Combustion: Flame Theory and Heat Produced

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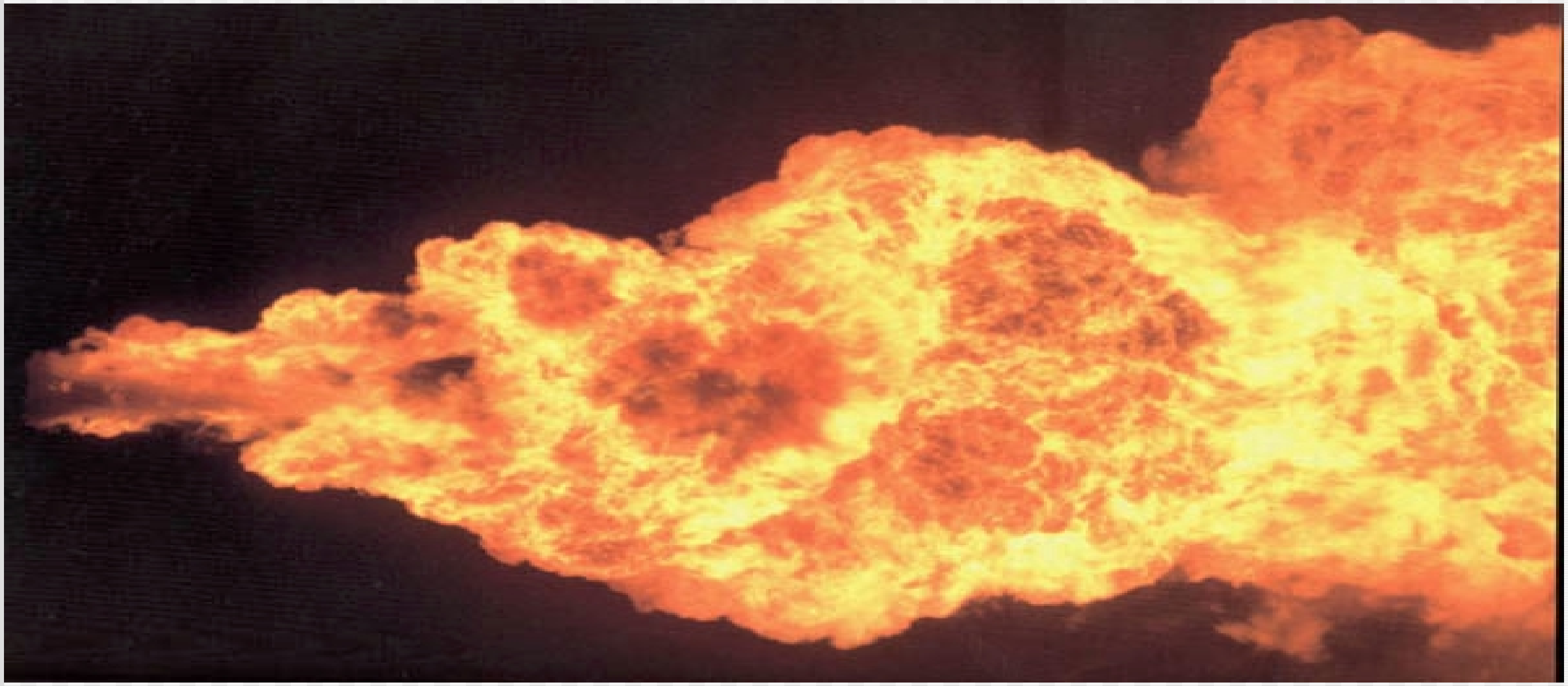
What is a Flame?

- Reaction Zone
- Thermo/Chemical characteristics

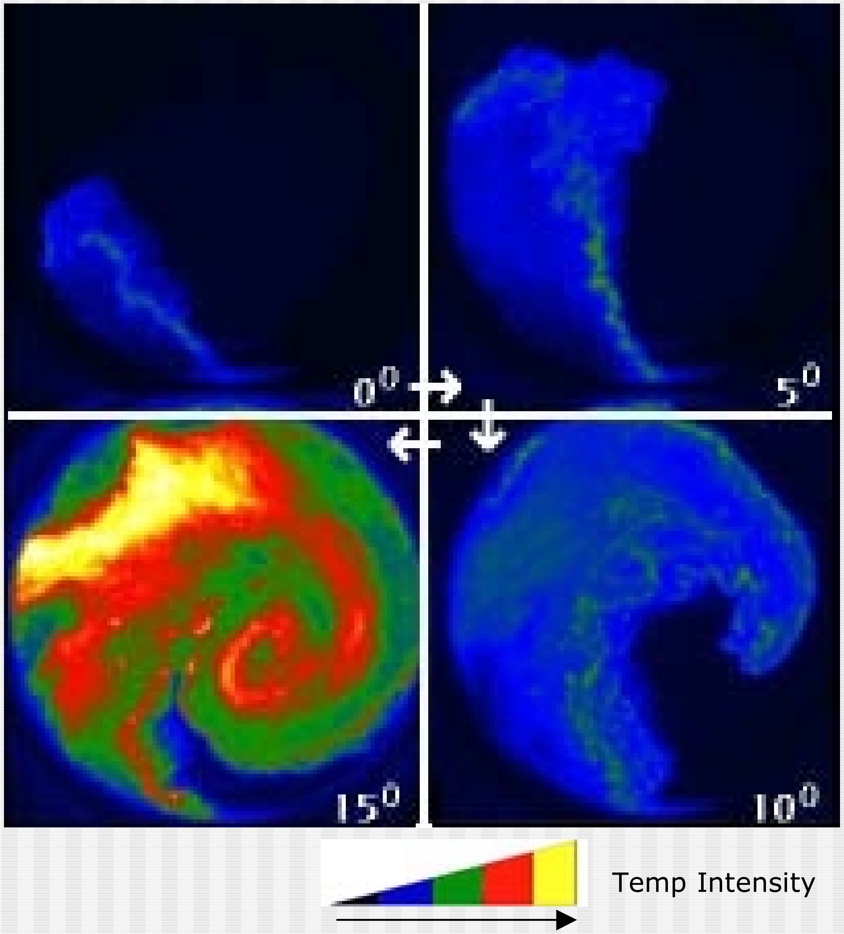


Types of Flame

- Premixed
- Diffusion
- Both can be Laminar or Turbulent

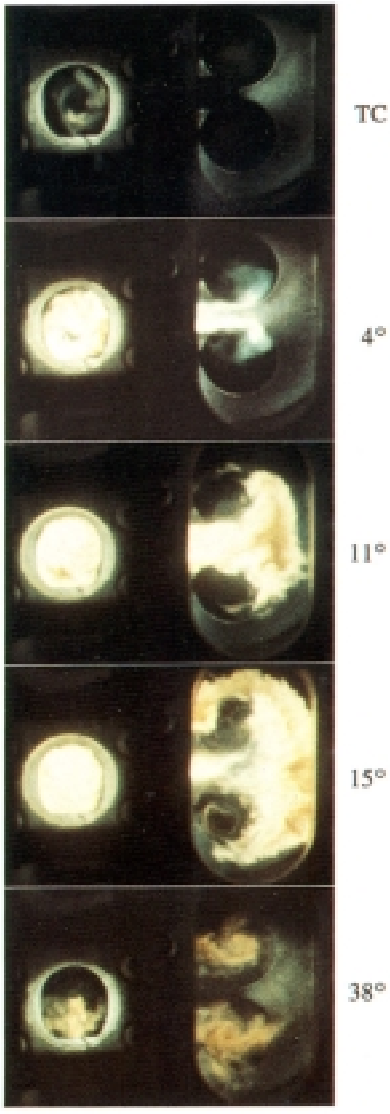
Premixed

- Mixed before Combustion
- Characteristics
  - Reacts Rapidly
  - Constant Pressure
  - Propagates as Thin Zone
- Ex: Spark Engine



Diffusion

- Mixed during Combustion
- Characteristics
  - Reaction occurs at Fuel/Air interface
  - Controlled by the Mixing of the Reactants
- Ex:Diesel Engines



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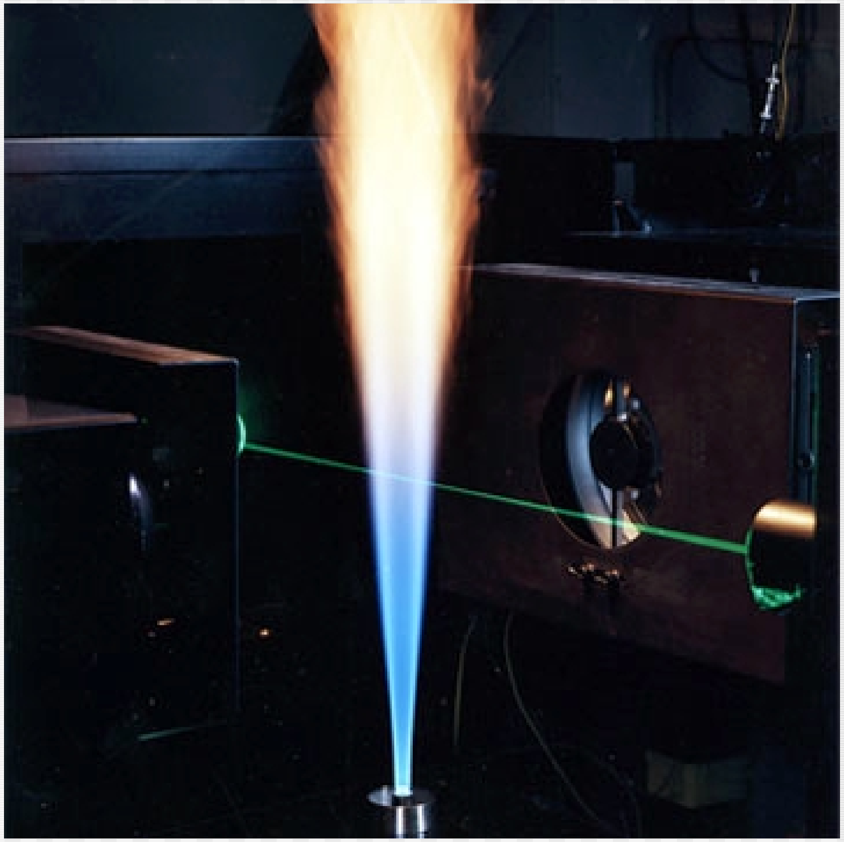
Laminar

- Premixed
  - Simplest flame type
  - Ex: Bunsen burner
- Diffusion
  - Ex: Candle

Turbulent



- Premixed
  - Faster heat release than laminar
  - Ex: Indirect fuel injection engines
- Diffusion
  - Ex: Direct fuel injection engines

Chemical Energy

- The energy inside fuel can be considered “potential energy”
- Combustion unleashes that “potential energy”
- How do we calculate the amount of energy released?

Basic Chemistry

- Hydrocarbon fuels
- Air
  - Nitrogen (79%)
  - Oxygen (21%)
  - 1 mol O_2:3.76 mol N_2
- Common Products: H_2O, CO_2, N_2

Basic Chemistry-Moles

- Amount of mass of an element or compound that contains Avogadro’s number of atoms or molecules
- Avogadro’s number = 6.022 E 23
- For example one mole of Hydrogen contains 6.022E 23 Hydrogen atoms.
- Molar mass is the amount of mass in one mole of a substance.

Basic Chemistry–Molar Mass

Mass is conserved in chemical equations

1 kmol H_2 + ½ kmol O_2 $\longrightarrow$ 1 kmolH_2O

$$1\text{kmol}\cdot H_2\left(\frac{2.016\text{kg}}{\text{kmol}\cdot H_2}\right)+\frac{1}{2}\cdot\text{kmol}\cdot O_2\left(\frac{32\text{kg}}{\text{kmol}\cdot O_2}\right)=1\text{kmol}\cdot H_2O\left(\frac{18.02\text{kg}}{\text{kmol}\cdot H_2O}\right)$$

$$18.02\text{kg} = 18.02\,\text{kg}$$

Balancing an Equation

Original Chemical Equation:

$$C_4H_{10} + a(O_2 + \ 3.76N_2) \longrightarrow \ bCO_2 + cH_20 + dN_2$$

Write equations for each element, solve:

C: $4 = b$

H: $10 = 2c$

$c = 5$

O: $2a = 2b + c$

$a = 6.5$

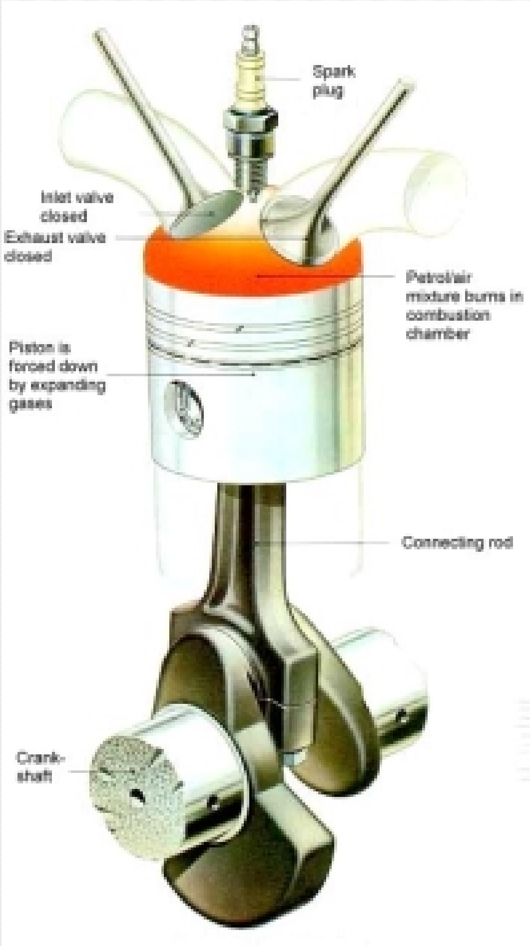
N: $2(3.76)a = 2d$

$d = 24.44$

Final Balanced Equation:

$$C_4H_{10} + 6.5(O_2 + \ 3.76N_2) \longrightarrow \ 4CO_2 + 5H_20 + 24.44N_2$$

Focusing on the Problem



- We have
  - Basics of Flame Theory
  - Balanced Equations
- What's Missing?

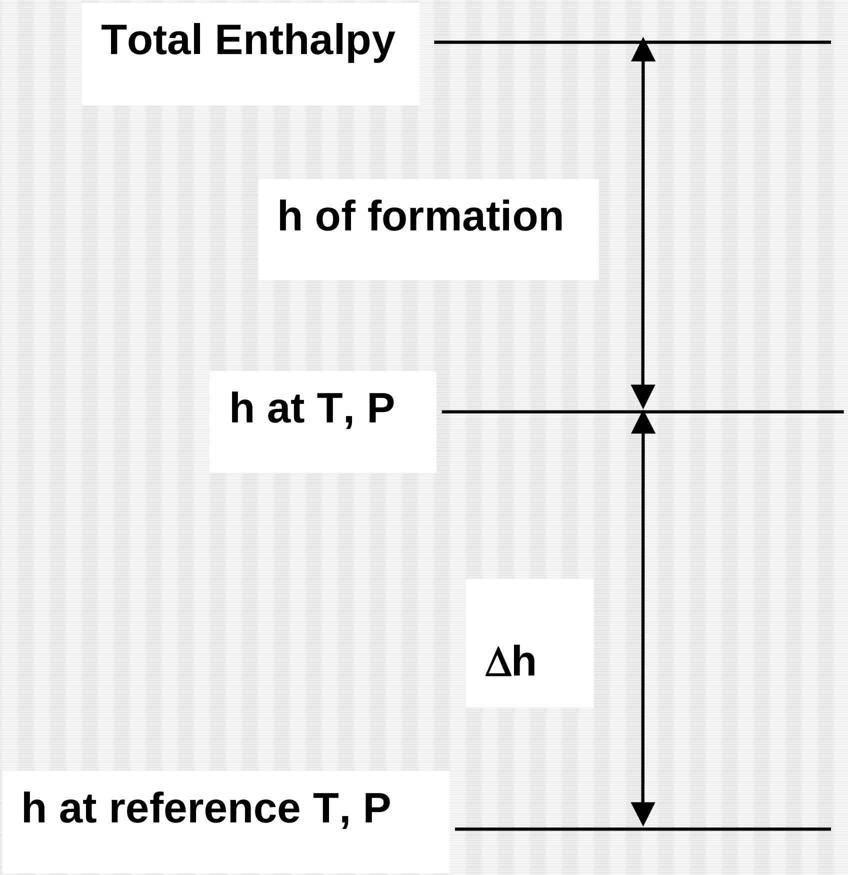
Enthalpy

- Definition $h = u + Pv$
- Reference State
    - 25 °C
    - 1 atm
- $\Delta h = h(T,P) - h(T,P)_{ref}$

Enthalpy

- Enthalpy of Formation
  - Energy exchanged during compound formation
  - N_2, O_2, & H_2 have $h_{form}=0$
- Total Enthalpy

  $h=h_{form} + \Delta h$



Total Enthalpy

h of formation

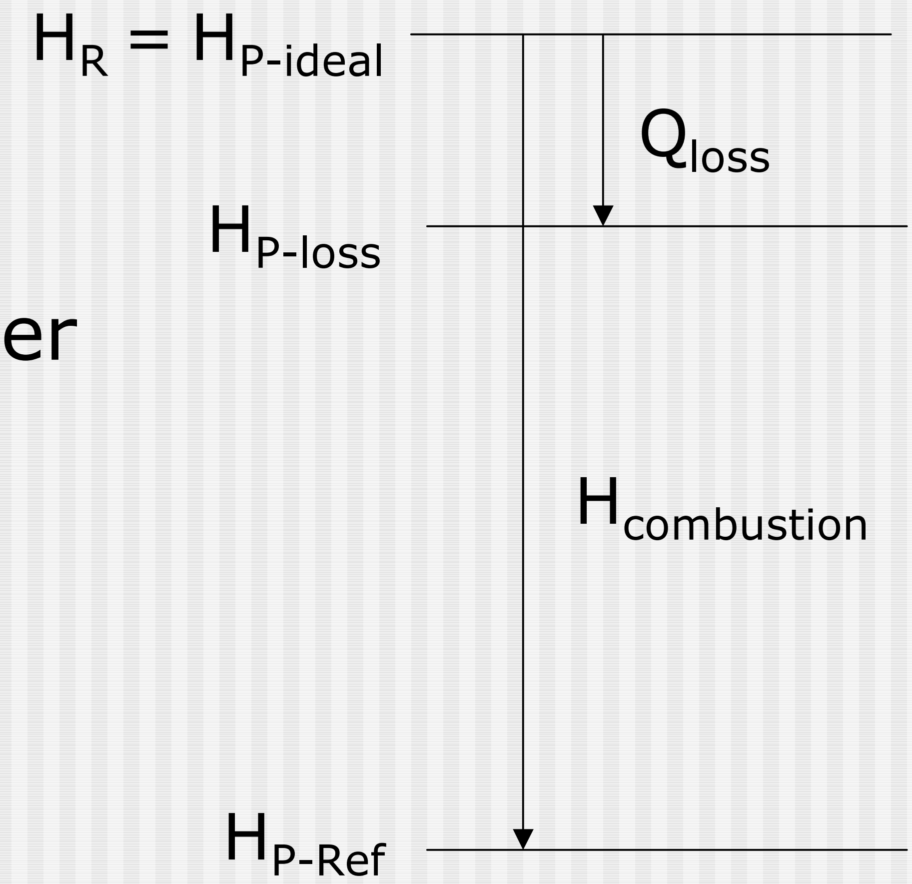
h at T, P

Δh

h at reference T, P

More Enthalpy

- Enthalpy of Combustion
- Higher and Lower Heating Values
  - Liquid H_2O
  - Vapor H_20



$H_R = H_{P\text{-ideal}}$

Q_{loss}

$H_{P\text{-loss}}$

$H_{combustion}$

$H_{P\text{-Ref}}$

Energy Equation

$Q-W = \Delta U$

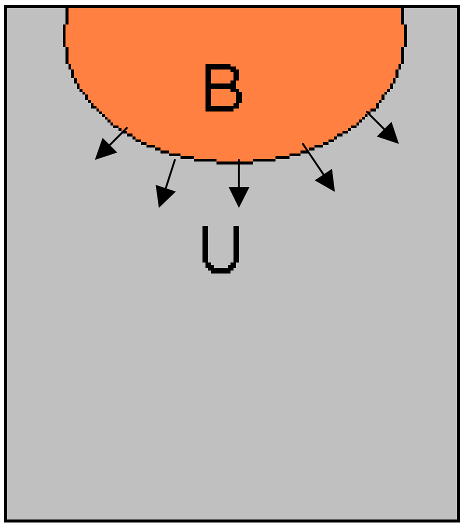
$Q= \Delta U+W= \Delta U+ P\Delta V$

$Q = \Delta H$

$Q = H_p - H_r$

Combustion Chamber

- Burned and Unburned regions
- Flame propagation
- Constant Pressure



Heat Loss Example

A mixture of 1kmol of gaseous methane and air, originally at reference state, burns completely in a combustion chamber, at constant pressure. Determine the amount of heat the chamber loses if the Product temperature measured after combustion is 890K.

$$CH_4 + \left(O_2 + 3.76 \cdot N_2\right) \longrightarrow CO_2 + H_2O + N_2$$

Balanced $$CH_4 + 2 \cdot \left(O_2 + 3.76N_2\right) \longrightarrow CO_2 + 2H_2O + 7.52N_2$$

$$Q = H_p - H_r$$

$$Q = \sum_{P} (n \cdot h) - \sum_{R} (n \cdot h)$$

Heat Loss Example

$$Q = H_p - H_r$$

$$Q = \sum_{P} (n \cdot h) - \sum_{R} (n \cdot h)$$

$$\sum_{P} (n \cdot h) = \underline{1 \cdot \left(h_{CO2}\right)} + 2\left(h_{H2O}\right) + 7.52\left(h_{N2}\right)$$

$$\sum_{R} (n \cdot h) = 1\left(h_{CH4}\right) + \underline{2 \cdot \left(h_{O2}\right)} + 7.52\left(h_{N2}\right)$$

$$h = h_{form} + \Delta h$$

$$h = h_{form} + \left(h(T) - h\left(T_{ref}\right)\right)$$

A lot of terms
Lets look at two of them.

Heat Loss Example-CO_2

$$H_{CO2} = 1\left(h_{CO2}\right) = h_{form} + \left(h\left(T_p\right) - h\left(T_{ref}\right)\right)$$

	$h°_f$ (kJ/kmol)	h at 298 K	h at 890 K
Carbon Dioxide CO_2	**-393,520**	**9364**	**36876**
Water Vapor H_2O	**-241,820**	**9904**	**31429**
Oxygen O_2	**0**	**8682**	**27584**
Nitrogen N_2	**0**	**8669**	**26568**
Methane Ch_4	**-74850**		
Octane C_8H_{18}	**-249910**		

$$H_{CO2} = -393520 + (36876 - 9364)$$

$$H_{CO2} = -366008 \text{ kJ}$$

Heat Loss Example-O_2

$$H_{O2} = 2\left(h_{O2}\right) = 2\left[h_{form} + \left(h\left(T_R\right) - h\left(T_{ref}\right)\right)\right]$$

	$h°_f$ (kJ/kmol)	h at 298 K	h at 890 K
Carbon Dioxide CO_2	-393,520	9364	36876
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Oxygen O_2	0	8682	27584
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Methane Ch_4	-74850		
Octane C_8H_{18}	-249910		

$$H_{O2} = 2[0 + (8682 - 8682)]$$

$$H_{O2} = 0$$

Heat Loss Example

The remaining terms are evaluated, using the above techniques.

$$Q = \left(h_{CO2} + 2h_{H2O} + 7.52\cdot h_{N2}\right) - \left(h_{CH4} + 2\cdot h_{O2} + 7.52\cdot h_{N2}\right)$$

$$Q = [\,(-366008) + 2(-220295) + 7.52\cdot(17899)\,] - [\,-74850 + 2(0) + 7.52\cdot(0)\,]$$

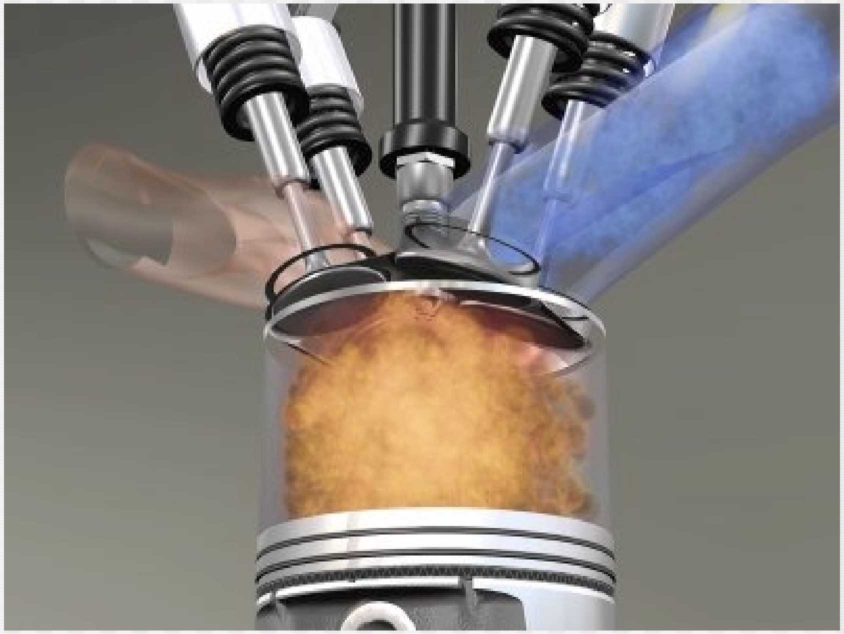
$$Q = -597148 \quad \text{kJ}$$

597148 kJ of heat was lost to the surroundings.

Departures From Ideal

- Combustion not always complete
  - Insufficient Mixing
  - Insufficient Air
- May Lead to Knocking

Adiabatic Flame Temperature



- Adiabatic Conditions
- Limiting Value of Flame Temperature
- Iterative Process

AFT Example

This problem has the same set of assumptions as the last problem. The only difference is that now we are assuming adiabatic flame conditions

$$CH_4 + 2(O_2 + 3.76N_2) \longrightarrow CO_2 + 2H_2O + 7.52\ N_2$$

$$\cancel{Q} = H_P - H_R$$

$$H_P = H_R$$

$$h_{CO2} + 2\cdot(h_{H2O}) + 7.52\cdot(h_{N2}) = (h_{CH4}) + 2\cdot(h_{O2}) + 7.52\cdot(h_{N2})$$

AFT Example

evaluate the products:

$$H_{CO2} = \left(h_{formCO2} + h_{CO2}\left(T_P\right) - h_{CO2}\left(T_{ref}\right)\right)$$

$$H_{H2O} = 2\left(h_{formH2O} + h_{H2O}\left(T_P\right) - h_{H2O}\left(T_{ref}\right)\right)$$

$$H_{N2} = 7.52\left(h_{formN2} + h_{N2}\left(T_P\right) - h_{N2}\left(T_{ref}\right)\right)$$

None of these enthalpy terms can be fully evaluated since T_p is unknown

Keeping it Real

- Efficiency
- How far does AFT fall from actual?
- Factors influencing
  - Dissociation
  - Chamber not really adiabatic

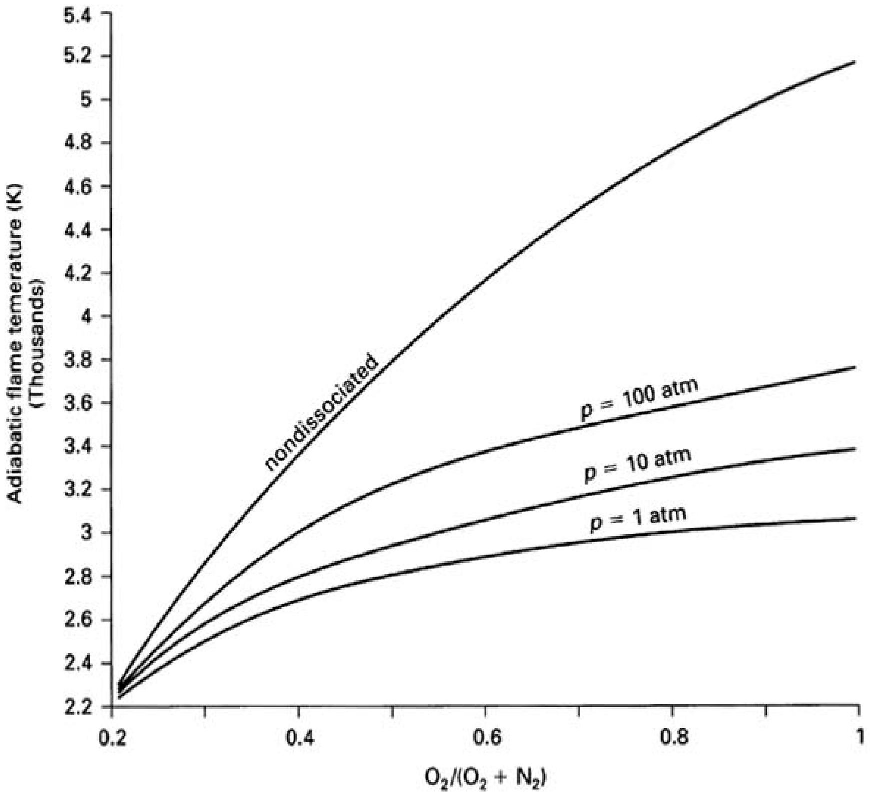


FIGURE 3.6
Adiabatic, constant-pressure flame temperature of stoichiometric methane-oxygen with nitrogen mixtures initially at 298 K.

Conclusion

- Premixed and Diffusion
  - Laminar and Turbulent
- Finding Qin
  - Balancing Chemical Equation
  - Energy Balance Equation
- Finding Adiabatic Flame Temperature
  - Gives Limit of Product Temperature
  - Dissociation, other factors decrease temperature