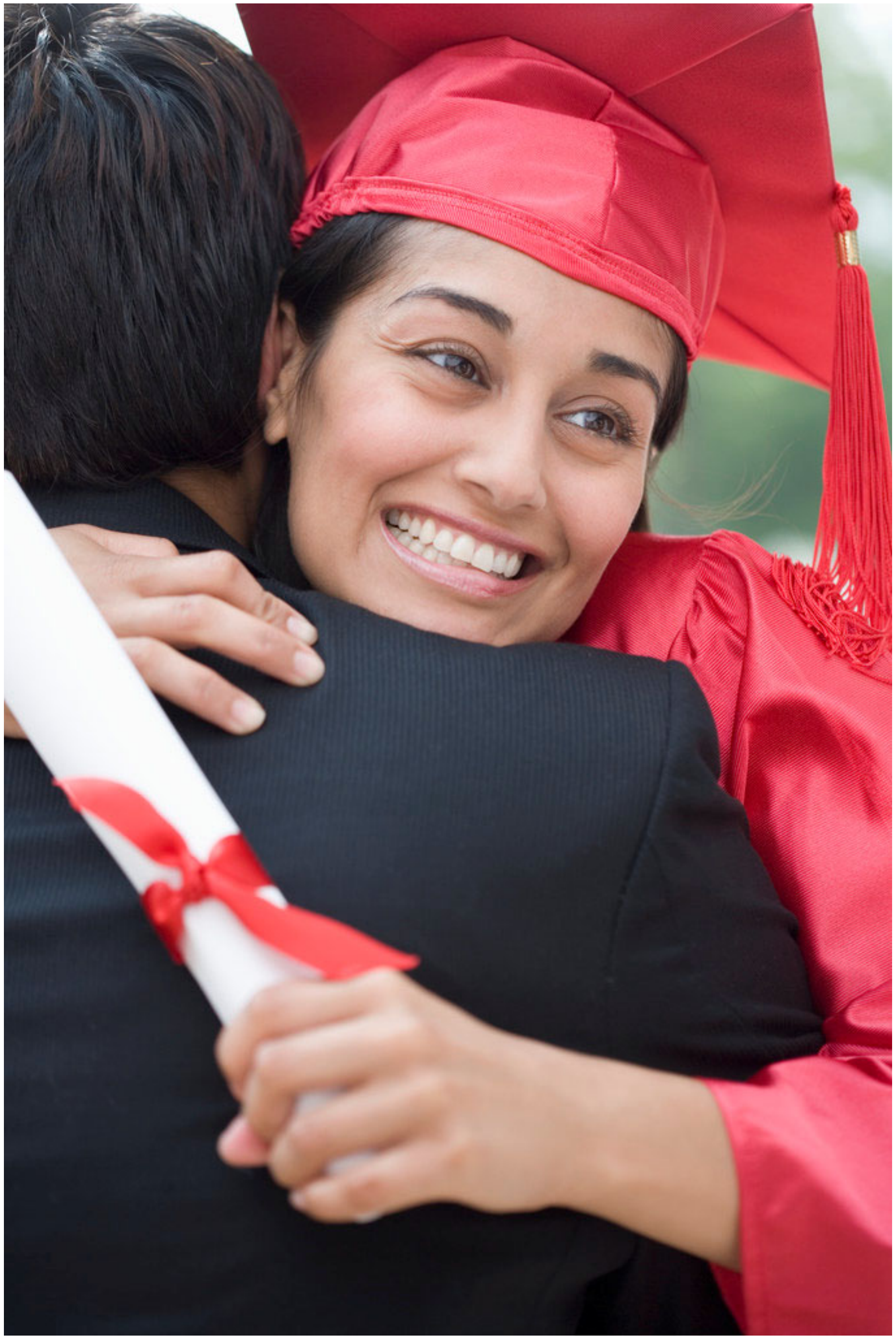


Last but not least…

- Counting today
  - 5 more class periods, including
    - 3 classes on Energy balances
    - 1 class on transient balances
    - Review for Exam 3… then Exam 3
  - Case Study (Ch. 14 problems)
  - Review for Final Exam
  - Final Exam

The End is Near!!

Goals Today

1. Energy Balance with ΔH_r^0 (single rxn)
2. Energy Balance with ΔH_f^0 (multiple rxns)

1. Energy Balance with only One Reaction

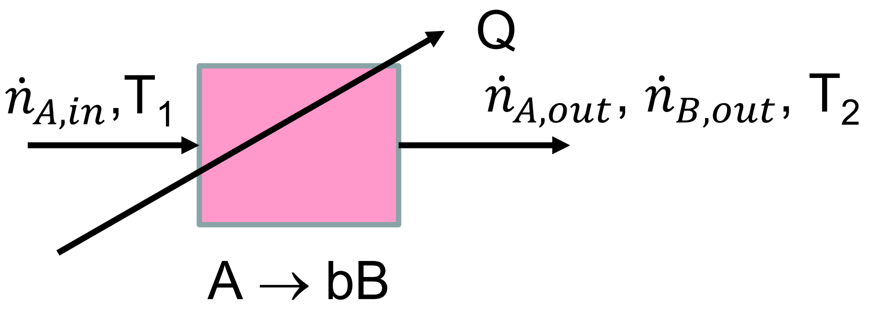
Board Problem

$A \rightarrow bB$

Path method, incomplete conversion

1. Energy Balance with only One Reaction

Path method, incomplete conversion



Q

$\dot{n}_{A,in}$, T_1

$\dot{n}_{A,out}$, $\dot{n}_{B,out}$, T_2

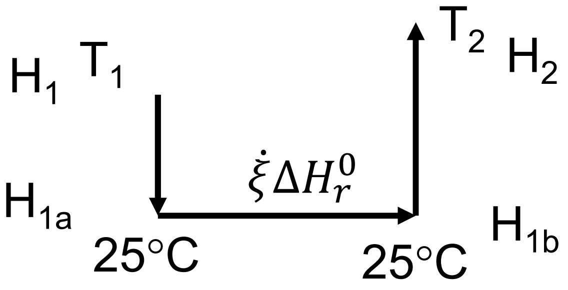
A → bB

Material Balance:

$$\dot{n}_{A,out} = \dot{n}_{A,in} + (-1)\dot{\xi}$$

$$\dot{n}_{B,out} = \dot{n}_{B,in} + (b)\dot{\xi} = b\dot{\xi}$$

Energy Balance: $\Delta\dot{H} = \Delta\dot{Q}$



H_1 T_1

T_2 H_2

H_{1a}

$\dot{\xi}\Delta H_r^0$

25°C

25°C

H_{1b}

$$\Delta H_r^0 = b\Delta H_{f,B}^0 - \Delta H_{f,A}^0$$

Wanted: H_2-H_1

$$\Delta\dot{H} = \dot{n}_{A,in}\int_{T_1}^{25°C} C_{p,A}\,dT + \dot{\xi}\Delta H_r^0 + \dot{n}_{A,out}\int_{25°C}^{T_2} C_{p,A}\,dT + \dot{n}_{B,out}\int_{25°C}^{T_2} C_{p,B}\,dT$$

Caution on Enthalpy Tables

Find $\hat{H}_{H2O,liq}$ at 25°C, 1 atm

1. Use steam tables (Table B.5)

   (104.8 kJ/kg)(kg/1000 g)(18g/mol) = 1.886 kJ/mol
   sat'd liquid (0.0317 bar)

2. Use ΔH_f^0

   Table B.1 says ΔH_f^0 = -285.84 kJ/mol at 25°C and 1 atm

What about VdP term since reference for steam tables is at 0.0317 bar?

$V\Delta P$ = (0.00101 m^3/kg)[1 atm - .0317 bar(atm/1.01325bar)](1.01325e5 N/m^2/atm)
= (99.1 N-m/kg)(kg/1000 g)(18 g/mol)(J/N-m)(kJ/1000J)
= 1.78e-3 kJ/mol (not enough to make a difference)

Bottom line: Do not mix and match enthalpies from different tables!

Look at Table B.7

- How does $\hat{H}_{\text{liq water}}$ change with pressure at 50°C? (use steam tables)
  - 0.5 bar → 209.3 kJ/kg
  - 1.0 bar → 209.3 kJ/kg
  - 5.0 bar → 209.7 kJ/kg (0.19% above 0.5 bar value)
- Pretty small change!! (for a liquid)
  - But relatively small change in pressure
- What about for steam?
  - At 350°C, $\Delta\hat{H}_{5\text{bar}}$ vs $\Delta\hat{H}_{0.5\text{bar}}$ = 0.28% decrease

2. Energy Balance with Multiple Reactions using ΔH_f^o

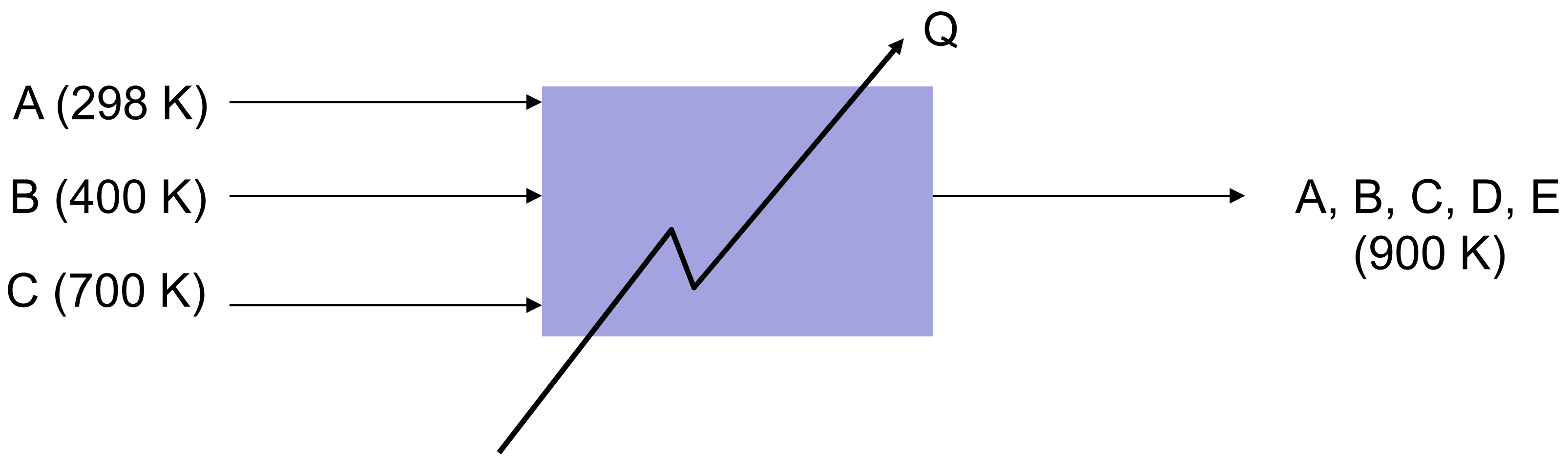
- Most common approach
- Most reliable approach

$$\Delta H + \Delta E_k + \Delta E_p = Q - W_s$$

$$\Delta \dot{H} + \Delta \dot{E}_k + \Delta \dot{E}_p = \dot{Q} - \dot{W}_s$$

- $\Delta \dot{H} = \dot{H}_{\text{out}} - \dot{H}_{\text{in}} = (\sum n_i \widehat{H}_i)_{out} - (\sum n_i \widehat{H}_i)_{in}$
- $\widehat{H}_i = \Delta \widehat{H}_{i,f}^0 + \int_{T_{ref}}^{T} \hat{C}_p dT$

Where is the ΔH_{rxn} term?



A (298 K)

B (400 K)

C (700 K)

Q

A, B, C, D, E
(900 K)

Idea: Construct a Table

In

Species	$\dot{n}_i$	T	$\hat{H}_i$	$\dot{n}_i\hat{H}_i$
A	2.0	298	?	?
B	1.0	400	?	?
C	0.5	700	?	?
D	0	-		
E	0	-		

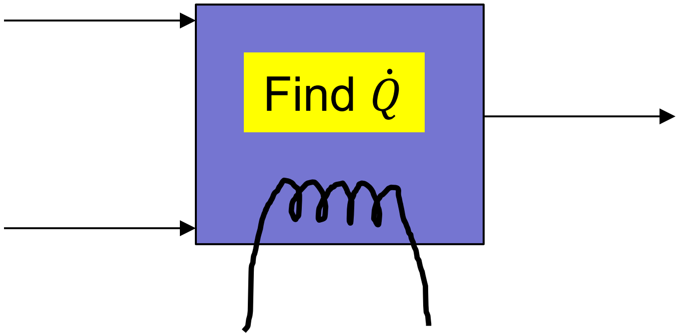
Out

Species	$\dot{n}_i$	T	$\hat{H}_i$	$\dot{n}_i\hat{H}_i$
A	0.5	900	?	?
B	0.1	900	?	?
C	0.05	900	?	?
D	1.0	900	?	?
E	1.3	900	?	?

Example: Problem 9.23

(9.20 in 3rd Ed.)

$$4\ NH_3 + 5\ O_2 \rightarrow 4\ NO + 6\ H_2O$$
$$2\ NH_3 + 3/2\ O_2 \rightarrow N_2 + 3\ H_2O$$



100 mol/min NH_3 (g)
25°C, 8 bar

900 mol/min air
150°C, 8 bar

Product gas
700°C, 8 bar
90 mol/min NO
150 mol/min H_2O (vapor)
716 mol/min N_2
69 mol/min O_2

Step 1: Write the mole balance (already done)

Step 2: Write the energy balance

Energy Balance with ΔH_f^o

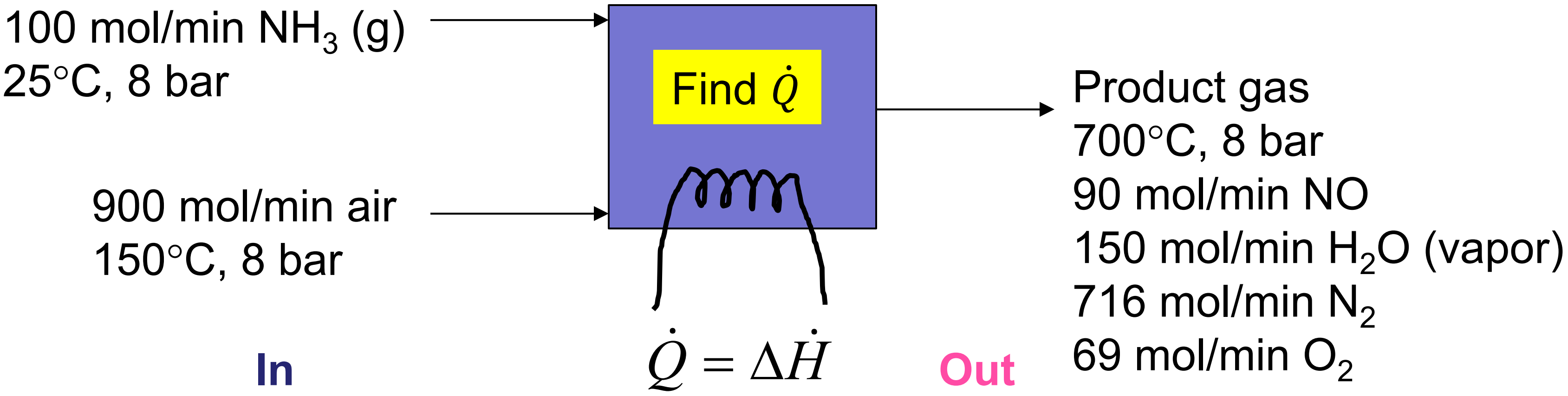
$$\Delta\dot{H} + \cancel{\Delta\dot{E}_k} + \cancel{\Delta\dot{E}_p} = \dot{Q} - \cancel{\dot{W}_s}$$

- $\Delta\dot{H} = \dot{H}_{\text{out}} - \dot{H}_{\text{in}} = \left(\sum n_i \widehat{H}_i\right)_{out} - \left(\sum n_i \widehat{H}_i\right)_{in}$
- $\widehat{H}_i = \Delta\widehat{H}_{i,f}^0 + \int_{T_{ref}}^{T} \hat{C}_p dT$

Example: Problem 9.23

(9.20 in 3rd Ed.)

$$4\ NH_3 + 5\ O_2 \rightarrow 4\ NO + 6\ H_2O$$
$$2\ NH_3 + 3/2\ O_2 \rightarrow N_2 + 3\ H_2O$$



100 mol/min NH_3 (g)
25°C, 8 bar

900 mol/min air
150°C, 8 bar

Find $\dot{Q}$

Product gas
700°C, 8 bar
90 mol/min NO
150 mol/min H_2O (vapor)
716 mol/min N_2
69 mol/min O_2

$$\dot{Q} = \Delta\dot{H}$$

In

Species	$\dot{n}_i$	T (°C)	$\hat{H}_i$	$\dot{n}_i\hat{H}_i$
NH_3	100	25	?	?
O_2	189	150	?	?
N_2	711	150	?	?
NO	0	-		
H_2O (g)	0	-		

Out

Species	$\dot{n}_i$	T (°C)	$\hat{H}_i$	$\dot{n}_i\hat{H}_i$
NH_3	0	-	-	-
O_2	69	700	?	?
N_2	716	700	?	?
NO	90	700	?	?
H_2O (g)	150	700	?	?

Excel Sheet

Homework: Problem 27.1

(a) $CaCO_3(s) \rightarrow CaO(s) + CO_2(g)$

- Given T's, find Q

(b) Additional reaction:

$CO(g) + 1/2\ O_2(g) \rightarrow CO_2(g)$

- Given T's, find Q

Homework: Problem 27.2

$$CO_2(g) + C(s) \rightarrow 2CO(g)$$

Draw schematic

Given $T_{in,}$ $T_{out,}$ Q, find conversion of C(s)

Hint: use ξ to solve for moles of outlet species so that energy balance is only a function of ξ. Use solver to find ξ, then calculate conversion (X_C).