Engineering Software

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Engineering Software is pleased to announce the introduction of ***Free Coursework Material***.

Engineering Software Coursework Material covers the following area:

Physical Properties
Single Species Approach

Single Species Approach

Introduction

This section provides a Physical Properties analysis for single species.

Analysis

In the presented Physical Properties analysis, only ten (10) basic species are considered behaving as an ideal gas -- ideal gas state equation is valid -- pv = RT.

For each reaction species, the thermodynamic functions specific heat, enthalpy and entropy as functions of temperature are given in the form of least squares coefficients as follows:

$$\mathbf{Cp/R = A1 + A2T + A3T^2 + A4T^3 + A5T^4}$$

$$\mathbf{H/(R*T) = A1 + A2T/2 + A3T^2/3 + A4T^3/4 + A5T^4/5 + A6/T}$$

$$\mathbf{S/R = A1lnT + A2T + A3T^2/2 + A4T^3/3 + A5T^4/4 + A7}$$

or

$$\mathbf{S/R = A1lnT + A2T + A3T^2/2 + A4T^3/3 + A5T^4/4 + A7 - lnp}$$

For each species, two sets of coefficients are included for two adjacent temperature intervals, 273 to 1,000 [K] and 1,000 to 5,000 [K]. The data have been constrained to be equal at 1,000 [K].

For example, physical properties for both reactants and combustion products are very important and need to be known in order to carry out successful combustion calculations.

The plot in Figure 1 depicts how the species enthalpy values change with the temperature. The physical properties provided in this plot come from the JANAF Thermochemical Data - Tables, 1970.

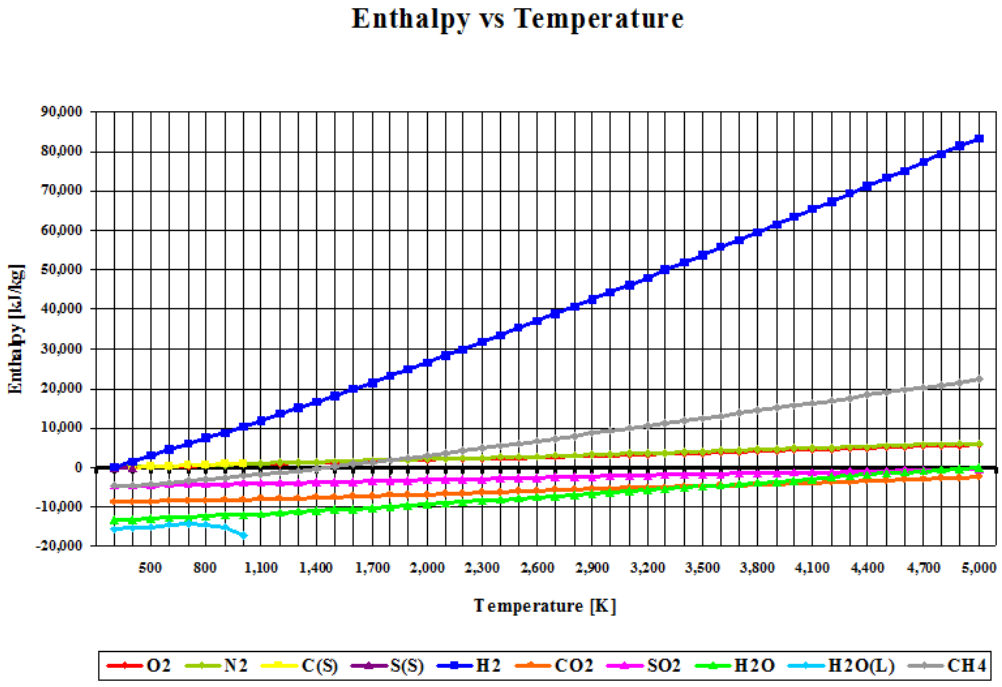

Figure 1 - Enthalpy vs Temperature

In general, enthalpy values increase with an increase in temperature.

It is interesting to note that the enthalpy value for basic combustion elements such as carbon (C), hydrogen (H_2), sulfur (S), oxygen (O_2) and nitrogen (N_2) is equal to zero at the standard combustion conditions of 298 [K] and 1 [atm].

Also, it should be mentioned that for ideal gas species, the enthalpy value is only dependent on the temperature.

Assumptions

Considered species behave as an ideal gas.

Governing Equations

For each reaction specie, the thermodynamic functions specific heat, enthalpy and entropy as functions of temperature are given in the form of least squares coefficients as follows:

$$\mathbf{Cp/R = A1 + A2T + A3T^2 + A4T^3 + A5T^4}$$

$$\mathbf{H/(R*T) = A1 + A2T/2 + A3T^2/3 + A4T^3/4 + A5T^4/5 + A6/T}$$

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For each species, two sets of coefficients are included for two adjacent temperature intervals, 273 to 1,000 [K] and 1,000 to 5,000 [K]. The data have been constrained to be equal at 1,000 [K].

Also,

U = H - p*v*MW or **U = H - R*T**

G = H - S*T

and

u = h - p*v or **u = h - R*T/MW**

g = h - s*T

Legend:

Cp -- Specific Heat [kJ/kmol*K]

cp -- Specific Heat [kJ/kg*K]

MW -- Molecular Weight [kg/kmol]

R -- Universal Gas Constant [kJ/kmol*K]

Gas Constant = R/MW [kJ/kg*K]

H -- Enthalpy [kJ/kmol]

h -- Enthalpy [kJ/kg]

T -- Temperature [K]

S -- Entropy [kJ/kmol*K]

s -- Entropy [kJ/kg*K]

p -- Pressure [atm]

U -- Internal Energy [kJ/kmol]

u -- Internal Energy [kJ/kg]

v -- Specific Volume [m^3/kg]

G -- Gibbs Free Energy [kJ/kmol]

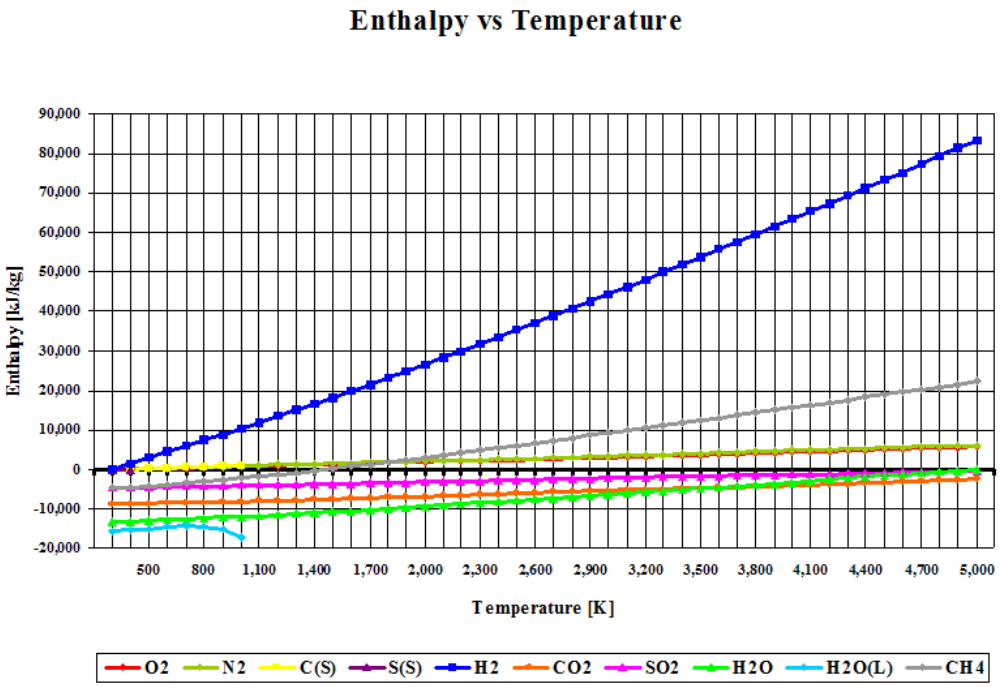
g -- Gibbs Free Energy [kJ/kg]

Input Data

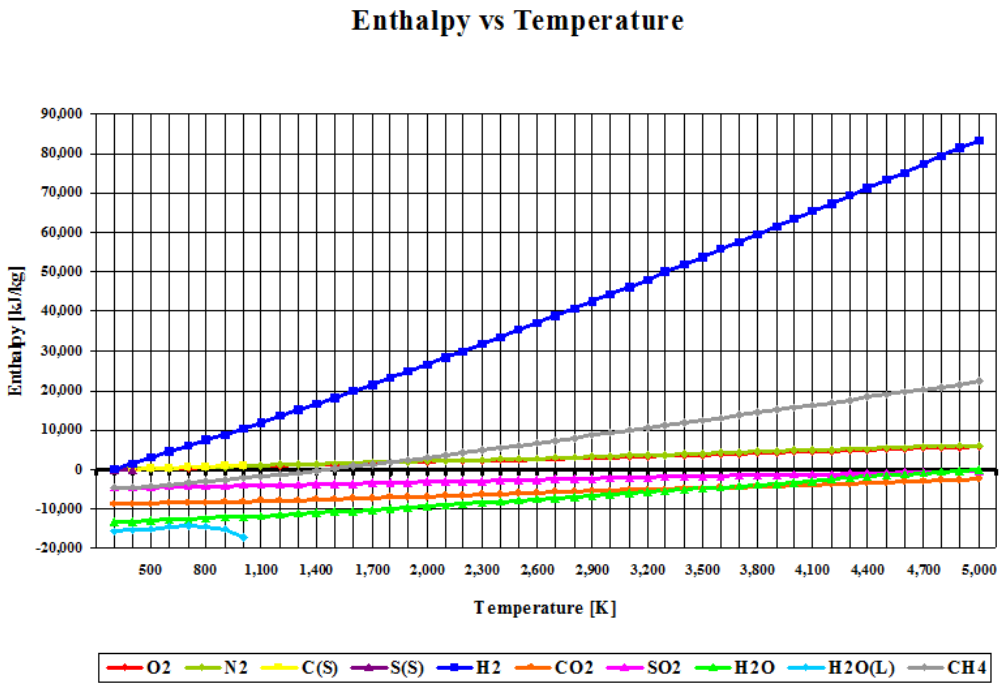
Enthalpy Values for Considered Species at Temperature of 298 [K] and Absolute Pressure of 1 [atm]

Species	***Enthalpy [kJ/kg]***
O_2	-0.15
N_2	-0.17
C(S)	0.13
S(S)	0.53
H_2	-0.67
CO_2	-8,947.21
SO_2	-4,640.06
H2O	-13,440.38
H_2O(L)	-15,887.63
CH_4	-4,682.15

Results


Enthalpy vs Temperature
Enthalpy [kJ/kg]
90,000
80,000
70,000
60,000
50,000
40,000
30,000
20,000
10,000
0
-10,000
-20,000
500
800
1,100
1,400
1,700
2,000
2,300
2,600
2,900
3,200
3,500
3,800
4,100
4,400
4,700
5,000
Temperature [K]
O2
N2
C(S)
S(S)
H2
CO2
SO2
H2O
H2O(L)
CH4

Figures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1,400
1,700
2,000
2,300
2,600
2,900
3,200
3,500
3,800
4,100
4,400
4,700
5,000
Temperature [K]
O2
N2
C(S)
S(S)
H2
CO2
SO2
H2O
H2O(L)
CH4

Conclusions

In general, enthalpy values increase with an increase in temperature.

It is interesting to note that the enthalpy value for basic combustion elements such as carbon (C), hydrogen (H_2), sulfur (S), oxygen (O_2) and nitrogen (N_2) is equal to zero at the standard combustion conditions of 298 [K] and 1 [atm].

Also, it should be mentioned that for ideal gas species, the enthalpy value is only dependent on the temperature.

References

JANAF Thermochemical Data - Tables, 1970