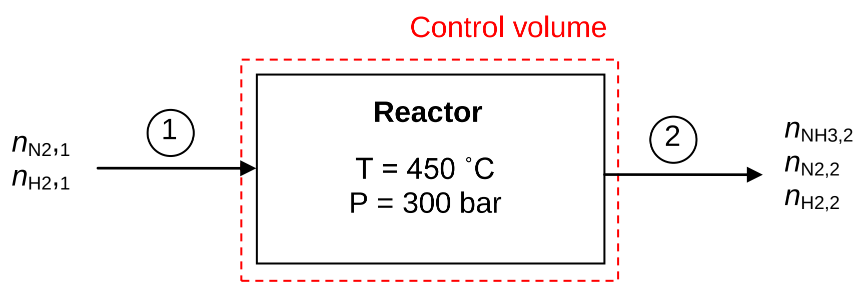
Given: The feed to an ammonia synthesis reactor contains a stoichiometric ratio of N_2 and H_2. The equilibrium relationship for this process is:

$$K_{eq} = \frac{{x_{NH_3}}^2}{x_{N_2}{x_{H_2}}^3} = 0.35 \quad \text{(at 450 °C and 300 bar)}$$

Predict: The maximum yield assuming that equilibrium is achieved in the reactor, and the fractional conversion for N_2 in this process.

Strategy: Mass balances with equilibrium relationships

Step 1: Draw PFD (note that the "dot" superscript has been omitted but all n_i indicate molar flow rates in units of *mol/h*.)



$N_2 + 3H_2 \leftrightarrow 2NH_3$

Step 2: Draw control volume: in this case, around the reactor.

Step 3: Choose a basis: Let's choose the output stream of $n_{NH3,2}$ = 100 *mol/h*

Step 4: What would be the maximum yield? This would be the yield achieved if the output stream from the reactor has reached equilibrium.

$$\text{(maximum)yield} = \frac{\text{actual yield (at equilibrium)}}{\text{theoretical yield if all of limiting reactant reacted}}$$

$$= \frac{\text{mol product formed (at equilibrium)}}{\text{mol product formed if all of limiting reactant reacted}}$$

We need to know $n_{N2,1}$ (or $n_{H2,1}$ since stoichiometric feed) to find the denominator. Ultimately, we will also need to know $n_{N2,2}$ to determine the fractional conversion of N_2. We have two types of relationships available to us in order to determine these values: the equilibrium relationship and mass balances on each species.

Mass Balances around CV: IN – OUT + GEN – CONS = ACC = 0 (since steady state)

$$N_2: \quad n_{N_2,1} - n_{N_2,2} + 0 - \frac{100\ mol\ NH_3}{h} \cdot \frac{1 mol\ N_2}{2\ mol\ NH_3} = 0$$

(i.e. 50 mol N_2/h consumed in reaction)

$$H_2: \quad n_{H_2,1} - n_{H_2,2} + 0 - \frac{100\ mol\ NH_3}{h} \cdot \frac{3 mol\ H_2}{2\ mol\ NH_3} = 0$$

(i.e. 150 mol H_2/h consumed in reaction)

Equilibrium Relationship:
The equilibrium constant K_{eq} tells us the composition of the output stream if equilibrium is reached. We can use this to determine the composition of the outlet stream (assuming our basis of 100 mol NH_3/h produced in the reactor). Because the equilibrium relationship is given in mole fractions, first calculate the relationships between *x*'s (mole fractions) and *n*'s (molar flow rates).

$$x_{NH_3,2} = \frac{n_{NH_3,2}}{n_{NH_3,2} + n_{N_2,2} + n_{H_2,2}}, x_{N_2,2} = \frac{n_{N_2,2}}{n_{NH_3,2} + n_{N_2,2} + n_{H_2,2}}, x_{H_2,2} = \frac{n_{H_2,2}}{n_{NH_3,2} + n_{N_2,2} + n_{H_2,2}}$$

- Because the feed stream has a stoichiometric ratio of N_2 and H_2, $n_{H2,1} = 3n_{N2,1}$.
- Because NH_3 synthesis is the only reaction occurring in the reactor, $n_{H2,2} = 3n_{N2,2}$.

Therefore:

$$x_{NH_3,2} = \frac{100\, {}^{mol}/_{h}}{100\, {}^{mol}/_{h} + 4n_{N_2,2}}, x_{N_2,2} = \frac{n_{N_2,2}}{100\, {}^{mol}/_{h} + 4n_{N_2,2}}, x_{H_2,2} = \frac{3n_{N_2,2}}{100\, {}^{mol}/_{h} + 4n_{N_2,2}}$$

Plug these into the given equilibrium relationship to obtain:

$$0.35 = \frac{\left(100\, {}^{mol}/_{h}\right)^2 \left(100\, {}^{mol}/_{h} + 4n_{N_2,2}\right)^2}{(n_{N_2,2})(3n_{N_2,2})^3}$$

Solve for $n_{N2,2}$: $n_{N_2,2} = 150\frac{mol}{h}$. Therefore, $n_{H_2,2} = 450\frac{mol}{h}$.

Combine:
We can plug these values into the mass balances to determine the molar flow rates of the feed stream:

$$n_{N_2,1} = 150\frac{mol}{h} + 50\frac{mol}{h} = 200\frac{mol}{h}$$
$$n_{H_2,2} = 450\frac{mol}{h} + 150\frac{mol}{h} = 600\frac{mol}{h}$$

Thus (without recycle):

$$\boxed{\text{(Maximum) Yield} = \frac{100\,\frac{\text{mol NH}_3}{\text{h}}}{200\,\frac{\text{mol N}_2}{\text{h}} \text{x} \frac{2\text{ mol NH}_3}{1\text{ mol N}_2}} = 0.25}$$

Calculate fractional conversion of N_2:

$$\boxed{\text{Fractional conversion of N}_2\ (\text{f}_{\text{N2}}) = \frac{\text{moles N}_2\textbf{reacted}}{\text{moles N}_2\textbf{fed}} = \frac{50\,\frac{\text{mol}}{\text{h}}}{200\,\frac{\text{mol}}{\text{h}}} = 0.25}$$