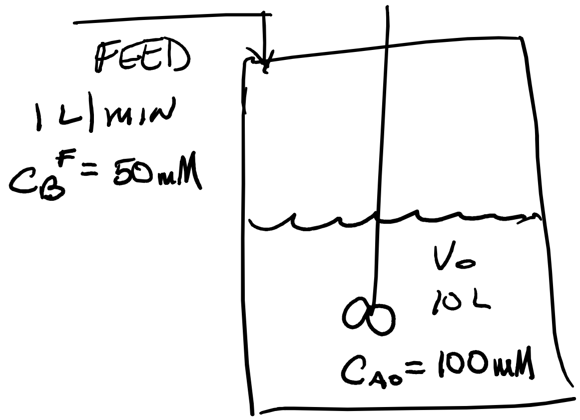
EXAMPLE WITH KINETIC EXPRESSION



20 L REACTOR CAPACITY

OVERALL BALANCE

ACC = IN − OUT

$$\frac{d(\rho V)}{dt} = Q^{IN} \rho^{IN}$$

$$\frac{dV}{dt} = Q^{IN} \Rightarrow \frac{dV}{dt} = 1$$

$$V - V_0 = t \qquad 0 \le t \le 10 \text{ min}$$

$$\boxed{V = t + 10}$$

"B" BALANCE

ACC = IN − OUT + GEN

$$\frac{d(c_B V)}{dt} = Q^F c_B^{IN} - 0 - V k c_B$$

$\frac{\left(\frac{mmoles}{L}\right)(L)}{min}$

$(L)\left(\frac{1}{min}\right)\left(\frac{mmoles}{L}\right)$

VOLUME IS NOT A CONSTANT

$$V\frac{dc_B}{dt} + c_B\frac{dV}{dt} = (1)(50) - V k c_B$$

$$(t+10)\frac{dc_B}{dt} + c_B(1) = 50 - (t+10) k c_B$$

$$\frac{dc_B}{dt} + \left[\frac{1 + k(t+10)}{(t+10)}\right] c_B = \frac{50}{t+10}$$

$$\frac{dc_B}{dt} + a(t)\, c_B = f(t)$$

INTEGRATING FACTOR ....

$$p(t) = e^{\int a(t)\,dt}$$

$$\frac{d}{dt}\left[p(t) c_B \right] = f(t)\,p(t)$$

$$a(t) = \frac{1 + k(t+10)}{t+10}$$

$$\int a(t)\,dt = \int \frac{1 + k(t+10)}{t+10}\,dt$$

$$= \int \frac{dt}{t+10} + \int k\,dt$$

$$= \ln(t+10) + kt$$

$$p(t) = e^{\ln(t+10) + kt} = e^{\ln(t+10)}\,e^{kt}$$

$$\boxed{p(t) = (t+10)\,e^{kt}}$$

$$\frac{d}{dt}\left[p(t)\, c_B\right] = f(t)\, p(t)$$

$$\frac{d}{dt}\left[(t+10)e^{kt} c_B\right] = \underbrace{\left(\frac{50}{t+10}\right)}_{f(t)}\underbrace{(t+10)e^{kt}}_{p(t)} = 50e^{kt}$$

$$\int d\left[(t+10)\, e^{kt} c_B\right] = 50\int e^{kt}\, dt$$

$$(t+10)\, e^{kt} c_B = \frac{50}{k} e^{kt} + C$$

THIS IS WHERE A CONSTANT OF INTEGRATION IS NEEDED!

$$(t+10)e^{kt}C_B = \frac{50}{k}e^{kt} + C$$

$$C_B = \frac{50}{k(t+10)} + \frac{C}{(t+10)}e^{-kt}$$

NOTE HOW CONSTANT OF INTEGRATION ENDS UP.

FIND C?

$t = 0 \quad C_B = 0$

$$0 = \frac{50}{k(10)} + \frac{C}{10}(1)$$

$$-\frac{50}{k(10)} = \frac{C}{10}$$

$$C = -50/k$$

$$C_B = \frac{50}{k(t+10)} - \frac{50}{k(t+10)}e^{-kt}$$

OR

$$\boxed{C_B = \frac{50}{k(t+10)}\left[1 - e^{-kt}\right]}$$

CONSIDER WHAT AN "A" BALANCE WOULD LOOK LIKE:

$t = 0$

$C_{A0} = 100$

ACC = IN − OUT + GEN

$$\frac{d(C_A V)}{dt} = 0 - 0 - Vk\,C_B$$

⋮

RESULTING EQUATION IS A BIT COMPLICATED

IF WE HAD AN "OUT" STREAM, THEN THAT TERM WOULD LOOK LIKE $Q^{out} C_A$

SOME CALCULATIONS:

MOLES OF B IN REACTOR AT ANY TIME $= C_B V = \left[\frac{50}{k(t+10)}\left(1-e^{-kt}\right)\right]\left[t+10\right]$

$$= \frac{50}{k}\left(1-e^{-kt}\right)$$

MOLES OF B THAT HAVE BEEN FED INTO REACTOR AT ANY TIME $= Q^{IN} C_B^{IN}\, t = 50t$

(NOTE: THE REACTOR STARTED WITH NO "B")

MOLES OF B REACTED + MOLES OF B UNREACTED = MOLES OF B FED

SO, MOLES OF B REACTED = MOLES OF B FED − MOLES OF B UNREACTED

$$= 50t - \frac{50}{k}\left(1 - e^{-kt}\right)$$

MOLES OF "A" REACTED = MOLES OF "B" REACTED = MOLES OF C FORMED

CONC OF C AT ANY TIMES = $\dfrac{\text{MOLES OF C FORMED}}{\text{VOLUME}} = \dfrac{50t - \frac{50}{k}\left(1 - e^{-kt}\right)}{t+10}$

$$\boxed{C_C = \frac{50t - \frac{50}{k}\left(1 - e^{-kt}\right)}{t+10}}$$

$$\text{MOLES OF "A" PRESENT} = \text{MOLES OF "A" INITIALLY} - \text{MOLES OF "A" REACTED}$$

$$\text{MOLES OF "A" PRESENT} = (100)(10) - \left[50t - \frac{50}{k}\left(1 - e^{-kt}\right)\right]$$

$$\boxed{C_A = \frac{\text{MOLES OF "A" PRESENT}}{\text{VOLUME}} = \frac{1000 - 50t + \frac{50}{k}\left(1 - e^{-kt}\right)}{t+10}}$$

@ $t = 10$ min $k = 0.9$ min^{-1}

$$C_B = \frac{50}{(0.9)(20)}\left[1 - e^{-9}\right] = 2.78 \text{ mmol/L}$$

$$C_C = \frac{(50)(10) - \frac{50}{0.9}\left[1 - e^{-9}\right]}{20} = 22.22 \text{ mmol/L}$$

$$C_A = \frac{1000 - 50(10) + \frac{50}{0.9}\left[1 - e^{-9}\right]}{20} = 27.79 \text{ mmol/L}$$

NOTE $C_A > C_B$ BY FACTOR OF 10.