

## **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*

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## *Single Species Approach*

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### *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:

$$C_p/R = A_1 + A_2T + A_3T^2 + A_4T^3 + A_5T^4$$

$$H/(R^*T) = A_1 + A_2T/2 + A_3T^2/3 + A_4T^3/4 + A_5T^4/5 + A_6/T$$

$$S/R = A_1 \ln T + A_2T + A_3T^2/2 + A_4T^3/3 + A_5T^4/4 + A_7$$

or

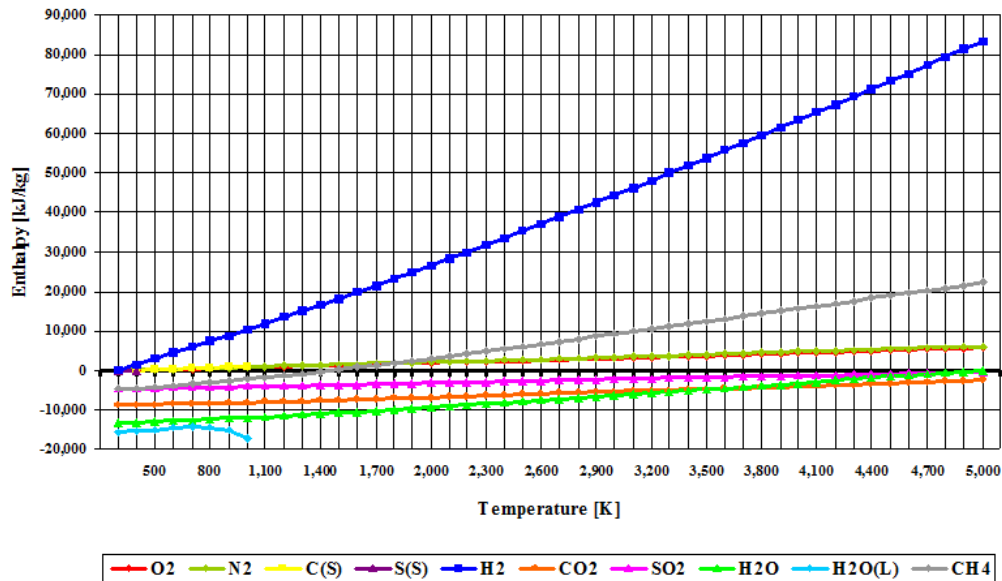
$$S/R = A_1 \ln T + A_2T + A_3T^2/2 + A_4T^3/3 + A_5T^4/4 + A_7 - \ln p$$

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.

## Enthalpy vs Temperature



**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<sub>2</sub>), sulfur (S), oxygen (O<sub>2</sub>) and nitrogen (N<sub>2</sub>) 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:

$$C_p/R = A_1 + A_2T + A_3T^2 + A_4T^3 + A_5T^4$$

$$H/(R^*T) = A_1 + A_2T/2 + A_3T^2/3 + A_4T^3/4 + A_5T^4/5 + A_6/T$$

$$S/R = A_1 \ln T + A_2T + A_3T^2/2 + A_4T^3/3 + A_5T^4/4 + A_7$$

or

$$S/R = A_1 \ln T + A_2T + A_3T^2/2 + A_4T^3/3 + A_5T^4/4 + A_7 - \ln p$$

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,

$$U = H - p^*v^*MW \text{ or } U = H - R^*T$$

$$G = H - S^*T$$

and

$$u = h - p^*v \text{ or } u = h - R^*T/MW$$

$$g = h - s^*T$$

Legend:

**C<sub>p</sub>** -- Specific Heat [kJ/kmol\*K]

**c<sub>p</sub>** -- 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<sup>3</sup>/kg]**

**G -- Gibbs Free Energy [kJ/kmol]**

**g -- Gibbs Free Energy [kJ/kg]**

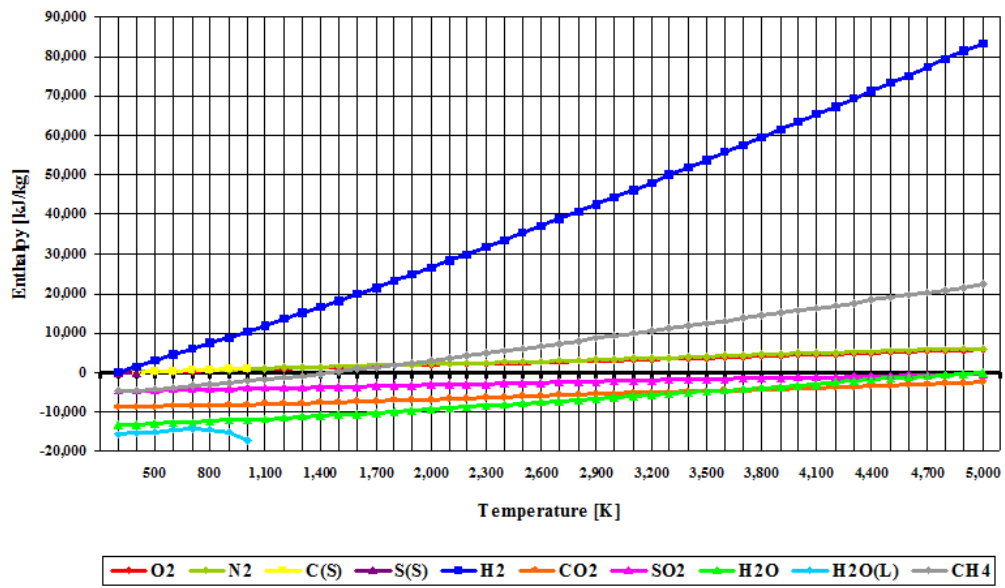
*Input Data*

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

<i>Species</i>	<i>Enthalpy [kJ/kg]</i>
O <sub>2</sub>	-0.15
N <sub>2</sub>	-0.17
C(S)	0.13
S(S)	0.53
H <sub>2</sub>	-0.67
CO <sub>2</sub>	-8,947.21
SO <sub>2</sub>	-4,640.06
H <sub>2</sub> O	-13,440.38
H <sub>2</sub> O(L)	-15,887.63
CH <sub>4</sub>	-4,682.15

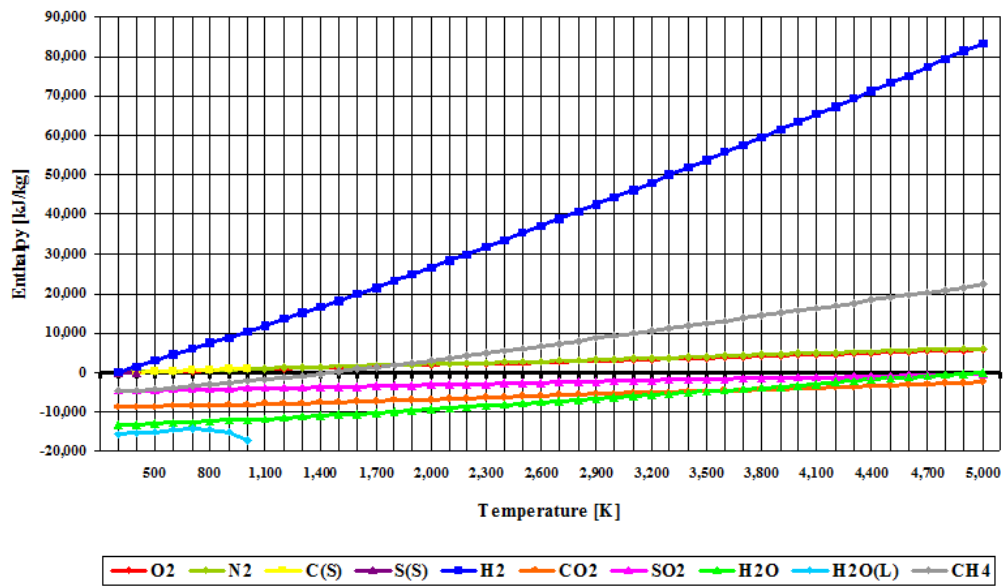
## Results

### Enthalpy vs Temperature



*Figures*

**Enthalpy vs Temperature**



### ***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<sub>2</sub>), sulfur (S), oxygen (O<sub>2</sub>) and nitrogen (N<sub>2</sub>) 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