4.40 **a.** $4\,NH_3 + 5\,O_2 \rightarrow 4\,NO + 6\,H_2O$

$$\frac{5 \text{ lb-mole } O_2 \text{ react}}{4 \text{ lb-mole NO formed}} = \underline{\underline{1.25 \text{ lb-mole } O_2 \text{ react / lb-mole NO formed}}}$$

b.

$$\left(n_{O_2}\right)_{\text{theoretical}} = \frac{100 \text{ kmol } NH_3}{\text{h}} \bigg| \frac{5 \text{ kmol } O_2}{4 \text{ kmol } NH_3} = 125 \text{ kmol } O_2$$

$$40\% \text{ excess } O_2 \Rightarrow \left(n_{O_2}\right)_{\text{fed}} = 1.40(125 \text{ kmol } O_2) = \underline{175 \text{ kmol } O_2}$$

c.

$$(50.0 \text{ kg } NH_3)(1 \text{ kmol } NH_3 / 17 \text{ kg } NH_3) = 2.94 \text{ kmol } NH_3$$

$$(100.0 \text{ kg } O_2)(1 \text{ kmol } O_2 / 32 \text{ kg } O_2) = 3.125 \text{ kmol } O_2$$

$$\left(\frac{n_{O_2}}{n_{NH_3}}\right)_{\text{fed}} = \frac{3.125}{2.94} = 1.06 < \left(\frac{n_{O_2}}{n_{NH_3}}\right)_{\text{stoich}} = \frac{5}{4} = 1.25$$

$\Rightarrow \underline{O_2 \text{ is the limiting reactant}}$

Required NH_3: $$\frac{3.125 \text{ kmol } O_2}{} \bigg| \frac{4 \text{ kmol } NH_3}{5 \text{ kmol } O_2} = 2.50 \text{ kmol } NH_3$$

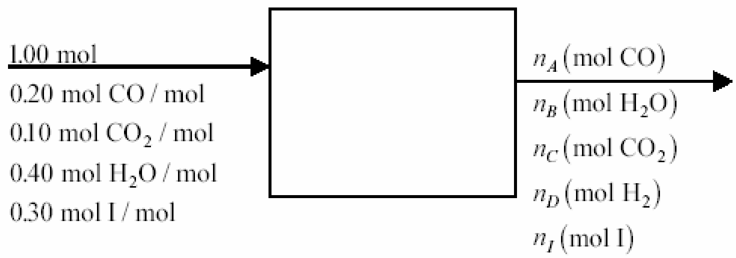
$$\underline{\%\text{excess } NH_3} = \frac{2.94 - 2.50}{2.50} \times 100\% = \underline{\underline{17.6\% \text{excess } NH_3}}$$

Extent of reaction: $n_{O_2} = \left(n_{O_2}\right)_0 - \nu_{O_2}\xi \Rightarrow 0 = 3.125 - (-5)\xi \Rightarrow \xi = 0.625 \text{ kmol} = \underline{625 \text{ mol}}$

Mass of NO: $$\frac{3.125 \text{ kmol } O_2}{} \bigg| \frac{4 \text{ kmol NO}}{5 \text{ kmol } O_2} \bigg| \frac{30.0 \text{ kg NO}}{1 \text{ kmol NO}} = \underline{\underline{75.0 \text{ kg NO}}}$$

4.47 a. $CO + H_2O \longleftrightarrow CO_2 + H_2$

(A) (B) (C) (D)



Degree of freedom analysis: 6 unknowns ($n_A, n_B, n_C, n_D, n_I, \xi$)

– 4 expressions for $n_i(\xi)$

– 1 balance on I

– 1 equilibrium relationship

0 DF

b. Since two moles are prodcued for every two moles that react,

$(n_{\text{total}})_{\text{out}} = (n_{\text{total}})_{\text{in}} = \underline{\underline{1.00\,(\text{mol})}}$

$n_A = 0.20 - \xi$ (1)

$n_B = 0.40 - \xi$ (2)

$n_C = 0.10 + \xi$ (3)

$n_D = \xi$ (4)

$n_I = 0.30$ (5)

$n_{tot} = 1.00\,\text{mol}$

At equilibrium: $\dfrac{y_C y_D}{y_A y_B} = \dfrac{n_C n_D}{n_A n_B} = \dfrac{(0.10+\xi)(\xi)}{(0.20-\xi)(0.40-\xi)} = 0.0247\exp\left(\dfrac{4020}{1123}\right) \Rightarrow \xi = 0.110\text{ mol}$

$y_D = n_D = \xi = \underline{\underline{0.110\,(\text{mol } H_2/\text{mol})}}$

c. The reaction has not reached equilibrium yet.

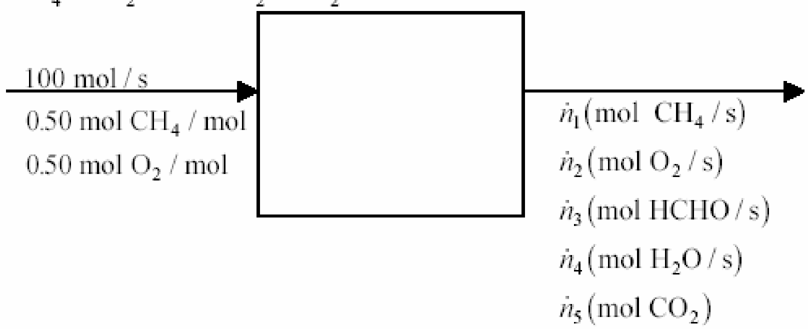
d.

T (K)	x (CO)	x (H_2O)	x (CO_2)	Keq	Keq (Goal Seek)	Extent of Reaction	y (H_2)
1223	0.5	0.5	0	0.6610	0.6610	0.2242	0.224
1123	0.5	0.5	0	0.8858	0.8856	0.2424	0.242
1023	0.5	0.5	0	1.2569	1.2569	0.2643	0.264
923	0.5	0.5	0	1.9240	1.9242	0.2905	0.291
823	0.5	0.5	0	3.2662	3.2661	0.3219	0.322
723	0.5	0.5	0	6.4187	6.4188	0.3585	0.358
623	0.5	0.5	0	15.6692	15.6692	0.3992	0.399
673	0.5	0.5	0	9.7017	9.7011	0.3785	0.378
698	0.5	0.5	0	7.8331	7.8331	0.3684	0.368
688	0.5	0.5	0	8.5171	8.5177	0.3724	0.372
1123	0.2	0.4	0.1	0.8858	0.8863	0.1101	0.110
1123	0.4	0.2	0.1	0.8858	0.8857	0.1100	0.110
1123	0.3	0.3	0	0.8858	0.8856	0.1454	0.145
1123	0.5	0.4	0	0.8858	0.8867	0.2156	0.216

The lower the temperature, the higher the extent of reaction. An equimolar feed ratio of carbon monoxide and water also maximizes the extent of reaction.

4.49 **a.** $CH_4 + O_2 \longrightarrow HCHO + H_2O$ (1)

$CH_4 + 2O_2 \longrightarrow CO_2 + 2H_2O$ (2)



7 unknowns ($\dot{n}_1, \dot{n}_2, \dot{n}_3, \dot{n}_4, \dot{n}_5, \dot{\xi}_1, \dot{\xi}_2$)

−5 equations for $\dot{n}_i\left(\dot{\xi}_1, \dot{\xi}_2\right)$

2 DF

b.

$$\dot{n}_1 = 50 - \dot{\xi}_1 - \dot{\xi}_2 \quad (1)$$

$$\dot{n}_2 = 50 - \dot{\xi}_1 - 2\dot{\xi}_2 \quad (2)$$

$$\dot{n}_3 = \dot{\xi}_1 \quad (3)$$

$$\dot{n}_4 = \dot{\xi}_1 + 2\dot{\xi}_2 \quad (4)$$

$$\dot{n}_5 = \dot{\xi}_2 \quad (5)$$

c.

Fractional conversion: $\dfrac{(50 - \dot{n}_1)}{50} = 0.900 \Rightarrow \dot{n}_1 = 5.00 \text{ mol } CH_4 / s$

Fractional yield: $\dfrac{\dot{n}_3}{50} = 0.855 \Rightarrow \dot{n}_3 = 42.75 \text{ mol HCHO} / s$

$$\left.\begin{array}{l} \text{Equation } 3 \Rightarrow \xi_1 = 42.75 \\ \text{Equation } 1 \Rightarrow \xi_2 = 2.25 \\ \text{Equation } 2 \Rightarrow \dot{n}_2 = 2.75 \\ \text{Equation } 4 \Rightarrow \dot{n}_4 = 47.25 \\ \text{Equation } 5 \Rightarrow \dot{n}_5 = 2.25 \end{array}\right\} \Rightarrow \begin{array}{l} y_{CH_4} = \underline{0.0500 \text{ mol } CH_4 / \text{mol}} \\ y_{O_2} = \underline{0.0275 \text{ mol } O_2 / \text{mol}} \\ y_{HCHO} = \underline{0.4275 \text{ mol HCHO / mol}} \\ y_{H_2O} = \underline{0.4725 \text{ mol } H_2O / \text{mol}} \\ y_{CO_2} = \underline{0.0225 \text{ mol } CO_2 / \text{mol}} \end{array}$$

Selectivity: $\dfrac{42.75 \text{ mol HCHO} / s}{2.25 \text{ mol } CO_2 / s} = \underline{19.0 \text{ mol HCHO} / \text{mol } CO_2}$