

Software Flow Chart for Octave-Fortran Hybrid Version

This version of the software avoids both Chemkin and Matlab fees, which can be substantial in a corporate setting. The purpose of this project was to simplify the Chemkin fuel mechanism modeling software as well as avoid its expensive fees, but Matlab also has expensive fees, Matlab's free cousin GNU Octave is great but slow. This therefore resulted in the Octave-Fortran hybrid version of my software.

Read mechanism file into intermediate variables using GNU Octave Numerical computing environment, a free Matlab alternative with parallel computing capabilities

Print hardcode functions in Fortran because much faster and best public domain ode solvers are written in it. Mechanism specific functions are printed to a file called mechsspecific.f

Compile using f95 compiler, run reactor code, results are printed to output.txt file

Use GNU Octave to read and plot results

What is Dassl?

Dassl is a Fortran ordinary differential equation solver written in 1983 by L. Petzold. Since it is in the public domain, it is therefore totally free to use. Dassl stands for differential algebraic system solver. It has a slightly different style from the Matlab ode solver in that instead of writing

$$\frac{dy}{dt} = \dot{w} \quad \text{You write} \quad \textit{delta} = \dot{w} - \frac{dy}{dt}$$