06-100: Recitation 3 Help

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Mass Balances with Reaction

- Given reaction

$$A + 2\,B \rightarrow C$$

- First step is to identify the limiting reactant
- Example: if the feed to the reactor contains 0.1 mol of A and 1 mol of B, who is the limiting reactant?

Stoichiometry: 1 mol of A reacts with 2 mol of B

Then 0.1 mol of A reacts with $2 \times 0.1 = 0.2$ mol of B

So B is in excess ($1 - 0.2 = 0.8$ mol excess) and A is the limiting reactant

- See textbook section 4.6b (starts on page 117)

Reaction Conversion

- Usually denoted by *X* (and generally defined on a **molar** basis)
- Two types
  - Single-Pass Conversion:

$$X = \frac{\text{reactant input to the reactor} - \text{reactant output from reactor}}{\text{reactant input to the reactor}}$$

  - Overall Conversion:

$$X = \frac{\text{reactant input to the process} - \text{reactant output from reactor}}{\text{reactant input to the process}}$$

- The real difference is whether we are considering the stream with reactant immediately entering the reactor of the process fresh feed. See textbook section 4.7f (page 135).

Conservation of Mass

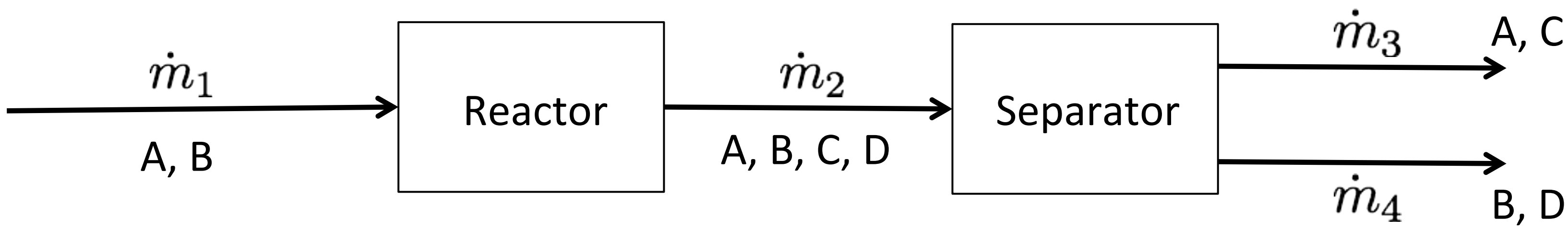
- I would strongly recommend writing out the conservation of mass equation when performing material balances

In − Out + Generation − Consumption = Accumulation

- In this course, we always use the steady-state assumption, *i.e.* quantities do not change with time. So Accumulation = 0.
- The information about the reaction is considered in the Generation and Consumption terms

Example

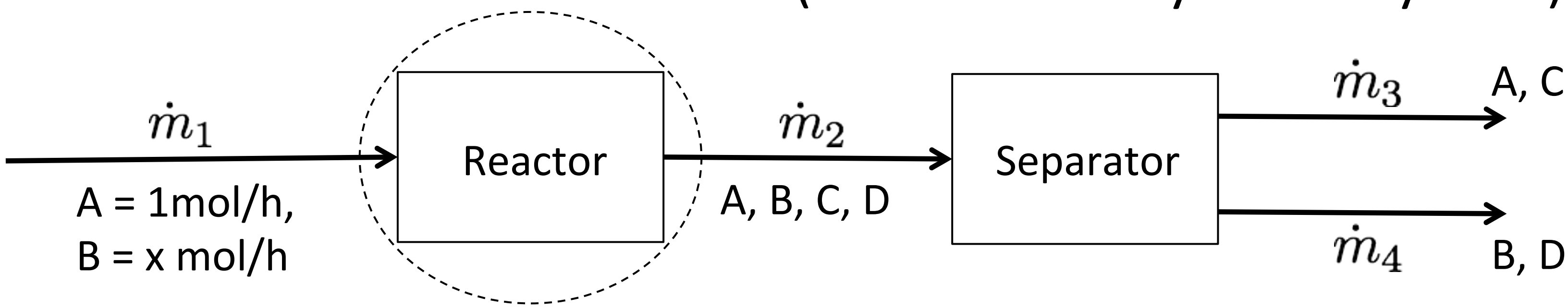
$$A + x\,B \rightarrow y\,C + z\,D$$



- Given
  - Fresh stream: 1 mol/h of A and *x* mol/h of B (stoichiometric proportions)
  - Reactor conversion: 90% = (moles reacted/moles in feed)
- Calculate
  - Output flowrates of A, B, C, and D from separator

Example: Solution (I)

- No reactant is in excess. Choose either A or B as limiting reactant. I will choose A (stoichiometric coefficient = 1, avoids fractions in mass balances as shown later).
- Mass balance around reactor (draw boundary → subsystem)



- Write out conservation of mass equation for each component
  - A:

0 => A is reactant

In – Out + Generation – Consumption = 0

$$\dot{m}_1^A - \dot{m}_2^A + 0 - \dot{m}_1^A X = 0$$

$$\dot{m}_2^A = \dot{m}_1^A (1 - X)$$

$$\dot{m}_2^A = (1)(1 - 0.9) = \boxed{0.1\,\mathrm{mol/h}}$$

Example: Solution (II)

- Write out conservation of mass equation for each component
  - B:

0 => B is reactant

In − Out + Generation − Consumption = 0

$$\dot{m}_1^B - \dot{m}_2^B + 0 - \dot{m}_1^A X x = 0$$

$$\dot{m}_2^B = \dot{m}_1^B - \dot{m}_1^A X x$$

$$\dot{m}_2^B = x - (1)(0.9)(x) = \boxed{0.1x\,\mathrm{mol/h}}$$

Note that the Consumption term is written with respect to the <u>limiting reactant</u> (A) and the stoichiometric ratio (B/A = *x*/1) is taken into account. The same applies to C and D.

  - C:

0 => C is product

In − Out + Generation − Consumption = 0

$$\dot{m}_1^C - \dot{m}_2^C + \dot{m}_1^A X y - 0 = 0$$

$$\dot{m}_2^C = \dot{m}_1^C + \dot{m}_1^A X y$$

$$\dot{m}_2^C = 0 + (1)(0.9)(y) = \boxed{0.9y\,\mathrm{mol/h}}$$

Example: Solution (III)

- Write out conservation of mass equation for each component
  - D:

In − Out + Generation − Consumption = 0

0 => D is product

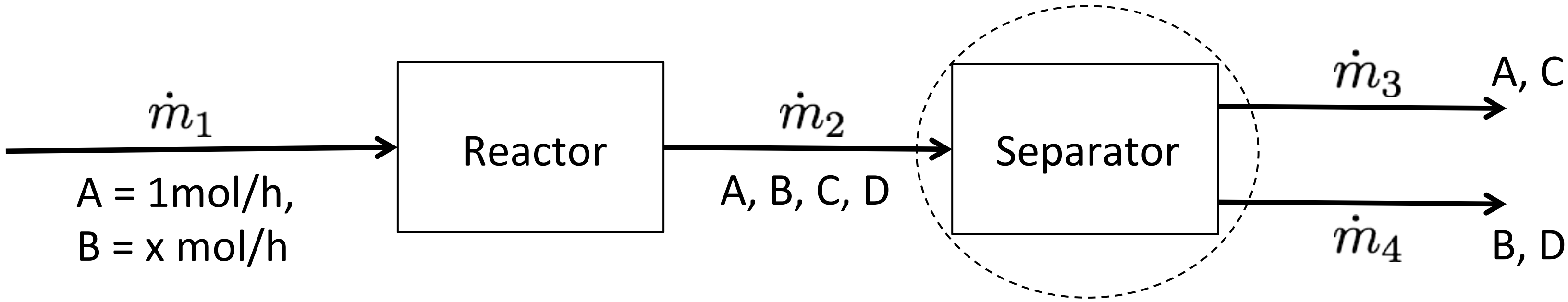
$$\dot{m}_1^D - \dot{m}_2^D + \dot{m}_1^A X z - 0 = 0$$

$$\dot{m}_2^D = \dot{m}_1^D + \dot{m}_1^A X z$$

$$\dot{m}_2^D = 0 + (1)(0.9)(z) = \boxed{0.9z \text{ mol/h}}$$

- The component output flowrates from the separator are the same as the ones calculated in the steps before (can you see why?). To illustrate, let us calculate the output flowrate of A from the separator.
- Draw a boundary around the separator (this is our new subsystem):

Example: Solution (IV)



- Write out conservation of mass equation for component A
  - A:

0 => no reaction takes place

In − Out + Generation − Consumption = 0

$$\dot{m}_2^A - \dot{m}_3^A + 0 - 0 = 0$$

$$\dot{m}_3^A = \dot{m}_2^A$$

$$\dot{m}_3^A = \boxed{0.1\,\mathrm{mol/h}}$$

- In fact, the reactor and separator could have been combined into a single subsystem.