Introduction to Chemical Engineering

Problem Sheet 4 – Week 6 – October 18 2024

Recap:

Mass Balance on Reative Systems (Atom Balance)

- Knowing that number of atoms of any given element does not change in any reaction:

$$\text{In} + \cancel{\text{Gen}}^{0} - \text{Out} - \cancel{\text{Cons}}^{0} = \cancel{\text{Acc}}^{0}$$

$$\underline{\text{In} - \text{Out} = 0} \quad \textit{Assume st.st.}$$

- When analyzing a reactive system, you must choose *either* an atom balance *or* a molecular species balance but **not both**
  - An atom balance often yields simpler algebra (especially for multiple reactions)
  - When doing **atom balances**, the extent of reaction does not count as an unknown, while with a molecular species balance it does
  - When you're doing an atom balance you should only include reactive species, not inert.

Defining the energy balance on a system

- Recall the mother of all equations for conservation of mass:

$$\text{Acc} = \text{In} - \text{Out} + \text{Gen} - \text{Cons}$$

Law of conservation of energy:

$$E_{accumulated} = E_{input} - E_{output} + E_{gen} + E_{transferred}$$

$$E_{in} = \Sigma_{input\ streams}\, m_j \hat{E}_j \quad , \quad E_{out} = \Sigma_{output\ streams}\, m_j \hat{E}_j$$

$$E_{transferred} = Q - W$$

Q: heat transferred **to the system** from its surrounding (+ sign: gain of energy)

W: work **done by system** on its surrounding (+ sign so that –W is negative)

Problem 1: Atom balances (Practice with familiar reactions)

You have previously solved the following 2 problems by balancing the molecular species. Form the respective expressions by balancing the atomic species (they should solve to yield the same answers as before).

a) **(Week 2 Problem 1)**
The chlorination of methane occurs by the following reaction:

$$CH_4 + Cl_2 \rightarrow CH_3Cl + HCl$$

Determine the product composition if the conversion of the limiting reactant is 67%, and the feed composition in mole % is given as: 40% CH_4, 50% Cl_2, and 10% N_2.

b) **(Week 2 Problem 3)**
Formaldehyde (CH_2O) is produced industrially by the catalytic oxidation of methanol according to the following reaction:

$$CH_3OH + \frac{1}{2}O_2 \rightarrow CH_2O + H_2O \quad \cdots (1)$$

Unfortunately, under the conditions used to produce formaldehyde at a profitable rate, a significant portion of the formaldehyde reacts with oxygen to produce CO and H_2O, that is:

$$CH_2O + \frac{1}{2}O_2 \rightarrow CO + H_2O \quad \cdots (2)$$

Assume that methanol is twice the stoichiometric amount of air needed for complete conversion of the CH_3OH to the desired products (CH_2O and H_2O) are fed to the reactor. Also, assume that 90% conversion of the methanol results, and that a 75% yield of the formaldehyde occurs based on the theoretical production of CH_2O by Reaction 1. Determine the composition of the product gas leaving the reactor.

Problem 2: Atomic Balances (Hydrocracking of Octane)

Hydrocracking is an important refinery process for converting low-valued heavy hydrocarbons into more valuable lower molecular weight hydrocarbons by exposing the feed to a zeolite catalyst at high temperature and pressure in the presence of hydrogen. Researchers in this field study the hydrocracking of pure components, such as octane (C_8H_{18}), to understand the behavior of cracking reactions.

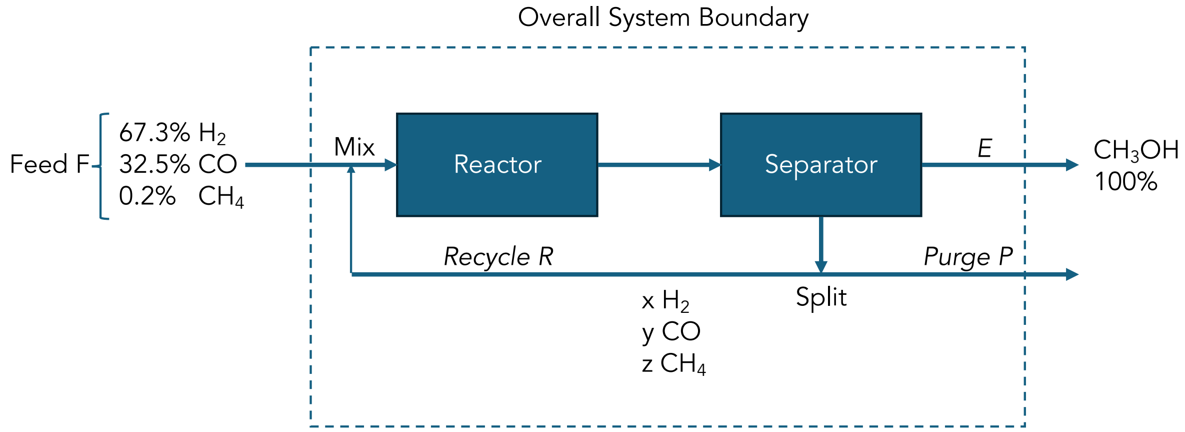
In one such experiment for the hydrocracking of octane, the cracked products had the following composition in mole percent: 19.5% C_3H_8, 59.4% C_4H_{10}, and 21.1% C_5H_{12}. Determine the molar ratio of hydrogen consumed to octane reacted for this process.

Problem 3: Purge stream

Considerable interest exists in the conversion of coal into more convenient liquid products for subsequent production of chemicals. Two of the main gases that can be generated under suitable conditions from in-situ (in the ground) coal combustion in the presence of steam (occurs naturally in the presence of ground water) are H_2 and CO. After cleanup, these two gases can be combined to yield methanol according to the following equation.

$$CO + H_2 \rightarrow CH_3OH$$

The diagram below illustrates a steady-state process for the production of methanol. All of the compositions are in mole fractions, or percent. The stream flows are in moles.



Note that some CH_4 enters the process, but does not participate in the reaction. A purge stream is used to maintain the CH_4 concentration in the exit from the separator at no more than 3.2 mol%, and prevent hydrogen buildup. The once-through conversion of CO in the reactor is 18%.

Calculate the following:

a) R, moles of Recycle
b) E, moles of CH_3OH produced
c) P
d) Purge gas composition

(Hint: the question says that the CH_4 concentration from the exit of the separator is no more than 3.2%, you can then ***assume*** *the composition of CH_4 in the exit stream is 3.2% for calculations)*

Problem 4: Energy Balance (Non-reactive systems)

Superheated steam at 40 bar absolute and 500°C flows at a rate of 250 kg/min to an adiabatic turbine, where it expands to 5 bar. The turbine develops 1500 kW. From the turbine, the steam flows to a heater, where it is reheated isobarically to its initial temperature. Neglect kinetic energy changes.

a) Write an energy balance on the turbine and use it to determine the outlet stream temperature.
b) Write an energy balance on the heater and use it to determine the required input (kW) to the steam.
c) Verify that an overall energy balance on the two-unit process is satisfied.
d) Suppose the turbine inlet and outlet pipes both have diameters of 0.5 meter. Show that it is reasonable to neglect the change in kinetic energy for this unit.