Simple Micromixing Models (one parameter or less) for a Stirrred Tank Reactor

These models apply to perfectly mixed continuous flow stirred tank with exponential residence time distribution that indicates no bypassing or stagnancy. i.e. $E(t) = \frac{1}{\bar{t}} e^{-t/\bar{t}}$. In the treatment below the rate of disappearance of reactant A is denoted by $(-R_A)$, and the tank has a mean residence time of $\bar{t}$.

The **Segregated Flow (SF) model** prediction for the exit reactant concentration in a stirred tank with exponential residence time density function is given below by equation (A).

$$\bar{C}_A = \frac{1}{\bar{t}} \int_0^\infty C_A(t) \exp(-t/\bar{t}) dt \qquad (A)$$

The evolution of the reactant A concentration with age t in a segregated fluid element is given by equation (1) with boundary (initial) condition (2), where C_{A0} is the reactant A concentration in the feed. The exit concentration of A, $\overline{C_A}$ is obtained by weighted averaging of the exit flow over all residence times.

$$\frac{dC_A}{dt} = -(-R_A) \qquad (1)$$

$$t = 0 \qquad C_A = C_{A_0} \qquad (2)$$

In the **Exchange in the Mean Model (EIM)** it is assumed that each segregated fluid element, while reacting, exchanges molecular content with all the elements in the system. This exchange rate is modeled as a product of an exchange coefficient, h, and a driving force, which is taken proportional to the difference in concentration of A in the element at any time and the mean steady state concentration in the reactor (which is the same as mean exit concentration), e.g. $(C_A - \overline{C_A})$. The model parameter is the exchange coefficient h.

Equations (A) still determines the exit average concentration while equation (1) for the concentration change in the individual segregated element is replaced by equation (1a) below which accounts for the finite rate of exchange between the segregated flow element and the contents of the tank at the mean concentration $\overline{C_A}$.

$$\frac{dC_A}{dt} = -(-R_A) - h(C_A - \overline{C_A}) \qquad (1a)$$

A trial and error solution is now needed for the mean (exit) concentration $\overline{C_A}$.

In the **Recycle Model (RM)** a recycle is superimposed on the CSTR, which is assumed in segregated flow, and complete mixing on molecular scale is assumed at the point M where the recycle stream carrying segregated flow elements from the CSTR at mean concentration $\overline{C_A}$ meets the fresh feed at C_{A0}. Thus, the initial reactant concentration of the elements that travel in segregated flow in the CSTR, is obtained by mixing the fresh feed with the final mean concentration in the tank (which is the same as the concentration of the exit stream). The model parameter is the recycle ratio R.

Hence, the differential equation for reactant concentration evolution in an element is still given by equation (1). The initial condition given by eq. (2) now is replaced by equation (2b):

$$t = 0 \quad C_A = C_{A_{in}} = \frac{C_{A_0} + R\overline{C_A}}{R+1} \qquad (2b)$$

Since the flow through the segregated flow section is now (R+1)Q ,and all the reactor volume is essentially in it, the pdf of residence times remains exponential but $\bar{t}$ is replaced by $\bar{t}/(R+1)$.

Thus equation (A) for the evaluation of the mean concentration in the system (and its outflow) must be replaced by equation (B):

$$\overline{C_A} = \frac{R+1}{\bar{t}} \int_0^\infty C_A(t)\exp(-(R+1)t/\bar{t})dt \qquad (B)$$

C_A(t) is obtained by solution of equation(1) using initial condition (2b) and the exit (mean) concentration is obtained by trial and error using equation (B) with equations (1) and (2b). Zwietering's general equation for the **Maximum Mixedness (MM) model** for the case of systems with exponential RTD is reduced to the standard equation for a perfectly mixed CSTR on the molecular level:

$$\bar{t} = \frac{C_{A_0} - C_A}{(-R_A)} \qquad (C)$$

The exit concentration from the CSTR is C_A.