Component Material Balance Equations (with or without reaction)

The previous discussion has been in terms of the total mass of the system, but most process streams, encountered in practice, contain more than one chemical species. Provided no chemical change occurs, the generalized dynamic equation for the conservation of mass can also be applied to each chemical component of the system. Thus for any particular component

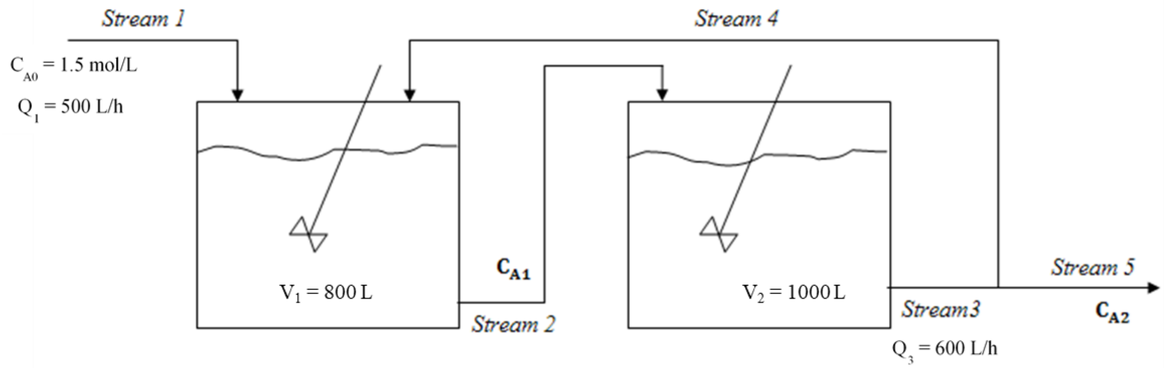
Rate of accumulation of mass of component , A, in the system = Mass flow rate of the component ,A into the system − Mass flow rate of the component ,A out of the system

Where a chemical reaction occurs, the change, due to reaction, can be taken into account by the addition of a reaction rate term into the component balance eequation. Thus in the case of material produced by the reaction

Rate of accumulation of mass of component , A, in the system = Mass flow rate of the component ,A into the system − Mass flow rate of the component ,A out of the system ± Rate of production/ consumption of the component ,A by the reaction

EXAMPLE (Component Material Balance Equations (with reaction)

A first order, liquid phase irreversible reaction takes place in series of continuous stirred reactors as shown in figure below.
$A \rightarrow B$



The rate of reaction in the reactors is;

$rA = -kCA$ with $k = 0.359\ h\text{-}1$

Determine the concentration of ***species A*** in each reactor **at steady state** if the feed to the first reactor contains 1.5 mol/L of A.

Assumptions:

-Steady state conditions prevail,

-Perfect mixing in the reactor, the concentrations and temperatures of the species within the reactor are uniform,

-Liquid density is constant

Overall material balance:

$$\dot{m}_{in} = \dot{m}_{out} \qquad \ldots(1)$$

Since the liquid density is constant, Eq.(1) simplifies to;

$$Q_{in} = Q_{out} \qquad \ldots(2)$$

Hence;

$$\boldsymbol{Q_1 = Q_5 = 500 L/h}$$

$$Q_3 = Q_4 + Q_5$$

$$600 = Q_4 + 500$$

$$\boldsymbol{Q_4 = 100\ L/h}$$

$$Q_2 = Q_1 + Q_4$$

$$\boldsymbol{Q_2 = 600\ L/h}$$

Component mass balance for species A around the first reactor:

$$Q_1 C_{A0} + Q_4 C_{A2} - Q_2 C_{A1} + r_A V_1 = \frac{d(C_{A1} V_1)}{dt} \quad \ldots (3)$$

$$Q_1 C_{A0} + Q_4 C_{A2} - Q_2 C_{A1} - k_1 C_{A1} V_1 = \frac{d(C_{A1} V_1)}{dt}$$

$$500\left(\frac{L}{h}\right) 1.5\left(\frac{mol}{L}\right) + 100\left(\frac{L}{h}\right) C_{A2} - 600\left(\frac{L}{h}\right) C_{A1} + (-0.359h^{-1}) C_{A1} 800(L) = 0$$

$$750 + 100 C_{A2} - 887.2\, C_{A1} = 0 \quad \ldots (4)$$

Component mass balance for species A around the second reactor:

$$Q_2C_{A1} - Q_3C_{A2} + r_{A2}V_2 = \frac{d(C_{A2}V_2)}{dt} \qquad \text{... (5)}$$

$$600C_{A1} - 600C_{A2} - \ k_2C_{A2}V_2 = 0$$

$$600C_{A1} - 600C_{A2} - \ 0.359\ C_{A2}1000 = 0$$

$$600C_{A1} - 959C_{A2} = 0 \qquad \text{... (6)}$$

$$C_{A1} = 1.60\ C_{A2} \qquad \text{... (7)}$$

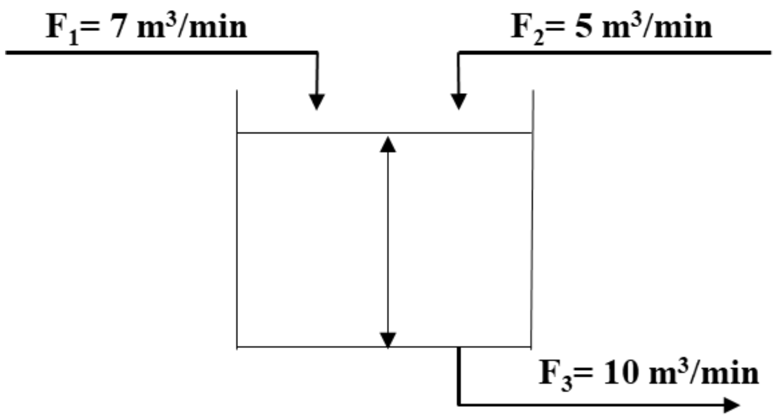
From Equation (4) by using Eq. (7);

C_{A2} = 0.57 mol/L and

C_{A1} = 0.91 mol/L

EXAMPLE (Component Material Balance Equations, without reaction)

There is a 4% NaCl solution in a 6 m^3 tank. This tank is fed pure water at a rate of 7 m^3/min and a 30% NaCl solution at a rate of 5 m^3/min and drains from the bottom of the tank at the flow rate of 10 m^3/min. The tank is completely mixed and density can be fixed. Take mathematical equations that change the time of the NaCl gradient in the tank.



Total Mass Balance:

$$\frac{dV\rho}{dt} = Q_1\rho + Q_2\rho - Q_3\rho$$

$$\frac{dV}{dt} = 7 + 5 - 10$$

$$\frac{dV}{dt} = 2 \qquad \dots(1)$$

$$V = 2t + C$$

Initial condition: t = 0 min, V = 6 m^3

$$\Rightarrow 6 = C$$

$$\Rightarrow V = 2t + 6 \qquad \dots(2)$$

Salt Balance:

V : volume in the tank

C_3 : salt concentration in the tank

Mass and salt concentration depend time. V = f(t), C_3 = f(t)

$$\frac{d(VC_3)}{dt} = V_1C_1 + V_2C_2 - V_3C_3$$

$$V\frac{dC_3}{dt} + C_3\frac{dV}{dt} = V_2C_2 - V_3C_3$$

C_1 = 0 (Stream 1 does not contain salt)

$$V\frac{dC_3}{dt} + C_3\frac{dV}{dt} = V_2C_2 - V_3C_3 \qquad \ldots(3)$$

Eq. (3) is rearranged by using Eq. (1) and Eq. (2).

$$\frac{dC_3}{dt} = \frac{1.5 - 12C_3}{2t + 6} \qquad \ldots(4)$$

$$\frac{dC_3}{dt} + \frac{12}{2t + 6}C_3 = \frac{1.5}{2t + 6} \qquad \ldots(5)$$

Eq. (5) is a first order linear differential equation.

$$\frac{dy}{dx} + P(x)y = Q(x), \qquad (y = C_3 \text{ and } \mathrm{x} = \mathrm{t})$$

Taking into account of Eq. (5);

$$P(x) = \frac{12}{2x+6} \quad \text{and} \quad Q(x) = \frac{1.5}{2x+6}$$

The general solution of a first order linear differential equation:

$$\lambda y = \int \lambda \; Q(x)dx + C$$

$$\lambda = e^{\int P(x)dx}$$

$$\lambda = e^{\int\left(\frac{12}{2x+6}\right)dx} = e^{6ln(x+3)} = (x+3)^6$$

$$(x+3)^6 y = \int\left((x+3)^6.\left(\frac{0.75}{x+3}\right)\right)dx + C$$

$$(x+3)^6 y = \int 0.75 * \ (x+3)^5\, dx + C$$

$$(x+3)^6 y = 0.75 * \int(x+100)dx + C$$

$$(x+3)^6 y = 0.75 * \frac{(x+3)^6}{6} + C$$

$$(x+3)^6 y = 0.125 * \ (x+3)^6 + C$$

$$y = \frac{0.125 * (x+3)^6}{(x+3)^6} + \frac{C}{(x+3)^6}$$

$$C_3 = \frac{0.125 * (t+3)^6}{(t+3)^6} + \frac{C}{(t+3)^6}$$

Initial condition: t = 0 min, C_3 = 0.04

$$0.04 = \frac{0.125 * (t+3)^6}{(t+3)^6} + \frac{C}{(t+3)^6}$$

$$\Rightarrow C = -61.965$$

$$y = 0.125 - \frac{61.965}{(x+3)^6}$$