Homework Hints

- See online hint for Problem 9-66 (9-56 in 3rd Ed.)

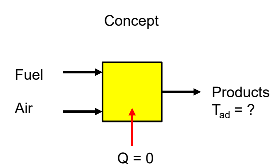
Class 33

Adiabatic Flame Temperatures

Review of Enthalpy

Term	Units	Explanation
H	J	
$\dot{H}$	J/s	
$\hat{H}$	J/mol or kJ/kg	
$\Delta H_f{}^0$	kJ/mol	
ΔH_{rxn}	kJ/mol	
ΔH_c	kJ/mol	
ΔH_{vap}	kJ/mol	
ΔH_m	kJ/mol	

Adiabatic Flame Temperature

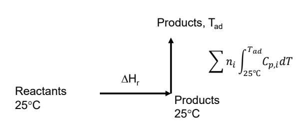


- Very useful in industry
  - Maximum T possible
  - Determines material used to confine the flame
- All energy from exothermic reaction goes into heating up products
- Iterative process because C_p = f(T)
- Numbers can be reasonable, but not with the C_p's in the text

Review of Enthalpy

Term	Units	Explanation
H	J	Total enthalpy (H = U + PV)
$\dot{H}$	J/s	Enthalpy per time
$\hat{H}$	J/mol or kJ/kg	Specific enthalpy (i.e., enthalpy per unit mass or mole)
$\Delta H_f{}^0$	kJ/mol	Standard heat of formation (^{0} means at 1 atm, 25°C)
ΔH_{rxn}	kJ/mol	Heat of reaction
ΔH_c	kJ/mol	Heat of combustion (in book, this corresponds to the high heating value with liquid H_2O as a product) (^{0} means reactants and products at 1 atm, 25°C)
ΔH_{vap}	kJ/mol	Heat of vaporization (liquid ⇒ vapor) (Value in Table B.1 at boiling temperature, 1 atm)
ΔH_m	kJ/mol	Heat of melting (Value in Table B.1 at melting temperature, 1 atm)

A. Path Method



- If reactants are at 25°C, then

Find

$$Q = 0 = n_{fuel} \Delta H_r + \sum_{products} n_i \int_{25°C}^{T_{ad}} C_{p,i} dT$$

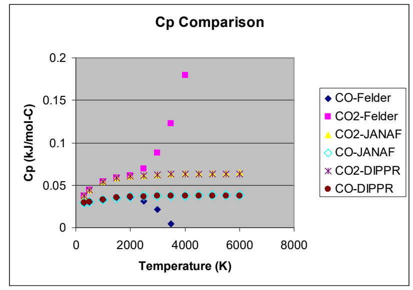
Good for simple reactions

B. In-Out Table to Calculate T_{ad}

1. Guess T_{ad}
2. Make H table on in and out streams based on T_{ad}
3. Compute $Q = \left(\sum n_i \hat{H}_i\right)_{out} - \left(\sum n_i \hat{H}_i\right)_{in}$
4. If $Q \neq 0$, go to step 1

- There are nice algorithms to make a series of guesses
- These are included in the solver in Excel and Mathcad

Heat Capacity Correlations Can Go Crazy at High Temperatures!



Example 1

- Fuel = methane at 25°C (basis: 1 mole of CH_4, stoichiometric air)
- T_{in} = 25°C

$CH_4 + 2\ O_2 \Rightarrow CO_2 + 2\ H_2O$

O_2 req'd
2 moles

- What is $T_{adiabatic}$ in stoichiometric air?
- What is $T_{adiabatic}$ in stoichiometric O_2?

N_2 req'd
$2 \times (79/21) = 7.524$ moles

See Excel Sheet

Then set $n_{N2} = 0$ and redo solver.

Spreadsheet with high T C_p's

http://www.et.byu.edu/~tom/classes/273/273.html

Spreadsheet

With More Complex Chemistry

CH4-Air Stoichimetric

Ar	0.84%
CO	0.85%
CO2	8.60%
H	0.04%
H2	0.34%
H2O	18.32%
NO	0.18%
N2	70.10%
O	0.02%
OH	0.30%
O2	0.43%

T_ad= 2212K

CH4-O2 Stoichimetric

CO	15.52%
CO2	11.36%
H	4.86%
HO2	0.01%
H2	7.15%
H2O	39.23%
O	3.78%
OH	9.93%
O2	8.18%

T_ad= 3048K

Example 2

- Fuel = 40 mol% CO, 60 mol% H_2 (basis: 100 moles of fuel)
- T_{in} = 25°C

$CO + ½O_2 \Rightarrow CO_2$

$H_2 + ½O_2 \Rightarrow H_2O$

O_2 req'd
20 moles
30 moles

- What is $T_{adiabatic}$ in stoichiometric air?
- What is $T_{adiabatic}$ in stoichiometric O_2?

N_2 req'd
$50 \times (79/21)$ = 188 moles

See Excel Sheet

Then set n_{N2} = 0 and redo solver.

40% CO, 60% H_2 Example

- In Air
  - T = 2649 K using Felder C_p's
  - T = 2584 K using JANAF C_p's
  - T = 2371 K using chemical equilibrium code
    - 6.10 mol% H_2
    - 0.99 mol% O_2
    - 0.11 mol% H
    - 0.07 mol% O
    - 0.61 mol% OH
    - 2.06 mol% CO
    - 0.37 mol% NO

Combined energy balance and chemical equilibrium calculation

Mistake Students Made on Exam

- Fuel = 40 mol% CO, 60 mol% H_2 (basis: 1 moles of fuel)
- $CO + H_2 + O_2 => CO_2 + H_2O$
- Rationalize: 1 mole of O_2 needed
- Problems with this idea:
  - There are actually 2 moles fuel in this equation (1 CO and 1 H_2)
  - There are not equal amounts of CO and H_2 (although this would not have caused the error)
- $4CO + 6H_2 + 5O_2 => 4 CO_2 + 6H_2O$
- Better to treat each fuel separately

40% CO, 60% H_2 Example

- In O_2
  - T = 5047 K using Felder C_p's
  - T = 5038 K using JANAF C_p's
  - T = 3009 K using chemical equilibrium code
    - 5.84 mol% H_2
    - 8.79 mol% O_2
    - 3.91 mol% H
    - 3.44 mol% O
    - 8.37 mol% OH
    - 17.41 mol% CO
    - Trace HO_2

Spreadsheet

Message:

- If temperatures get too hot, other species (like radical species) become stable, lowering the flame temperature!
- In particular, CO is as stable as CO_2 at high temperatures (above 2700 K)

Special Problem 9c

Help on Special Problem 9c

$CH_4 + 2\,O_2 \rightarrow CO_2 + 2\,H_2O$ (ξ_1)

$CH_4 + 1.5\,O_2 \rightarrow CO + 2\,H_2O$ (ξ_2)

$$SR = \frac{n_{oxidizer}}{n_{fuel}} \Big/ \left(\frac{n_{oxidizer}}{n_{fuel}}\right)_{stoich}$$

But $\left(\frac{n_{oxidizer}}{n_{fuel}}\right)_{stoich}$ = (2/1) = 2 (based only on first reaction!)

Therefore, $SR = \frac{n_{oxidizer}}{n_{fuel}}/2$

Assuming $n_{CH4,0} = 1$, then $n_{O2,0} = 2*SR$

Assuming all O_2 and CH_4 react (fuel-rich case),

$$n_{O2} = 0 = n_{O2,0} - 2\,\xi_1 - 1.5\,\xi_2$$

$$n_{CH4} = 0 = n_{CH4,0} - \xi_1 - \xi_2$$

$$\xi_2 = \frac{2 - n_{O2,0}}{0.5} \text{ (prove this)}$$

$$\xi_1 = 1 - \xi_2 \text{ (prove this)}$$

Questions?

- Enthalpy
- Heat Capacities
- Heat of Formation
- Heat of Vaporization, Heat of Melting
- Heat of Combustion
- Energy Balances
- Adiabatic Flame Temperature

Help on Special Problem 9c

$CH_4 + 2\,O_2 \rightarrow CO_2 + 2\,H_2O$ (ξ_1)

$CH_4 + 1.5\,O_2 \rightarrow CO + 2\,H_2O$ (ξ_2)

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But $\left(\frac{n_{oxidizer}}{n_{fuel}}\right)_{stoich}$ = (2/1) = 2 (based only on first reaction!)

Therefore, $SR = \frac{n_{oxidizer}}{n_{fuel}}/2$

Assuming $n_{CH4,0} = 1$, then $n_{O2,0} = 2*SR$

Assuming all CH_4 reacts and there is excess O_2 (O_2-rich case),

$$n_{O2} = 0 = n_{O2,0} - n_{O2,stoich} = n_{O2,0} - 2$$

No CO is formed (all CH_4 forms only CO_2)

$$\xi_2 = 0$$

$$\xi_1 = 1$$