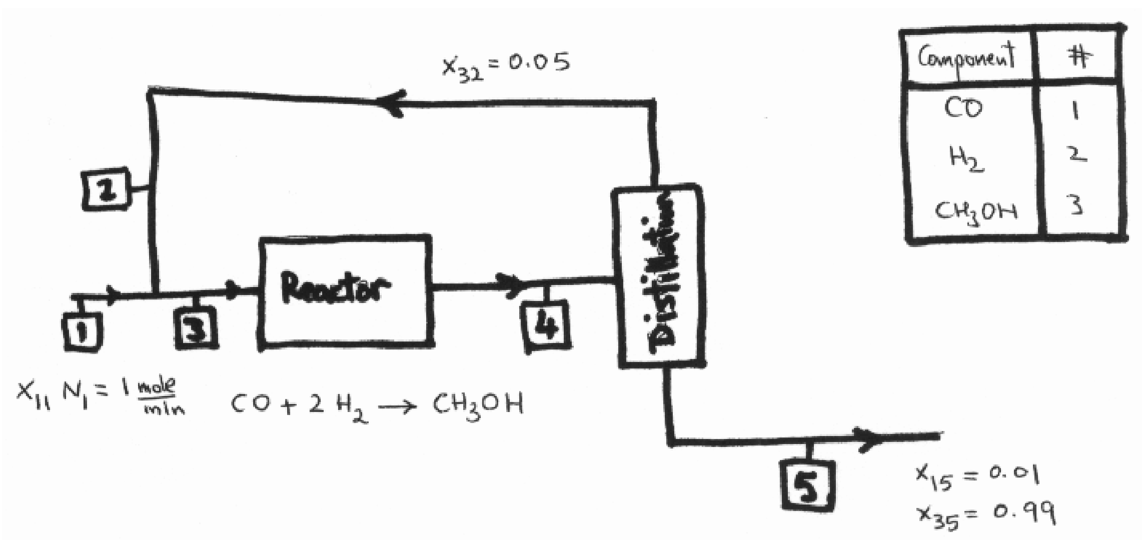
## Problem 10 10.213

Before we start solving the problem, we need to agree on the nomenclature.

$x_{ij}$ is the mole fraction of component i in stream j.
$N_j$ is the molar flow rate of stream j.
$x_{ij} * N_j$ is the molar flow rate of component i in stream j

This simplifies the notation because we use numbers to identify components instead of writing the chemical formulae in the subscript. So CO is component 1, $H_2$ is component 2, and $CH_3OH$ is component 3. We also know from the stoichiometry of the reaction that
$\nu_1 = -1$, $\nu_2 = -2$, and $\nu_3 = 1$

Let us draw the flow chart.




a) The flow rate of hydrogen in the feed stream (stream 1)

We will use an atom balance about the overall process

**Atom balance**
(# of atoms per molecule of component i * Molar flow rate of component i)$_{in}$
= (# of atoms per molecule of component i * Molar flow rate of component i)$_{out}$

**C balance**
C in CO in feed = C in $CH_3OH$ in product + C in CO in product
$1 * 1 = 1 * 0.99 * N_5 + 1 * 0.01 * N_5$

Therefore, the molar flow rate of the product stream (stream 5)
$N_5 = 1/(0.99+0.01) = 1$ mole/min

**H Balance**
H in $H_2$ in feed = H in $CH_3OH$ in product
$2 * (x_{21} * N_1) = 4 * 0.99 * 1$

Therefore, the molar flow rate of $H_2$ in feed

**$x_{21} * N_1 = 1.98$ mole/min**

b) <u>The molar flow rate of stream 3 ($N_3$)</u>

Since this is a variable inside the recycle loop, we have to solve the mass balance equations on all the units inside the loop. We will do it in a way to save us from solving so many simultaneous equations. It is important to note that there are many possible methods to solve this problem.

We will get the extent of the reaction first by doing mass balance on the $CH_3OH$ (component 3)

**<u>MB about the mixing point</u>**

$x_{31} N_1 + x_{32} N_2 = x_{33} N_3$ (1)

Since there is no $CH_3OH$ in feed, the above equation simplifies to

$x_{32} N_2 = x_{33} N_3$ (2)

**<u>MB about the reactor</u>**

$x_{33} N_3 + \nu_3 \varepsilon = x_{34} N_4$ (3)

**<u>MB about the separation unit</u>**

$x_{34} N_4 = x_{32} N_2 + x_{35} N_5$ (4)

Eliminating $x_{34} N_4$ using equations 3 and 4

$x_{33} N_3 + \nu_3 \varepsilon = x_{32} N_2 + x_{35} N_5$ (6)

Eliminating $x_{33} N_3$ using equations 2 and 6

$x_{32} N_2 + \nu_3 \varepsilon = x_{32} N_2 + x_{35} N_5$ (7)

The amount of $CH_3OH$ in stream 5 ($x_{35} N_5$) is known to be 0.99 mole/min. Substituting in equation 7 and solving for $\varepsilon$, knowing that $\nu_3$ is 1,

$\varepsilon = 0.99$ mole/min

We know that half of the reactants are consumed in each pass. That means that the amount consumed of CO in the reactor equals to half of the amount of CO in the feed to the reactor. The same applies to H2

$dn_1 = 0.5\, x_{13} N_3$

$dn_2 = 0.5\, x_{23} N_3$

We know that

$\varepsilon = dn_i/|\nu_i| = 0.99$

$0.99 = 0.5\, x_{13} N_3 / (1) = 0.5\, x_{23} N_3 / (2)$

Therefore

$x_{13} = x_{32} / 2$ (8)

$x_{13} N_3 = 1.98$ (9)

$x_{23} N_3 = 3.96$ (10)

It is also known that the mole fraction of $CH_3OH$ in the recycle stream (2) equals 0.05. Since the summation of all mole fractions in one stream equals 1, we have

$x_{12} + x_{22} = 0.95$ (11)

**MB about the mixing point on CO**
$X_{11} N_1 + x_{12} N_2 = x_{13} N_3$

Using 9 and the given information about CO in the feed stream, we get
$1 + x_{12} N_2 = 1.98$
$x_{12} N_2 = 0.98$ (12)

**MB about the mixing point on $H_2$**
$x_{21} N_1 + x_{22} N_2 = x_{23} N_3$

Using 10 and the results of part a, we get
$1.98 + x_{22} N_2 = 3.96$

Using 11 to remove x22, we get
$1.98 + (0.95-x_{12}) N_2 = 3.96$
$1.98 + 0.95 N_2 – x_{12} N_2 = 3.96$

Using 12, we get
$1.98 + 0.95 N_2 – 0.98 = 3.96$

Therefore,
$N_2 = (3.96- 1.98 + 0.98) / 0.95 = 3.116$ mole /min

And we know from part a,
$N_1 = 1 + 1.98 = 2.98$ mole/min
Now we can calculate $N_3$ (the total feed to the reactor),
$N_3 = N_1 + N_2$

$$\mathbf{N_3 = 2.98 + 3.116 = 6.096 \text{ mole/min}}$$

c) Molar flow rate from the reactor ($N_4$)

**MB on the separation unit**
$N_4 = N_2 + N_5$

$N_5$ is known from part a,
$N_5 = 1$ mole/min

$N_2$ is known from part b,
$N_2 = 3.116$ mole/min

Therefore,

$$\mathbf{N_4 = 3.116 + 1 = 4.116 \text{ mole/min}}$$

d) The composition of the recycle stream ($x_{12}$, $x_{22}$, and $x_{32}$)

Using 12,

$$\mathbf{x_{12} = 0.98 / N_2 = 0.98 / 3.116 = 0.315}$$

Using 11,

$$\mathbf{x_{22} = 0.95 – x_{12} = 0.95 – 0.315 = 0.635}$$

And we already know that

$$\mathbf{x_{32} = 0.05}$$