# 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.

$$2\ CH_4 + 2\ O_2 + 7.52\ N_2 \rightarrow 2\ CO_2 + 2\ H_2O + 7.52\ N_2$$

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

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

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

## Stoichiometry

Number of moles of reactants and products

$N_{r\_CH4} := 1\ \mathbf{mol}$ $\quad N_{p\_CO2} := 1\ \mathbf{mol}$

$N_{r\_O2} := 2\ \mathbf{mol}$ $\quad N_{p\_H2O} := 2\ \mathbf{mol}$

$N_{r\_N2} := 7.52\ \mathbf{mol}$ $\quad N_{p\_N2} := 7.52\ \mathbf{mol}$

## Thermochemical Data

Get data from ThermophysicalData package

Property := ThermophysicalData:-Chemicals:-Property

Enthalpy as a function of temperature

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

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

$h_{H2O}$ := Property( "Hmolar", "H2O(g)", "temperature" = T )

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

Enthalpy of formation at 298 K

$h_{f\_CH4} := \text{Property}(\text{"HeatOfFormation"}, \text{"CH4(g)"}, \text{useunits})$

$h_{f\_O2} := \text{Property}(\text{"HeatOfFormation"}, \text{"O2(g)"}, \text{useunits})$

$h_{f\_N2} := \text{Property}(\text{"HeatOfFormation"}, \text{"N2(g)"}, \text{useunits})$

$h_{f\_H2O} := \text{Property}(\text{"HeatOfFormation"}, \text{"H2O(g)"}, \text{useunits})$

$h_{f\_CO2} := \text{Property}(\text{"HeatOfFormation"}, \text{"CO2(g)"}, \text{useunits})$

Reference enthalpies

$h_{r\_CO2} := \text{eval}(h_{CO2}, T = 298.15\,\mathbf{K}) = -3.94 \times 10^{2}\,\frac{\mathbf{kJ}}{\mathbf{mol}}$

$h_{r\_H2O} := \text{eval}(h_{H2O}, T = 298.15\,\mathbf{K}) = -2.42 \times 10^{2}\,\frac{\mathbf{kJ}}{\mathbf{mol}}$

$h_{r\_N2} := \text{eval}(h_{N2}, T = 298.15\,\mathbf{K}) = 9.92 \times 10^{-9}\,\frac{\mathbf{kJ}}{\mathbf{mol}}$

## Heat Balance

Gas constant

$R := 8.314\,\mathbf{J \cdot mol^{-1} \cdot K^{-1}}$

Enthalpy of reactants and products

$H_{reactants} := N_{r\_CH4} \cdot h_{f\_CH4} + N_{r\_O2} \cdot h_{f\_O2} + N_{r\_N2} \cdot h_{f\_N2} = -7.46 \times 10^{1}\,\mathbf{kJ}$

$$H_{products} := N_{p\_CO2} \cdot (h_{CO2} + h_{f\_CO2} - h_{r\_CO2}) + N_{p\_H2O} \cdot (h_{H2O} + h_{f\_H2O} - h_{r\_H2O}) + N_{p\_N2} \cdot (h_{N2} + h_{f\_N2} - h_{r\_N2})$$

$$HeatBalance := H_{reactants} - H_{products} - R \cdot \left( (N_{r\_CH4} + N_{r\_O2} + N_{r\_N2}) \cdot 298.15\,\mathbf{K} - (N_{p\_CO2} + N_{p\_H2O} + N_{p\_N2}) \cdot T \right) = 0$$

## Numerical Solution

Adiabatic flame temperature at constant volume

$\text{fsolve}(HeatBalance, T = 1000\,\mathbf{K}) = 2818.19\,\mathbf{K}$