## Problem Set III

1. Hydrogen is produced from steam by water gas shift reaction
$\mathrm{CO}+\mathrm{H}_{2} \mathrm{O} \longrightarrow \mathrm{CO}_{2}+\mathrm{H}_{2}$
If the feed to the reactor contains 30 moles of $\mathrm{CO}, 12$ moles of $\mathrm{CO}_{2}$ and 35 moles of steam per hour and 18 moles of hydrogen are produced per hour, Calculate
a) The limiting reactant
b) The excess reactant
c) The fractional conversion of steam to $\mathrm{H}_{2}$
d) The degree of completion oft he reaction
e) The kg of hydrogen to be yield per kg of steam fed
f) The composition of the product
2. The reaction between ethylene $\left(\mathrm{C}_{2} \mathrm{H}_{4}\right)$ and HBr to form ethyl bromide $\left(\mathrm{C}_{2} \mathrm{H}_{5} \mathrm{Br}\right)$ is carried out in a continous reactor. The product stream is analyzed and is found to contain $50 \%$ $\mathrm{C}_{2} \mathrm{H}_{5} \mathrm{Br}$ an $33.3 \% \mathrm{HBr}$ by mole. The feed to the reactor contains only ethylene and hydrogen bromide. Calculate:
a) The fractional conversion of the limiting reactant
b) The percentage of the excess reactant
3. Methan $\left(\mathrm{CH}_{4}\right)$ and oxygen react to form formaldehyde $\left(\mathrm{CH}_{2} \mathrm{O}\right)$. In a side reaction, some of methane is oxidized to carbon dioxide and water

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\begin{aligned}
& \mathrm{CH}_{4}+\mathrm{O}_{2} \longrightarrow \mathrm{CH}_{2} \mathrm{O}+\mathrm{H}_{2} \mathrm{O} \\
& \mathrm{CH}_{4}+2 \mathrm{O}_{2} \longrightarrow \mathrm{CO}_{2}+2 \mathrm{H}_{2} \mathrm{O}
\end{aligned}
$$

The feed to the reactor contains $50 \%$ methane and $50 \%$ oxygen in moles. The fractional conversion of methane is 0.95 and the fractional yield of formaldehyde is 0.90 .
a) Calculate the molar composition of the reactor output stream and the selectivity of formaldehyde production relative to carbon dioxide production.
b) Calculate conversion of $\mathrm{O}_{2}$
4. Five kilograms of bismuth ( $\mathrm{MW}=209$ ) is reacted with one kilogram of sulfur ( $\mathrm{MW}=32$ ) to form $\mathrm{Bi}_{2} \mathrm{~S}_{3}(\mathrm{MW}=514)$. At the end of the reaction, output is taken out of the reactor and is found to contain $5 \mathrm{wt} \%$ free sulfur. Reaction is,

$$
2 \mathrm{Bi}+3 \mathrm{~S} \longrightarrow \mathrm{Bi}_{2} \mathrm{~S}_{3}
$$

Determine:
a) the limiting reactant,
b) the percent excess reactant,
c) the percent conversion of sulfur to $\mathrm{Bi}_{2} \mathrm{~S}_{3}$,
d) percent conversion of Bi to $\mathrm{Bi}_{2} \mathrm{~S}_{3}$.
5. When propylene $\left(\mathrm{C}_{3} \mathrm{H}_{6}\right)$ is mixed with chlorine $\left(\mathrm{Cl}_{2}\right)$, the following reactions take place.
$\mathrm{C}_{3} \mathrm{H}_{6}(\mathrm{~g})+\mathrm{Cl}_{2}(\mathrm{~g}) \rightarrow \mathrm{C}_{3} \mathrm{H}_{5} \mathrm{Cl}(\mathrm{g})+\mathrm{HCl}(\mathrm{g})$
(a)
$\mathrm{C}_{3} \mathrm{H}_{6}(\mathrm{~g})+\mathrm{Cl}_{2}(\mathrm{~g}) \rightarrow \mathrm{C}_{3} \mathrm{H}_{6} \mathrm{Cl}_{2}(\mathrm{~g})$

Molecular weights of $\mathrm{C}_{3} \mathrm{H}_{6}, \mathrm{C}_{3} \mathrm{H}_{5} \mathrm{Cl}$, and $\mathrm{C}_{3} \mathrm{H}_{6} \mathrm{Cl}_{2}$ are 42.0, 76.5, and 113.0 respectively. The species in the product are listed in the following table.

| Species | gmol |
| :--- | :--- |
| $\mathrm{Cl}_{2}$ | 141.0 |
| $\mathrm{C}_{3} \mathrm{H}_{6}$ | 651.0 |
| $\mathrm{C}_{3} \mathrm{H}_{5} \mathrm{Cl}$ | 4.6 |
| $\mathrm{C}_{3} \mathrm{H}_{4} \mathrm{Cl}_{2}$ | 24.5 |
| HCl | 4.6 |

assuming that there are only propylene and chlorine in feed, calculate the following:
(a) How much propylene and chlorine are fed to the reactor in gmol?
(b) What was the limiting reactant?
(c) What was the excess reactant and excess percentage of the excess reactant on the basis of reaction (a) ?
(d) What was the fractional conversion of $\mathrm{C}_{3} \mathrm{H}_{6}$ to $\mathrm{C}_{3} \mathrm{H}_{5} \mathrm{Cl}$ ?
(e) What was the selectivity of $\mathrm{C}_{3} \mathrm{H}_{5} \mathrm{Cl}$ relative to $\mathrm{C}_{3} \mathrm{H}_{6} \mathrm{Cl}_{2}$ ?
(f) What was the yield of $\mathrm{C}_{3} \mathrm{H}_{5} \mathrm{Cl}$ expressed in gmol $\mathrm{C}_{3} \mathrm{H}_{5} \mathrm{Cl}$ to the gmol of $\mathrm{C}_{3} \mathrm{H}_{6}$ fed to the reactor?
(g) What was the extent of reaction of the first and second reactions?
6. In a process for the manufacture of chlorine by direct oxidation of HCl with air over a catalyst to form $\mathrm{Cl}_{2}$ and $\mathrm{H}_{2} \mathrm{O}$ (only), the exit product is composed of $\mathrm{HCl}(4.4 \%), \mathrm{Cl}_{2}$ (19.8\%), $\mathrm{O}_{2}$ (4.0\%), and $\mathrm{N}_{2}$ ( $52.0 \%$ ). What was
(a) The limiting reactant?
(b) The percent excess air?
(c) The degree of completion of the reaction?
7.Consider a continous, steady -state process in which the following reactions take place :

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\begin{aligned}
& \mathrm{C}_{6} \mathrm{H}_{12}+6 \mathrm{H}_{2} \mathrm{O} \rightarrow 6 \mathrm{CO}+12 \mathrm{H}_{2} \\
& \mathrm{C}_{6} \mathrm{H}_{12}+\mathrm{H}_{2} \xrightarrow{\rightarrow} \mathrm{C}_{6} \mathrm{H}_{14}
\end{aligned}
$$

In the process 250 moles $/ \mathrm{h}$ of $\mathrm{C}_{6} \mathrm{H}_{12}$ and $800 \mathrm{moles} / \mathrm{h}$ of $\mathrm{H}_{2} \mathrm{O}$ are fed into reactor . The yield of $\mathrm{H}_{2}$ is $40 \%$. Yield is defined as the mole of $\mathrm{H}_{2}$ obtained divided by the theoretical maximum $\mathrm{H}_{2}$ that would be obtained based on the limiting reactant being comletely consumed). The selectivity of $\mathrm{H}_{2}$ relative to $\mathrm{C}_{6} \mathrm{H}_{14}$ is 12 .
(a) What is limiting reactant?
(b) Calculate the molar flow rates of all five components in output stream.

Note: Use extent of reaction method.
(c) Calculate the fractional conversion of $\mathrm{H}_{2} \mathrm{O}$.
(d) What was the conversion of $\mathrm{C}_{6} \mathrm{H}_{12}$ to $\mathrm{C}_{6} \mathrm{H}_{14}$ ?

