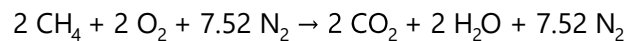


Constant Volume Adiabatic Flame Temperature of the Combustion of Methane in Air

This application calculates the constant volume adiabatic flame temperature of the combustion of methane in air.



The constant volume flame temperature T_{ad} is given by a heat balance on the reactants and products.

$$\sum_{\text{reac}} N_i h_i - \sum_{\text{prod}} N_i h_i - R_u (N_{\text{reac}} T_{\text{init}} - N_{\text{prod}} T_a) = 0$$

The resulting equation is solved numerically for T_{ad} .

Stoichiometry

Number of moles of reactants and products

$$N_{r,\text{CH}_4} := 1 \text{ mol}$$

$$N_{p,\text{CO}_2} := 1 \text{ mol}$$

$$N_{r,\text{O}_2} := 2 \text{ mol}$$

$$N_{p,\text{H}_2\text{O}} := 2 \text{ mol}$$

$$N_{r,\text{N}_2} := 7.52 \text{ mol}$$

$$N_{p,\text{N}_2} := 7.52 \text{ mol}$$

Thermochemical Data

Get data from ThermophysicalData package

Property := ThermophysicalData:-Chemicals:-Property

Enthalpy as a function of temperature

$$h_{\text{CH}_4} := \text{Property}(\text{"Hmolar", "CH4(g)", "temperature"} = T)$$

$$h_{\text{CO}_2} := \text{Property}(\text{"Hmolar", "CO2(g)", "temperature"} = T)$$

$$h_{\text{H}_2\text{O}} := \text{Property}(\text{"Hmolar", "H2O(g)", "temperature"} = T)$$

$$h_{\text{N}_2} := \text{Property}(\text{"Hmolar", "N2(g)", "temperature"} = T)$$

Enthalpy of formation at 298 K

$$h_{f,CH_4} := \text{Property}(\text{"HeatOfFormation"}, \text{"CH4(g)"}, \text{useunits})$$

$$h_{f,O_2} := \text{Property}(\text{"HeatOfFormation"}, \text{"O2(g)"}, \text{useunits})$$

$$h_{f,N_2} := \text{Property}(\text{"HeatOfFormation"}, \text{"N2(g)"}, \text{useunits})$$

$$h_{f,H_2O} := \text{Property}(\text{"HeatOfFormation"}, \text{"H2O(g)"}, \text{useunits})$$

$$h_{f,CO_2} := \text{Property}(\text{"HeatOfFormation"}, \text{"CO2(g)"}, \text{useunits})$$

Reference enthalpies

$$h_{r,CO_2} := \text{eval}(h_{CO_2}, T = 298.15 \text{ K}) = -3.94 \times 10^2 \frac{\text{kJ}}{\text{mol}}$$

$$h_{r,H_2O} := \text{eval}(h_{H_2O}, T = 298.15 \text{ K}) = -2.42 \times 10^2 \frac{\text{kJ}}{\text{mol}}$$

$$h_{r,N_2} := \text{eval}(h_{N_2}, T = 298.15 \text{ K}) = 9.92 \times 10^{-9} \frac{\text{kJ}}{\text{mol}}$$

Heat Balance

Gas constant $R := 8.314 \text{ J} \cdot \text{mol}^{-1} \cdot \text{K}^{-1}$

Enthalpy of reactants and products

$$H_{\text{reactants}} := N_{r,CH_4} \cdot h_{f,CH_4} + N_{r,O_2} \cdot h_{f,O_2} + N_{r,N_2} \cdot h_{f,N_2} = -7.46 \times 10^1 \text{ kJ}$$

$$H_{\text{products}} := N_{p,CO_2} \cdot (h_{CO_2} + h_{f,CO_2} - h_{r,CO_2})$$

$$+ N_{p,H_2O} \cdot (h_{H_2O} + h_{f,H_2O} - h_{r,H_2O})$$

$$+ N_{p,N_2} \cdot (h_{N_2} + h_{f,N_2} - h_{r,N_2})$$

$$\text{HeatBalance} := H_{\text{reactants}} - H_{\text{products}}$$

$$- R \cdot ((N_{r,CH_4} + N_{r,O_2} + N_{r,N_2}) \cdot 298.15 \text{ K}$$

$$- (N_{p,CO_2} + N_{p,H_2O} + N_{p,N_2}) \cdot T) = 0$$

Numerical Solution

Adiabatic flame temperature at constant volume $\text{fsolve}(\text{HeatBalance}, T = 1000 \text{ K}) = 2818.19 \text{ K}$