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.

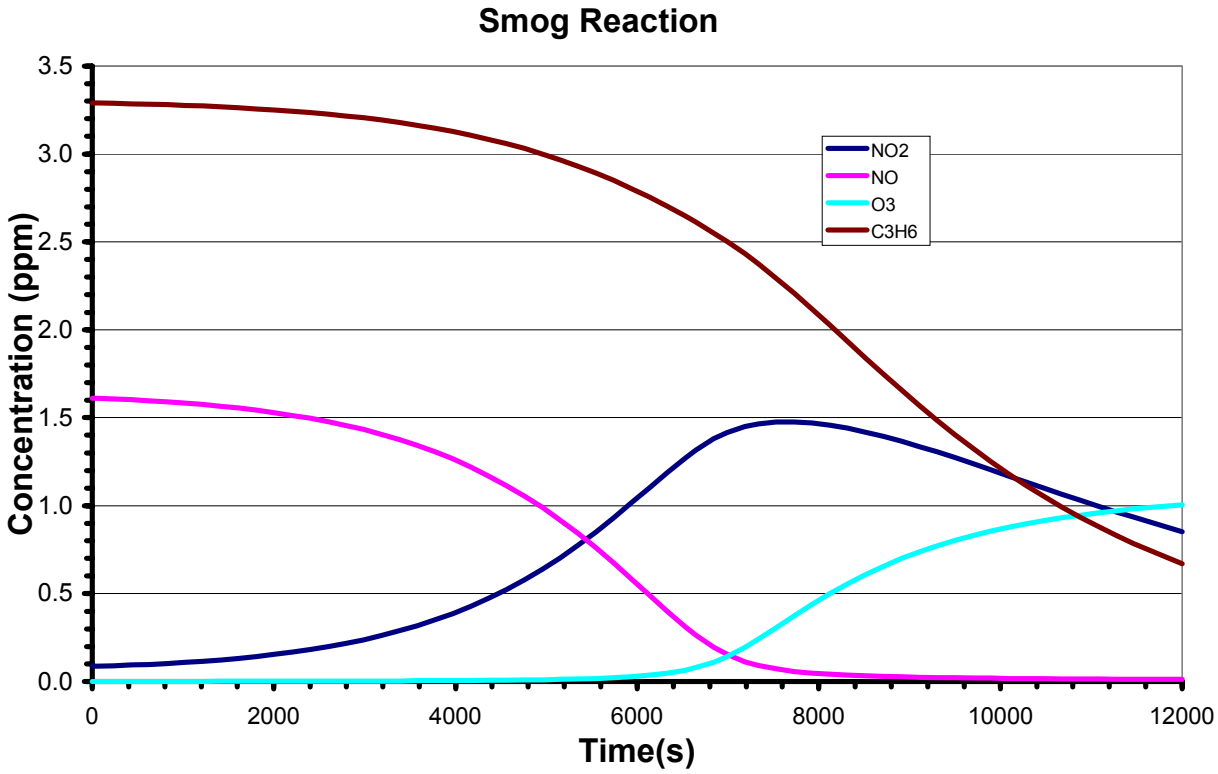
Simple Sample Model Runs

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].

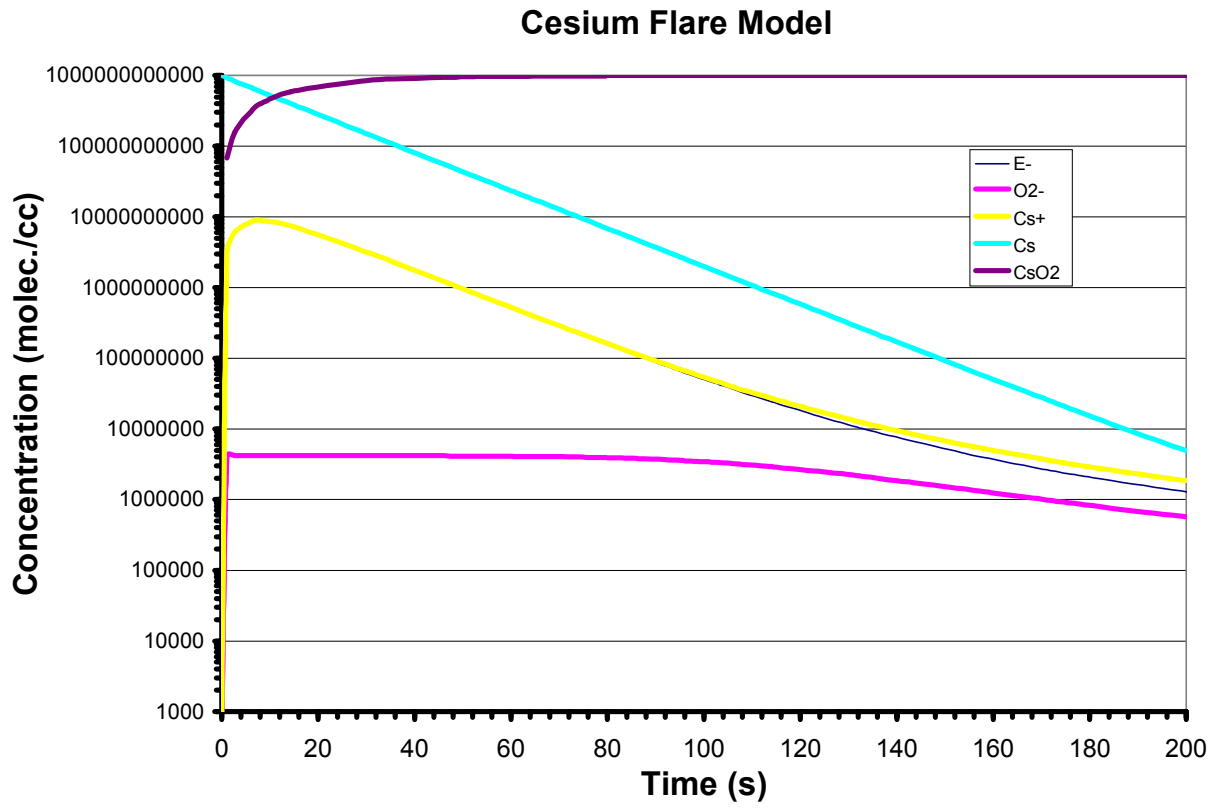
MODSMOG.TX2 - The kinetics reactions
SPECSMOG.TX2 - The species involved
PARMSMOG.TX2 - The parameters used
CONCSMOG.TXT - A simulation run.
SMOG.BAT - A very simple one line batch file that will run the above model producing the concentration profile equal to CONCSMOG.TXT.



The Cesium Flare Model

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

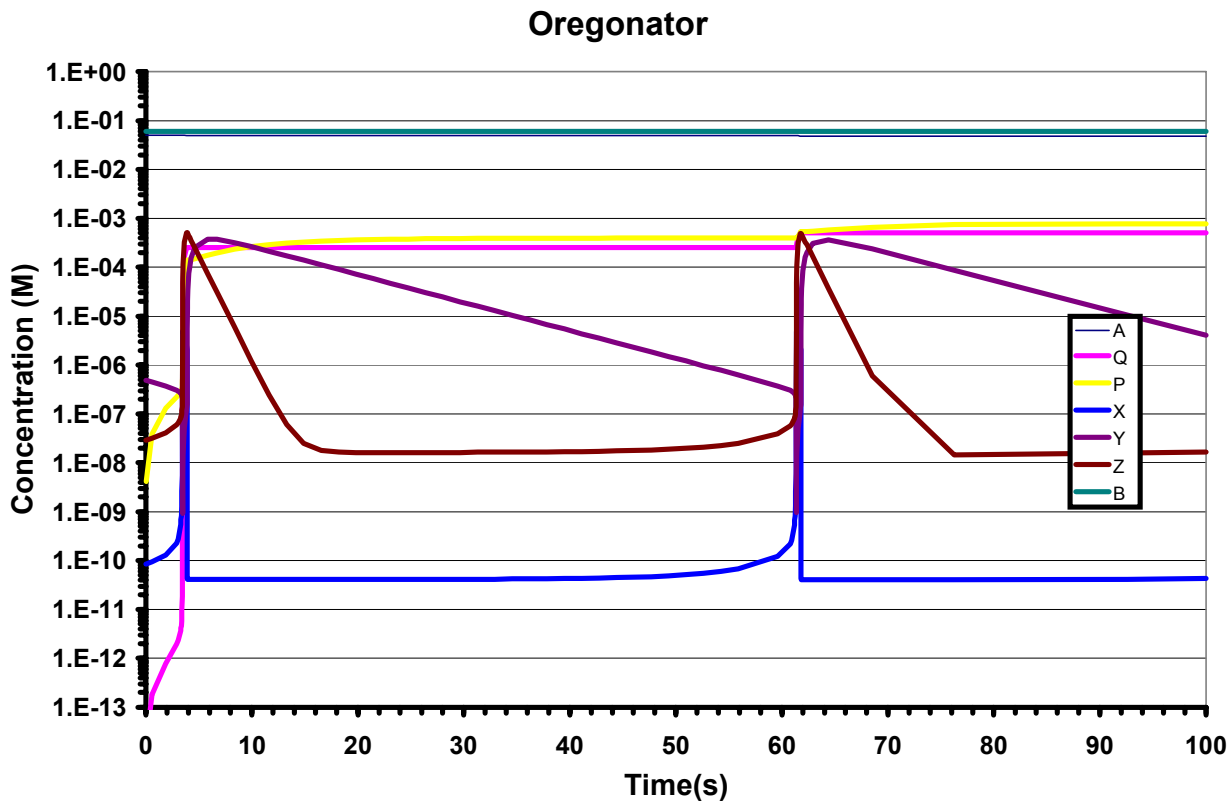
NAMECES.TX2 - A species name file containing common names and their MW.
MODCES.TX2 - The kinetics reactions
SPECCES.TX2 - The species involved
PARMCES.TX2 - The parameters used
CONCCES.TXT - A simulation run.
CES.BAT - A very simple one line batch file that will run the above model producing the concentration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



The Oscillating Oregonator

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

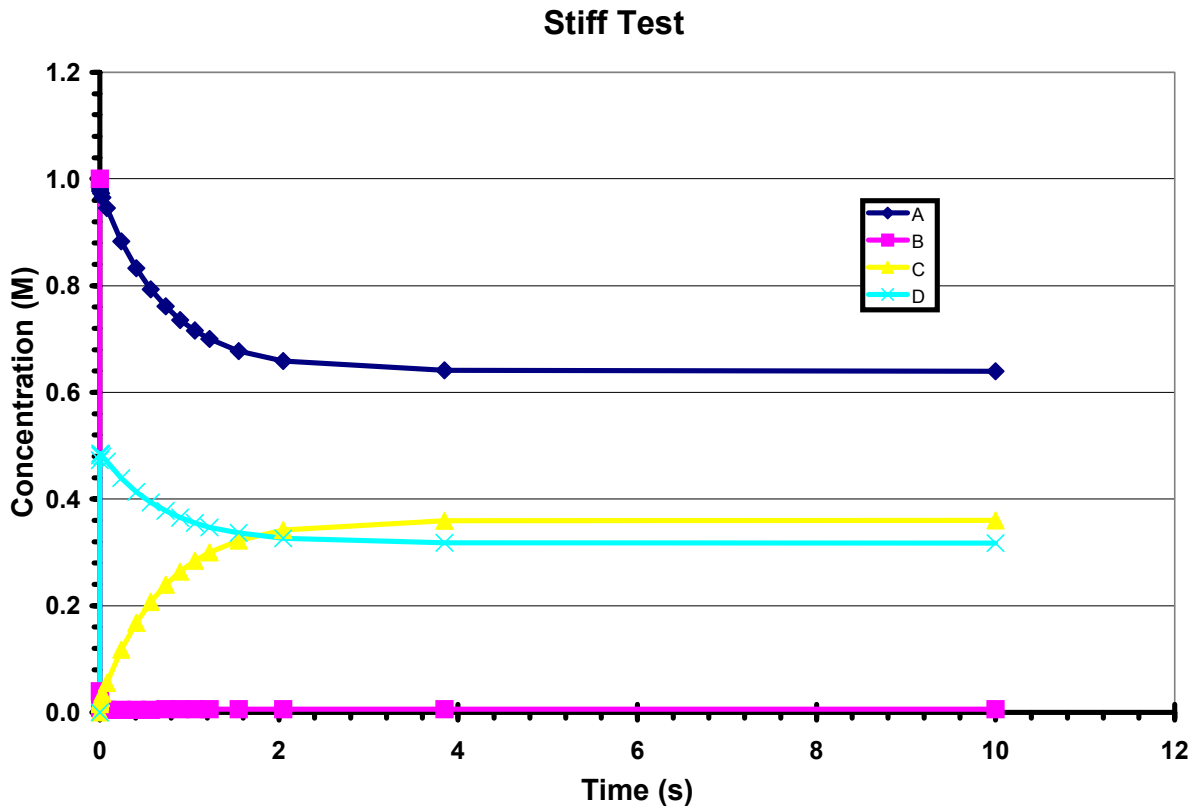
MODOREG.TX2 - The kinetics reactions
SPECOREG.TX2 - The species involved
PARMOREG.TX2 - The parameters used
CONCOREG.TXT - A simulation run.
OREG.BAT - A very simple one line batch file that will run the above model producing the concentration profile equal to CONCOREG.TXT.



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.