CH4 + H2O ↔ CO + 3 H2

Calculation of Heat of Reactor

gmol := mole

Basis := 1 gmol

kJ := J·10^3

$$n := \begin{pmatrix} -1 \\ -1 \\ 1 \\ 3 \end{pmatrix} \cdot gmol$$

$$Cpc := \begin{pmatrix} 34.31 & 5.469 & 0.3661 & -11 \\ 33.46 & 0.6880 & 0.7604 & -3.593 \\ 28.95 & 0.4110 & 0.3548 & -2.220 \\ 28.84 & 0.00765 & 0.3288 & -0.8698 \end{pmatrix}$$

$$\Delta Hf := \begin{pmatrix} -74.84 \\ -241.826 \\ -110.52 \\ 0 \end{pmatrix} \cdot \frac{kJ}{gmol}$$

$$\Delta Hf_1 = -7.484 \times 10^4 \ \frac{kg \cdot m^2}{s^2 \cdot mol}$$

a := Cpc^⟨1⟩

$$n_1 = -1 \ mol$$

$$a = \begin{pmatrix} 34.31 \\ 33.46 \\ 28.95 \\ 28.84 \end{pmatrix}$$

b := Cpc^⟨2⟩·10^−2

$$b = \begin{pmatrix} 0.055 \\ 6.88 \times 10^{-3} \\ 4.11 \times 10^{-3} \\ 7.65 \times 10^{-5} \end{pmatrix}$$

c := Cpc^⟨3⟩·10^−5

$$c = \begin{pmatrix} 3.661 \times 10^{-6} \\ 7.604 \times 10^{-6} \\ 3.548 \times 10^{-6} \\ 3.288 \times 10^{-6} \end{pmatrix}$$

$$d := Cpc^{\langle 4 \rangle} \cdot 10^{-9}$$

$$d = \begin{pmatrix} -1.1 \times 10^{-8} \\ -3.593 \times 10^{-9} \\ -2.22 \times 10^{-9} \\ -8.698 \times 10^{-10} \end{pmatrix}$$

$$T := 900$$

$$Tref := 500$$

$$\Delta H_1 := n_1 \cdot \left[\int_{Tref}^{T} \left(a_1 + b_1 \cdot T + c_1 \cdot T^2 + d_1 \cdot T^3 \right) dT \cdot \frac{J}{gmol} + \Delta Hf_1 \right]$$

$$\Delta H_1 = 44.261 \cdot BTU$$

$$\Delta H_2 := n_2 \cdot \left[\int_{Tref}^{T} \left(a_2 + b_2 \cdot T + c_2 \cdot T^2 + d_2 \cdot T^3 \right) dT \cdot \frac{J}{gmol} + \Delta Hf_2 \right]$$

$$\Delta H_2 = 213.75 \cdot BTU$$

$$\Delta H_3 := n_3 \cdot \left[\int_{Tref}^{T} \left(a_3 + b_3 \cdot T + c_3 \cdot T^2 + d_3 \cdot T^3 \right) dT \cdot \frac{J}{gmol} + \Delta Hf_3 \right]$$

$$\Delta H_3 = -92.321 \cdot BTU$$

$$\Delta H_4 := n_4 \cdot \left[\int_{Tref}^{T} \left(a_4 + b_4 \cdot T + c_4 \cdot T^2 + d_4 \cdot T^3 \right) dT \cdot \frac{J}{gmol} + \Delta Hf_4 \right]$$

$$\Delta H_4 = 34.378 \cdot BTU$$

$$\Delta H = \begin{pmatrix} 44.261 \\ 213.75 \\ -92.321 \\ 34.378 \end{pmatrix} \cdot BTU$$

$$\Delta H := \sum \Delta H$$

$$\Delta H = 211.083 \cdot kJ$$

WATER GAS SHIFT REACTION

CO + H2O ↔ CO2 + H2

$$n := \begin{pmatrix} -1 \\ -1 \\ 1 \\ 1 \end{pmatrix} \cdot gmol$$

$$Cpc := \begin{pmatrix} 28.95 & 0.4110 & 0.3548 & -2.220 \\ 33.46 & 0.6880 & 0.7604 & -3.593 \\ 36.11 & 4.233 & -2.887 & 7.464 \\ 28.84 & 0.00765 & 0.3288 & -0.8698 \end{pmatrix}$$

$$\Delta Hf := \begin{pmatrix} -110.52 \\ -241.826 \\ -393.51 \\ 0 \end{pmatrix} \cdot \frac{kJ}{gmol}$$

$$\Delta Hf_1 = -1.105 \times 10^5 \frac{kg \cdot m^2}{s^2 \cdot mol}$$

$$a := Cpc^{\langle 1 \rangle}$$

$$n_1 = -1\ mol$$

$$a = \begin{pmatrix} 28.95 \\ 33.46 \\ 36.11 \\ 28.84 \end{pmatrix}$$

$$b := Cpc^{\langle 2 \rangle} \cdot 10^{-2}$$

$$b = \begin{pmatrix} 4.11 \times 10^{-3} \\ 6.88 \times 10^{-3} \\ 0.042 \\ 7.65 \times 10^{-5} \end{pmatrix}$$

$$c := Cpc^{\langle 3 \rangle} \cdot 10^{-5}$$

$$c = \begin{pmatrix} 3.548 \times 10^{-6} \\ 7.604 \times 10^{-6} \\ -2.887 \times 10^{-5} \\ 3.288 \times 10^{-6} \end{pmatrix}$$

$$d := Cpc^{\langle 4 \rangle} \cdot 10^{-9}$$

$$d = \begin{pmatrix} -2.22 \times 10^{-9} \\ -3.593 \times 10^{-9} \\ 7.464 \times 10^{-9} \\ -8.698 \times 10^{-10} \end{pmatrix}$$

$$T := 900$$

$$Tref := 500$$

$$\Delta H_1 := n_1 \cdot \left[\int_{Tref}^{T} \left(a_1 + b_1 \cdot T + c_1 \cdot T^2 + d_1 \cdot T^3 \right) dT \cdot \frac{J}{gmol} + \Delta Hf_1 \right]$$

$$\Delta H_1 = 92.321 \cdot BTU$$

$$\Delta H_2 := n_2 \cdot \left[\int_{Tref}^{T} \left(a_2 + b_2 \cdot T + c_2 \cdot T^2 + d_2 \cdot T^3 \right) dT \cdot \frac{J}{gmol} + \Delta Hf_2 \right]$$

$$\Delta H_2 = 213.75 \cdot BTU$$

$$\Delta H_3 := n_3 \cdot \left[\int_{Tref}^{T} \left(a_3 + b_3 \cdot T + c_3 \cdot T^2 + d_3 \cdot T^3 \right) dT \cdot \frac{J}{gmol} + \Delta Hf_3 \right]$$

$$\Delta H_3 = -352.511 \cdot BTU$$

$$\Delta H_4 := n_4 \cdot \left[\int_{Tref}^{T} \left(a_4 + b_4 \cdot T + c_4 \cdot T^2 + d_4 \cdot T^3 \right) dT \cdot \frac{J}{gmol} + \Delta Hf_4 \right]$$

$$\Delta H_4 = 11.459 \cdot BTU$$

$$\Delta H = \begin{pmatrix} 92.321 \\ 213.75 \\ -352.511 \\ 11.459 \end{pmatrix} \cdot BTU$$

$$\Delta H := \sum \Delta H$$

$$\Delta H = -36.906 \cdot kJ$$