BT209

Bioreaction Engineering

27/04/2023

Non ideal reactor

Prediction of conversion in non-ideal reactors,

(Segregation model, Tanks-in-series model)

Conversion in Non ideal reactors

- RTD tells us **how long the various fluid elements** have been in the reactor
- Knowledge of **RTD is not sufficient** to predict **conversion** because it **does not** tell us anything about the **exchange of matter between the fluid elements** (i.e., *mixing*)
- **Degree of mixing of molecules must be known** in addition to how long each molecule spends in the reactor (except 1st order reaction)
- The mixing of reacting species is one of the major factors controlling the behavior of chemical reactors

✓ **Need: Models that account for the mixing of molecules** inside the reactor.

RTD + kinetics + mixing model ⇒ **Exit conversion or exit concentration**

Mixing in Non ideal reactors

- Required information about ***micromixing*** in addition to that of ***macromixing***.

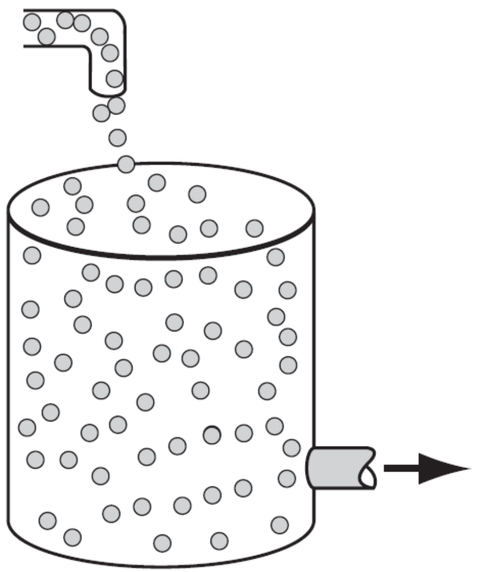
- **Macromixing** produces a distribution of residence times *without*, however, specifying how **molecules of different ages encounter one another** in the reactor.

- **Micromixing**, on the other hand, describes how molecules of different ages encounter one another in the reactor.

- There are **two extremes of *micromixing***:
  - (i) **complete segregation :** all **molecules of the same age group remain together** as they travel through the reactor and are not mixed with any other age until they exit the reactor (**segregation model**)
  - (ii) **complete micromixing: molecules of different age groups are completely mixed** at the molecular level as soon as they enter the reactor

- For a given state of **macromixing (i.e., a given RTD)**, these **two extremes of micromixing** will give the **upper and lower limits on conversion** in a non ideal reactor.

Segregation model

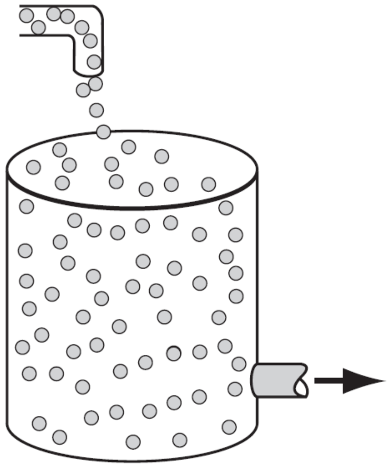


- In the segregated flow model we visualize the flow through the reactor to consist of a continuous series of globules.
- These globules retain their identity; that is, they do not interchange materia with other globules in the fluid during their period of residence in the reactio environment, i.e., they remain segregated.
- In addition, each globule spends a different amount of time in the reactor.
- In essence, what we are doing is lumping all the molecules that have exactly the same residence time in the reactor into the same globule.
- Because there is no molecular interchange between globules, each acts essentially as its own batch reactor. The reaction time in any one of these tiny batch reactors is equal to the time that the particular globule spends in the reaction environment. The distribution of residence times among the globules is given by the RTD of the particular reactor.

Cont..

- To determine the **mean conversion in the effluent stream ($\bar{X}$)**, we must **average the conversions of all of the various globules in the exit stream**

$$\begin{bmatrix} \text{Mean} \\ \text{conversion} \\ \text{of those globules} \\ \text{spending between} \\ \text{time } t \text{ and } t+dt \\ \text{in the reactor} \end{bmatrix} = \begin{bmatrix} \text{Conversion} \\ \text{achieved in a globule} \\ \text{after spending a time } t \\ \text{in the reactor} \end{bmatrix} \times \begin{bmatrix} \text{Fraction} \\ \text{of globules that} \\ \text{spend between } t \\ \text{and } t+dt \text{ in the} \\ \text{reactor} \end{bmatrix}$$



then

$$d\bar{X} = X(t) \times E(t)\, dt$$

$$\boxed{\frac{d\bar{X}}{dt} = X(t)E(t)}$$

$$\boxed{\bar{X} = \int_0^\infty X(t)E(t)\, dt}$$

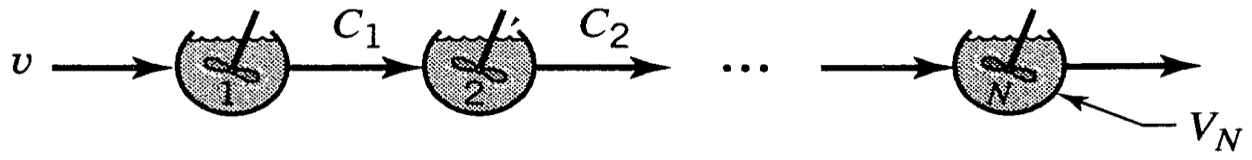
- Consequently, if we have the **batch reactor equation for *X*(*t*) and measure the RTD experimentally**, we can find the **mean conversion** in the exit stream.

Tanks-in series (TIS) Model

- In Real reactor flow is close to plug flow, close to mixed or **somewhere in between. Typically not perfect plug flow or mixed flow.**

- Models are useful for representing flow in real vessels, **to predict conversion** and for scale up.

- In TIS model **it is assume the real (non-ideal) reactor (volume V) is a connection of 'N' number of CSTR in series ($V_1+V_2+V_3+......V_N=V$)**



- **RTD is analyzed to determine the number of ideal tanks, N, in series that will give approximately the same RTD as the non-ideal reactor.**
- Here **tracer experiment is performed to get RTD of the real reactor** and **compare with the predicted RTD of 'N' number CSTR in series to get the number of CSTR (i.e. 'N')**

- If N→ 1 : ideal CSTR
- If N→ infinity : ideal PFR

✓ **Number of parameter of TIS model =1 (N, number of tanks)**

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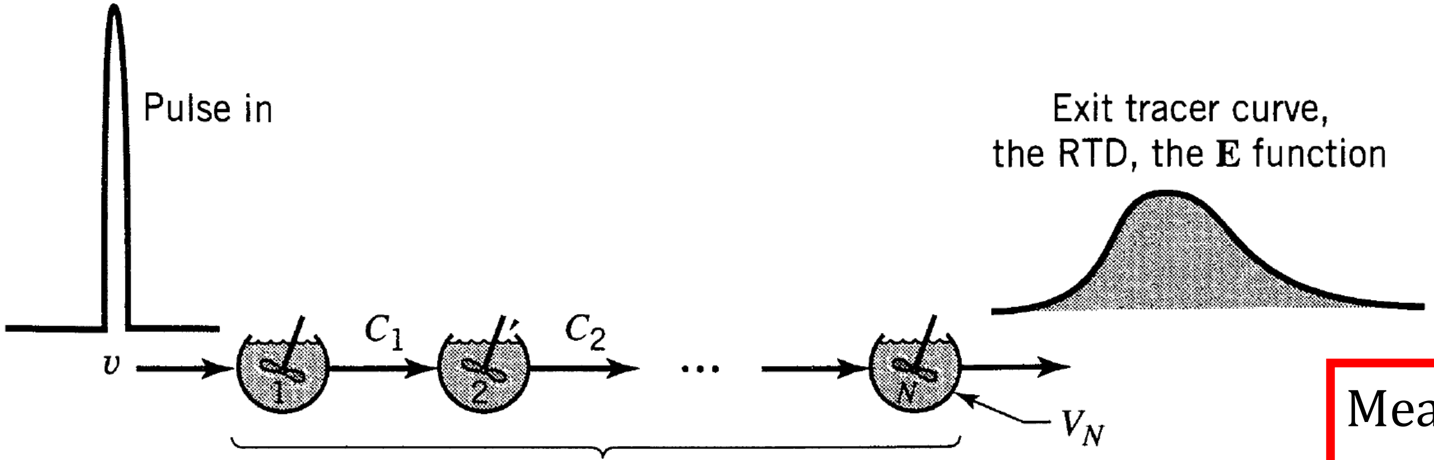
Prediction on RTD of N number ideal CSTR in series by tracer experiment



$\tau = N\tau_i =$ **Mean residence time of all tanks**

Assume the volume of each reactors are same,

$V_1 = V_2 = V_3 = \ldots\ldots\ldots = V_N$

Also $V_1 + V_2 + V_3 + \ldots\ldots V_N = V$ (real reactor volume)

Mean residence time of real reactors (or all tanks)

$$\tau = \frac{V}{v}$$

Mean residence time of each reactors (τ_i)

$$\tau_i = \frac{V_1}{v} = \frac{V_2}{v} = \frac{V_3}{v} = \cdots = \frac{V_N}{v}$$

A material balance on an **inert tracer** that has been injected **as a pulse** at time ***t*=0 into a yields for *t* > 0**

Inert Tracer material balance in 1st reactor for *t* > 0

$$V_1\frac{dC_1}{dt} = 0 - vC_1 \quad \Rightarrow \int_{C_0}^{C_1}\frac{dC_1}{C_1} = -\frac{1}{\tau_i}\int_0^t dt \quad \Rightarrow C_1 = C_0 e^{-\frac{t}{\tau_i}} \quad and\ \ E(t) = \frac{C_1(t)}{\int_0^\infty C_1(t)dt} = \frac{1}{\tau_i}e^{-\frac{t}{\tau_i}}$$

Cont..

Inert Tracer material balance in 2nd reactor (at *t* >0)

$$V_2 \frac{dC_2}{dt} = vC_1 - vC_2 \qquad C_2 = \frac{C_0 t}{\tau_i} e^{-t/\tau_i} \qquad E(t) = \frac{C_2(t)}{\int_0^\infty C_2(t)dt} = \frac{C_0 \frac{t}{\tau_i} e^{-\frac{t}{\tau_i}}}{\int_0^\infty C_0 \frac{t}{\tau_i} e^{-\frac{t}{\tau_i}}} = \frac{t}{\tau_i^2} e^{-\frac{t}{\tau_i}}$$

Inert Tracer material balance in 3rd reactor (at *t* >0)

$$V_3 \frac{dC_3}{dt} = vC_2 - vC_3 \qquad C_3 = \frac{C_0 t^2}{2\tau_i^2} e^{-t/\tau_i} \qquad E(t) = \frac{C_3(t)}{\int_0^\infty C_3(t)dt} = \frac{C_0 t^2/(2\tau_i^2)e^{-t/\tau_i}}{\int_0^\infty \frac{C_0 t^2 e^{-t/\tau_i}}{2\tau_i^2}dt} = \frac{t^2}{2\tau_i^3} e^{-t/\tau_i}$$

Do balances for 4th, 5th, …….Nth reactor (at *t* >0)

Cont..

E (t) - curve for one ideal CSTR (N=1)

$$E(t) = \frac{1}{\tau_i} e^{-\frac{t}{\tau_i}}$$

E (t) - curve for TWO ideal CSTR in series (N=2)

$$E(t) = \frac{t}{\tau_i^2} e^{-\frac{t}{\tau_i}}$$

E (t) - curve for three ideal CSTR in series (N=3)

$$E(t) = \frac{t^2}{2\tau_i^3} e^{-\frac{t}{\tau_i}}$$

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E (t) - curve for N number ideal CSTR in series

$$E(t) = \frac{t^{N-1}}{(N-1)!\,\tau_i^N} e^{-\frac{t}{\tau_i}}$$

$$\sigma^2 = \int_0^\infty (t-\tau)^2 E(t)dt$$

$$= \int_0^\infty t^2 E(t)dt - 2\tau \int_0^\infty tE(t)dt + \int_0^\infty \tau^2 E(t)dt$$

$$= \int_0^\infty t^2 E(t)dt - 2\tau^2 + \tau^2$$

$$= \int_0^\infty t^2 E(t)dt - \tau^2$$

$$= \int_0^\infty t^2 \frac{t^{N-1}}{(N-1)!\,\tau_i^N} e^{-\frac{t}{\tau_i}} dt - \tau^2$$

$$= \frac{\tau^2}{N}$$

Steps for Prediction of conversion using TIS model

Step 1: Calculate mean residence time of the reactor $\tau = \frac{V}{v} = \frac{volume\ of\ reactor}{volumetric\ flow\ rate}$

Step 2: Do tracer experiment in the reactor to get RTD (E-curve)

i. Get C_{tracer} vs t curve

ii. $E(t) = \frac{C_{tracer}(t)}{\int_0^\infty C_{tracer}(t)dt}$

Step 3: Calculate variance, $\sigma^2 = \int_0^\infty (t-\tau)^2 E(t)dt$

Step 4: Calculate number of ideal tanks, $N = \frac{\tau^2}{\sigma^2}$

Step 5: calculate conversion (X) if N number of CSTRs of equal volume are connected in serie

- Example: for 1st order reaction, $X = 1 - \frac{C_A}{C_{A0}} = 1 - \frac{1}{\left(1+k\tau_i\right)^N}$ $where, \tau_i = \frac{\tau}{N}$
- For 2nd order reaction you can also calculate