Remaining Schedule

- Today – Adiabatic Flame Temperature
- Wed – Transient Balance Review
- Fri, Nov. 18 – Exam 3 Review
  - Practice Exam 3 now available on Learning Suite
  - No formal class on Mon, Nov. 22
  - Due Tuesday, November 22, 9 am
- Tues, Nov 22 – Class will be for you to start the case study with your team
  - Due in class on Wed, Dec 7
- Wed, Dec 7 – Final Exam Review
- Tues, Dec 13 – Final Exam, 7 am, in class
  - Practice Final now available on Learning Suite

1

Some anthropologists believe that the discoveries of fire, shelter, and language were almost simultaneous.

COMBUSTION

2

A fire started on some grasslands near a farm. The county fire department was called to put out the fire. The fire was more than the county fire department could handle. Someone suggested that a nearby volunteer group be called. Despite some doubt that the volunteer outfit would be of any assistance, the call was made.

The volunteers arrived in a dilapidated old fire truck. They rumbled straight towards the fire, drove right into the middle of the flames and stopped! The firemen jumped off the truck and frantically started spraying water in all directions. Soon they had snuffed out the center of the fire, breaking the blaze into two easily-controlled parts.

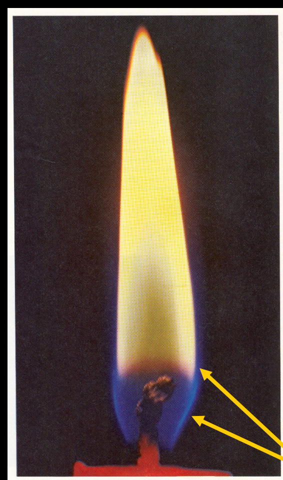
Watching all this, the farmer was so impressed with the volunteer fire department's work and was so grateful that his farm had been spared, that right there on the spot he presented the volunteers with a check for $1,000.

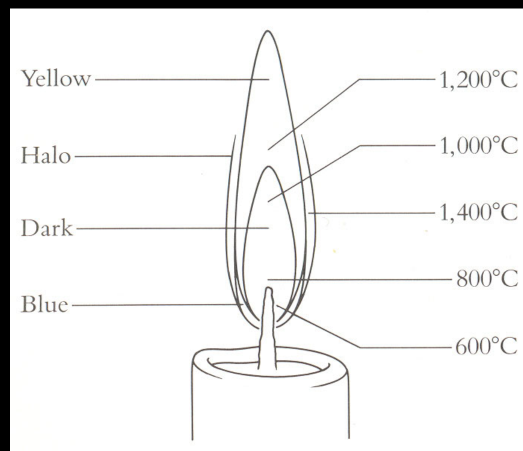
A local news reporter asked the volunteer fire captain what the department planned to do with the funds. "That ought to be obvious" he responded, wiping ashes off his coat. "The first thing we're gonna do is get the brakes fixed on our fire truck!"

3

4

A. Temperatures





Hottest areas

Figures from Fire, by J. W. Lyons (1985)

5

Energy Flow

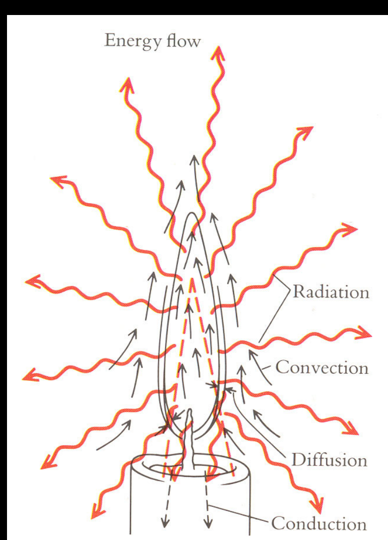


Figure from Fire, by J. W. Lyons (1985)

- 25% of energy lost to radiation
- 4% of radiation melts wax at top of candle
- Liquid wax moves up wick (capillary action)
- Wax vaporizes from wick
- Wax vapor cracks into smaller molecules
- Small hydrocarbon molecules combust at edge of flame

6

Colors

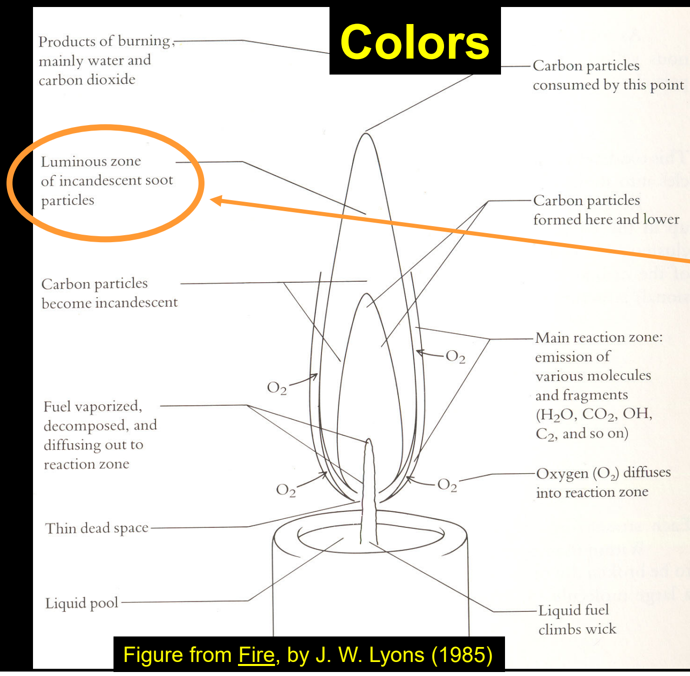


Figure from Fire, by J. W. Lyons (1985)

Yellow – Soot (hot solid)

Blue – CH_2 and CH

7

Class 33

Adiabatic Flame Temperatures

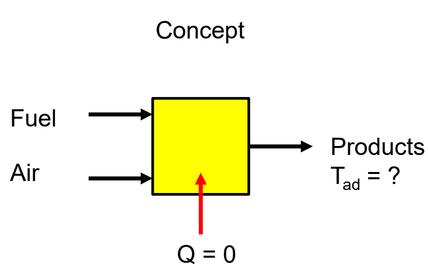
8

Thought Questions

- Which will have a higher temperature:
  - CH_4-air flame or CH_4-O_2 flame?
    - Why?
  - Fuel-rich flame, stoichiometric flame, or fuel-lean flame?
    - Why?
- Why do fuel-lean and fuel-rich flammability limits exist?

9

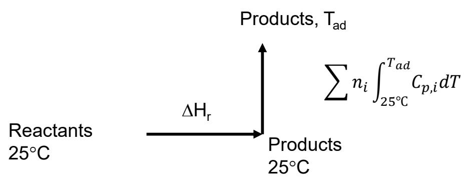
Adiabatic Flame Temperature



- 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

10

A. Path Method



Find

- If reactants are at 25°C, then

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

Good for simple reactions

11

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 Python

12

Example 1

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

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

<u>O_2 req'd</u>
2 moles

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

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

See Excel Sheet

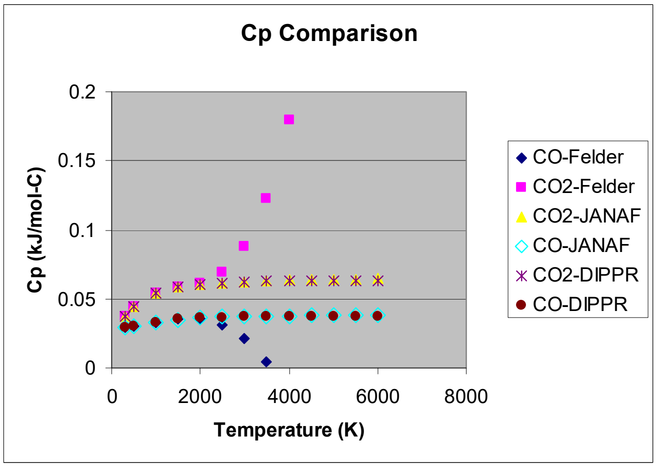
Then set $n_{N2} = 0$ and redo solver.

13

Spreadsheet

14

Heat Capacity Correlations Can Go Crazy at High Temperatures!



15

Spreadsheet with high T C_p's

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

16

With More Complex Chemistry

CH4-Air Stoichiometric

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 Stoichiometric

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

17

Example 2

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

$$CO + \frac{1}{2}O_2 \Rightarrow CO_2$$

$$H_2 + \frac{1}{2}O_2 \Rightarrow H_2O$$

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×(79/21) = 188 moles

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

18

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

19

Spreadsheet

20

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

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

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)
- The NASA-CEA program is one of many equilibrium programs

https://cearun.grc.nasa.gov/

23

Help on HW Problem 30.1
(fuel-rich)

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

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

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

$\xi_2 = \frac{2 - n_{O2,0}}{0.5}$ (prove this, remembering $n_{CH4,0} = 1$)

$\xi_1 = 1 - \xi_2$ (prove this)

24

Help on HW Problem 30.1

(fuel-lean)

$CH_4 + 2\ O_2 \rightarrow CO_2 + 2\ H_2O$ (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 CH_4 reacts and there is excess O_2 (O_2-rich case),

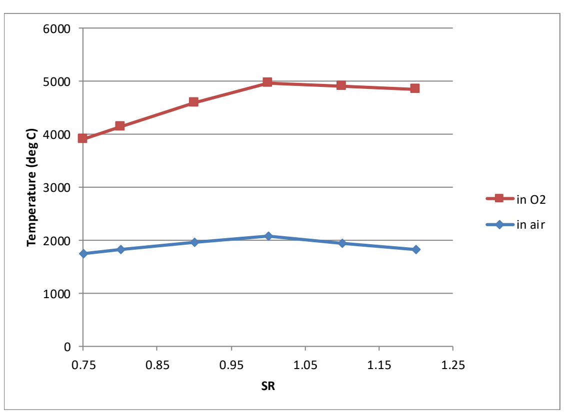
$n_{O2} \neq 0 = n_{O2,0} - n_{O2,stoich} = n_{O2,0} - 2$

No CO is formed (all CH_4 forms only CO_2)

$\xi_2 = 0$

$\xi_1 = 1$

Answer to Problem 30.1



27

Questions?

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

28