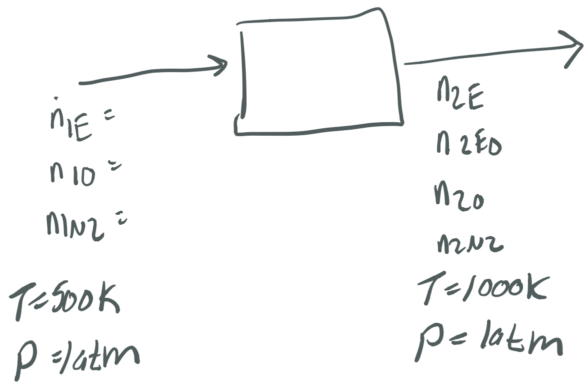
Problem 1 - 25 points

$2E + O \rightarrow 2EO$

a)



Additional info : $n_{E} = n_{1N_2}$ equimolar

$2n_{1E} = n_{1O}$ stoichiometric

$f_E = 0.30 = \frac{n_{2E} - n_{1E}}{n_{1E}}$ fractional conversion of E

Want to know: $\dot{Q}$

b) <u>DOF analysis</u>

7 unknowns (n_{1E} n_{1O} n_{1N_2} n_{2E} n_{2EO} n_{2O} n_{2N_2})

+ 1 chemical rxn (ξ)

-4 ind. material balances (4 species – N_2, E, EO, O)

-4 additional equations (f_E, equimolar, stoich, assume a basis)

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0 DOF - can solve for all listed unknowns!

c) $\dot{Q} - \cancel{\dot{W}_s}^{\,0} = \cancel{\Delta \dot{E}_k}^{\,0} + \cancel{\Delta \dot{E}_p}^{\,0} + \Delta \dot{H}$

no moving parts
no Δheight
no Δvelocity

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

$$\dot{Q} = \sum_{out} n_i H_i - \sum_{in} n_i H_i$$

Heat of formation method

$$\dot{Q} = \left[n_{2N_2} \hat{H}_{2N_2} + n_{2EO} \hat{H}_{2EO} + n_{2O} \hat{H}_{2O} + n_{2E} \hat{H}_{2E} \right] - \left[n_{1N_2} \hat{H}_{1N_2} + n_{1O} \hat{H}_{1O} + n_{1E} \hat{H}_{1E} \right]$$

heat of reaction method

$$\dot{Q} = \xi \Delta H_{rxn} + \left[n_{2N_2} \hat{H}_{2N_2} + n_{2EO} \hat{H}_{2EO} + n_{2O} \hat{H}_{2O} + n_{2E} \hat{H}_{2E} \right] - \left[n_{1N_2} \hat{H}_{1N_2} + n_{1O} \hat{H}_{1O} + n_{1E} \hat{H}_{1E} \right]$$

d) Heat of reaction Method

Ref states: E (g, 298K, 1atm)
O (g, 298K, 1atm)
EO (g, 298K, 1atm)
N_2 (g, 600K, 1atm)

Heat of reaction theoretical paths

Inlet Stream

N_2:

$N_2(g, 600K, 1atm)$

$N_2(g, 600K, 1atm)$

E:

$E(g, 298K, 1atm)$

$E(g, 600K, 1atm)$

O_2:

$O_2(g, 298K, 1atm)$

$O_2(g, 600K, 1atm)$

Outlet Stream

N_2:

$N_2(g, 600K, 1atm)$

$N_2(g, 1000K, 1atm)$

$E(g, 298K, 1atm)$

$E(g, 1000K, 1atm)$

$O_2(g, 298K, 1atm)$

$O_2(g, 1000K, 1atm)$

$EO(g, 298K, 1atm)$

$EO(g, 1000K, 1atm)$

e/f)

$\hat{H}_{1N_2} = 0$ because its the reference state

$\hat{H}_{1O_2} = \int_{298K}^{600K} Cp_{O_2}\, dT$

$\hat{H}_{1E} = \int_{298K}^{600K} Cp_{E}\, dT$

$\hat{H}_{2N_2} = \int_{600K}^{1000K} Cp_{N_2}\, dT$

$\hat{H}_{2O_2} = \int_{298K}^{1000K} Cp_{O_2}\, dT$

$\hat{H}_{2E} = \int_{298K}^{1000K} Cp_{E}\, dT$

$\hat{H}_{2EO} = \int_{298K}^{1000K} Cp_{EO}\, dT$

$$\Delta H^{\circ}_{rxn} = \underbrace{\sum \nu_i \Delta H^{\circ}_f}_{\text{products}} - \underbrace{\sum \nu_i \Delta H^{\circ}_f}_{\text{reactants}}$$

according to Hess's rule, we need to use the coefficients here.

$$\Delta H^{\circ}_{rxn} = 2\Delta H^{\circ}_{f\,EO} - 2\Delta H^{\circ}_{f\,E} - \Delta H^{\circ}_{f\,O_2}$$

$\Delta H^{\circ}_{f\,EO} = -52$ kJ/mol NIST chemical webbook

$\Delta H^{\circ}_{f\,E} = 52$ kJ/mol Table B.1

$\Delta H^{\circ}_{f\,O_2} = 0$ Diatomic species

Heat Capacity Expressions

$$\left.\begin{array}{ll} Cp_{N_2} = 29\times10^{-3} + 0.22\times10^{-5}\,T & T \text{ in } ^{\circ}C \\ Cp_{O_2} = 29.10\times10^{-3} + 1.16\times10^{-5}\,T & T \text{ in } ^{\circ}C \\ Cp_{E} = 40\times10^{-3} + 11.47\times10^{-5}\,T & T \text{ in } ^{\circ}C \end{array}\right\}\text{Table B.2}$$

$Cp_{EO} = -23 + \frac{276}{1000}T$ T in K ← NIST Chemical webbook.

g) 1. First, I would solve the material balances to get all $\dot{n}_i$ and ξ

$$0.3 = \frac{n_{2E} - n_{1E}}{n_{2E}}$$

N_2: $n_{2N_2} = n_{1N_2}$

O_2: $n_{2O_2} = n_{1O_2} - \xi$

E: $n_{2E} = n_{1E} - 2\xi$

EO: $n_{2EO} = 2\xi$

$n_{1E} = n_{1N_2}$

$2n_{1E} = n_{1O}$

Assume a basis!

$n_{2EO} = 100\ mol/s$

because its easy.

- EO balance to calc ξ
- E balance w/ f_E to calc n_{2E} and n_{1E}
- Add. equations to calc n_{1N_2} and n_{1O}
- N2 balance to calc n_{2N_2}
- O2 balance to calc n_{2O_2}

2. I would integrate and evaluate all $\int C_p$ expressions, and pay attention to the units of T needed for each form. I would convert any T(K) to T(°C) by subtracting 273K. Calculate all $\hat{H}_i$

3. Plug in all $\dot{n}_i$, ξ and tabulated values into the energy balance in part d.

4. Calculate $\dot{Q}$

Problem 2 – 12 points

Heat of formation method

$$\dot{Q} = \left[n_{2N_2}\hat{H}_{2N_2} + n_{2EO}\hat{H}_{2EO} + n_{2O}\hat{H}_{2O} + n_{2E}\hat{H}_{2E}\right] - \left[n_{1N_2}\hat{H}_{1N_2} + n_{1O}\hat{H}_{1O} + n_{1E}\hat{H}_{1E}\right]$$

d) Ref. States

C, H, O (298K, g, 1atm)

N_2 (600K, g, 1atm)

Theoretical paths using heat of formation method

Inlet Stream

N_2: N_2(g, 600K, 1atm)
N_2(g, 600K, 1atm)

E: C, H (g, 298K, 1atm)
E (g, 298K, 1atm)
E (g, 600K, 1atm)

O_2: O_2 (g, 298K, 1atm)
O_2(g, 600K, 1atm)

Outlet Stream

N_2:

$N_2(g, 600K, 1atm)$
$N_2(g, 1000K, 1atm)$

$C, H(g, 298K, 1atm)$
$E(g, 298K, 1atm)$
$E(g, 1000K, 1atm)$

$O_2(g, 298K, 1atm)$
$O_2(g, 1000K, 1atm)$

$C, H, O(g, 298K, 1atm)$
$EO(g, 298K, 1atm)$
$EO(g, 1000K, 1atm)$

e/f)

$$\hat{H}_{1N_2} = 0$$

$$\hat{H}_{1O_2} = 0 + \int_{298K}^{600K} Cp_{O_2}\, dT$$

$$\hat{H}_{1E} = \Delta H^{o}_{fE} + \int_{298K}^{600K} Cp_{E}\, dT$$

$$\hat{H}_{2N_2} = 0 + \int_{600K}^{1000K} Cp_{N_2}\, dT$$

$$\hat{H}_{2O_2} = 0 + \int_{298K}^{1000K} Cp_{O_2}\, dT$$

$$\hat{H}_{2E} = \Delta H^{o}_{fE} + \int_{298K}^{1000K} Cp_{E}\, dT$$

$$\hat{H}_{2EO} = \Delta H^{o}_{fEO} \int_{298K}^{1000K} Cp_{EO}\, dT$$

* In this step, all ΔH_f° and C_p expressions are the same as $\boxed{\text{Problem 1 part e/f}}$ *