

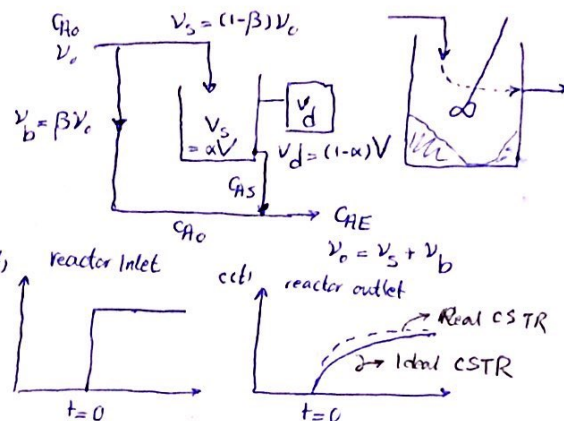
① Multiparameter Models

- These models consider the reactor as different regions (plug, dispersed plug, mixed, deadzone) interconnected in various ways
- Typical RTD behavior for these models is given in text.
- parameters of the model are obtained from RTD (i.e. $\frac{V_1}{V_2}$ and $\frac{V_m}{V}$ for that last case)
- Note that the above simple models do not allow for transfer between different parts

② Compartmental Models

- go to Levenspiel p. 284-286

- Liquid-phase CSTR with deadzone and by-passing
 - $\beta \triangleq$ fraction of v_0 by-passing the reactor
 - $\alpha \triangleq$ total reactor volume used
 - To examine the RTD behavior for such a reactor, it is more convenient to do a step pulse tracer study.



fraction of reactor effluent with residence time between 0 and t

$$= \int_0^t E(t) dt = \frac{c(t)}{C_0}$$

$$\Rightarrow E(t) = \left. \frac{d}{dt} \left(\frac{c(t)}{C_0} \right) \right|_{t=0}$$

- MBE for well-mixed deadzone

in - out + generation = accumulation

$$v_s C_{T_0} - v_s C_{T_s} = V_s \frac{dC_{T_s}}{dt} \Rightarrow dt = \frac{V_s}{v_s} \frac{dC_{T_s}}{C_{T_0} - C_{T_s}} \Rightarrow t - 0 = -\frac{V_s}{v_s} \ln(C_{T_0} - C_{T_s}) \Big|_0^{C_{T_s}}$$

$$\Rightarrow t = -\frac{V_s}{v_s} \ln\left(\frac{C_{T_0} - C_{T_s}}{C_{T_0}}\right) \Rightarrow \exp\left(-\frac{v_s}{V_s} t\right) = 1 - \frac{C_{T_s}}{C_{T_0}} \Rightarrow \frac{C_{T_s}}{C_{T_0}} = 1 - \exp\left(-\frac{v_s}{V_s} t\right)$$

$$\frac{C_{T_s}}{C_{T_0}} = 1 - \exp\left(-\frac{(1-\beta)v_0}{\alpha V} t\right) \xrightarrow{\tau = \frac{V}{v_0}} \frac{C_{T_s}}{C_{T_0}} = 1 - \exp\left(-\frac{(1-\beta)}{\alpha \tau} t\right) \quad (A)$$

- MBE for by-pass stream

$$\gamma_0 C_T = \gamma_0 (1-\beta) C_{T_s} + \gamma_0 \beta C_{T_0} \Rightarrow \frac{C_T}{C_{T_0}} = \beta + (1-\beta) \frac{C_{T_s}}{C_{T_0}}$$

$$\xrightarrow{(A)} \frac{C_T}{C_{T_0}} = \beta + (1-\beta) \left[1 - \exp\left(-\frac{(1-\beta)}{\alpha \tau} t\right) \right] = 1 - (1-\beta) \exp\left(-\frac{(1-\beta)}{\alpha \tau} t\right)$$

$$\rightarrow 1 - \frac{C_T}{C_{T_0}} = \frac{C_{T_0} - C_T}{C_{T_0}} = (1-\beta) \exp\left(-\frac{(1-\beta)}{\alpha \tau} t\right) \xrightarrow{or} \frac{C_{T_0}}{C_{T_0} - C_T} = \frac{1}{1-\beta} \exp\left(\frac{(1-\beta)}{\alpha \tau} t\right)$$

$$\ln \frac{C_{T_0}}{C_{T_0} - C_T} = \underbrace{\ln\left(\frac{1}{1-\beta}\right)}_{\text{intercept}} + \underbrace{\left(\frac{1-\beta}{\alpha \tau}\right)}_{\text{slope}} t$$

- [ex. 0]
- > liquid phase, $A \rightarrow B$, $-r_A = kC_A$, $k = 0.5 \text{ min}^{-1}$
 - > feed pure A, $C_{A_0} = 1000 \text{ mol/m}^3$, $V = 1 \text{ m}^3$, $v_0 = 0.1 \text{ m}^3/\text{min}$
 - > Tracer test for a step input, $C_{T_0} = 1 \text{ mol/m}^3$

C_T (mol/m^3)	t (min)	$\ln\left(\frac{C_{T_0}}{C_{T_0} - C_T}\right)$
0.5	5	0.693
0.667	10	1.098
0.8	15	1.609
0.875	20	2.079
0.925	25	2.550

- Solution of Ex. 01

from plot $\ln \frac{1}{1-\beta} = 0.23 \Rightarrow \beta = 0.205$
 $\frac{1-\beta}{\alpha \tau} = 0.092 \text{ min}^{-1} \Rightarrow \tau = \frac{V}{v_0} = 10 \text{ min} \Rightarrow \alpha = 0.864$

For conversion, we must use V_S
 $\frac{F_{A0} - F_{AS}}{V_S} = k_1 C_{AS} \Rightarrow \frac{v_0(1-\beta)C_{A0} - v_0(1-\beta)C_{AS}}{\alpha V} = k_1 C_{AS}$

$\Rightarrow C_{A0} - C_{AS} = \frac{\alpha V}{v_0(1-\beta)} k_1 C_{AS} \Rightarrow C_{AS} = \frac{C_{A0}}{1 + \frac{\alpha V}{v_0(1-\beta)} k_1}$

MB after reactor: $v_0 C_{AE} = v_0(1-\beta)C_{AS} + v_0 \beta C_{A0} \Rightarrow C_{AE} = \frac{(1-\beta)C_{A0}}{1 + \frac{\alpha V}{v_0(1-\beta)} k_1} + \beta C_{A0}$

$\Rightarrow C_{AE} = 123.56 + 205 = 328.56 \text{ mol m}^{-3}$

$x_{AE} = \frac{C_{A0} - C_{AE}}{C_{A0}} = 0.671$

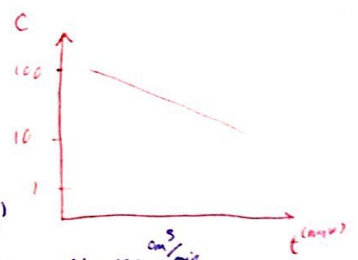
- Ex. 02

Gas phase rxn, $A \rightarrow 2R$, $-r_A = k C_A$, $v_0 = 100 \text{ cm}^3/\text{min}$, $V = 100 \text{ cm}^3$
 Feed: 0.75 A, 0.25 inert, $x_{AE} = 0.6$, find k

- Solution of Ex. 02

note from stoichiometry
 $\Rightarrow v_E = (1 + \frac{x_{AE}}{4}) v_0 = 1.15 v_0$

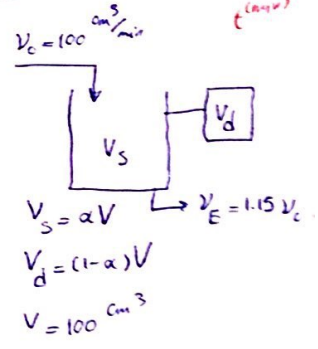
comp.	@ inlet	@ exit
A	F_{A0}	$F_{A0}(1-x_{AE})$
B	-	$2 F_{A0} x_{AE}$
I	$F_{I0} = 3 F_{A0}$	$3 F_{A0}$
total:	$4 F_{A0}$	$F_{A0}(4+x_{AE})$



consider the model as a CSTR with deadzone.

balance for tracer using a pulse input: $-v_E C = V_S \frac{dC}{dt}$
 $\Rightarrow dt = -\frac{V_S}{v_E} \frac{dC}{C} \int \Rightarrow t = -\frac{V_S}{v_E} \ln \frac{C}{C_0}$, $C_{T0} = 100$

(from the fig.) @ $t = 2 \text{ min} \Rightarrow C = 10 \Rightarrow V_S = 99.89 \text{ cm}^3$
 $V_d = 0.11 \text{ cm}^3 \rightarrow$ almost an Ideal CSTR



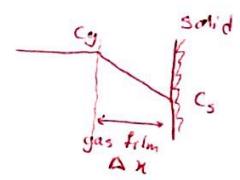
for an Ideal CSTR:

$-r_{AE} = \frac{F_{A0} x_{AE}}{V_S} = k C_{AE} = k \frac{F_{A0}(1-x_{AE})}{F_{A0}(4+x_{AE})} \cdot C_{TE} \Rightarrow k = 1.727 \text{ min}^{-1}$

③ Introduction to Design for Heterogeneous Systems

- Rate eq.
 - we have more than one phase present.
 - Hence, we need to consider mass transfer between phases
 - In the general rate expression, we have both mass transfer and chemical kinetics terms.
- Contacting patterns for 2 phase systems
 - Each phase could be in plug or mixed flow
 - phases may be discontinuous (droplets or solid particles, or bubbles)
 - performance eq. depends on the contacting pattern.
- Overall rate expression
 - Q: How can we incorporate processes involving both physical transport and chemical rxn into one overall rate expression?
 - for parallel paths: $r_{overall} = \sum_{i=1}^n r_i$
 - for processes in series
 - at steady state, all these rates will proceed at the same rate.
 - $r_{overall} = r_1 = r_2 = \dots = r_n$
- Points to consider
 - one.oh
 - rates for different processes should be expressed on the same basis.
 - rates of mass transfer: $Q_{transfer} = \frac{1}{S} \frac{dN_A}{dt}$ (mol/2.s)
 - for chemical rxn: $Q_{rxn} = r_A = \frac{1}{S} \frac{dN_A}{dt}$ (mol/2.s)
 - two.oh
 - In combining rates to obtain an overall rate expression, we do not know the concentration of materials at intermediate positions.
 - we need to eliminate the intermediate concentrations and express them in terms of bulk phase concentration.

- Ex. 03 $A_{(g)} + B_{(s)} \rightarrow R_{(g)}$, $C_g \triangleq$ concentration of g A in the gas phase
 $C_s \triangleq$ ~ ~ ~ ~ ~ surface



$Q_g = \frac{1}{S} \frac{dN_A}{dt} = -D \frac{\Delta C}{\Delta x} = -D \frac{C_g - C_s}{\Delta x} = -k_g (C_g - C_s)$
 (cm²/s) Diffusivity of A in gas film → mass transfer coefficient in the gas phase (cm/s)

$Q_s = \frac{1}{S} \frac{dN_A}{dt} = -k_s C_s$ → rate constant for surface rxn

at SS: $Q_s = Q_g \Rightarrow k_g (C_g - C_s) = k_s C_s \Rightarrow C_s = \frac{k_g C_g}{k_g + k_s}$ (C_s has been eliminated)

thus: $Q_g = Q_s = \frac{1}{S} \frac{dN_A}{dt} = -\frac{k_s k_g}{k_s + k_g} C_g = -\frac{1}{\frac{1}{k_s} + \frac{1}{k_g}} C_g$

If surface rxn was of 2nd order: $k_g (C_g - C_s) = k_s C_s^2 \Rightarrow C_s = \frac{-k_g + \sqrt{k_g^2 + 4k_s k_g C_g}}{2k_s}$

- Rate Controlling step
 - one step provides the major resistance to the overall change (i.e. slowest step)
 - If chemical rxn is rate controlling: $Q_s = Q_g = k_s C_s^2$ $k_s \ll k_g$
 - ~ mass transfer ~ ~ ~ : $Q_s = Q_g = k_g C_g$ ($C_s = 0$) $k_s \gg k_g$
- Contacting Patterns
 - (I) Both phases in plug flow $\rightleftharpoons \rightleftharpoons \rightleftharpoons$
 - (II) One phase in plug flow, another in mixed flow
 - Macrofluid → complete segregation
 - Microfluid → no segregation
 - (III) Both phases in mixed flow
 - Applications
 - I, II for fluid-fluid systems (tower, mixer-settler)
 - II, III for fluid-solid ~ (fluidized beds, continuous belt)