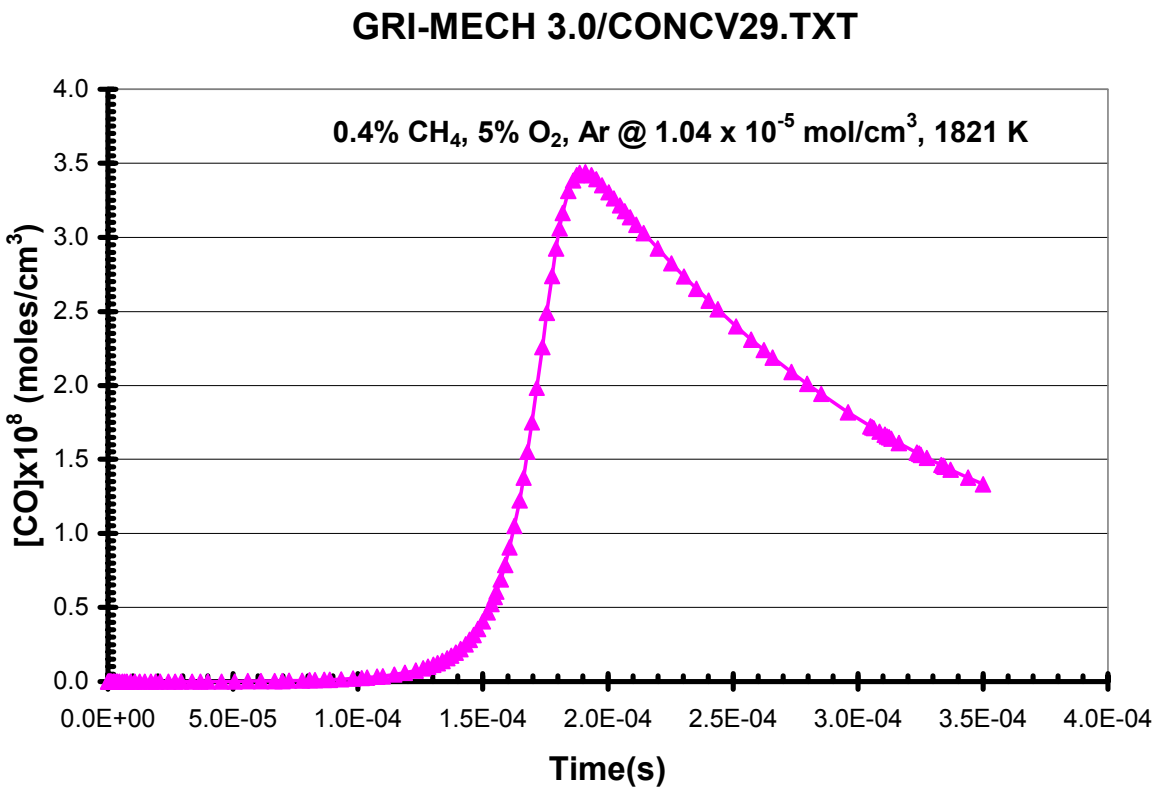


GRI-MECH RUN 0.4% CH_4 5% O_2

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.

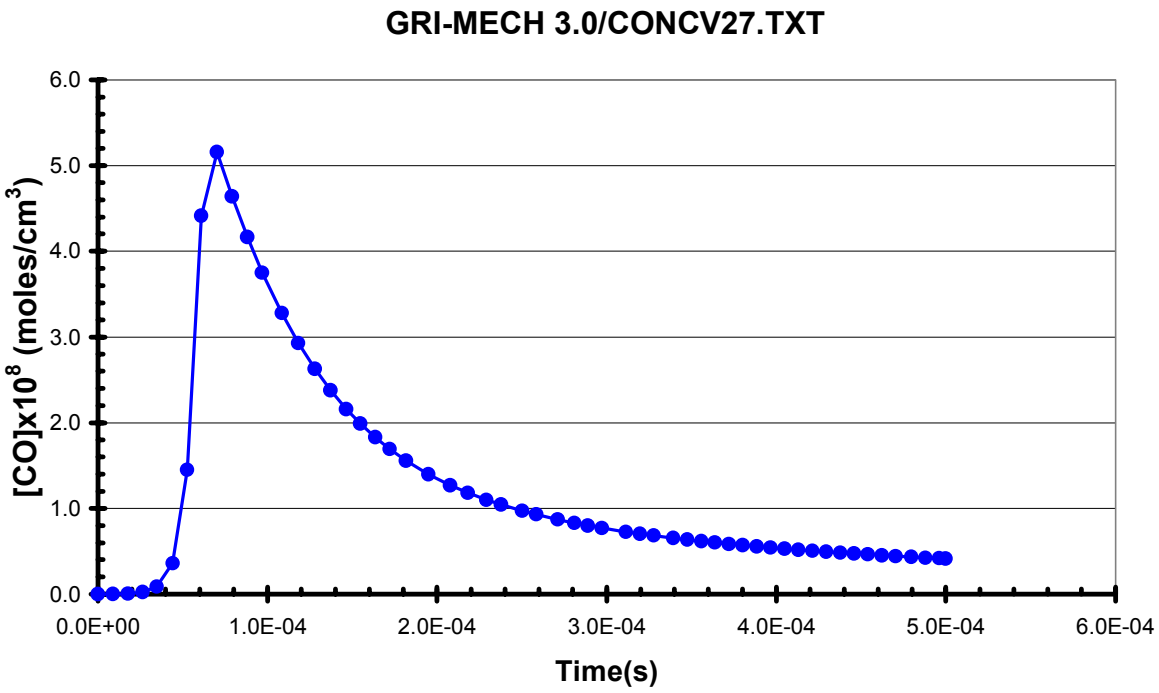


GRI-MECH RUN 0.4% CH_4 5% O_2

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.

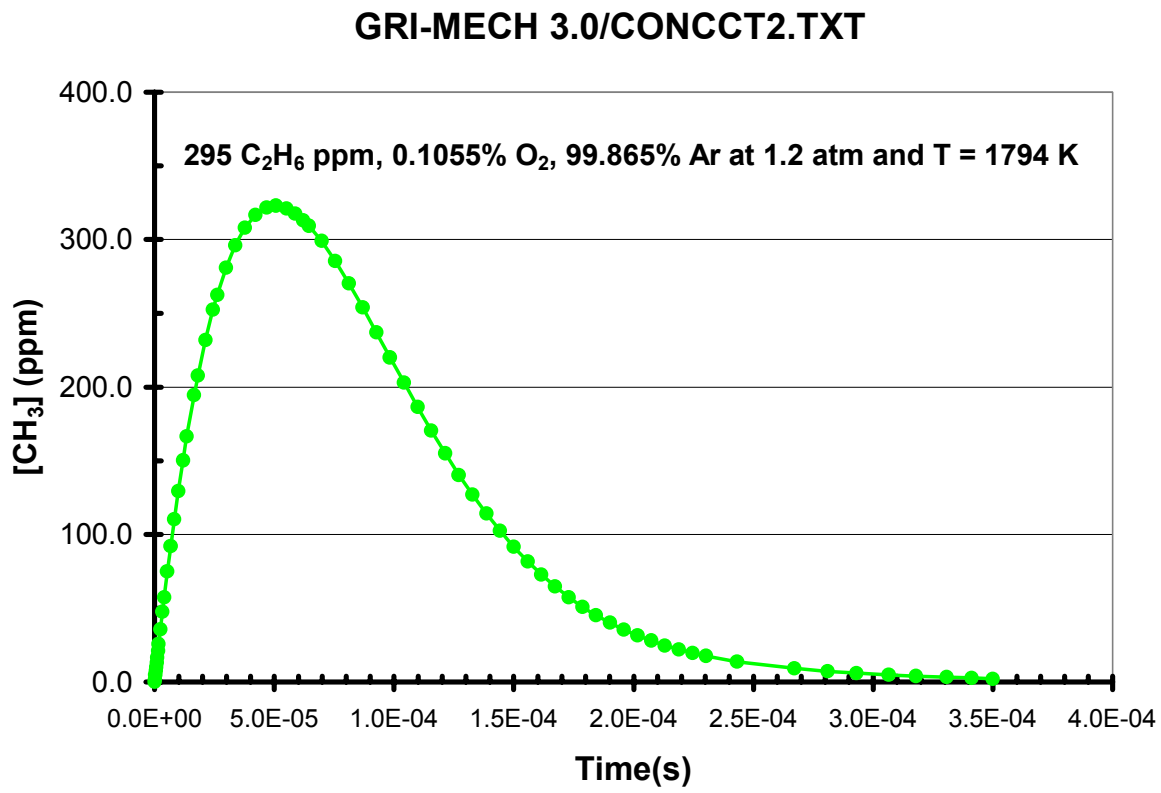


GRI-MECH RUN 295 C_2H_6 ppm, 0.1055% O_2, 99.865% Ar

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.

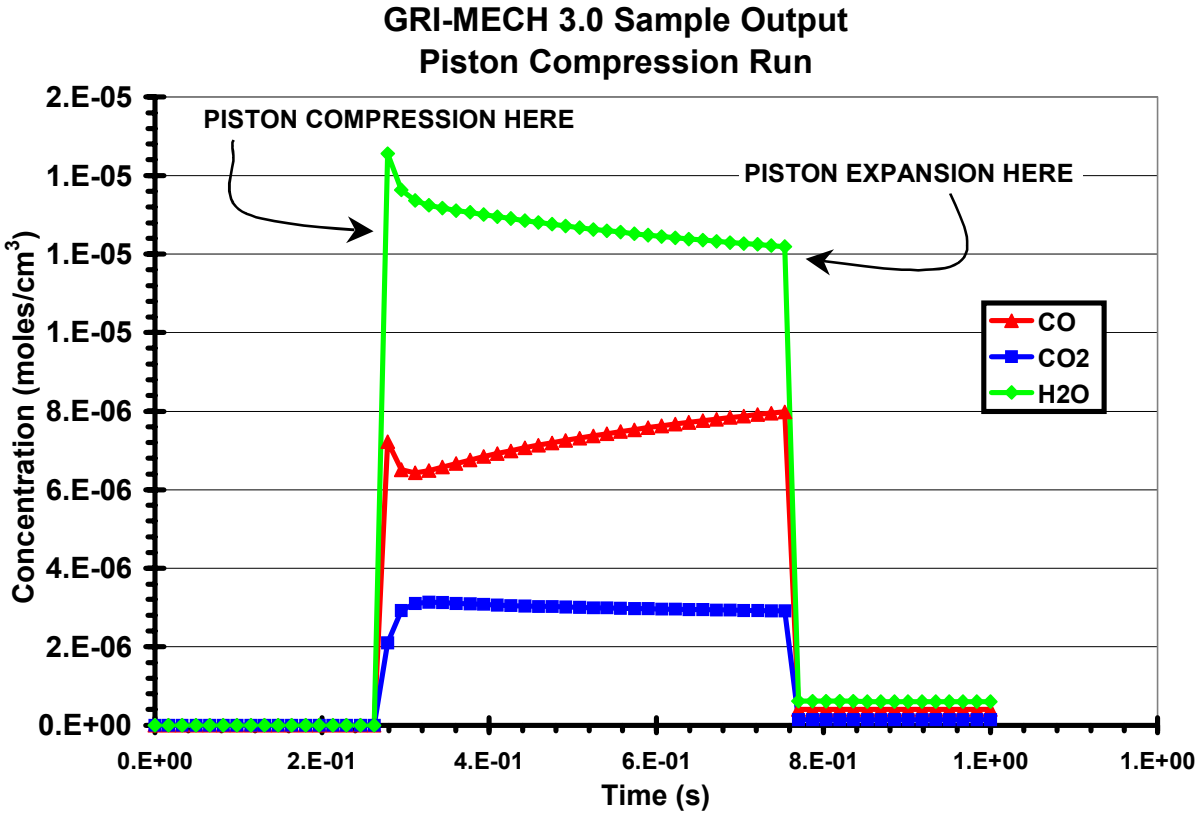


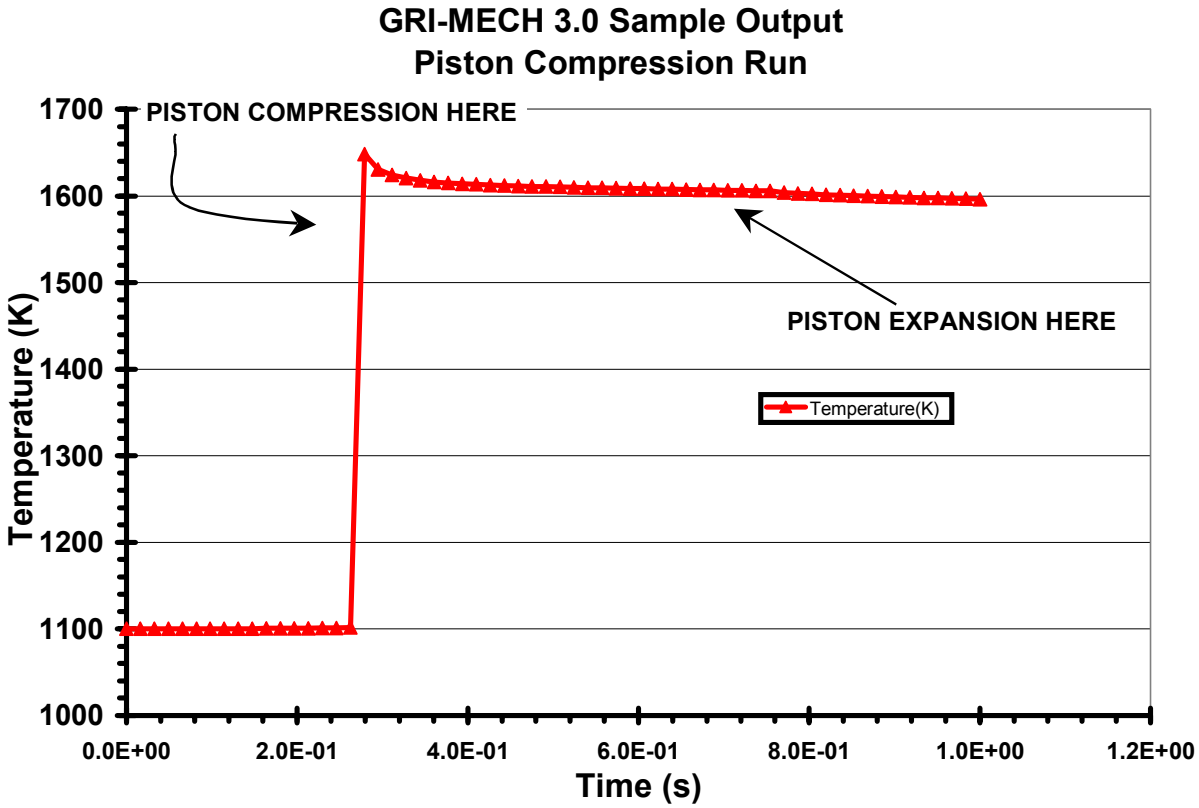
GRI-MECH PISTON COMPRESSION RUN

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

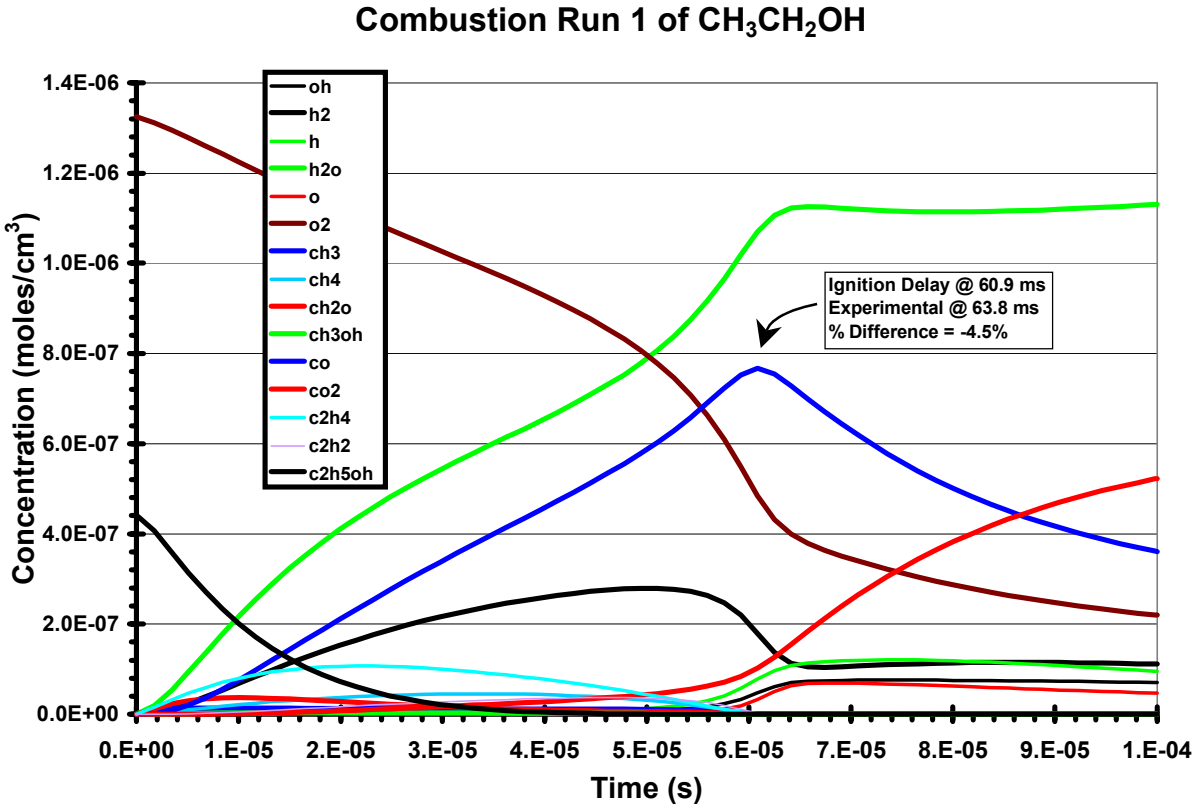
The ignition delay obtained from the output concentration file, CONCETH1.TXT, matches the experimental results given by Dunphy and Simmie [15]. Dunphy and Simmie correlated their experimental ignition times with the expression:

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

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

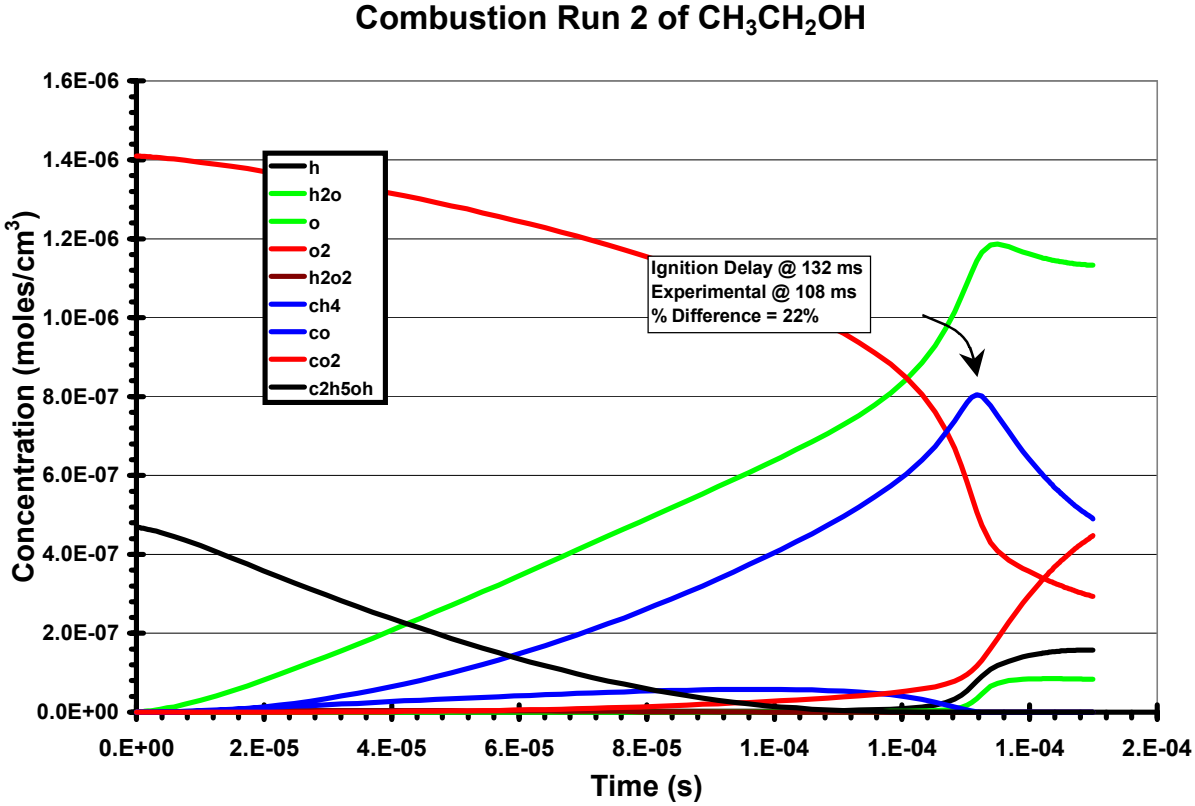
The ignition delay obtained from the output concentration file, CONCETH2.TXT, matches the experimental results given by Dunphy and Simmie [15]. Dunphy and Simmie correlated their experimental ignition times with the expression:

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

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

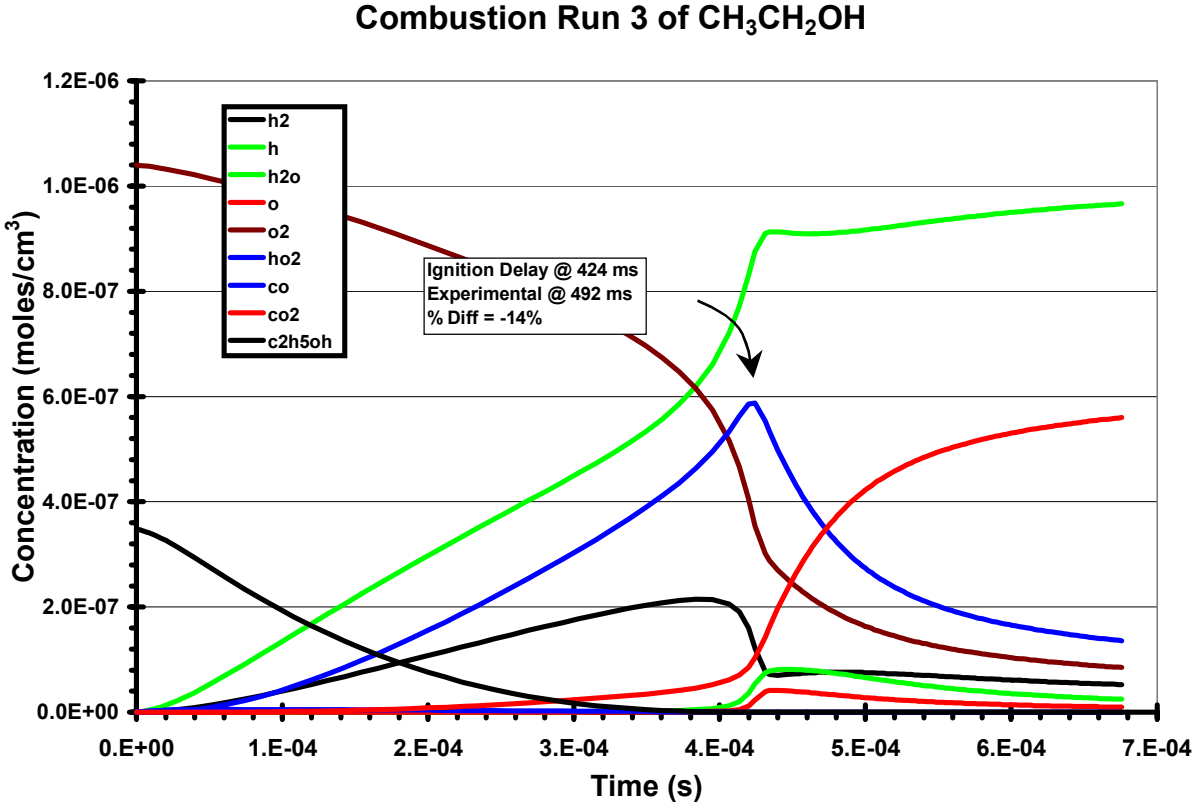
The ignition delay obtained from the output concentration file, CONCETH1.TXT, matches the experimental results given by Dunphy and Simmie [15]. Dunphy and Simmie correlated their experimental ignition times with the expression:

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

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.

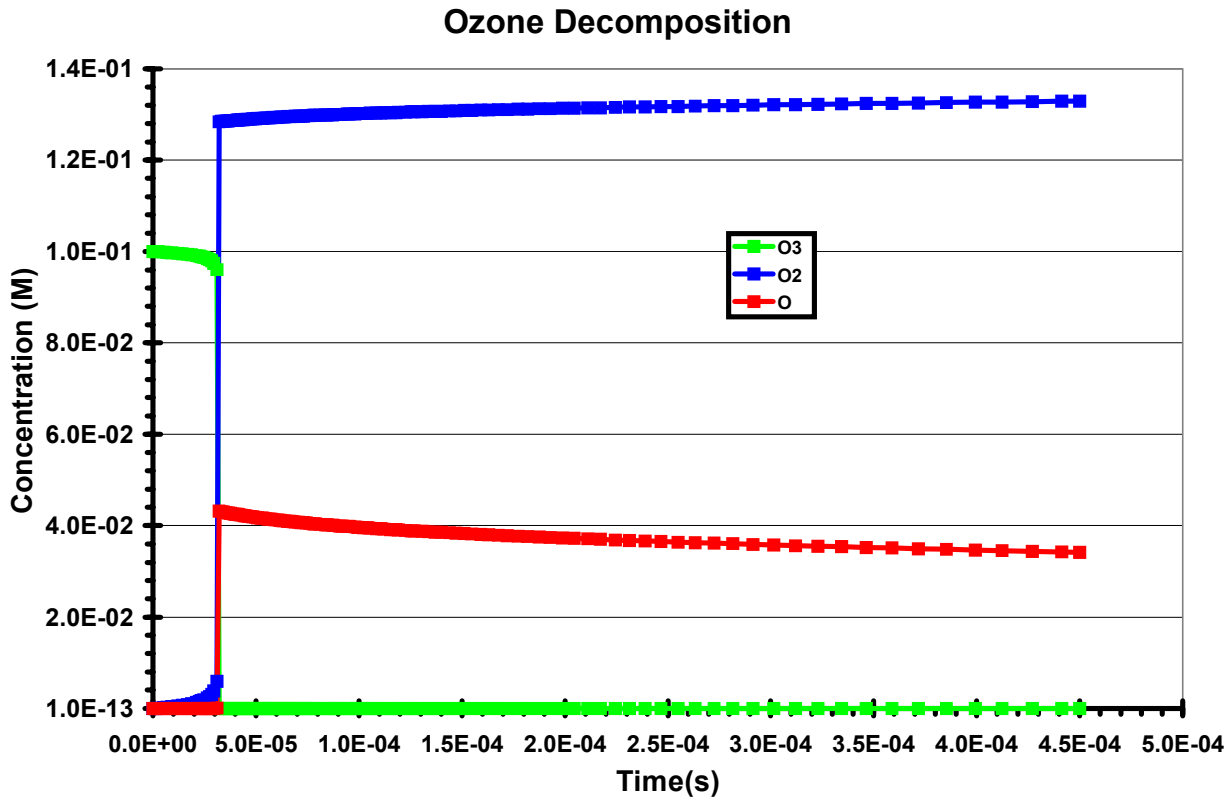


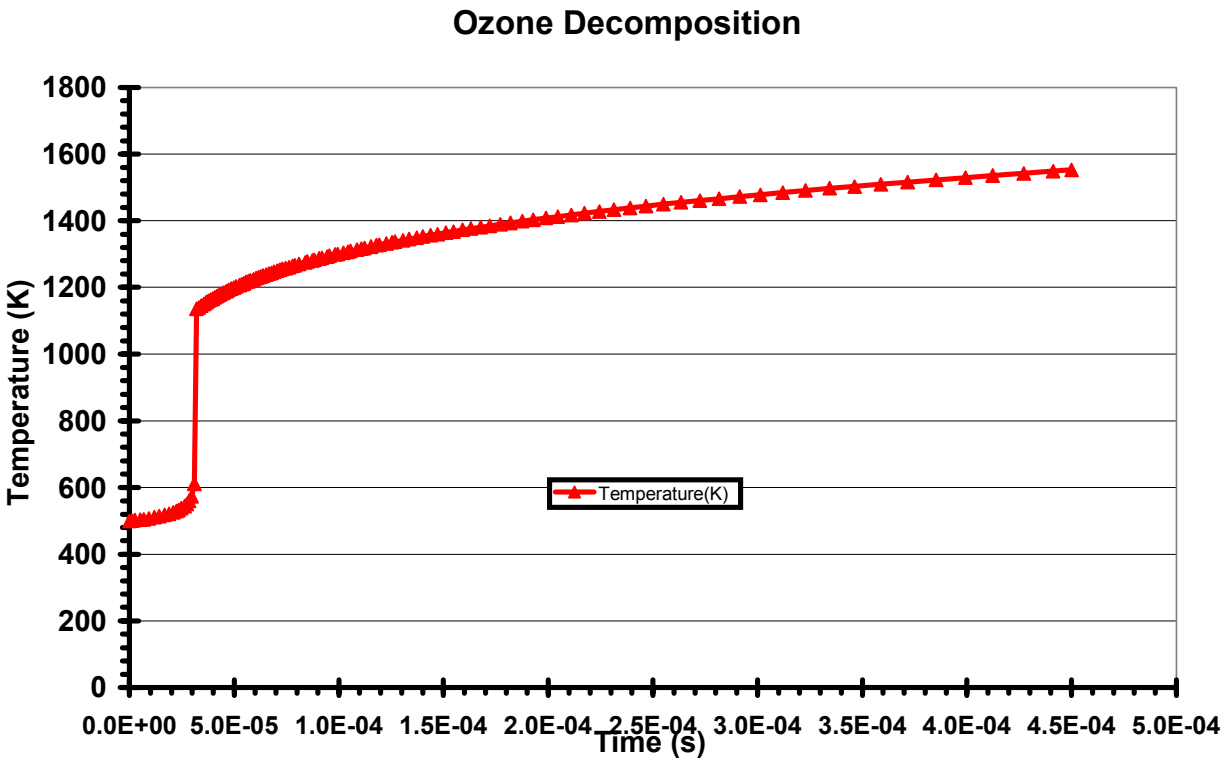
Ozone Decomposition

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.



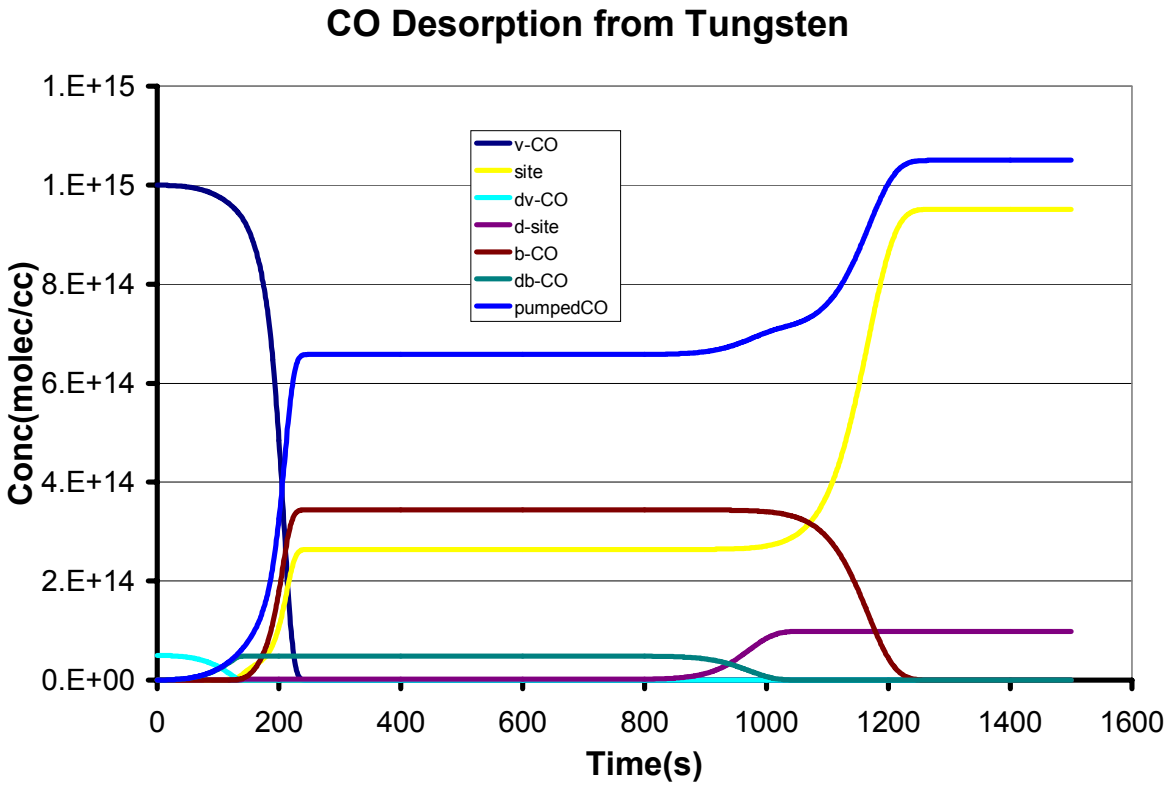

Ozone Decomposition
1800
1600
1400
1200
1000
800
600
400
200
0
Temperature (K)
Temperature(K)
0.0E+00
5.0E-05
1.0E-04
1.5E-04
2.0E-04
2.5E-04
3.0E-04
3.5E-04
4.0E-04
4.5E-04
5.0E-04
Time (s)

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.

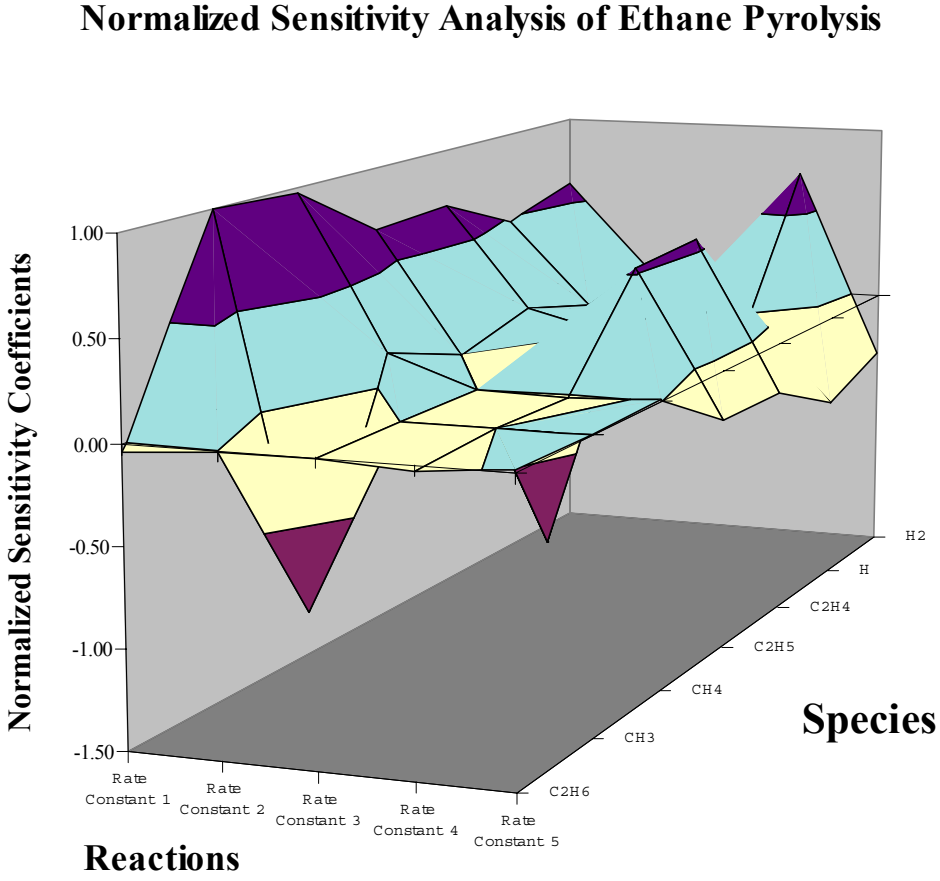
Sensitivity Analysis Sample Runs

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.

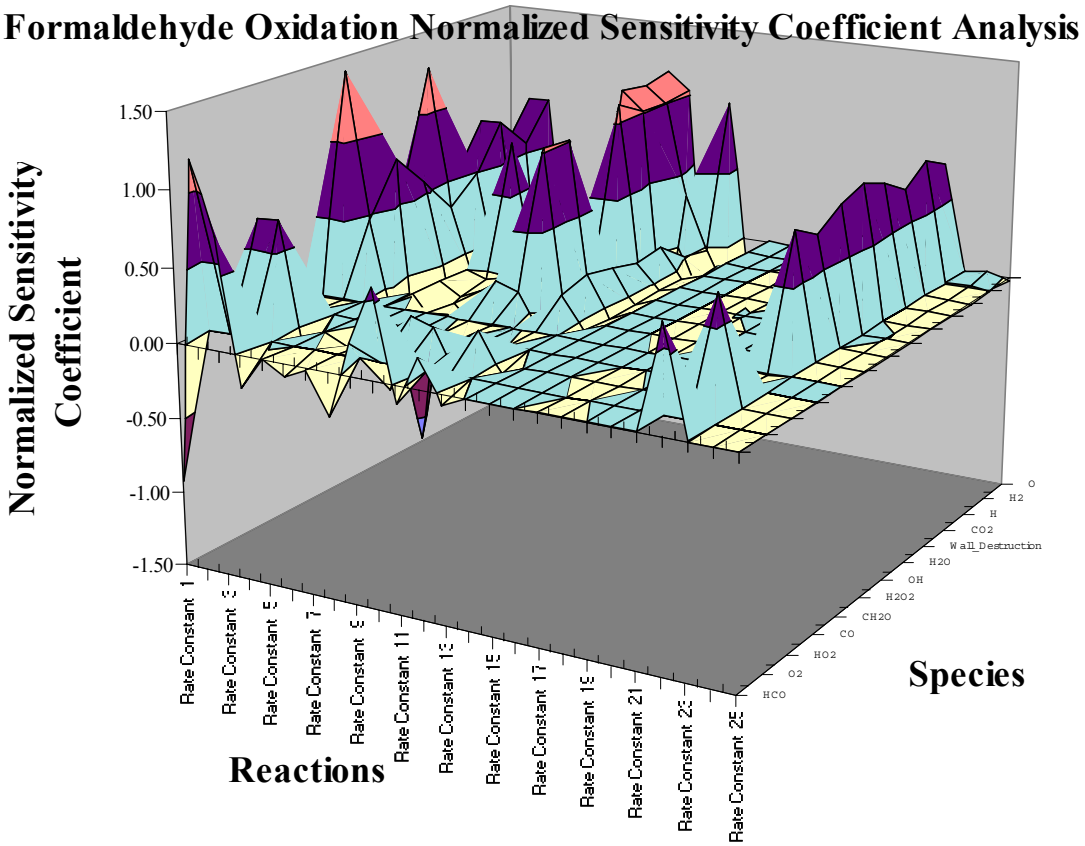


Sensitivity Analysis of the Oxidation of Formaldehyde Mechanism

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.