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Parsing and visualizing Chemkin formatted database in GNU Octave

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INTRODUCTION

- Molar Enthalpy, Entropy, Specific Heat of gases are significant in combustion reactions. Thermo chemistry deals with heat change in chemical reactions, which is a phenomena to be considered in simulation of combustions.

OBJECTIVE

- A parser to read all polynomial coefficients for a gas species from the Chemkin formatted database.
- Using the polynomials to calculate c_p , H^0 , S^0 in a given temperature using NASA defined formula
- Study their thermodynamic behavior in a range of temperature.

Database file

```
THERMO
   300.000  1000.000  5000.000
! GRI-Mech Version 3.0 Thermodynamics released 7/30/99
! NASA Polynomial format for CHEMKIN-II
! see README file for disclaimer
O                 L 1/90O   1               G   200.000  3500.000  1000.000    1
 2.56942078E+00-8.59741137E-05 4.19484589E-08-1.00177799E-11 1.22833691E-15    2
 2.92175791E+04 4.78433864E+00 3.16826710E+00-3.27931884E-03 6.64306396E-06    3
-6.12806624E-09 2.11265971E-12 2.91222592E+04 2.05193346E+00                   4
O2                TPIS89O   2               G   200.000  3500.000  1000.000    1
 3.28253784E+00 1.48308754E-03-7.57966669E-07 2.09470555E-10-2.16717794E-14    2
-1.08845772E+03 5.45323129E+00 3.78245636E+00-2.99673416E-03 9.84730201E-06    3
-9.68129509E-09 3.24372837E-12-1.06394356E+03 3.65767573E+00                   4
H                 L 7/88H   1               G   200.000  3500.000  1000.000    1
 2.50000001E+00-2.30842973E-11 1.61561948E-14-4.73515235E-18 4.98197357E-22    2
 2.54736599E+04-4.46682914E-01 2.50000000E+00 7.05332819E-13-1.99591964E-15    3
 2.30081632E-18-9.27732332E-22 2.54736599E+04-4.46682853E-01                   4
H2                TPIS78H   2               G   200.000  3500.000  1000.000    1
 3.33727920E+00-4.94024731E-05 4.99456778E-07-1.79566394E-10 2.00255376E-14    2
-9.50158922E+02-3.20502331E+00 2.34433112E+00 7.98052075E-03-1.94781510E-05    3
 2.01572094E-08-7.37611761E-12-9.17935173E+02 6.83010238E-01                   4
OH                RUS 78O   1H  1           G   200.000  3500.000  1000.000    1
 3.09288767E+00 5.48429716E-04 1.26505228E-07-8.79461556E-11 1.17412376E-14    2
```

Coefficients for 'O'

T_{min} T_{max} T_{mean}

Species

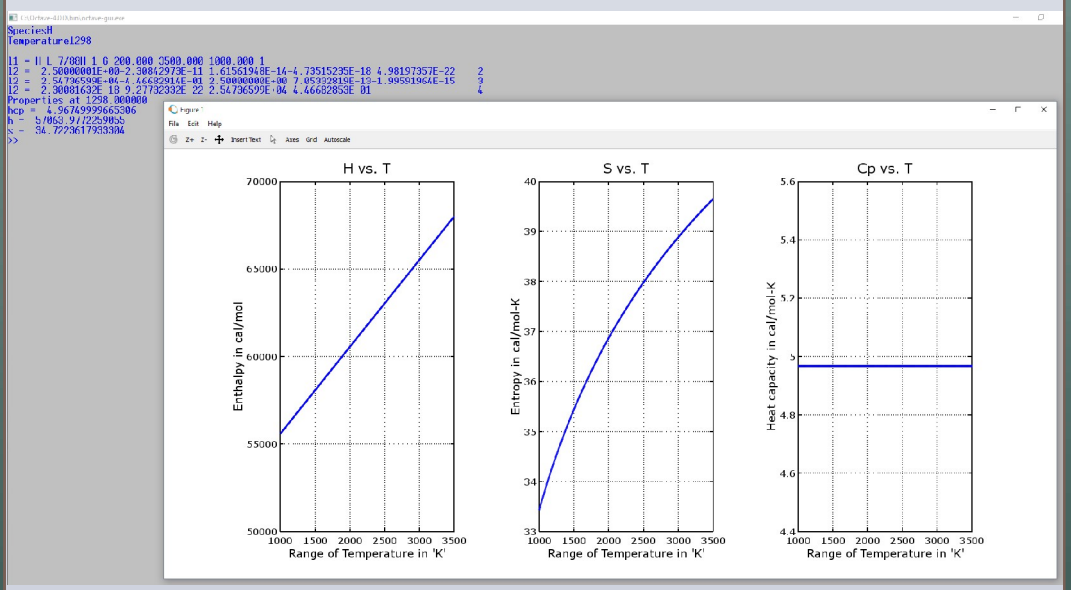
The NASA polynomials have the form:

$$Cp/R = a1 + a2\ T + a3\ T^2 + a4\ T^3 + a5\ T^4$$

$$H/RT = a1 + a2\ T /2 + a3\ T^2 /3 + a4\ T^3 /4 + a5\ T^4 /5 + a6/T$$

$$S/R = a1\ lnT + a2\ T + a3\ T^2 /2 + a4\ T^3 /3 + a5\ T^4 /4 + a7$$

Plot for H @ 1298 K

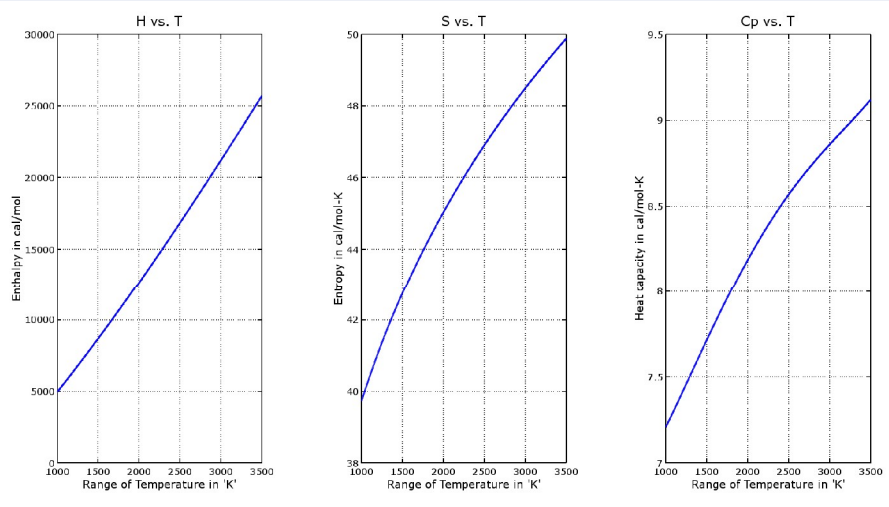


Units : H – cal/mol 1 mol = 4.18 J

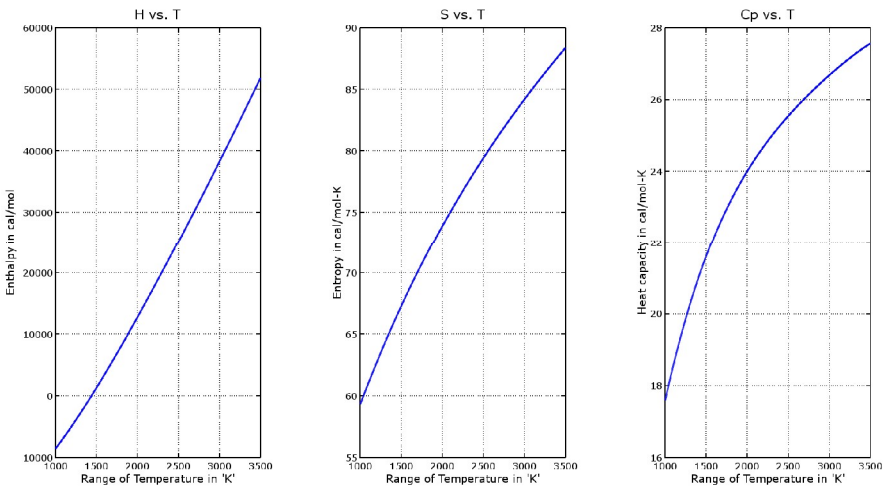
S – cal/mol-k 1 mol = $Grams/Mol.wt$

c_p – cal/mol-k 1 mol(O) = 15.9994 gms

Plot for H2 @ 1298 K



Plot for CH4 @ 2000 K



RESULTS AND DISCUSSIONS

- Molar Enthalpy of 'H' is always more than that of ' H_2 '@ same temperature.
- This says, more energy is involved in reactions with H.

- The thermodynamic properties for gaseous species are visualized by parsing the database and can further be used in other simulation analyses.

REFERENCES

1.https://www.gnu.org/software/octave/doc/v4.0.0/
2.http://www.edxengine.com

ACKNOWLDEGEMENTS

- Mechanical department- Velammal Engineering College
- Edxengine ,www.edxengine.com