

## Tutorial 2 – Reactors in Series

A reactor not that ideal...

An isothermal plug flow reactor is designed to give 85% conversion of A for a second-order liquid phase reaction  $A \rightarrow B$ . The feed consists of 75% A, 25% inert. The total concentration of the inlet stream is  $1 \text{ kmol/m}^3$  and is fed at a flow rate of  $5 \text{ m}^3/\text{hr}$ . The rate constant for the reaction at a specified operating temperature is  $0.5 \text{ m}^3/\text{kmol/hr}$ .

When the reactor is actually operated based on this design, it was found that 30% of the initial reactor behaved as a CSTR while the remaining behaved as a plug flow reactor. Calculate the conversion obtained in such a reactor.

(Answer:  $X = 82.9\%$ )



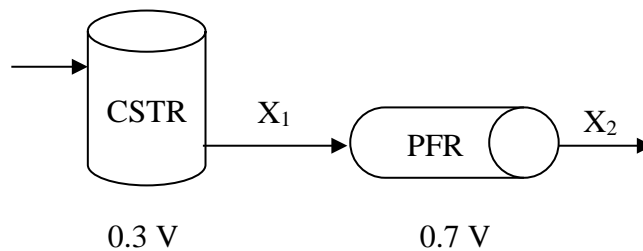
### Solution of Tutorial 2

Answer:

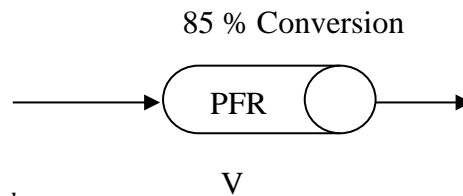
Remark: One possible way to solve this problem, which is what I believe many of you did, is to first calculate the volume using the data given. In the solution below, you will see that we can actually solve this problem without calculating the volume of the reactor (and hence not using many of the info given).

A → B

Equivalent to:



Initially design:



$$V_{\text{real,PFR}} = F_{A0} \int_0^x \frac{dx}{-r_A}$$

$$-r_A = kC_A^2$$

$$V_{\text{real,PFR}} = \int_0^{0.85} \frac{F_{A0} dx}{kC_A^2}$$

Stoichiometric table:

Species	Feed	Change	Exit
A	$F_{A0}$	$F_{A0} X$	$F_{A0} (1-X)$
B	0	$F_{A0} X$	$F_{A0} X$
I	$F_I$	$F_I$	$F_I$

Assume constant volume.

$$C_A = \frac{F_A}{v} = \frac{F_{A0}(1-x)}{v_0} = C_{A0}(1-x)$$



$$V_{\text{real,PFR}} = \int_0^{0.85} \frac{F_{AO} dx}{kC_{AO}^2(1-x)^2} = \frac{F_{AO}}{kC_{AO}^2} \int_0^{0.85} \frac{dx}{(1-x)^2}$$

Take integration,

$$V_{\text{real,PFR}} = \frac{F_{AO}}{kC_{AO}^2} \left[ \frac{1}{1-x} \right]_0^{0.85} \rightarrow V_{\text{real,PFR}} = \frac{5.667F_{AO}}{kC_{AO}^2}$$

Real Reactor:

CSTR

$$0.3 V_{\text{real,PFR}} = \frac{F_{AO} x_1}{-r_A} = \frac{F_{AO} x_1}{kC_{AO}^2(1-x_1)^2} \rightarrow 0.3 \frac{V_{\text{real,PFR}} kC_{AO}^2}{F_{AO}} (1-x_1)^2 = x_1$$

$$1.7(1-x_1)^2 = x_1 \rightarrow 1.7x_1^2 - 4.4x_1 + 1.7 = 0 \rightarrow x_1^2 - 2.588x_1 + 1 = 0$$

A=1, B= -2.588, C=1

$$X = \frac{-B \pm \sqrt{B^2 - 4AC}}{2A} \rightarrow \frac{-(-2.588) \pm \sqrt{(2.588)^2 - 4(1)(1)}}{2(1)} \rightarrow = 0.4726$$

PFR

We know

$$0.7 V_{\text{real,PFR}} = \frac{F_{AO}}{kC_{AO}^2} \left[ \frac{1}{1-x} \right]_0^{x_2} \rightarrow 0.7 \frac{V_{\text{real,PFR}} kC_{AO}^2}{F_{AO}} = \frac{1}{1-x_2} - \frac{1}{1-0.4726}$$

$$0.7(5.667) = \frac{1}{1-x_2} - \frac{1}{1-0.4726} \rightarrow 3.9669 = \frac{1}{1-x_2} - 1.896$$

$$\frac{1}{1-x_2} = 5.8629 \rightarrow 0.17 = 1-x_2 \rightarrow x_2 = 0.829 \rightarrow x_2 = 82.9\%$$