**Moving bed reactor:**

Consider the case when the reactor bed moves from up to down and the reactant is also fed at the top, i.e. They movement is cocurrent.

The catalyst decays with time and the decay is independent of reactant concentrations, but is first order wrt 'a'. i.e. \( \frac{da}{dt} = k_d a \). The reaction is second order i.e. \( r_A^* = -kC_A^2 \). The reaction is \( A \rightarrow B \).

Given, \( k' = 0.60 \text{ lit}^2/(\text{g-cat. Mol. min}) \) and \( k_d = 0.72 \text{ min}^{-1} \). The reactor contains 22 kg catalyst, and it moves at 10 kg/min. Reactant is fed at 0.075 mol/lit concentration and \( F_{A0} = 30 \text{ mol/min} \). Determine the conversion under steady state conditions.

**Variation:** (Problem 10.18). The reaction is \( A \rightarrow B \). The reaction is zero order and the decay is also zero order. \( k = 1 \text{ mol/kg cat/min} \) and \( k_d = 2 \text{ min}^{-1} \). The reactor can contain 1 kg catalyst. \( F_{A0} = 1 \text{ mol/min} \). The feed is inexpensive (cost is zero) and the process cost such as pumping, separation etc. is also negligible (zero). The product can be sold at Rs. 8000/mole and the catalyst cost is Rs 500 /kg catalyst. What is the optimal feed rate of catalyst?

**Solution:**

Mass balance at any location ‘Z’, or ‘W’ is given by

\[
F_A|_W + a \times r_A^* \times \Delta W = F_A|_{W+\Delta W}
\]

Note that the activity is a function of location (or W).

The time the catalyst is in contact with reactants is given by \( t = \frac{W}{F_s} \)

Therefore, \( dt = \frac{dW}{F_s} \). From the decay law we can write \( -\frac{da}{dW} = \frac{k_d}{F_s} a \)

Hence \( a = e^{-\frac{k_dW}{F_s}} \)

The mass balance is written as

\[
\frac{dF_A}{dW} = a \times r_A^* = -e^{-\frac{k_dW}{F_s}} kC_A^2 = -e^{-\frac{k_dW}{F_s}} kC_{A0}^2 (1 - x)^2
\]

\[
\frac{dx}{(1 - x)^2} = e^{-\frac{k_dW}{F_s}} kC_{A0}^2 F_{A0} dW
\]

\[
\frac{1}{(1 - x)} = -e^{-\frac{k_dW}{F_s}} kC_{A0}^2 F_{A0} k_d + C
\]
At $W=0$, $x=0$, means $C = 1+\frac{kC_{A_0}^2 F_x}{F_{A_0} k_d}$. 

Hence \[
\frac{x}{1-x} = \frac{kC_{A_0}^2 F_x}{F_{A_0} k_d} \left(1-e^{-\frac{k_d W}{F_x}}\right).
\]

For the given values, \[
\frac{x}{1-x} = \frac{0.60 \times 0.075^2}{30} \times 10 \left(1-e^{-\frac{0.72 \times 22}{10}}\right) = 1.2419
\]

Therefore, $x$ is approximately 55.39%.

**Variation:**

**Solution:**

Decay is of zero order, therefore \[-\frac{da}{dt} = k_d\]. Since $t = \frac{W}{F_x}$ we have \[-\frac{da}{dW} = \frac{k_d}{F_x}\]. This results in \[a = 1 - \frac{k_d W}{F_x}\].

Reaction is of zero order, therefore \[F_{A_0} W + a \times r_A \times \Delta W = F_{A_0} W + \Delta W\] simplifies to \[\frac{dF_A}{dW} = -F_{A_0} \frac{dx}{dW} = a \times r_A = -\left(1 - \frac{k_d W}{F_x}\right) k\].

Integrating we get \[x = \left(W - \frac{k_d W^2}{2 F_x}\right) \frac{k}{F_{A_0}}\].

For the given values, \[x = \left(1 - \frac{2 \times 1^2}{2 F_x}\right) \frac{1}{1} = 1 - \frac{1}{F_x}\].

Net profit = product selling price – catalyst cost

\[= (F_{A_0} x) \times \text{(price of product)} - F_x \times \text{(cost of catalyst)}\]

\[= \left(1 - \frac{1}{F_x}\right) \times (8000) - F_x \times (500) = 8000 - \frac{8000}{F_x} - 500 \times F_x\]

This is a maximum when \[
\frac{8000}{F_x^2} - 500 = 0
\]
i.e. when $F_x = 4$ kg/min. At this condition, the conversion is $x = 0.75$

**Variation 2:** What if $k = 5$ mol/kgcat/min (instead of 1 mol/kgcat/min) and if the feed and the catalyst are fed at opposite ends?
Solution:

The mass balance equation is given by \( F_A \bigg|_W + a \times r_A' \times \Delta W = F_A \bigg|_{W+\Delta W} \)

The time a catalyst spends in the bed is given by \( t = \frac{W_{\text{max}} - W}{F_s} \). Therefore, \( dt = -\frac{dW}{F_s} \)

The decay law is \( -\frac{da}{dt} = k_d \). Therefore, \( \frac{da}{dW} = \frac{k_d}{F_s} \). The initial condition is at \( W = W_{\text{max}}, \ a = 1 \).

This results in \( a = \frac{k_d}{F_s}(W - W_{\text{max}}) + 1 \) This is with the understanding that the activity will not go to negative values, i.e. zero order decay is valid and the \( F_s, k_d \) and \( W_{\text{max}} \) are such that \( \frac{k_d W_{\text{max}}}{F_s} \leq 1 \)

The mass balance becomes

\[
\frac{dF_A}{dW} = -F_{A0} \frac{dx}{dW} = a \times r_A' = -\left( \frac{k_d}{F_s} (W - W_{\text{max}}) + 1 \right) k
\]

Integrating we get \( x = \left( \frac{k_d}{F_s} \left( \frac{W}{2} - W_{\text{max}} \right) + 1 \right) \frac{kW}{F_{A0}} \)

For the given values,
\[ x = \left( \frac{1}{F_s} \left( \frac{1}{2} - 1 \right) + 1 \right) \frac{5 \times 1}{1} = 5 \times \left( 1 - \frac{1}{2F_s} \right) \]

\[ = (F_{A0})^x \times \text{(price of product)} - F_s \times \text{(cost of catalyst)} \]

\[ = 5 \times \left( 1 - \frac{1}{2 \times F_s} \right) \times (8000) - F_s \times (500) = 40000 - \frac{20000}{F_s} - 500 \times F_s \]

This is a maximum when \( \frac{20000}{F_s^2} - 500 = 0 \), i.e. when \( F_s = 20 \) kg/min. The profit is Rs. 29,000/min. At this condition, the conversion is 4.8750. Impossible!

This is because we are using ‘zero order reaction’. In zero order reaction, if we blindly use the kinetics expression, we can get negative concentrations, and conversion exceeding 1. \textit{Always} watch out for unrealistic results when you work with zero or negative order kinetics.