Adiabatic Flame Temperature

- The temperature of product mixture obtained when the combustion is done in an adiabatic system
- Highest temperature obtained
- 2 types
  - Constant pressure adiabatic flame temperature
  - Constant volume adiabatic flame temperature

Const. Press. Adiab. Flame Temp.

- From 1st Law

$$H_{react}(T_i, P) = H_{prods}(T_{ad}, P)$$

Const. Vol. Adiab. Flame Temp.

- From 1st Law

$$U_{react}(T_i, P_i) = U_{prods}(T_{ad}, P_f)$$

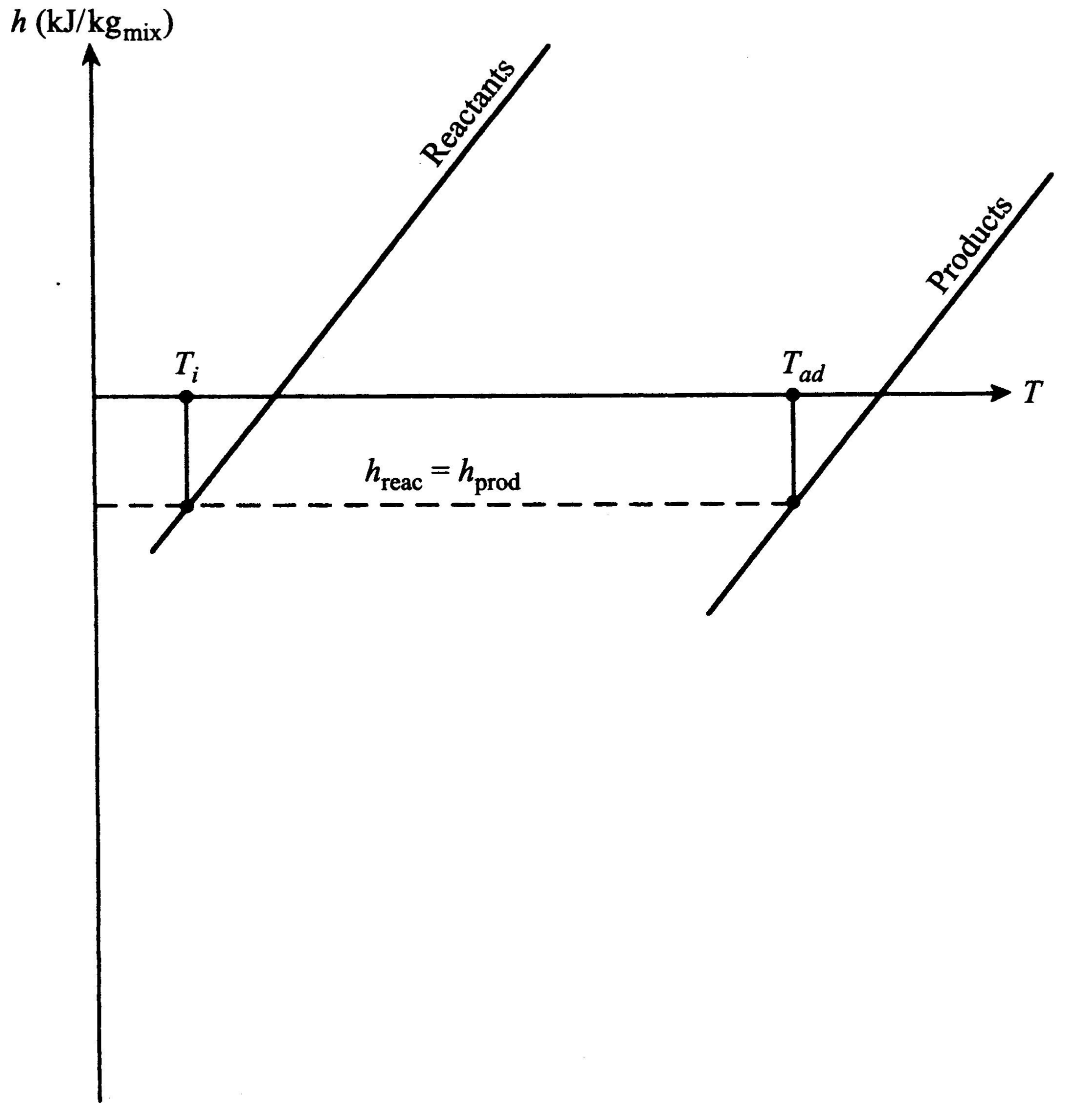

Figure 2.10 Illustration of constant-pressure adiabatic flame temperature on *h*–*T* coordinates.

Specific Heats

- C_p varies with temperature
- Non trivial to determine T_{adiab} since temp is implicit in c_p

$$\bar{h}_i = \bar{h}^o_{f,i} + \int_{298}^{T} \bar{c}_{p,i}\, dT$$

- We may
  - Integrate c_p
  - Use an average c_p value $\bar{h}_i = \bar{h}^o_{f,i} + \bar{c}_{p,i,avg}(T_{ad} - 298)$
  - Both methods need an initial guess of T_{adiab}

$$T_{adiab} \approx 2100\,K$$

Example 2.5

Estimate the constant-pressure adiabatic flame temperature for the combustion of a stoichiometric CH_4–air mixture. The pressure is 1 atm and the initial reactant temperature is 298 K.

Use the following assumptions:

1. "Complete combustion" (no dissociation), i.e., the product mixture consists of only CO_2, H_2O, and N_2.
2. The product mixture enthalpy is estimated using constant specific heats evaluated at 1200 K ($\approx 0.5(T_i + T_{ad})$, where T_{ad} is guessed to be about 2100 K).

Solution

Mixture composition:

$$CH_4 + 2(O_2 + 3.76N_2) \rightarrow 1\,CO_2 + 2H_2O + 7.52N_2$$

$$N_{CO_2} = 1,\ N_{H_2O} = 2,\ N_{N_2} = 7.52.$$

Properties (Appendices A and B):

Species	Enthalpy of Formation @ 298 K $\bar{h}^o_{f,i}$ (kJ/kmol)	Specific Heat @ 1200 K $\bar{c}_{p,i}$ (kJ/kmol-K)
CH_4	−74,831	—
CO_2	−393,546	56.21
H_2O	−241,845	43.87
N_2	0	33.71
O_2	0	—

First law (Eqn. 2.40):

$$\begin{aligned}
H_{\text{react}} &= \sum_{\text{react}} N_i \bar{h}_i = H_{\text{prod}} = \sum_{\text{prod}} N_i \bar{h}_i \\
H_{\text{react}} &= (1)(-74{,}831) + 2(0) + 7.52(0) \\
&= -74{,}831\ \text{kJ} \\
H_{\text{prod}} &= \sum N_i[\bar{h}^o_{f,i} + \bar{c}_{p,i}(T_{ad} - 298)] \\
&= (1)[-393{,}546 + 56.21(T_{ad} - 298)] \\
&\quad + (2)[-241{,}845 + 43.87(T_{ad} - 298)] \\
&\quad + (7.52)[0 + 33.71(T_{ad} - 298)].
\end{aligned}$$

Equating H_{react} to H_{prod} and solving for T_{ad} yields

$$\boxed{T_{ad} = 2318\ \text{K}}$$

Example 2.6

Estimate the constant-volume adiabatic flame temperature for a stoichiometric CH_4–air mixture using the same assumtions as in Example 2.5. Initial conditions are $T_i = 298$ K, $P = 1$ atm $(= 101{,}325$ Pa).

Solution

The same composition and properties used in Example 2.5 apply here. We note, however, that the $c_{p,i}$ values should be evaluated at a temperature somewhat greater than 1200 K, since the constant-volume T_{ad} will be higher than the constant-pressure T_{ad}. Nonetheless, we will use the same values as before.

First law (Eqn. 2.43):

$$H_{\text{reac}} - H_{\text{prod}} - R_u(N_{\text{reac}} T_{\text{init}} - N_{\text{prod}} T_{ad}) = 0$$

or

$$\sum_{\text{reac}} N_i \bar{h}_i - \sum_{\text{prod}} N_i \bar{h}_i - R_u(N_{\text{reac}} T_{\text{init}} - N_{\text{prod}} T_{ad}) = 0.$$

Substituting numerical values, we have

$$\begin{aligned} H_{\text{react}} &= (1)(-74{,}831) + 2(0) + 7.52(0) \\ &= -74{,}831\ \text{kJ} \\ H_{\text{prod}} &= (1)[-393{,}546 + 56.21(T_{ad} - 298)] \\ &\quad + (2)[-241{,}845 + 43.87(T_{ad} - 298)] \\ &\quad + (7.52)[0 + 33.71(T_{ad} - 298)] \\ &= -877{,}236 + 397.5(T_{ad} - 298)\ \text{kJ} \end{aligned}$$

and

$$R_u(N_{\text{reac}} T_{\text{init}} - N_{\text{prod}} T_{ad}) = 8.315(10.52)(298 - T_{ad}),$$

where $N_{\text{reac}} = N_{\text{prod}} = 10.52$ kmol.

Reassembling Eqn. 2.43 and solving for T_{ad} yields

$$\boxed{T_{ad} = 2889\ \text{K}}$$