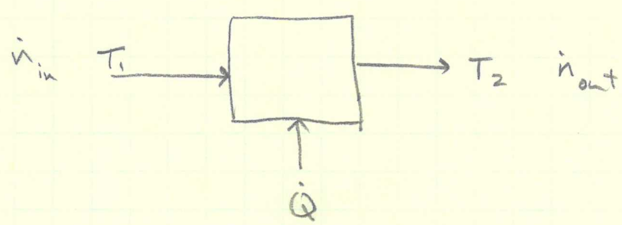
Energy Balances with Reaction

<u>Goals</u>: ① Energy balances w/ ΔH_r° (single rxns)

② Energy balances w/ ΔH_f° (multiple rxns)

A. Energy balances with ΔH_r°

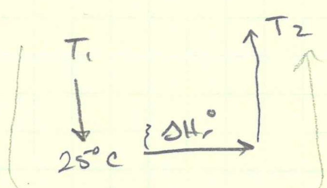
$A \longrightarrow bB$ not fully reacted!



<u>Material Balance</u>

$$\dot{n}_A = \dot{n}_{A,0} - \dot{\xi}$$
$$\dot{n}_B = 0 + b\dot{\xi}$$

<u>Energy Balance</u>



follow the path!

$$\Delta \dot{H} = \dot{n}_{A_0}\int_{T_1}^{25°C} C_{P_A}\,dT + \dot{\xi}\Delta H_r^\circ + \dot{n}_B\int_{25}^{T_2} C_{P_B}\,dT + \dot{n}_A\int_{25}^{T_2} C_{P_A}\,dT$$

where $\Delta H_r^\circ = \Delta H_{f,B}^\circ - \Delta H_{f,A}^\circ$; $\dot{n}_B = b\dot{\xi}$; $\dot{n}_A = \dot{n}_{A_0} - \dot{\xi}$

- this method only works well with one reactant species
- For multiple species and/or inerts, use different method

Caution Enthalpy tables are self consistent, but often not consistent with heat of formation tables

(what?)

Example: Find $\hat{H}_{H_2O,l}$ (sat'd liquid) at 25°C and 1 atm

ppt

(a) Use steam Tables

Table B.5 $\Rightarrow$ $\hat{H} = \left(104.8 \frac{kJ}{kg}\right)\left(\frac{kg}{1000\ g}\right)\left(\frac{18\ g}{mol}\right) = 1.886 \frac{kJ}{gmol}$

$+ \hat{V}\Delta P = \left(.00101 \frac{m^3}{kg}\right)(1\ atm - .0317\ bar)$

$= 1.78 \times 10^{-3}$ kJ/mol more

(b) use ΔH_f°

Table B.1 $\Rightarrow$ $\Delta H_f^\circ = -285.84 \frac{kJ}{gmol}$

$\hat{H} = \Delta H_f^\circ + \int_{25}^{25} C_p\, dT = \Delta H_f^\circ$

Why? Ref for steam tables $\Rightarrow$ $\hat{H}_{H_2O}$ at triple pt. = 0 (0.01°C, 0.00611 bar)

Ref for ΔH_f° is $\Delta H^\circ_{f,H_2} = 0$, $\Delta H^\circ_{f,O_2} = 0$ at 25°C, 1 bar

$H_2 + \frac{1}{2}O_2 \rightarrow H_2O(g)$

$H_2O(g) \rightarrow H_2O(l)$

By the way, Section 9.5 is off limits

Tables B.8 & B.9 are off limits $\Rightarrow$ ref = $\hat{H}_{25°C,i} = 0$

(unless entire problem is from Table)

$$\hat{V}\Delta P = \left(.00101\ \frac{m^3}{kg}\right)\left[1\ atm - .0317\ bar\left(\frac{atm}{1.01325\ bar}\right)\right]\left[\frac{1.01325\times10^5\ N/m^2}{atm}\right]$$

$$= \left(99.1\ \frac{N\text{-}m}{kg}\right)\left(\frac{kg}{1000\ g}\right)\left(\frac{18\ g}{mol}\right)\left(\frac{J}{N\text{-}m}\right)\left(\frac{kJ}{1000\ J}\right)$$

$$= 1.78\times10^{-3}\ \frac{kJ}{mol}$$

PPT

look at Table B.7, liquid at 50°C, see how $\hat{H}$ changes with pressure

0.5 bar → 209.3
1.0 bar → 209.3
5.0 bar → 209.7

pretty small change!

B. Energy balances with ΔH_f° & C_p's

$$\Delta \dot{H}_{sys} + \Delta \dot{E}_p + \Delta \dot{E}_K = \dot{Q} - \dot{W}_s$$

$$\Delta \dot{H}_{sys} = \left(\Sigma \dot{n}_i \hat{H}_i\right)_{out} - \left(\Sigma \dot{n}_i \hat{H}_i\right)_{in}$$

$$\hat{H}_i = \Delta \hat{H}^\circ_{f,i} + \int_{25^\circ C}^{T} \hat{C}_{p_i}\, dT$$

Construct Table

IN

species	$\dot{n}_i$	T	$\hat{H}_i$	H_i
A	✓	✓	✓	✓
B	✓	✓	✓	✓
C	✓	✓	✓	✓
R (products)	0	—	—	—
Q (products)	0	—	—	—
S (products)	0	—	—	—

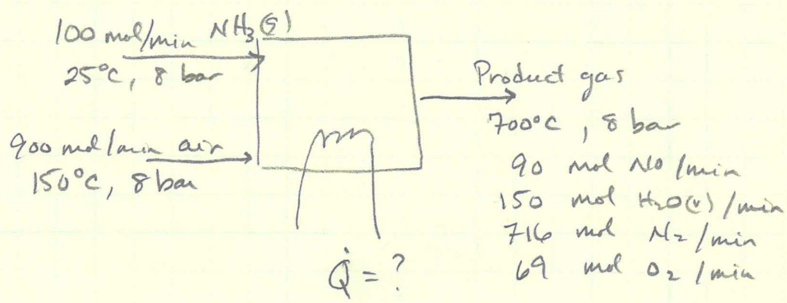
Out

species	$\dot{n}_i$	T	$\hat{H}_i$	H_i
A	✓	✓	✓	✓
B	✓	✓	✓	✓
C	✓	✓	✓	✓
R	✓	✓	✓	✓
Q	✓	✓	✓	✓
S	✓	✓	✓	✓

- This method does <u>not</u> calculate ΔH_{rxn}
- <u>Much</u> better for multiple reactions

Example: (9.20)

$$4\,NH_3 + 5\,O_2 \rightarrow 4\,NO + 6\,H_2O$$
$$2\,NH_3 + \tfrac{3}{2}\,O_2 \rightarrow N_2 + 3\,H_2O$$



(a) make enthalpy chart

IN

	$\dot{n}$	T(°C)	$\hat{H}$	H
NH_3	100	25	○	
O_2	189	150	○	
N_2	711	150	○	
NO	0	–	–	–
H_2O (v)	0	–	–	–

OUT

	$\dot{n}$	T(°C)	$\hat{H}$	H
NH_3	0	–	–	–
O_2	69	700	○	
N_2	716	700	○	
NO	90	700	○	
H_2O (v)				

$$\hat{H} = \Delta H^\circ_{f,i} + \int_{25}^{700} C_{p,i}\,dT$$

$$\dot{Q} = \left(\Sigma n_i \hat{H}_i\right)_{out} - \left(\Sigma n_i \hat{H}_i\right)_{in}$$

see spreadsheet