

-1.302 x 10-8

with T in kelvin and with coefficients c_i given in the table below:

Species	c_0	c_1	c_2	c_3	c_4
CH ₄	4.568	-0.008975	0.00003631	-3.407×10^{-8}	1.091×10^{-11}
H ₂ O	4.395	-0.004186	0.00001405	-1.564×10^{-8}	6.32×10^{-12}
CO	3.912	-0.003913	0.00001182	1.302×10^{-8}	5.15×10^{-12}
H ₂	2.883	0.003681	-7.72×10^{-6}	6.920×10^{-9}	-2.13×10^{-12}

Since all heat capacities are given by the same mathematical form, a fourth-order polynomial in T , ΔC_P can also be expressed in the same polynomial form with coefficients c'_i calculated as

$$c'_i = \sum_k \nu_k c_i^{(k)}.$$

Here $c_i^{(k)}$ is the coefficient of T^i in the heat capacity of species k . Applying this formula we obtain

$$\frac{\Delta C_P^\circ}{R} = 3.598 + 0.020291 T - 0.0000617 T^2 + 5.745 \times 10^{-8} T^3 - 1.847 \times 10^{-11} T^4$$

in which all coefficients are calculated by the same equation as ΔC_P° .

The standard heat of reaction at 800 °C is

$$\Delta H_{1073}^\circ = \Delta H_{298}^\circ + \int_{T_0}^T \Delta C_P dT.$$

add "o" as superscript to match

The enthalpy of reaction at 298 K was obtained in the previous example where we found $\Delta H_{298}^\circ = 205,813$ J/mol. The integral of ΔC_P° is

$$(8.314 \text{ J/mol K}) \int_{273.15}^{1073.15} \left(3.598 + 0.020291 T - 0.0000617 T^2 + 5.745 \times 10^{-8} T^3 - 1.847 \times 10^{-11} T^4 \right) dT = 19,820 \text{ J}$$

289.15

Therefore, the enthalpy of reaction at 1073.15 K is

$$\Delta H_{1073}^\circ = (205,813) + (19,820) = 225,633 \text{ J per mol of methane reacted.}$$

This is about 10% higher than the value at 25 °C.

14.3 Energy Balances in Reacting Systems

A chemical reactor is a vessel in which a reaction takes place. Industrial reactors come in a variety of designs, shapes and sizes. Liquid-phase reactors are usually