PQI-3401 – Engenharia de Reações Químicas II

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ANALYSIS OF NON-IDEAL REACTORS

ANÁLISE DE REATORES NÃO IDEAIS

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Analysis of Nonideal Reactors

OBJECTIVES

- To study deviations from the ideal reactors (CSTR, PFR)
  - Identification/diagnosis (qualitative)
  - Models for nonideal reactors (quantitative)

- Ideal reactors
  - Limiting behavior (total mixing/no-mixing)
  - Easier to math. model
  - Fairly good approx. for many real systems

Ref.

H.S. Fogler,

Elements of Chemical Reaction Engineering,

3rd ed., Prentice-Hall, 1999.

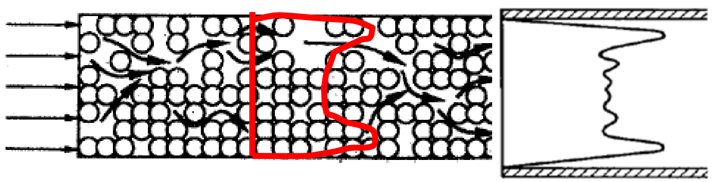
(Cap. 13 & 14)

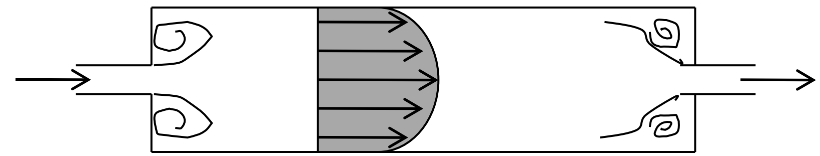
O. Levenspiel,

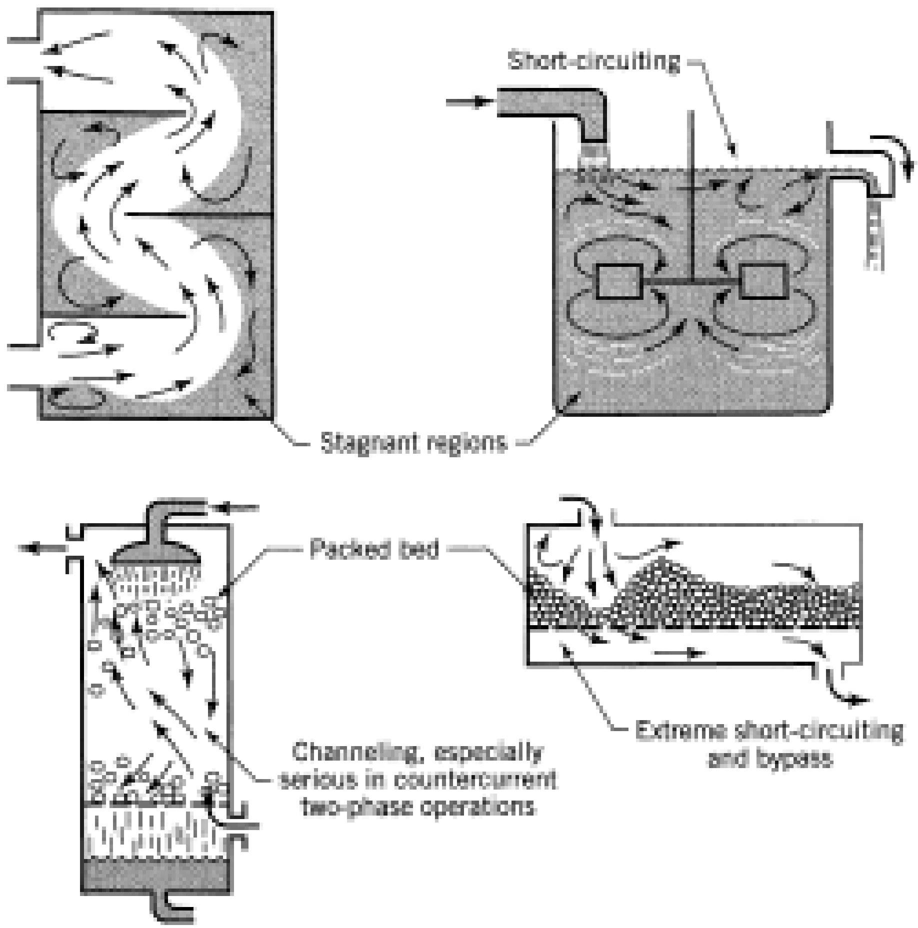
Chemical Reaction Engineering,

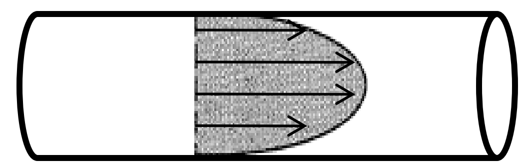
3rd ed., Wiley, 1999

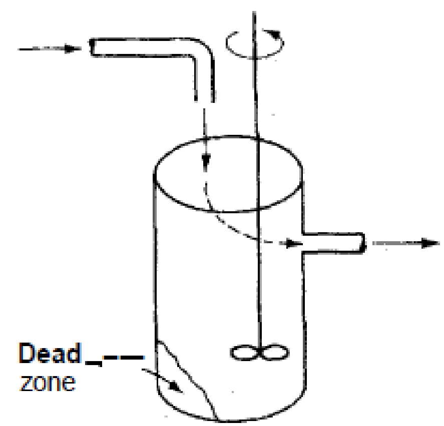
Deviations of the ideal reactor behavior





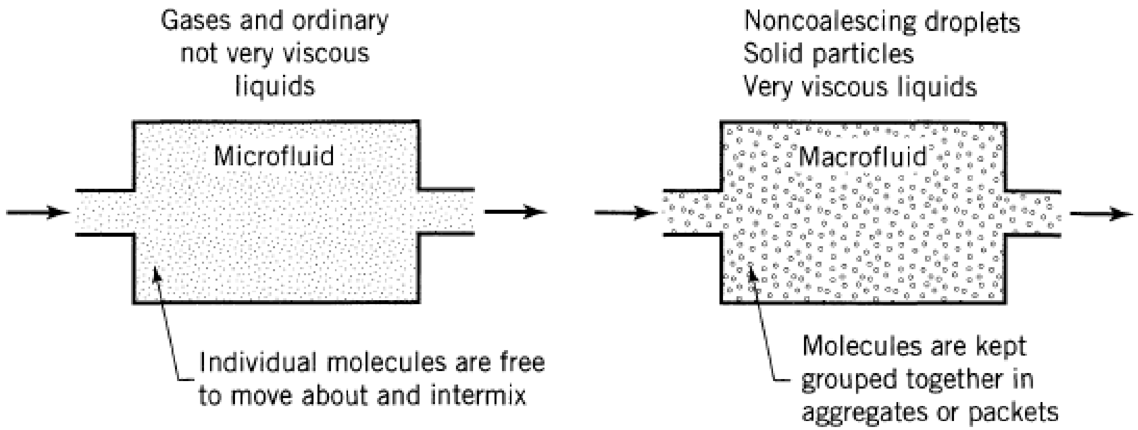




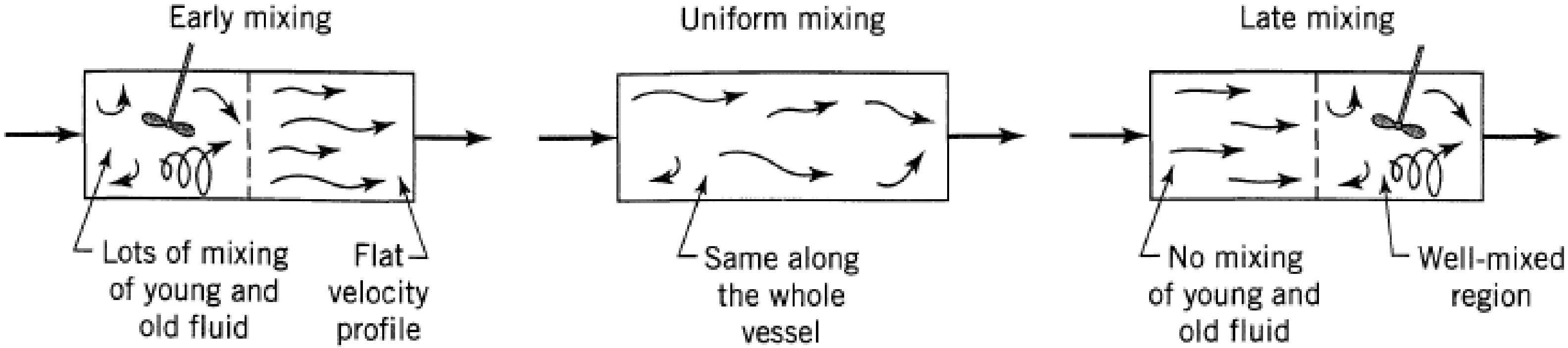


Factors affecting nonideal behavior

- the **RTD** or **residence time distribution** of material which is flowing through the vessel
- the **state of aggregation of the flowing material, its tendency to clump and** for a group of molecules to move about together

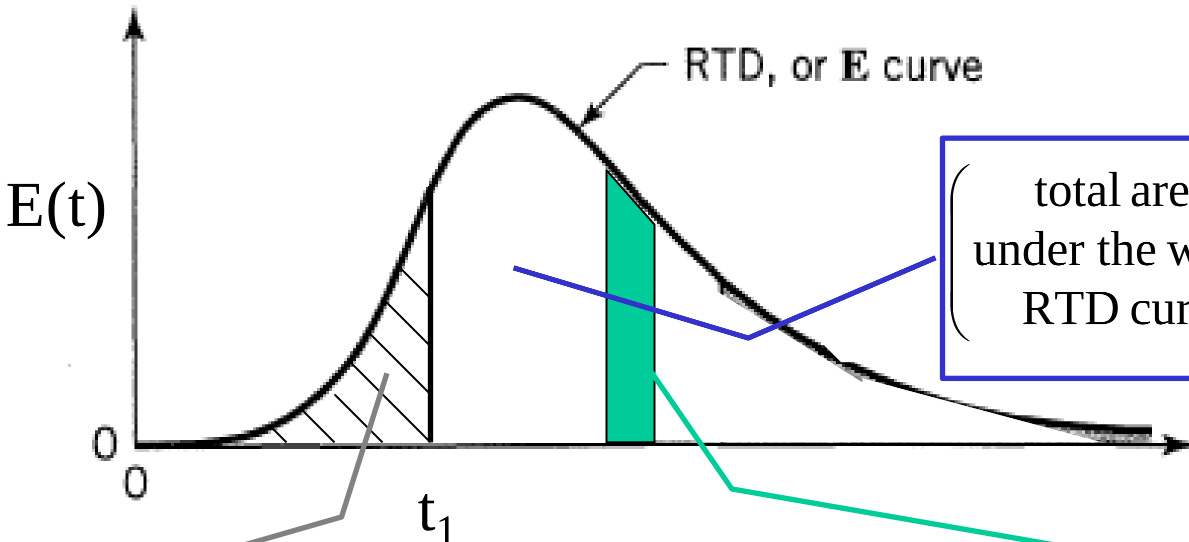


- the **earliness and lateness of mixing of material in the vessel.**



RTD

Residence Time Distribution



$$\begin{pmatrix} \text{total area} \\ \text{under the whole} \\ \text{RTD curve} \end{pmatrix} = \int_0^{\infty} E(t).dt = 1$$

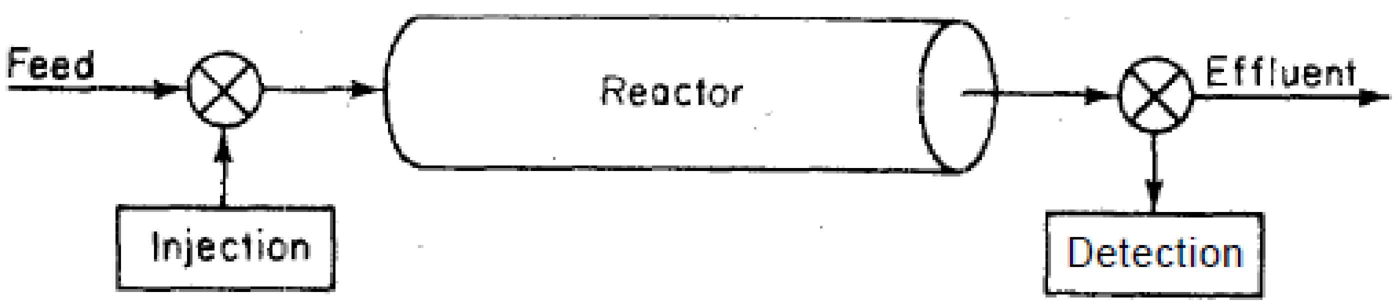
$$\begin{pmatrix} \text{fraction of the} \\ \text{exit stream with} \\ \text{RT} \le t_1 \end{pmatrix} = \int_0^{t_1} E(t).dt$$

$$\begin{pmatrix} \text{fraction of the} \\ \text{exit stream with} \\ \text{RT between} \\ t \text{ and } t + dt \end{pmatrix} = E(t).dt$$

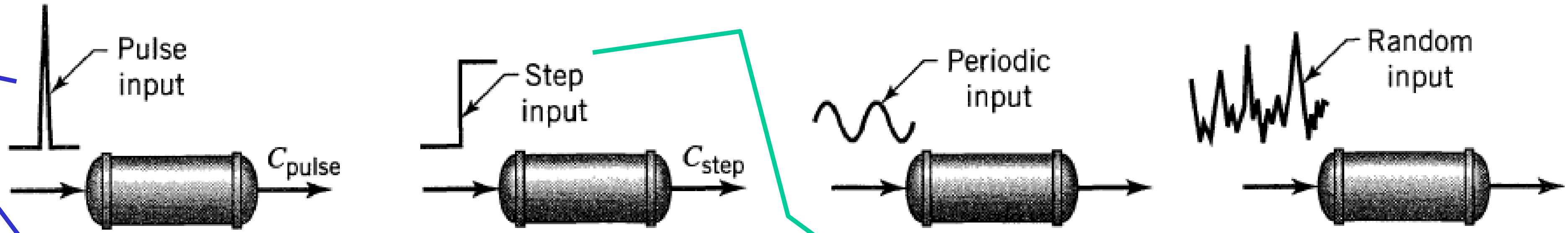
How to measure the RTD ?

Stimulus-response experiment using a **tracer**

Tracer requirements:
Physical properties similar to the reacting mixture
Completely soluble in the reacting mixture
Should not adsorb on the reactor walls and other surfaces
Easily detectable
Usually nonreactive



How to measure the RTD ?



pulse = Dirac´s delta function

$$\delta(t-t_0) = \begin{cases} 0 & \text{for } t \neq t_0 \\ \infty & \text{for } t = t_0 \end{cases}$$

$$\int_0^{\infty} \delta(t-t_0)dt = 1$$

a property of delta function :

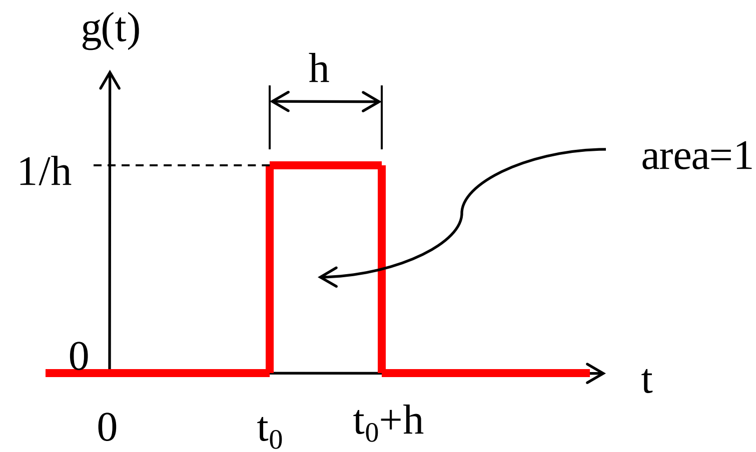
$$\int_a^b f(t)\delta(t-t_0)dt = \begin{cases} f(t_0) & \text{for } a \le t_0 \le b \\ 0 & \text{otherwise} \end{cases}$$

$$g(t) = \begin{cases} (1/h) & \text{for } t_0 \le t \le t_0 + h \\ 0 & \text{otherwise} \end{cases}$$

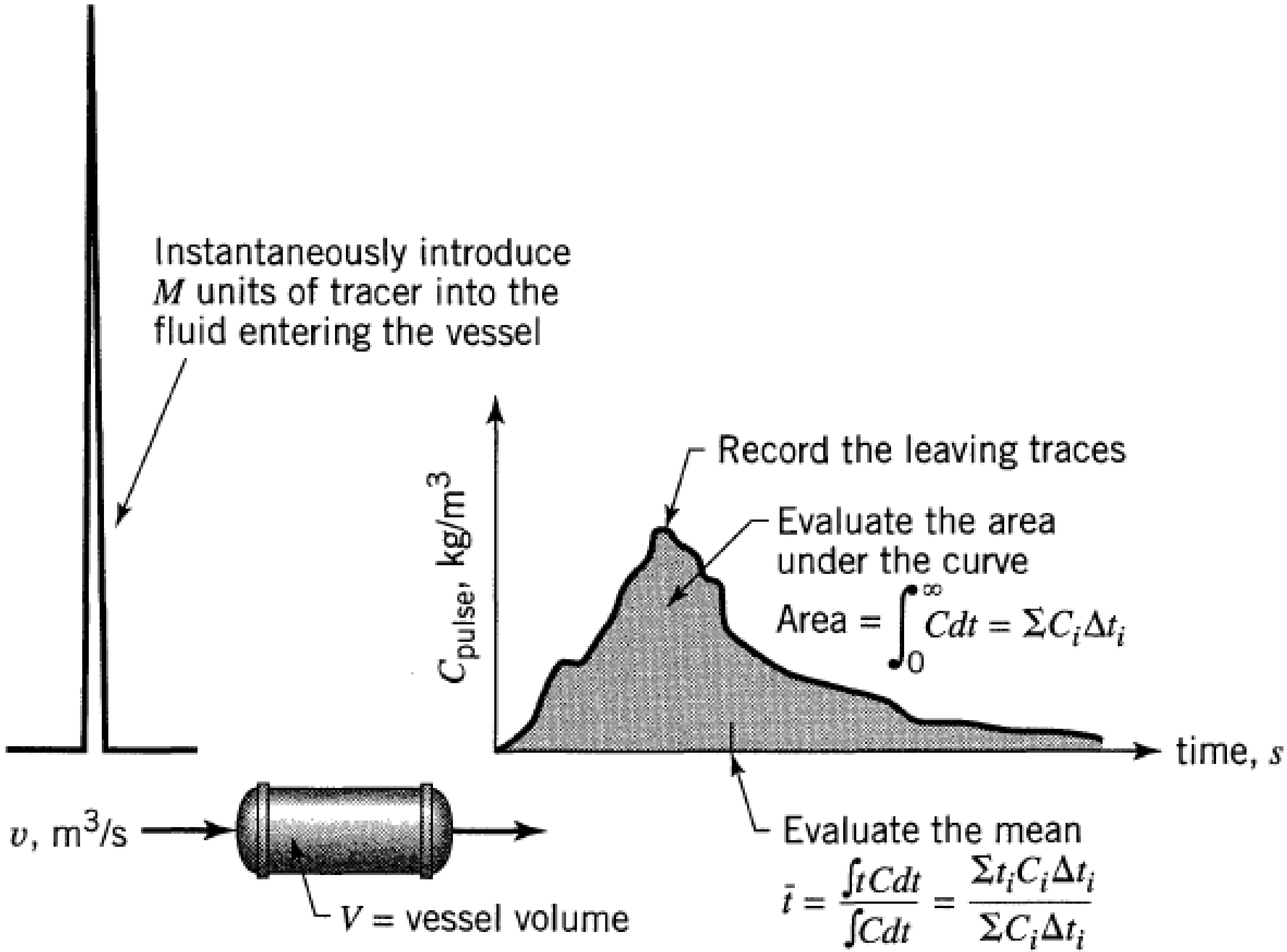
$$\delta(t-t_0) = \lim_{h \to 0} g(t)$$

step function

$$step(t-t_0) = \begin{cases} 0 & \text{for } t < t_0 \\ C_0 & \text{for } t \ge t_0 \end{cases}$$



The pulse experiment (input = pulse)



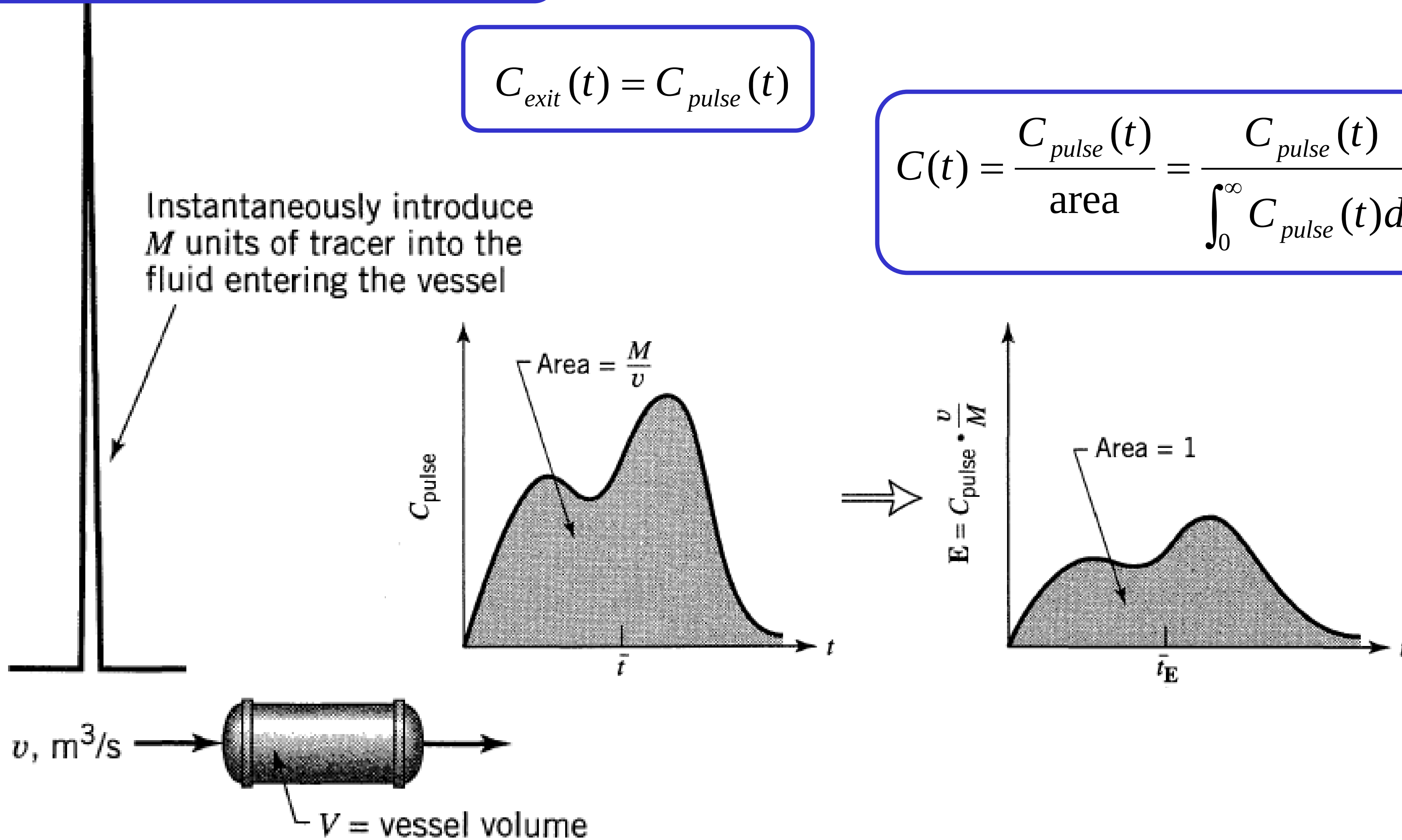
O. Levenspiel, Chemical Reaction Engineering, 3rd ed., Wiley, 1999.

The pulse experiment

$$C_{input}(t) = \delta(t-0) = \begin{cases} \infty & \text{for } t = 0 \\ 0 & \text{for } t \neq 0 \end{cases}$$

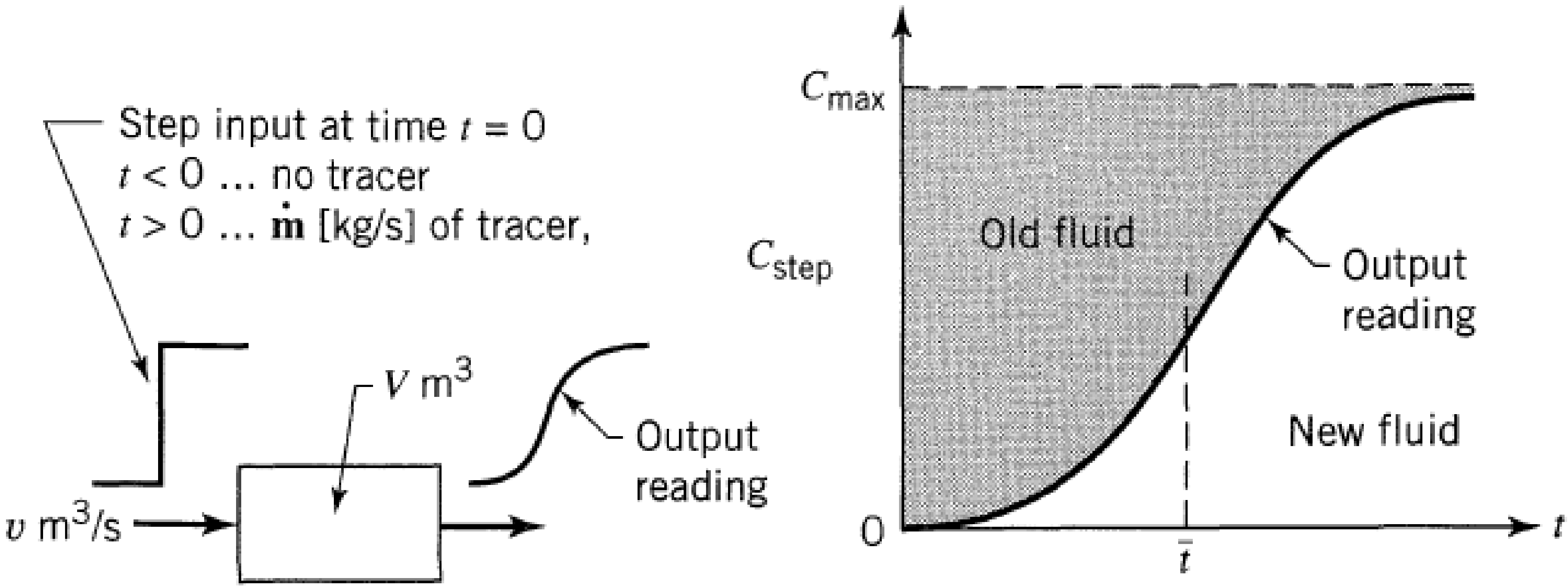
$$C_{exit}(t) = C_{pulse}(t)$$

$$C(t) = \frac{C_{pulse}(t)}{\text{area}} = \frac{C_{pulse}(t)}{\int_0^\infty C_{pulse}(t)dt}$$



O. Levenspiel, Chemical Reaction Engineering, 3rd ed., Wiley, 1999.

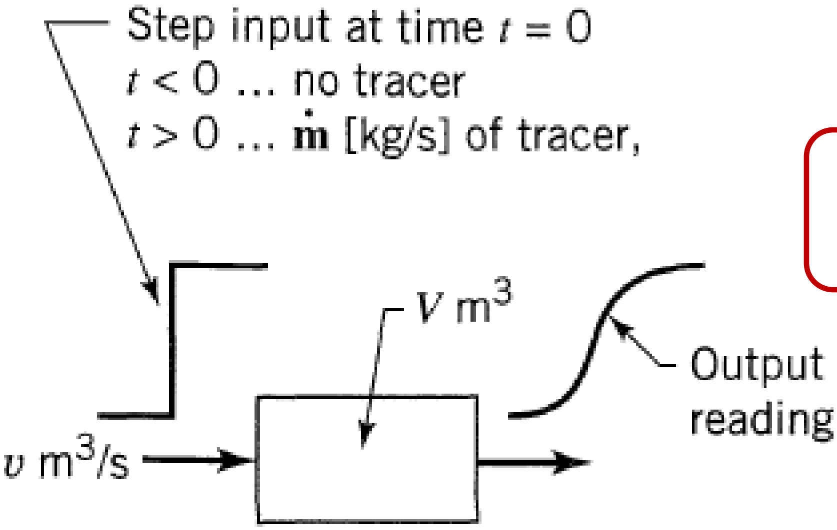
The step experiment (input = step)



O. Levenspiel, Chemical Reaction Engineering, 3rd ed., Wiley, 1999.

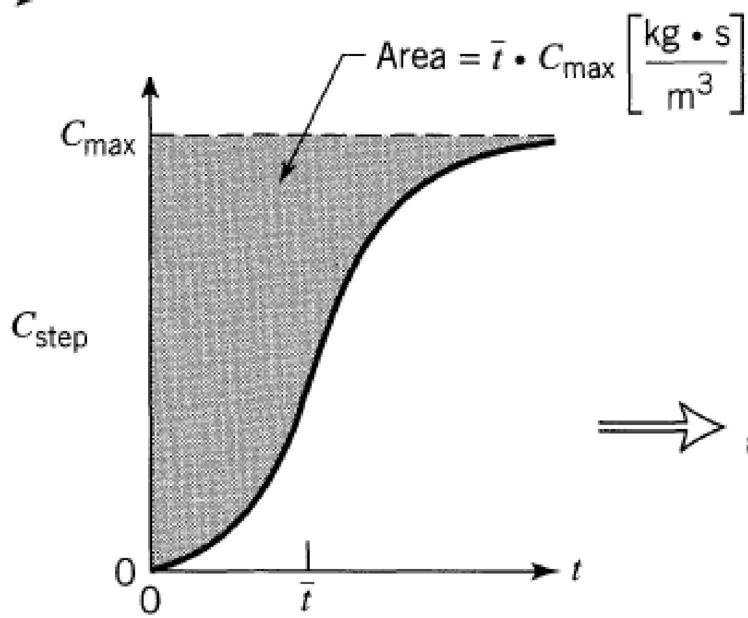
The step experiment

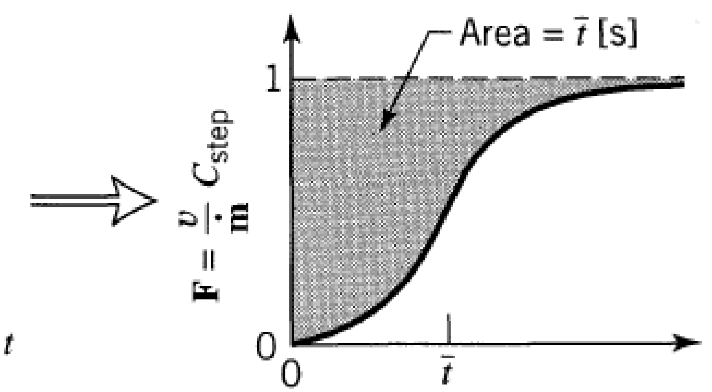
$$C_{input}(t) = \begin{cases} 0 & \text{for } t < t_0 \\ C_{\max} & \text{for } t \geq t_0 \end{cases}$$



$$C_{exit}(t) = C_{step}(t)$$

$$F(t) = \frac{C_{step}(t)}{C_{\max}}$$





O. Levenspiel, Chemical Reaction Engineering, 3rd ed., Wiley, 1999.

Relationship between
C(t) = response to pulse
F(t) = response to step
and
E(t) = RTD

PULSE EXPERIMENT

all tracer entered at t = 0
then
amount of tracer exiting the reactor
at time t has RT = t

$$\begin{pmatrix} \text{fraction of tracer} \\ \text{exiting the reactor} \\ \text{at time } t \end{pmatrix} = \begin{pmatrix} \text{fraction of} \\ \text{tracer that} \\ \text{has RT} = t \end{pmatrix}$$

$$C(t) = E(t)$$

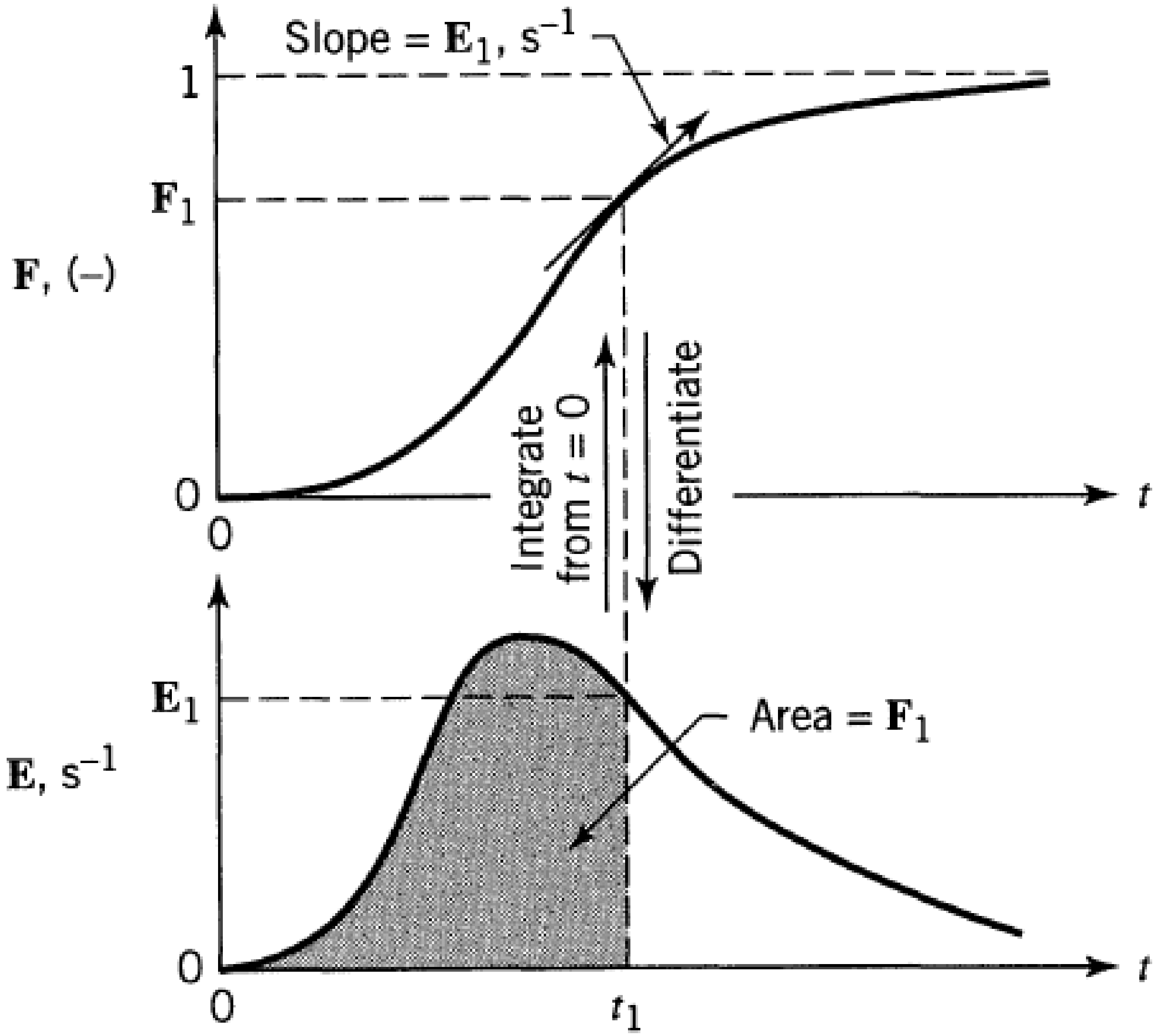
STEP EXPERIMENT

tracer exiting the reactor at time t_1
entered in the reactor
at a time between 0 and t_1

$$\begin{pmatrix} \text{fraction of tracer} \\ \text{exiting the reactor} \\ \text{at time} = t_1 \end{pmatrix} = \begin{pmatrix} \text{fraction of} \\ \text{tracer} \\ \text{with RT} \leq t_1 \end{pmatrix}$$

$$F(t_1) = \int_0^{t_1} E(t).dt$$

$$E(t) = \frac{dF(t)}{dt}$$



$$F(t_1) = \int_0^{t_1} E(t).dt$$

$$E(t)\Big|_{t_1} = \frac{dF(t)}{dt}\bigg|_{t_1}$$

O. Levenspiel, Chemical Reaction Engineering, 3rd ed., Wiley, 1999.

Characteristics of the RTD curve

$$\begin{pmatrix}\text{mean}\\ \text{residence}\\ \text{time}\end{pmatrix} = t_m = \frac{\int_0^\infty t.E(t).dt}{\int_0^\infty E(t).dt} = \int_0^\infty t.E(t).dt$$

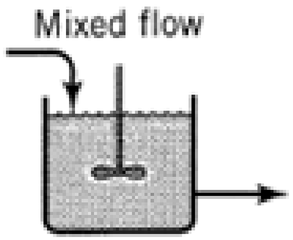
$$\text{variance} = \sigma^2 = \int_0^\infty (t - t_m)^2.E(t).dt$$

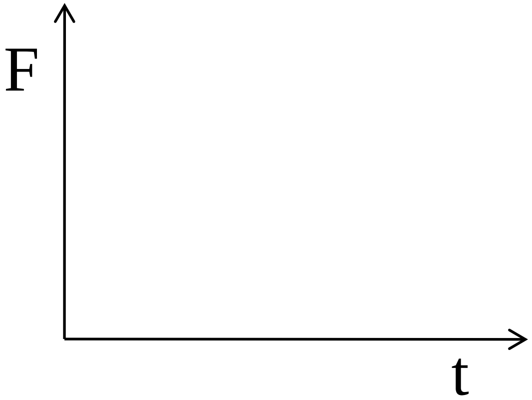
$$\text{skewness} = s^3 = \frac{1}{\sigma^{3/2}}\int_0^\infty (t - t_m)^3.E(t).dt$$

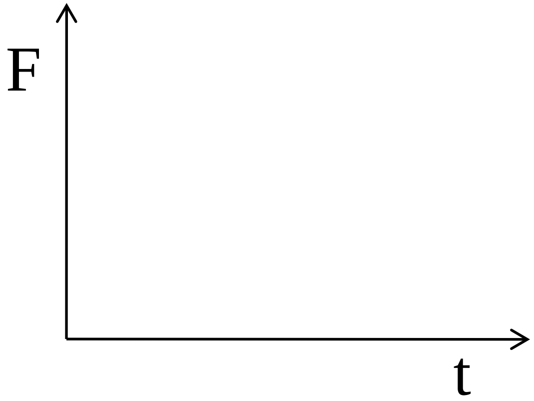
for a fluid of constant density (constant volumetric flow rate)

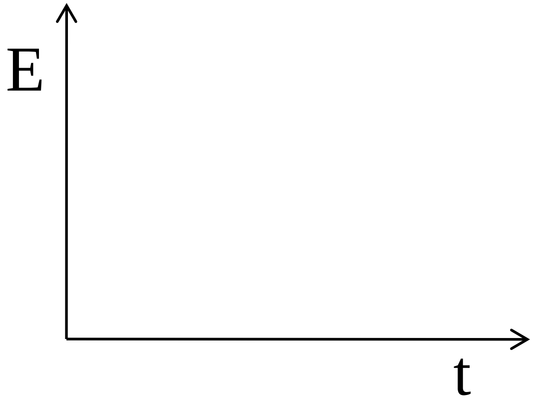
$$\begin{pmatrix}\text{mean}\\ \text{residence}\\ \text{time}\end{pmatrix} = t_m = \tau = \frac{V}{v_o}$$

RTD of the ideal reactors

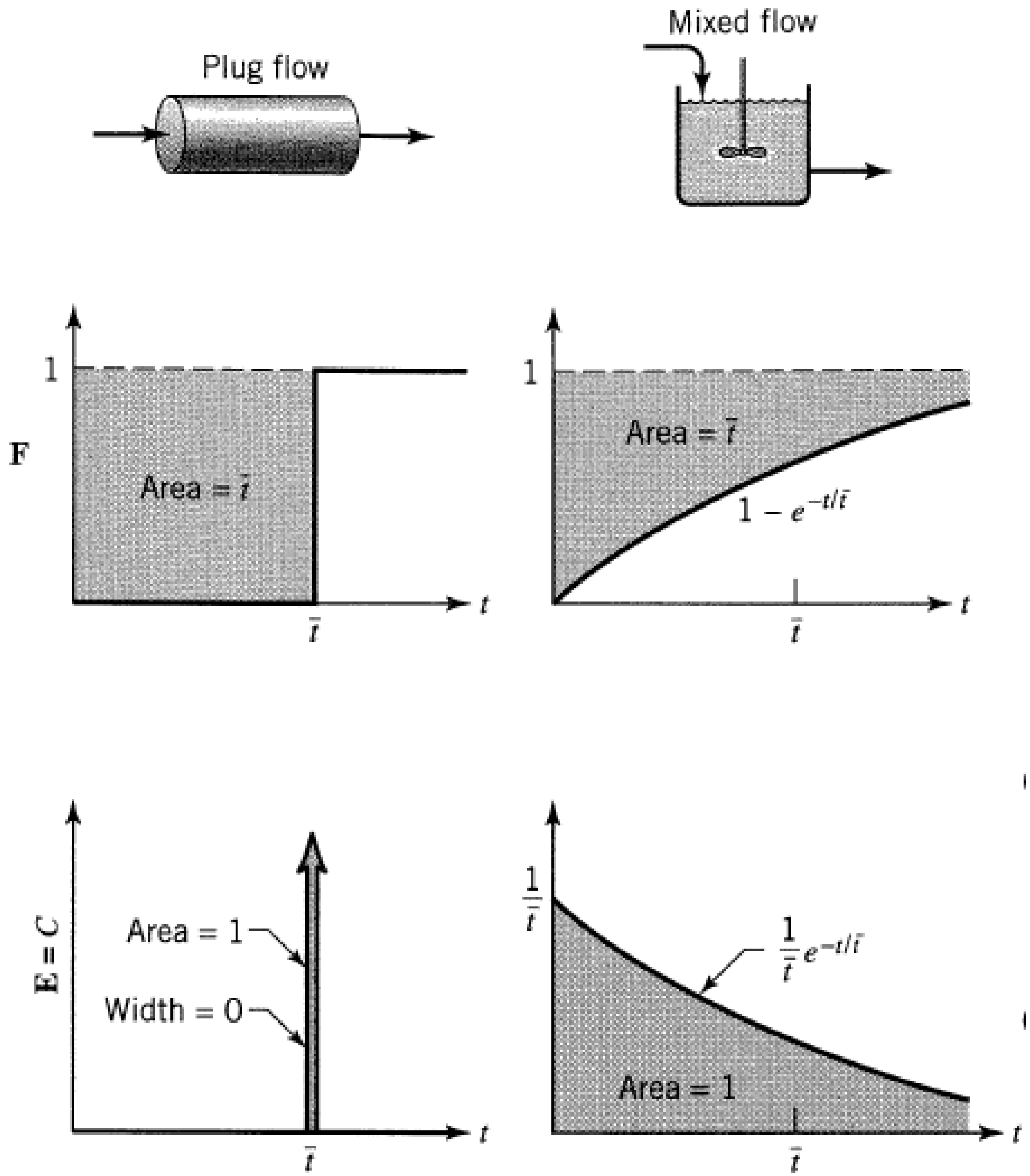








RTD of the ideal reactors

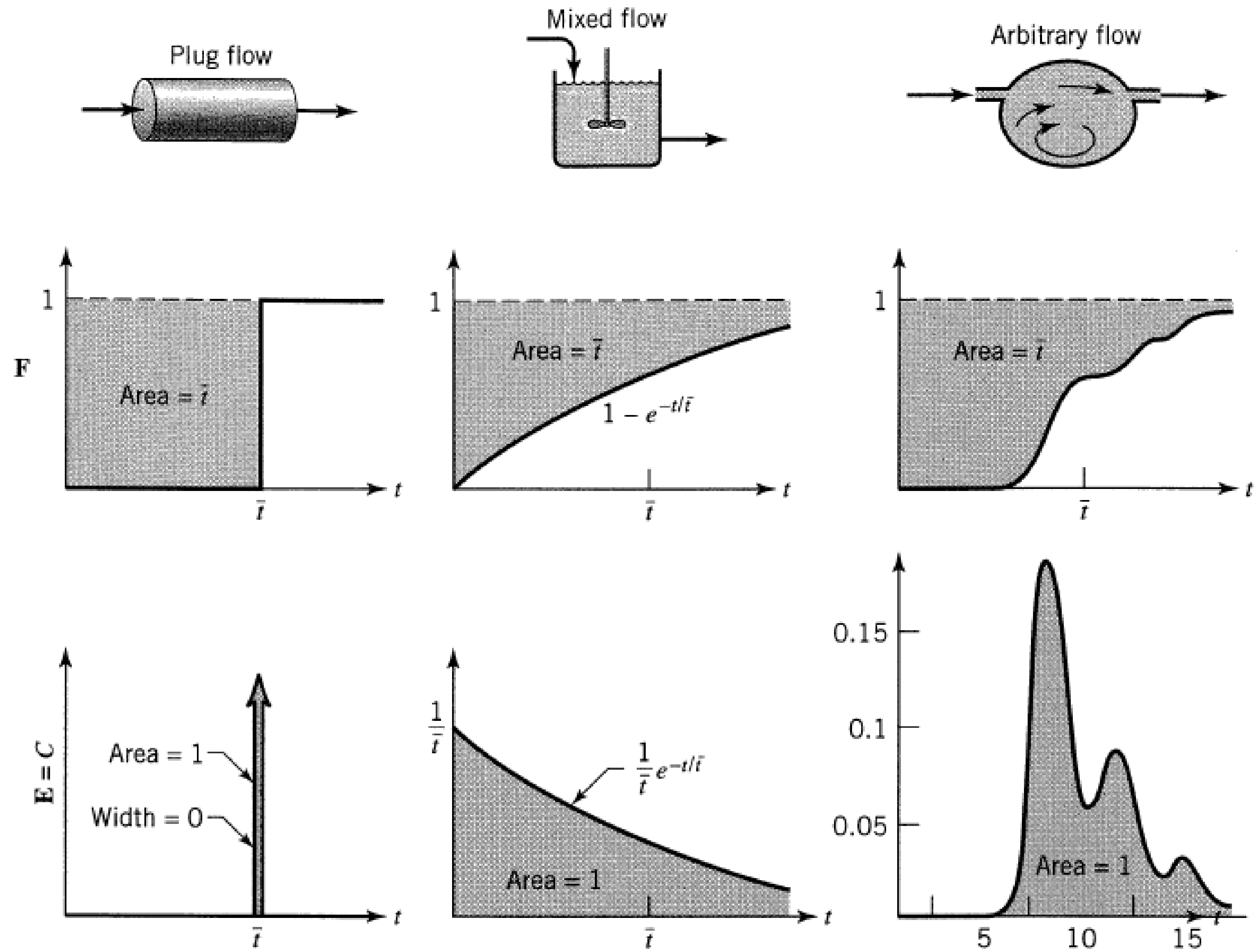


Assignment #1

Derive the RTD curve (E(t)) for the ideal reactors (PFR and CSTR)

Use “though experiment” and
mass balances

Using RTD to detect flow nonidealities



Using RTD to detect flow nonidealities

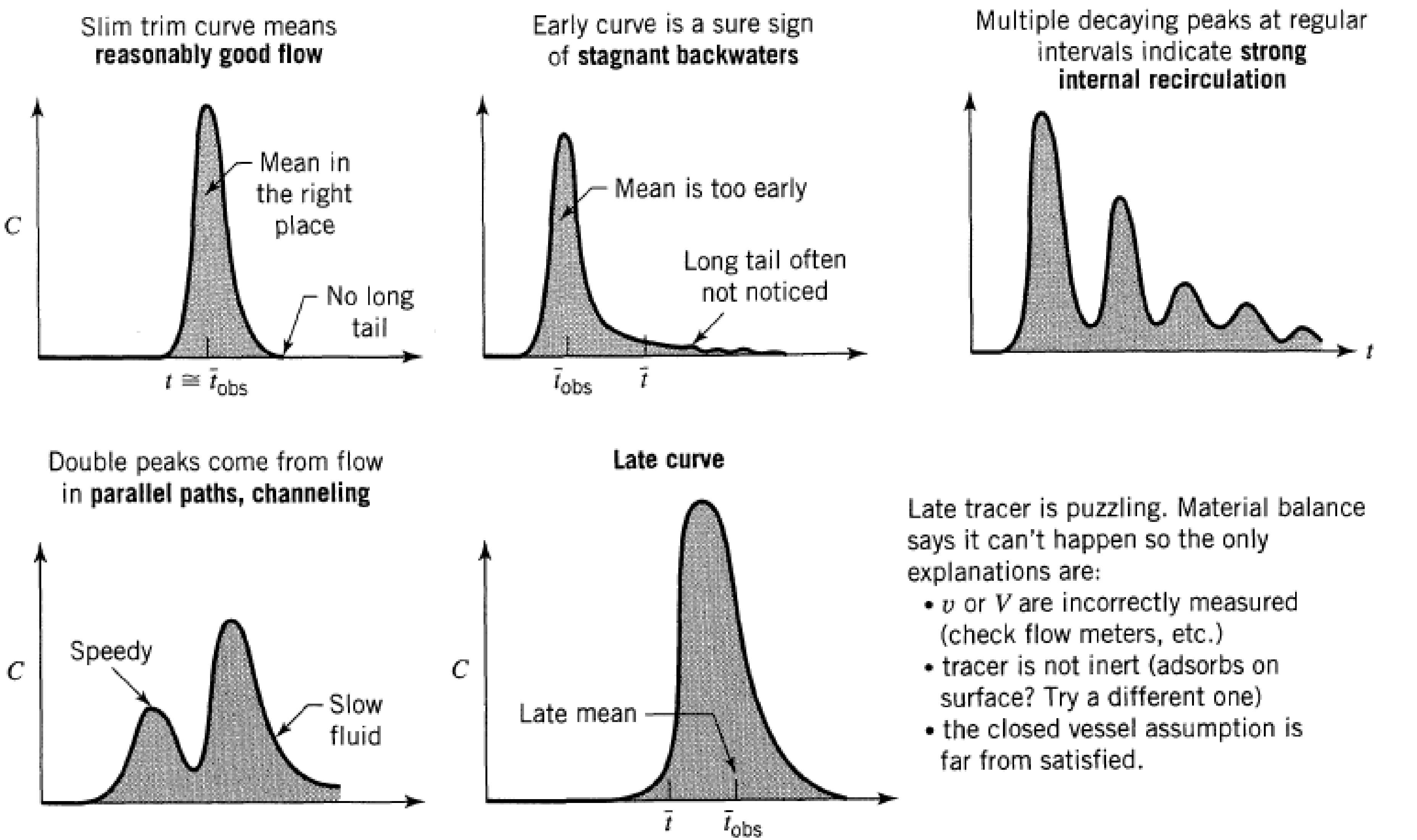


Figure 12.3 Misbehaving plug flow reactors.

O. Levenspiel, Chemical Reaction Engineering, 3rd ed., Wiley, 1999.

Using RTD to detect flow nonidealities

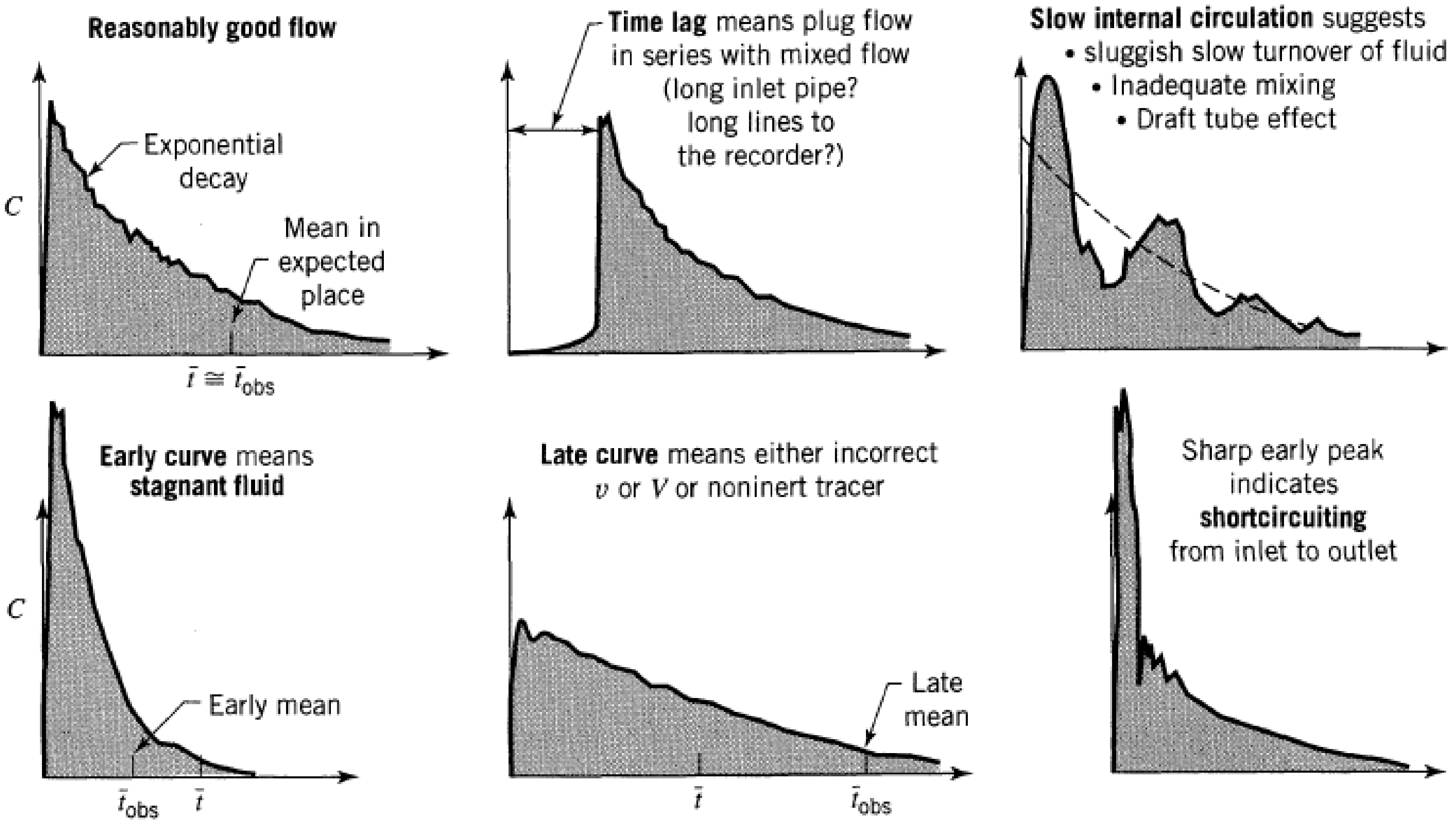
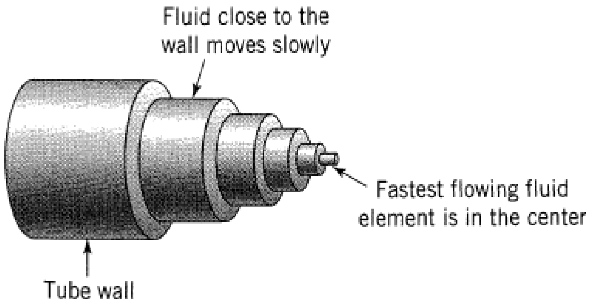


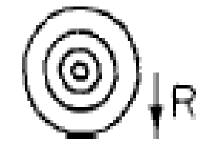
Figure 12.4 Misbehaving mixed flow reactors.

O. Levenspiel, Chemical Reaction Engineering, 3rd ed., Wiley, 1999.

MODELS FOR NONIDEAL REACTORS

Laminar flow reactor





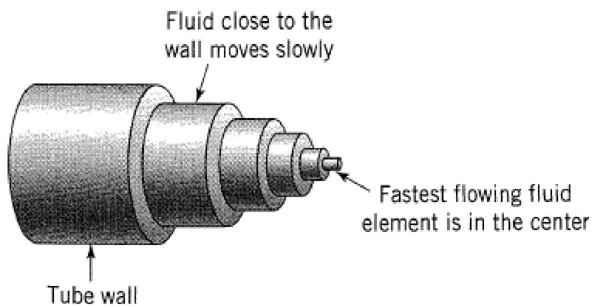
$$u(r) = u_{\max}\left[1-\left(\frac{r}{R}\right)^2\right] = 2u_{medio}\left[1-\left(\frac{r}{R}\right)^2\right] = 2\frac{v_0}{\pi R^2}\left[1-\left(\frac{r}{R}\right)^2\right]$$

$$t(r) = \frac{L}{u(r)} = \frac{L\pi R^2}{2u_{medio}\pi R^2\left[1-(r/R)^2\right]} = \frac{V}{2v_0\left[1-(r/R)^2\right]} = \frac{\tau}{2\left[1-(r/R)^2\right]}$$

$$dt = \frac{\tau}{2R^2}\frac{2.r.dr}{\left[1-(r/R)^2\right]^2}\frac{(\tau/2)^2}{(\tau/2)^2} = \frac{4}{\tau R^2}\left[\frac{\tau/2}{1-(r/R)^2}\right]^2 r.dr = \frac{4t^2}{\tau R^2}r.dr$$

$$\begin{pmatrix}\text{fraction of fluid}\\ \text{flowing between}\\ \text{r and r + dr}\end{pmatrix} = \frac{dv}{v_o} = \frac{u(r).2\pi.r.dr}{v_o} = \frac{L}{t}\frac{2\pi}{v_o}\frac{\tau R^2}{4t^2}dt = \frac{\tau^2}{2t^3}dt$$

Laminar flow reactor



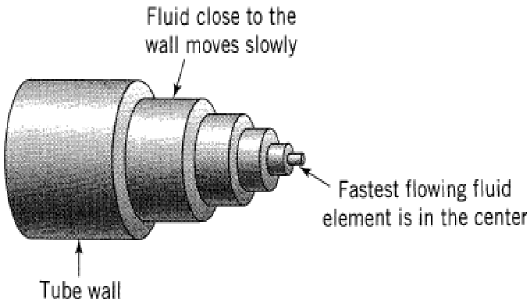
$$\begin{pmatrix} \text{fraction of fluid} \\ \text{flowing between} \\ \text{r and r + dr} \end{pmatrix} = \frac{\tau^2}{2t^3}dt = \begin{pmatrix} \text{fraction of fluid} \\ \text{flowing with RT} \\ \text{between} \\ \text{t and t + dt} \end{pmatrix} = E(t).dt$$

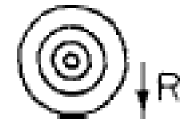
minimum residence time (at the tube center) is

$$t_{\min} = \frac{L}{u_{\max}} = \frac{L}{2.u_{medio}}\left(\frac{\pi R^2}{\pi R^2}\right) = \frac{V}{2v_0} = \frac{\tau}{2}$$

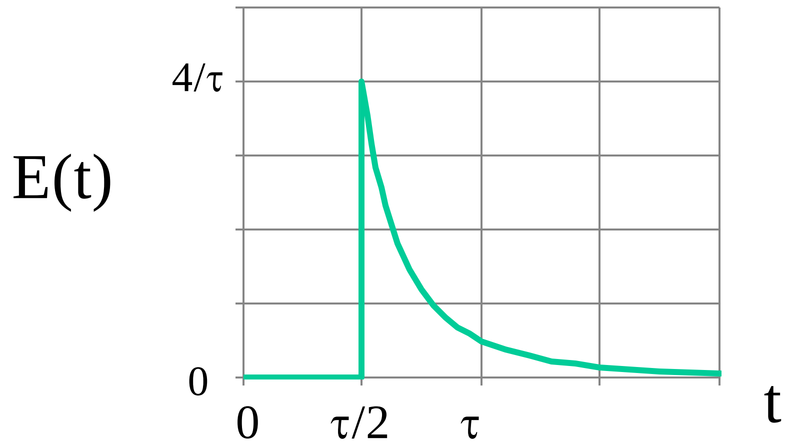
$$E(t) = \begin{cases} 0 & \text{for } t < \dfrac{\tau}{2} \\ \dfrac{\tau^2}{2t^3} & \text{for } t < \dfrac{\tau}{2} \end{cases} \qquad F(t) = \int_0^t E(t)dt = \begin{cases} 0 & \text{for } t < \dfrac{\tau}{2} \\ 1 - \dfrac{\tau^2}{4t^2} & \text{for } t < \dfrac{\tau}{2} \end{cases}$$

Laminar flow reactor

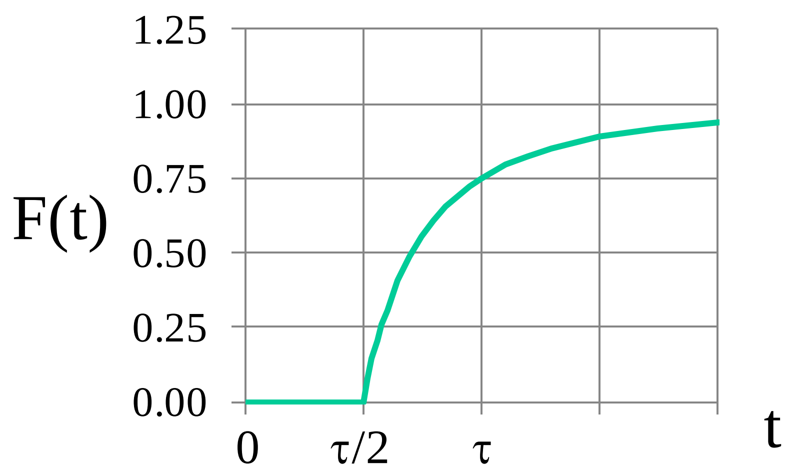




$$E(t) = \begin{cases} 0 & \text{for } t < \dfrac{\tau}{2} \\ \dfrac{\tau^2}{2t^3} & \text{for } t < \dfrac{\tau}{2} \end{cases}$$

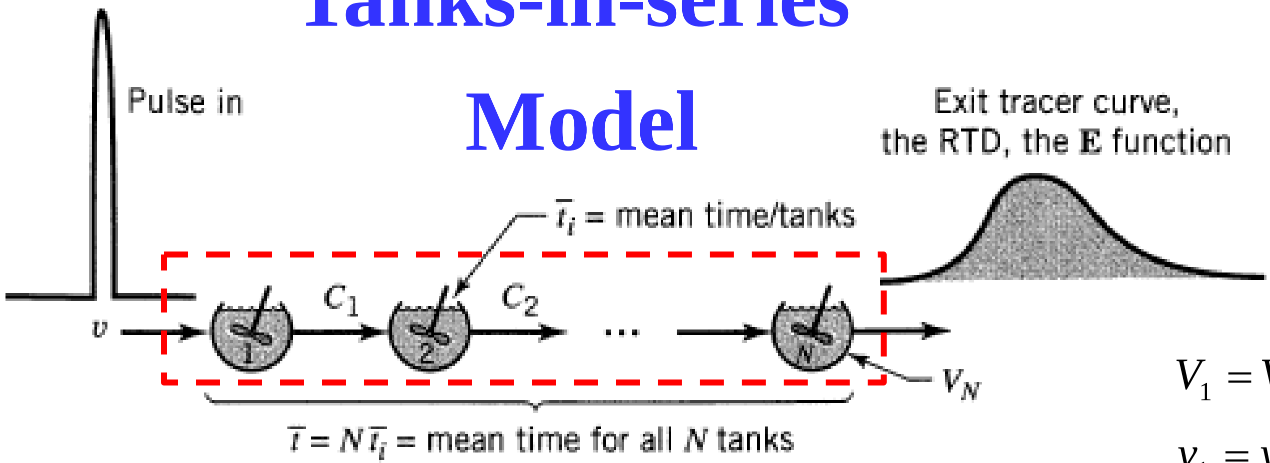


$$F(t) = \int_0^t E(t)dt = \begin{cases} 0 & \text{for } t < \dfrac{\tau}{2} \\ 1 - \dfrac{\tau^2}{4t^2} & \text{for } t < \dfrac{\tau}{2} \end{cases}$$



Tanks-in-series Model

Tanks-in-series Model



$$V_1 = V_2 = V_3 = \ldots = V_N = \frac{V}{N} = V_i$$

$$v_1 = v_2 = v_3 = \ldots = v_N = v_o$$

$$\tau_1 = \tau_2 = \tau_3 = \ldots = \tau_N = \frac{\tau}{N} = \tau_i$$

$$V_1 \frac{dC_1}{dt} = v_o\left(C_0 - C_1\right) \qquad C_1(t=0) = N_o / V_1 \qquad C_1 = \frac{N_o}{V_i}\exp\left(-\frac{t}{\tau_i}\right)$$

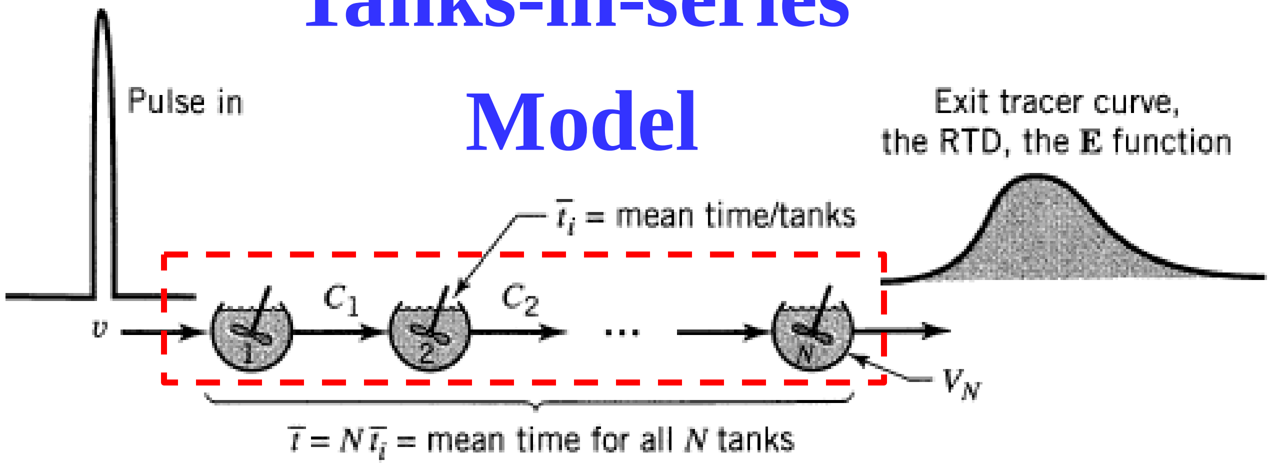
$$V_2 \frac{dC_2}{dt} = v_o\left(C_1 - C_2\right) \qquad C_2(t=0) = 0 \qquad C_2 = \frac{N_o}{V_i}\left(\frac{t}{\tau_i}\right)\exp\left(-\frac{t}{\tau_i}\right)$$

$$V_3 \frac{dC_3}{dt} = v_o\left(C_2 - C_3\right) \qquad C_3(t=0) = 0 \qquad C_3 = \frac{N_o}{V_i}\frac{1}{2}\left(\frac{t}{\tau_i}\right)^2\exp\left(-\frac{t}{\tau_i}\right)$$

$$\vdots \qquad\qquad \vdots$$

$$V_N \frac{dC_N}{dt} = v_o\left(C_{N-1} - C_N\right) \qquad C_N(t=0) = 0 \qquad C_N = \frac{N_o}{V_i}\frac{1}{(N-1)!}\left(\frac{t}{\tau_i}\right)^{N-1}\exp\left(-\frac{t}{\tau_i}\right)$$

Tanks-in-series Model



$$V_1 = V_2 = V_3 = \ldots = V_N = \frac{V}{N} = V_i$$

$$v_1 = v_2 = v_3 = \ldots = v_N = v_o$$

$$\tau_1 = \tau_2 = \tau_3 = \ldots = \tau_N = \frac{\tau}{N} = \tau_i$$

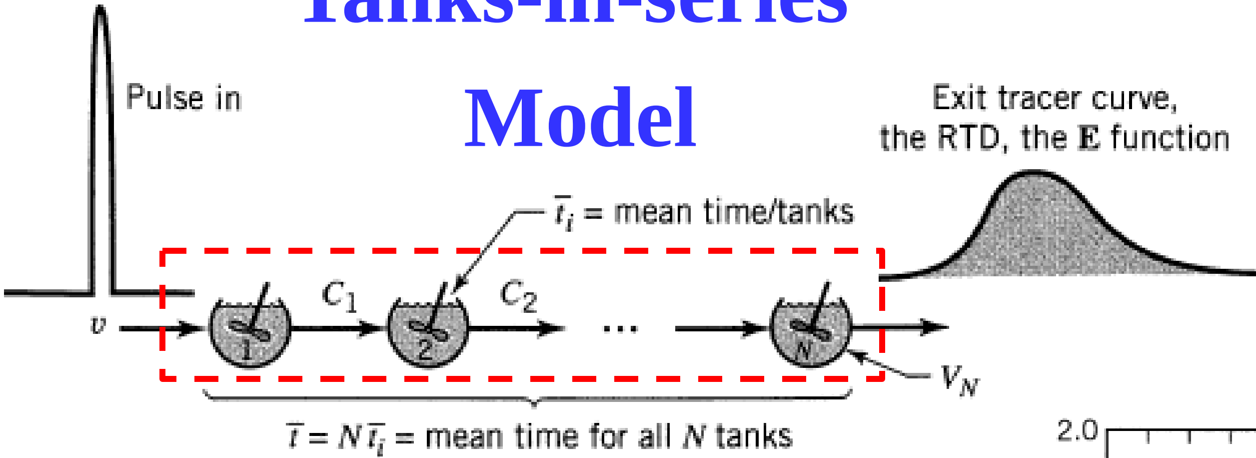
$$C_N = \frac{N_o}{V_i}\frac{1}{(N-1)!}\left(\frac{t}{\tau_i}\right)^{N-1}\exp\left(-\frac{t}{\tau_i}\right)$$

$$E(t) = \frac{C_N(t)}{\int_0^\infty C_N(t)dt} = \frac{C_N(t)}{N_o/v_o} = \frac{v_o C_N(t)}{C_o V} \Rightarrow \boxed{E(t) = \frac{t^{N-1}}{(N-1)!(\tau/N)^N}\exp\left(-\frac{t}{\tau/N}\right)}$$

$$\theta = \frac{t}{\tau} \qquad E_\theta = \tau.E(t) \qquad E_\theta = \frac{N(N\theta)^{N-1}}{(N-1)!}\exp(-N\theta)$$

$$\frac{\sigma^2}{\tau^2} = \frac{1}{N},\quad \text{N} = \text{parameter that quantifies nonideality}\begin{cases} N = 1 & \text{CSTR} \\ 1 < N < \infty & \text{real reactor} \\ N \to \infty & \text{PFR} \end{cases}$$

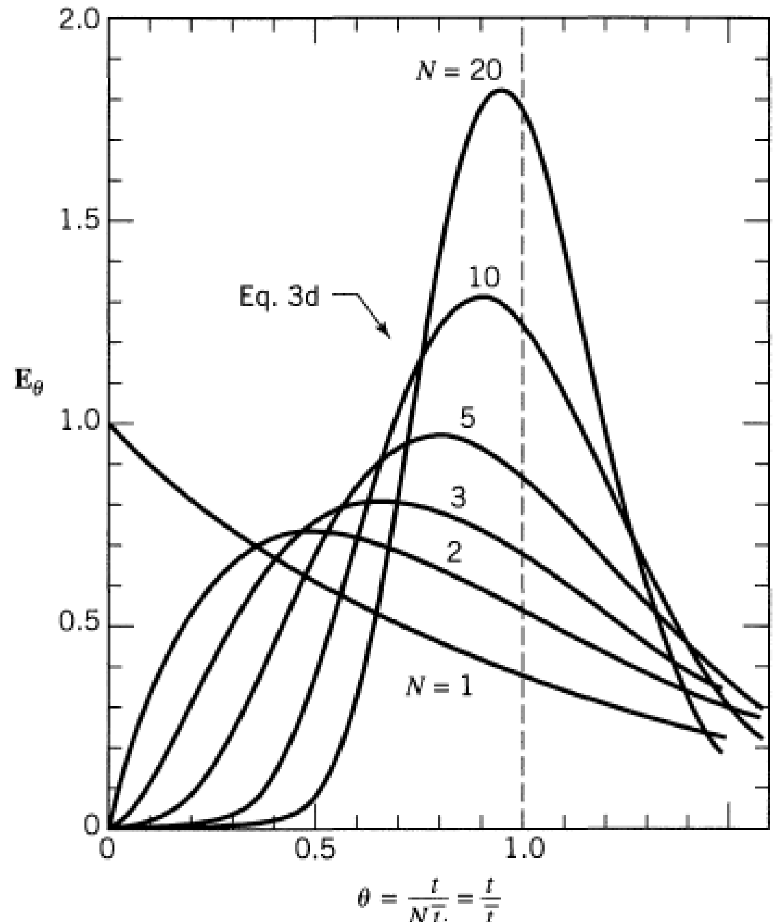
Tanks-in-series Model



$$V_1 = V_2 = V_3 = \ldots = V_N = \frac{V}{N} = V_i$$

$$v_1 = v_2 = v_3 = \ldots = v_N = v_o$$

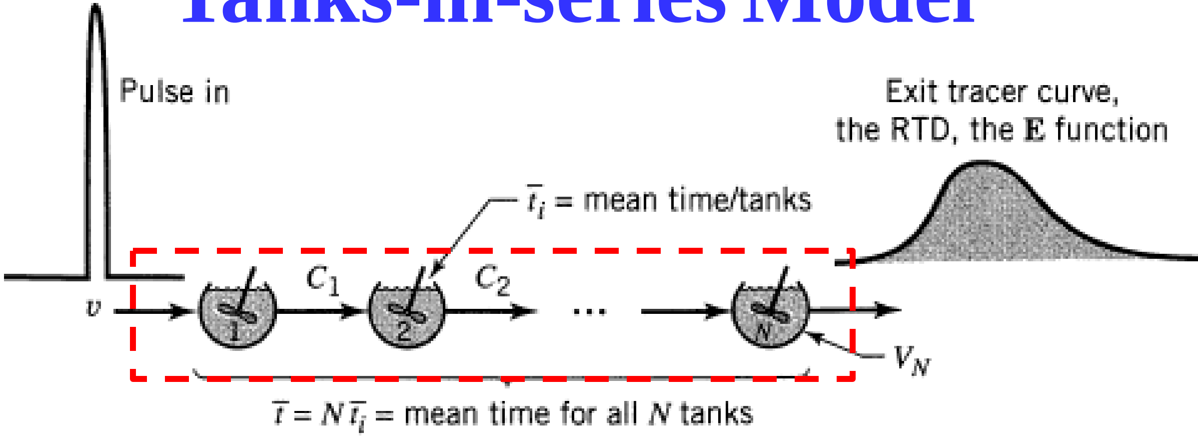
$$\tau_1 = \tau_2 = \tau_3 = \ldots = \tau_N = \frac{\tau}{N} = \tau_i$$



$$E(t) = \frac{t^{N-1}}{(N-1)!(\tau/N)^N}\exp\left(-\frac{t}{\tau/N}\right)$$

$$E_\theta = \frac{N(N\theta)^{N-1}}{(N-1)!}\exp(-N\theta)$$

Tanks-in-series Model



$$E(t) = \frac{t^{N-1}}{(N-1)!(\tau/N)^N}\exp\left(-\frac{t}{\tau/N}\right)$$

$$E_\theta = \frac{N(N\theta)^{N-1}}{(N-1)!}\exp(-N\theta)$$

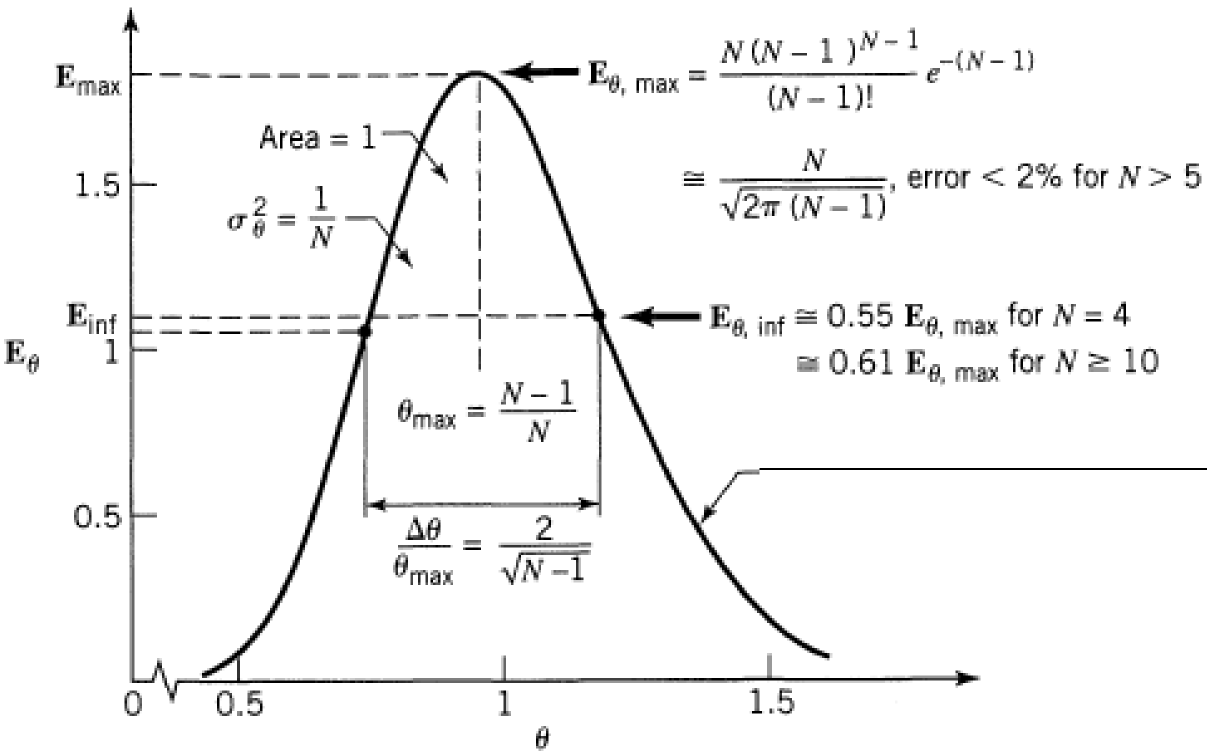
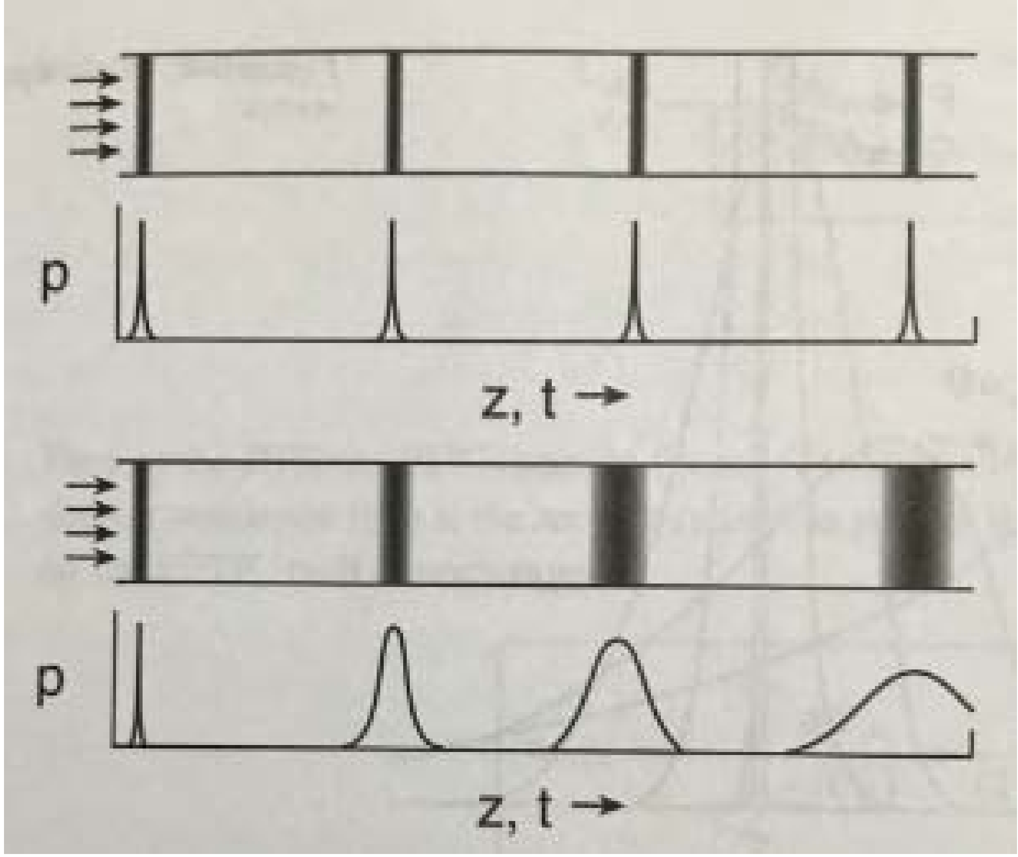


Figure 14.3 Properties of the RTD curve for the tanks-in-series model.

O. Levenspiel,
Chemical Reaction
Engineering,
3rd ed.,
Wiley, 1999.

Axial dispersion Model



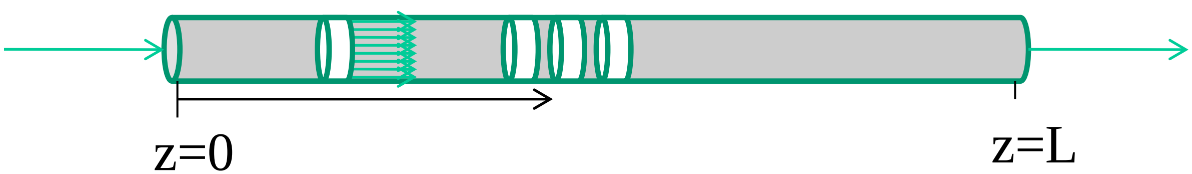
PFR

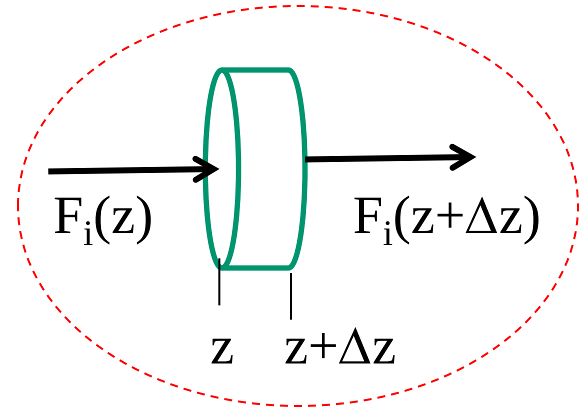
Axial dispersion model

Axially-Dispersed Tubular Reactor (ADPFR)

- No changes in radial and angular direction, only axial variations (z)
- Flow in direction z (v_r=0 , v_θ = 0) and some mixing in axial direction (similar to diffusion)
- Plug flow (piston-like velocity profile)
  (v_z = constant, no changes with r)
- Steady state

$\Delta V = A_c . \Delta z$





$$\frac{dF_i}{dV} = \frac{dF_i}{A_c.dz} = r_i \Rightarrow \frac{dF_i}{dz} = A_c r_i$$

- Mixing flow in the axial direction
- Account for different phenomena
- D_A = effective axial dispersion coefficient

$$F_i = \underbrace{A_c u C_i}_{\text{convective flow}} + \underbrace{A_c J_i}_{\text{axial mixing flow}} \qquad J_i = -D_A \frac{dC_i}{dz}$$

$$\frac{dF_i}{dz} = A_c \frac{d}{dz}\left(v_z C_i - D_A \frac{dC_i}{dz} \right) = A_c r_i$$

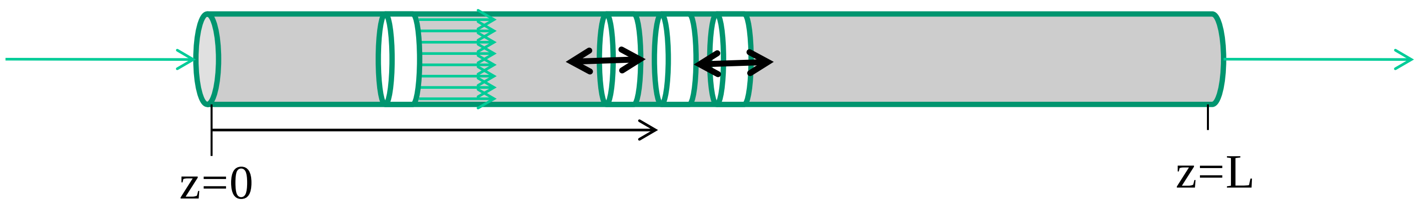
$$\boxed{v_z \frac{dC_i}{dz} = D_A \frac{d^2 C_i}{dz^2} + r_i}$$

Reator tubular com dispersão axial

- Mesmas hipóteses do reator PFR, exceto que agora se considera a ocorrência de mistura na direção z (dispersão axial). O fluxo de mistura axial é modelado como uma difusão:

$$\vec{j}_A = -D_A \vec{\nabla} C_A$$

$$\frac{\partial C_A}{\partial t} + \vec{\nabla} \bullet (\vec{v} C_A) = \vec{\nabla} \bullet \left(D_a \vec{\nabla} C_A \right) + r_A$$



$$\frac{\partial C_A}{\partial t} + \cancel{v_r \frac{\partial C_A}{\partial r}} + \cancel{\frac{v_\theta}{r} \frac{\partial C_A}{\partial \theta}} + v_z \frac{\partial C_A}{\partial z} = D_A \left[\cancel{\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial C_A}{\partial r} \right)} + \cancel{\frac{1}{r^2} \frac{\partial^2 C_A}{\partial \theta^2}} + \frac{\partial^2 C_A}{\partial z^2} \right] + R_{V_A}$$

$$\boxed{\frac{\partial C_A}{\partial t} = -v_z \frac{\partial C_A}{\partial z} + D_A \frac{\partial^2 C_A}{\partial z^2} + r_i}$$

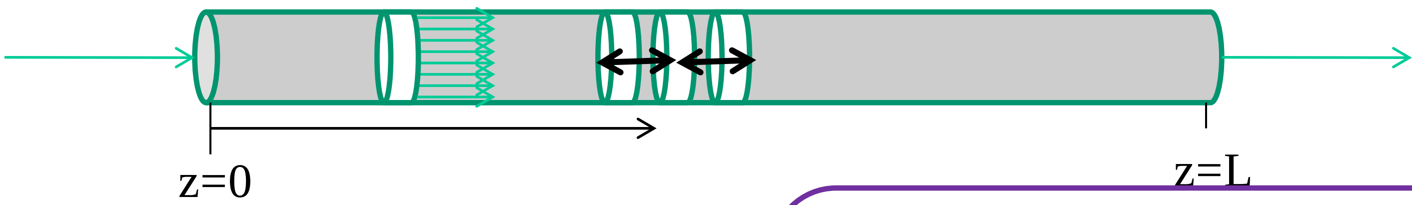
Esta equação diferencial tem, agora, derivadas de 2ª ordem, então requer 2 condições de contorno em z

Condições de contorno de Danckwerts

$$z = 0 \qquad c_A\Big|_{z=0} = c_{A,e} + \frac{D_a}{v_z} \frac{dc_A}{dz}\Big|_{z=0}$$

$$z = L \qquad \frac{dc_A}{dz}\Big|_{z=L} = 0$$

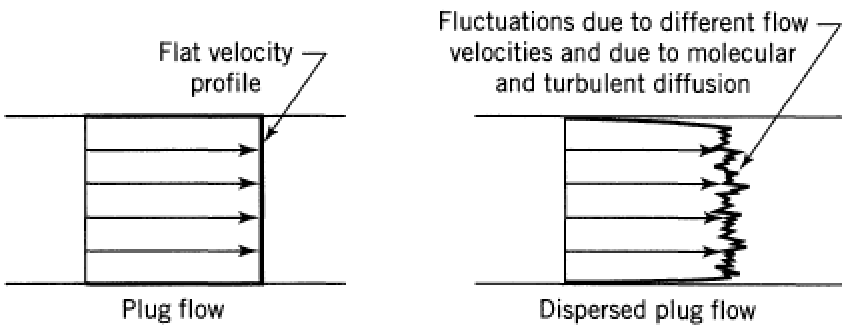
Axial Dispersion Model



$$\frac{\partial C_A}{\partial t} = -v_z \frac{\partial C_A}{\partial z} + D_A \frac{\partial^2 C_A}{\partial z^2} + r_i$$

$$z = 0 \qquad c_A\Big|_{z=0} = c_{A,e} + \frac{D_a}{v_z} \frac{dc_A}{dz}\Big|_{z=0}$$

$$z = L \qquad \frac{dc_A}{dz}\Big|_{z=L} = 0$$



$$Pe = \frac{uL}{D_A}$$

The axial dispersion coefficient is the parameter that quantifies the nonideality

- $D_A = 0$ $Pe \rightarrow \infty$ ....PFR
- $D_A \rightarrow \infty$ $Pe = 0$ ....CSTR

Axial Dispersion Model

$$\frac{\partial C_A}{\partial t} = -u\frac{\partial C_A}{\partial z} + D_A\frac{\partial^2 C_A}{\partial z^2} + r_i$$

$$z = 0 \qquad c_A\big|_{z=0} = c_{A,e} + \frac{D_a}{u}\frac{dc_A}{dz}\bigg|_{z=0}$$

$$z = L \qquad \frac{dc_A}{dz}\bigg|_{z=L} = 0$$

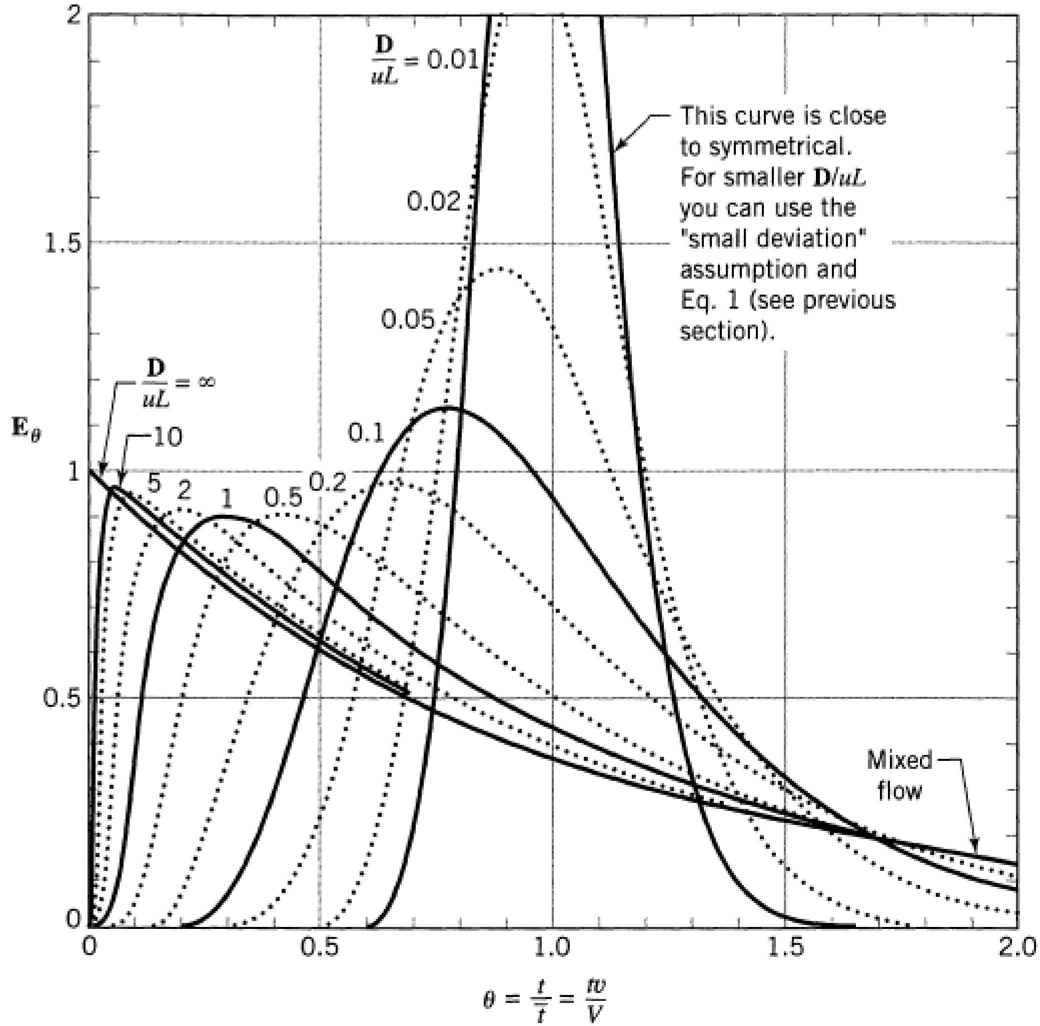
for odd i = 1,3,5,....

$$\tan\left(\frac{\alpha_i}{2}\right) = \frac{Pe}{4(\alpha_i/2)}$$

for even i = 2,4,6,...

$$\operatorname{cotg}\left(\frac{\alpha_i}{2}\right) = \frac{-Pe}{4(\alpha_i/2)}$$

$$\boxed{Pe = \frac{uL}{D_A}}$$



$$\frac{C_s(t)}{M/V} = E(\theta) = e^{Pe/2}\sum_{i=1}^{\infty}\frac{(-1)^{i+1}8\alpha_i^2}{4\alpha_i^2 + 4Pe + Pe^2}\exp\left(\frac{-\theta(Pe^2 + 4\alpha_i^2)}{4Pe}\right)$$

Axial Dispersion Model

$$\frac{C_s(t)}{M/V} = E(\theta) = e^{Pe/2} \sum_{i=1}^{\infty} \frac{(-1)^{i+1} 8\alpha_i^2}{4\alpha_i^2 + 4Pe + Pe^2} \exp\left(\frac{-\theta(Pe^2 + 4\alpha_i^2)}{4Pe} \right)$$

for odd i = 1,3,5,....

$$\tan\left(\frac{\alpha_i}{2}\right) = \frac{Pe}{4(\alpha_i/2)}$$

for even i = 2,4,6,...

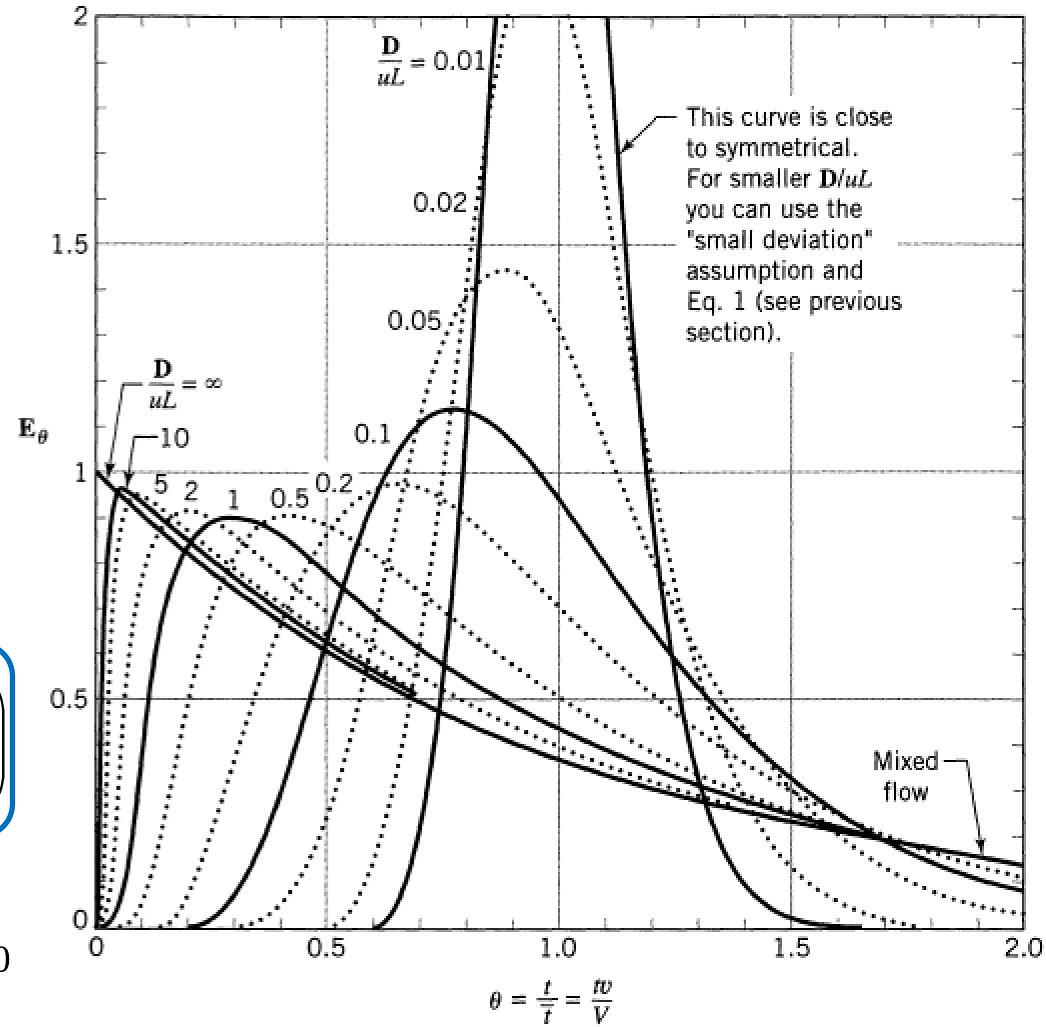
$$\mathrm{cotg}\left(\frac{\alpha_i}{2}\right) = \frac{-Pe}{4(\alpha_i/2)}$$

$\cong$

An excellent approximation for the infinite-series solution is

$$E(\theta) \cong \left(\frac{Pe+1}{4\pi\theta^3} \right)^{1/2} \exp\left(\frac{-(Pe+1)(1-\theta)^2}{4\theta} \right)$$

Gouvea, Park, & Giudici, Estimação de coeficientes de dispersão axial em leitos fixos. *18. Encontro sobre Escoamento em Meios Porosos*. Nova Friburgo. 1990



Axial dispersion model

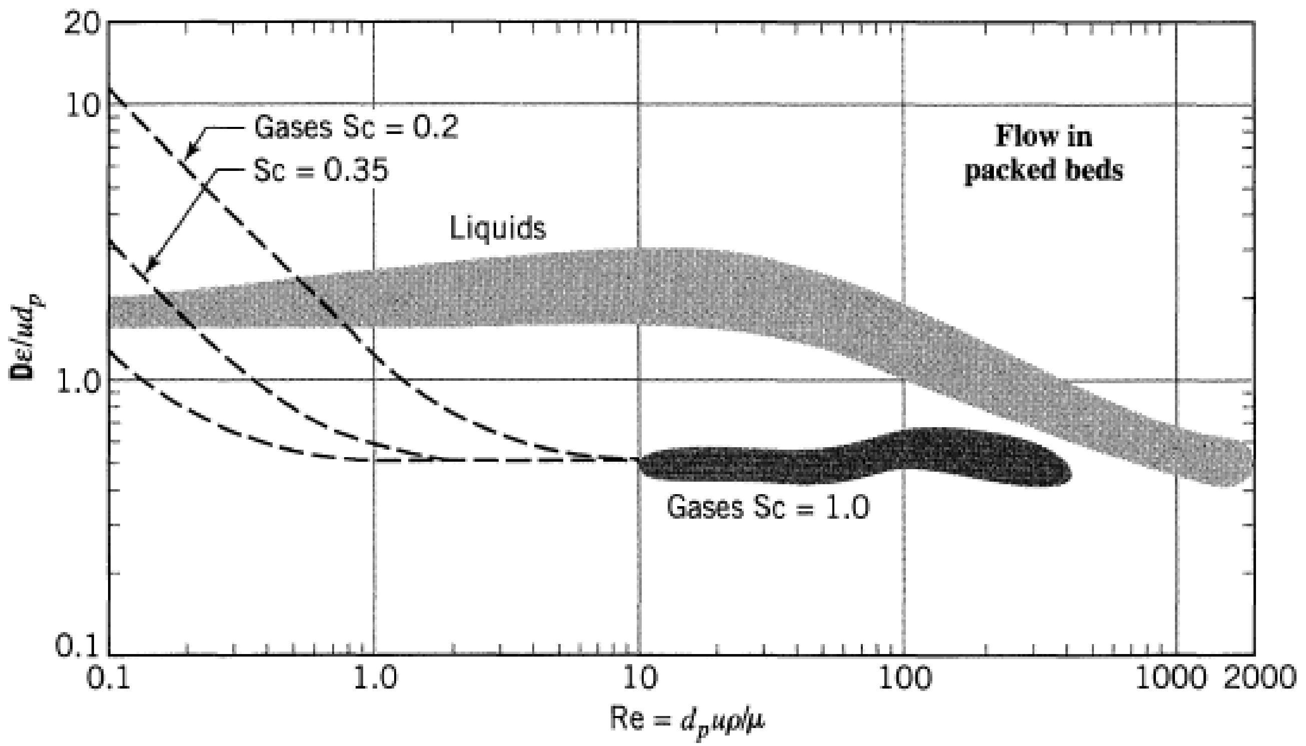


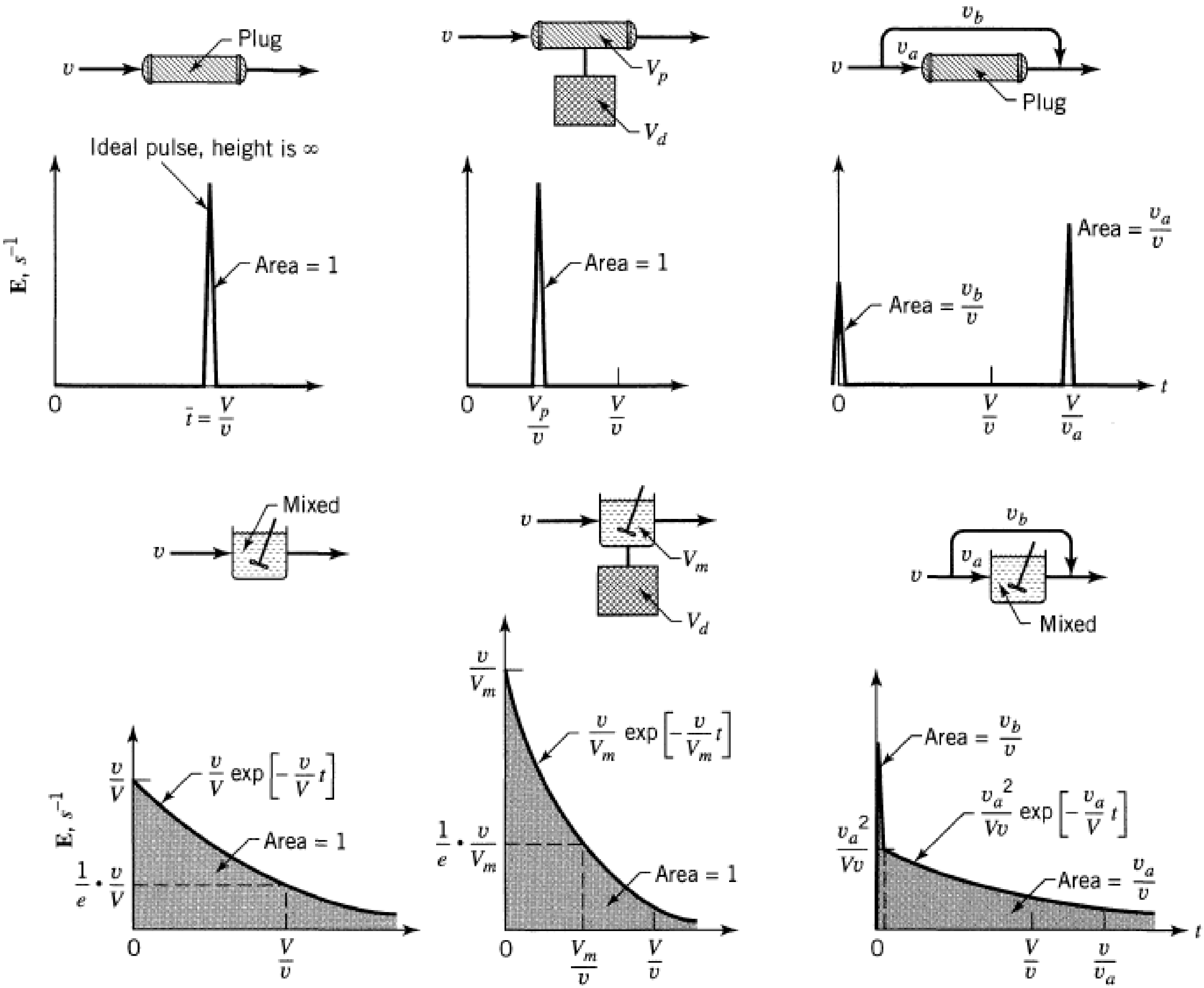
Figure 13.17 Experimental findings on dispersion of fluids flowing with mean axial velocity *u* in packed beds; prepared in part from Bischoff (1961).

Chung & Wen (1968) correlation

$$\varepsilon . Pe_L \frac{d_p}{L} = \varepsilon . \left(\frac{uL}{D_{ea}} \right) \frac{d_p}{L} = \varepsilon . \left(\frac{ud_p}{D_{ea}} \right) = 0.2 + 0.008 \, \mathrm{Re}^{0.48}$$

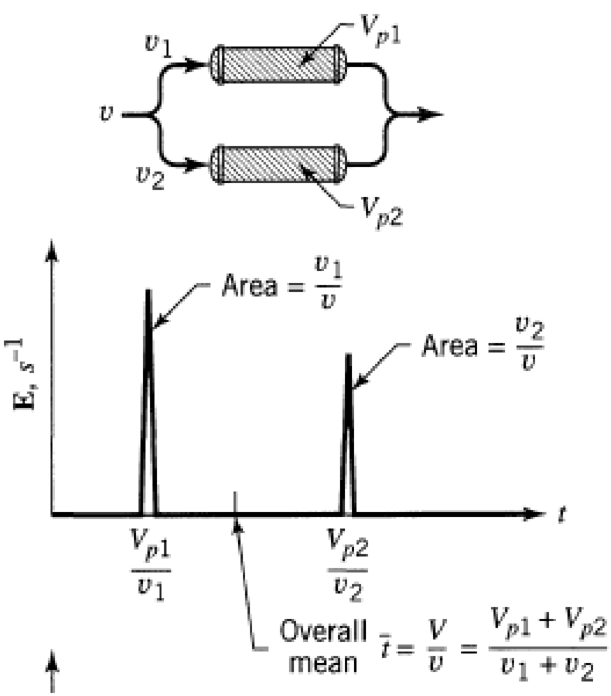
Compartment Models

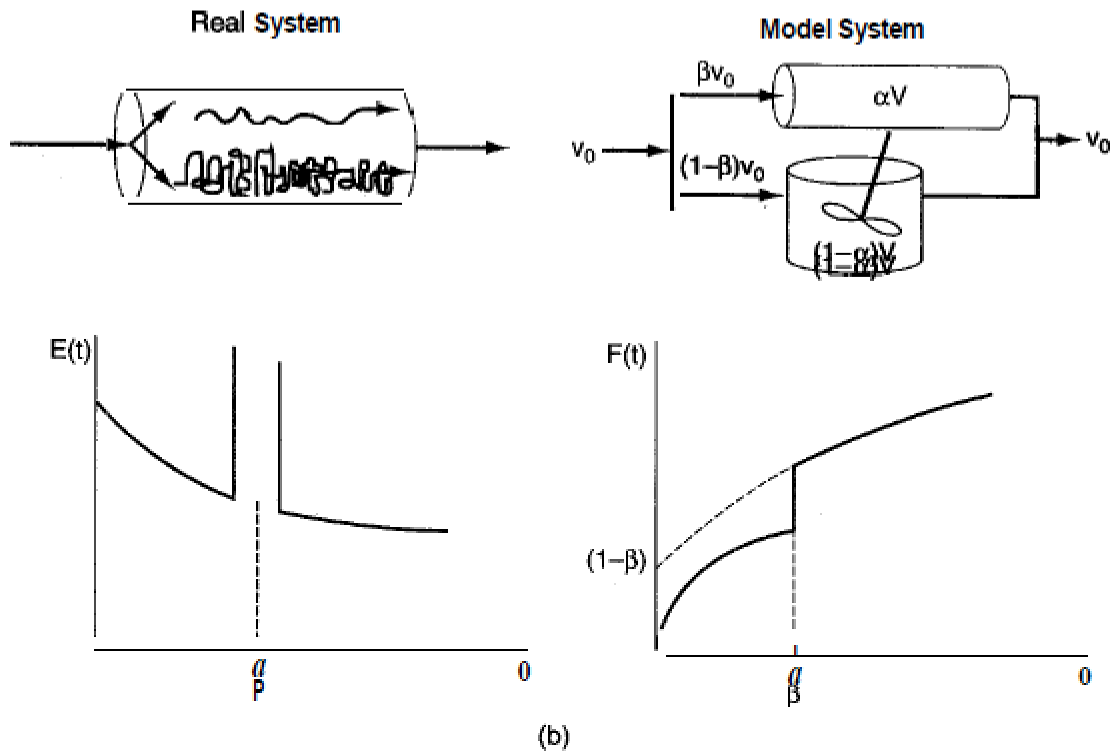
Compartment Models



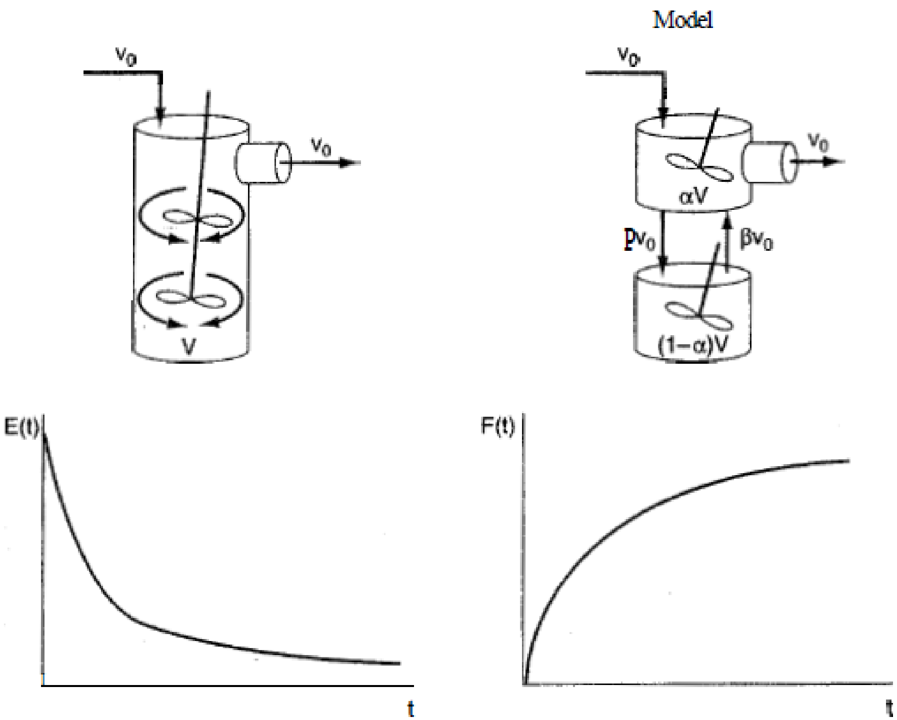
O. Levenspiel, Chemical Reaction Engineering, 3rd ed., Wiley, 1999.

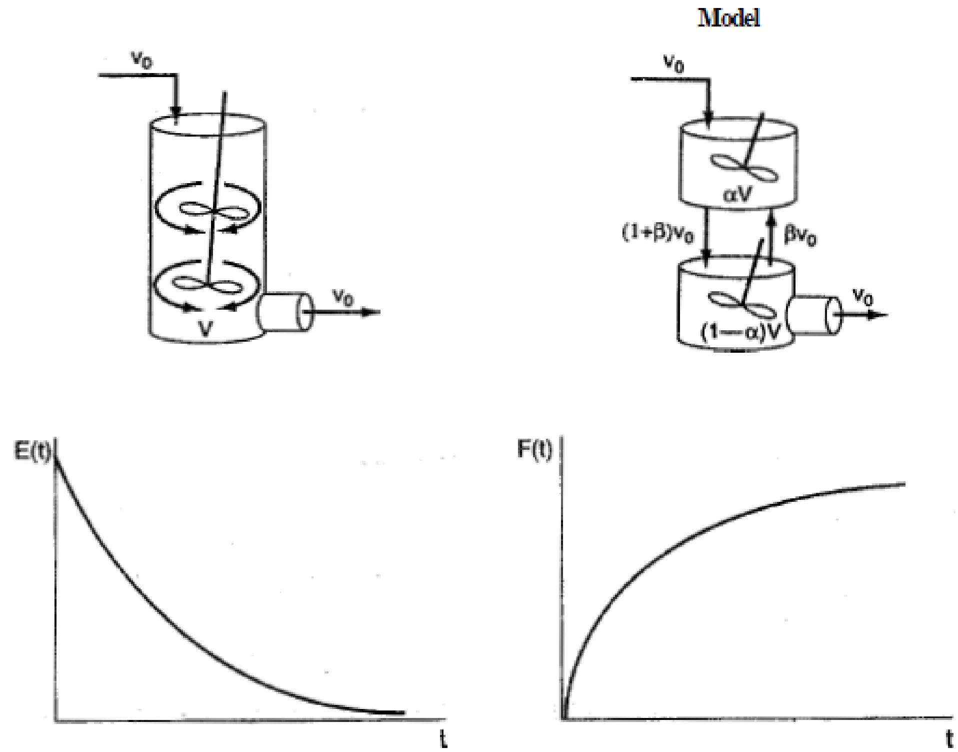
Compartment Models





Compartment Models





(b)

Compartment Models

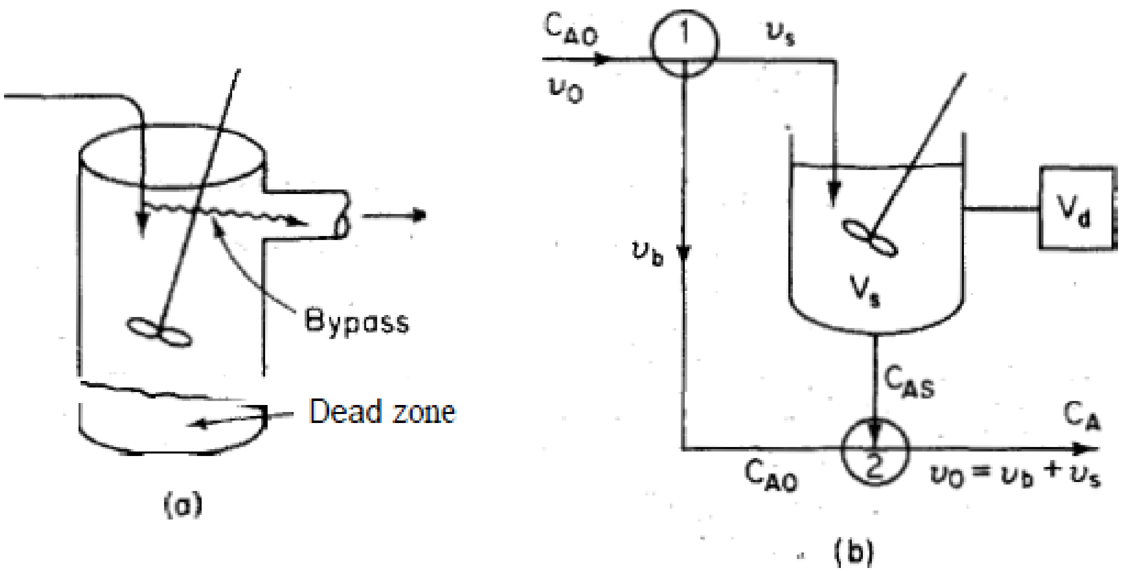
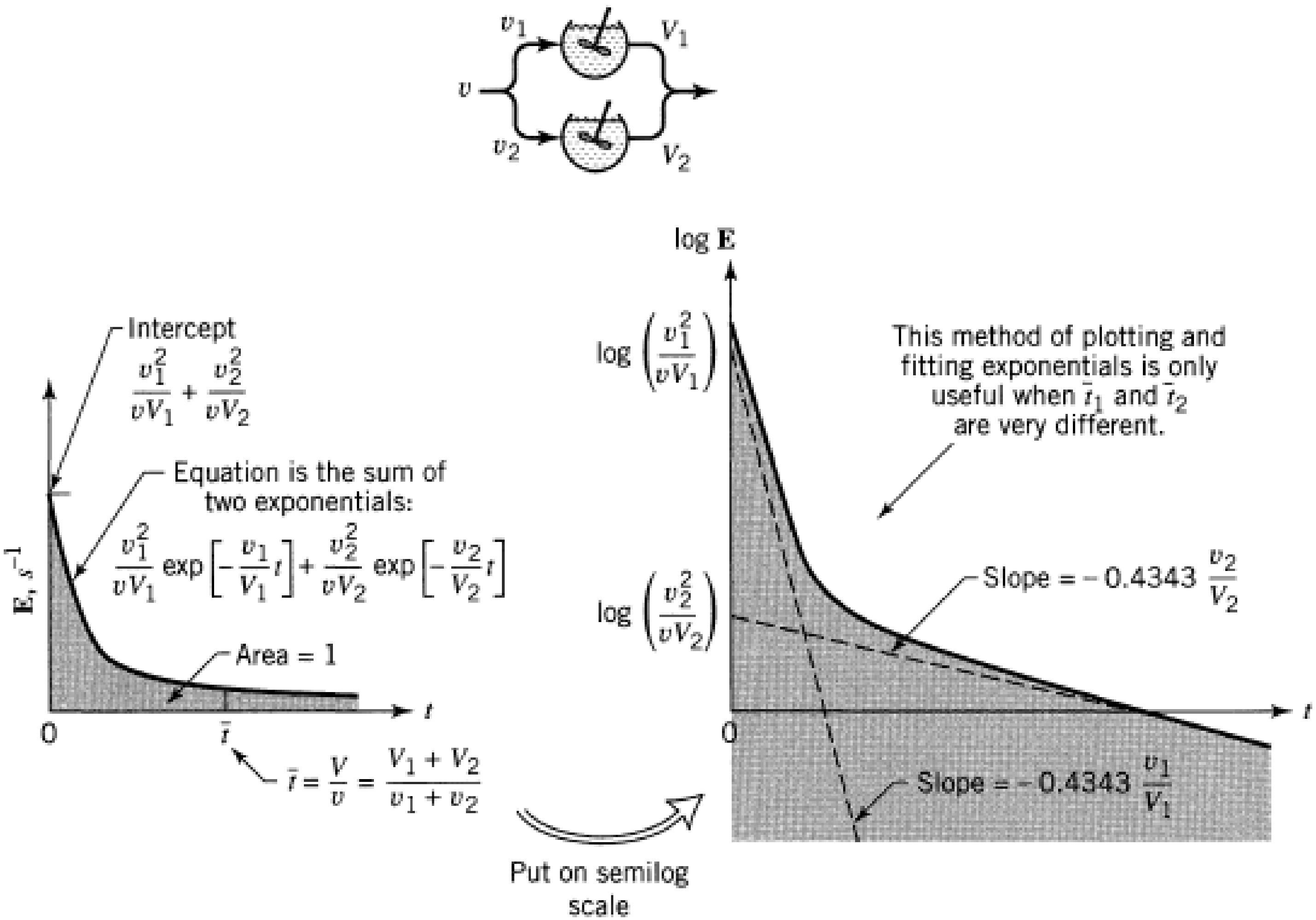


Figure 14-11 (a) Real system; (b) model system.

$$E(t) = \left(\frac{v_b}{v_0}\right)\delta(t) + \left(\frac{v_a^2}{V_s v_0}\right)\exp\left(-\frac{v_a}{V_s}t\right) = \beta.\delta(t) + \frac{(1-\beta)^2}{\alpha\tau}\exp\left(-\frac{(1-\beta)}{\alpha\tau}t\right)$$

$$F(t) = 1 - \left(\frac{v_a}{v_0}\right)\exp\left(-\frac{v_a}{V_s}t\right) = 1-(1-\beta)\exp\left(-\frac{(1-\beta)}{\alpha\tau}t\right)$$

Compartment Models



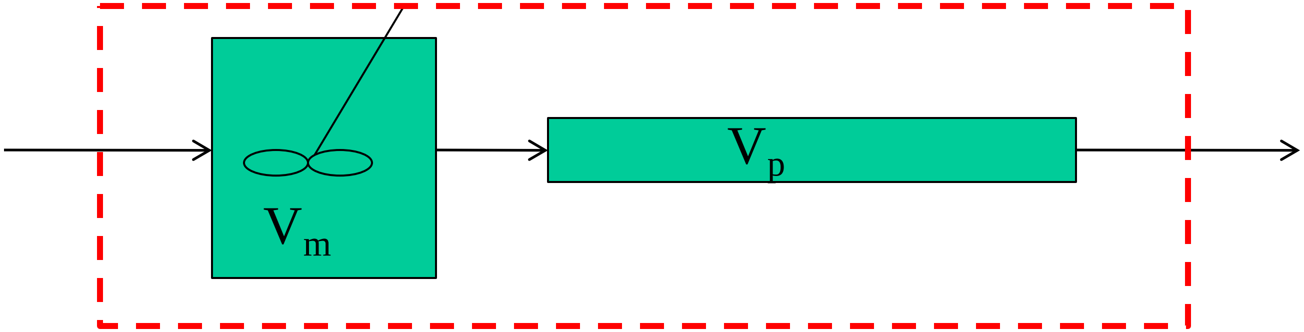
Compartment Models

Assignment #2:

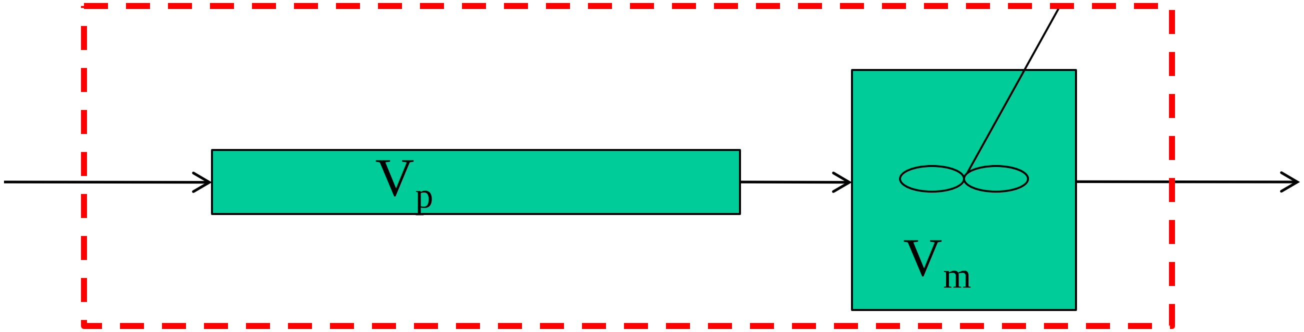
Draw the RTD curves E(t) for the systems shown bellow.

Explain your results (via mass balances and via “thought experiment”)

- (a) a system formed by a CSTR followed by a PFR.

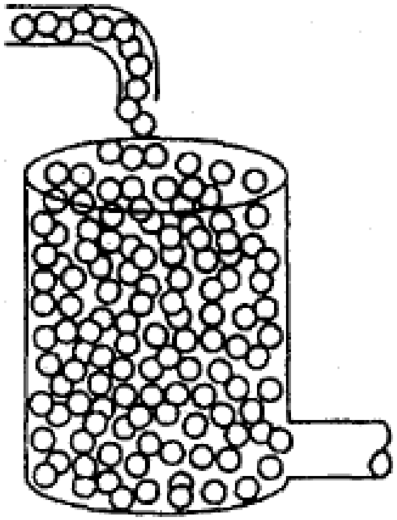


- (b) a system formed by a PFR followed by a CSTR.



Conversion directly from the RTD for Segregated Flow

Segregated Flow



MACROFLUID:

- mixing at the level of macroscopic portions of fluid
- molecules flow together in groups (globules) and they are not mixed until they exit the reactor
- different from a microfluid (where mixing occurs at the molecular level)
- each globule is a closed system (batch reactor)

$$\begin{pmatrix} \text{mean conversion} \\ \text{of all globules} \\ \text{exiting} \\ \text{the reactor} \end{pmatrix} = \sum_{\substack{\text{all} \\ \text{globules} \\ \text{exiting} \\ \text{the reactor}}} \begin{pmatrix} \text{conversion} \\ \text{achieved in} \\ \text{a globule} \\ \text{that spend} \\ \text{a time } t \\ \text{in the reactor} \end{pmatrix} \times \begin{pmatrix} \text{fraction of} \\ \text{globules that} \\ \text{spend between} \\ \text{time} \\ t \text{ and } t + dt \\ \text{in the reactor} \end{pmatrix}$$

$$\boxed{\bar{X} = \int_0^\infty \underbrace{X_{batch}(t)}_{\substack{\text{batch} \\ \text{reactor}}} E(t)\,dt}$$

Assignments RTD
(laboratory activity, gathering real data)

Assignment #3: Given the experimental data (absorbance versus time) of a pulse RTD experiment (fluid = water) in a real tubular reactor (L=90 cm, D=4 cm) packed with 0,8 cm Raschig rings (void fraction of the packed bed ϕ=0,70).

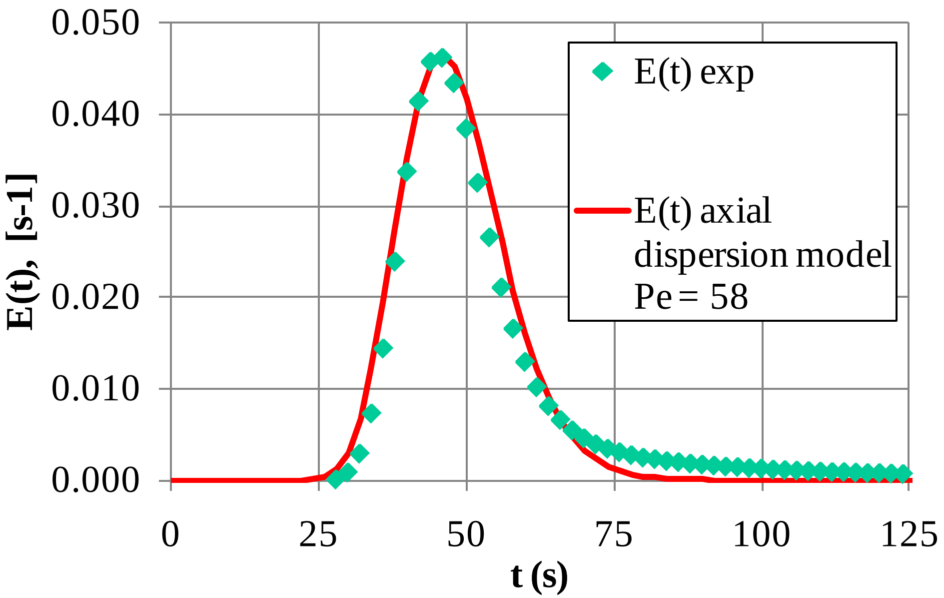
(a) Fit the axial dispersion model to the data and determine the value of Peclet number, Pe =u.L/D_A and τ. Compare the obtained Peclet value with literature values (see slide 37). Use the approximated solution for the RTD of the axial dispersion model.

$$E(t) \cong \frac{1}{\tau}\left(\frac{Pe+1}{4\pi(t/\tau)^3}\right)^{1/2} \exp\left(\frac{-(Pe+1)[1-(t/\tau)]^2}{4(t/\tau)}\right)$$

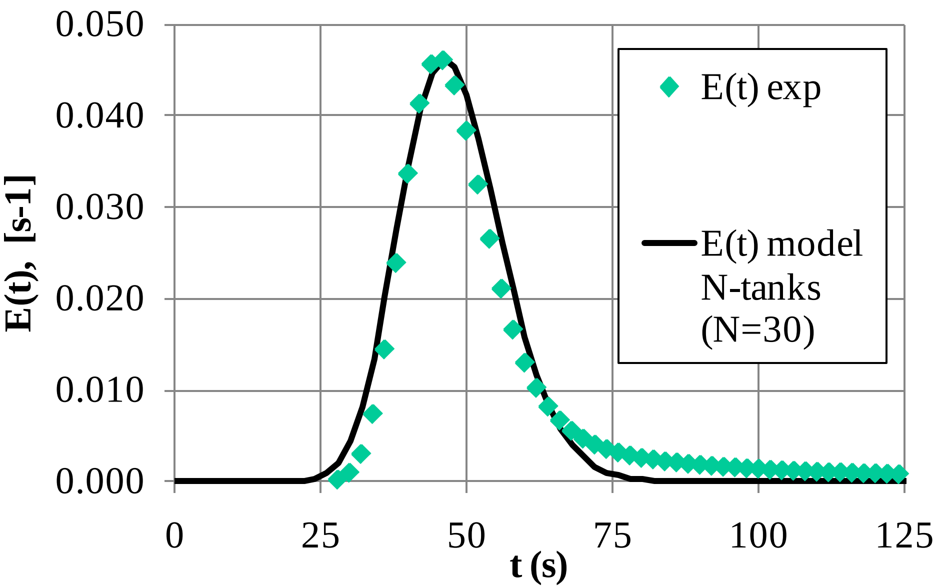
(a) Fit the N-tanks-in-series model to the exp. data and determine N and τ

$$E(t) = \frac{N\left(N\dfrac{t}{\tau}\right)^{N-1}}{\tau(N-1)!}\exp\left(-N\frac{t}{\tau}\right) = \frac{t^{N-1}}{(N-1)!(\tau/N)^N}\exp\left(-N\frac{t}{\tau}\right)$$

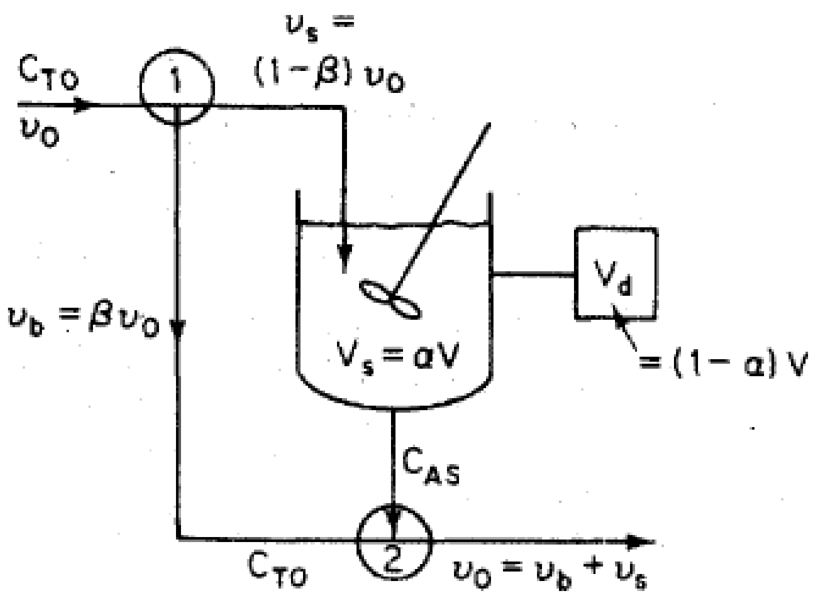
$$E(t) \cong \frac{1}{\tau}\left(\frac{Pe+1}{4\pi\left(\frac{t}{\tau}\right)^3}\right)^{1/2} \exp\left(\frac{-(Pe+1)\left[1-\left(\frac{t}{\tau}\right)\right]^2}{4\left(\frac{t}{\tau}\right)}\right)$$



$$E(t) = \frac{t^{N-1}}{(N-1)!\left(\tau / N\right)^N}\exp\left(-N\frac{t}{\tau}\right)$$

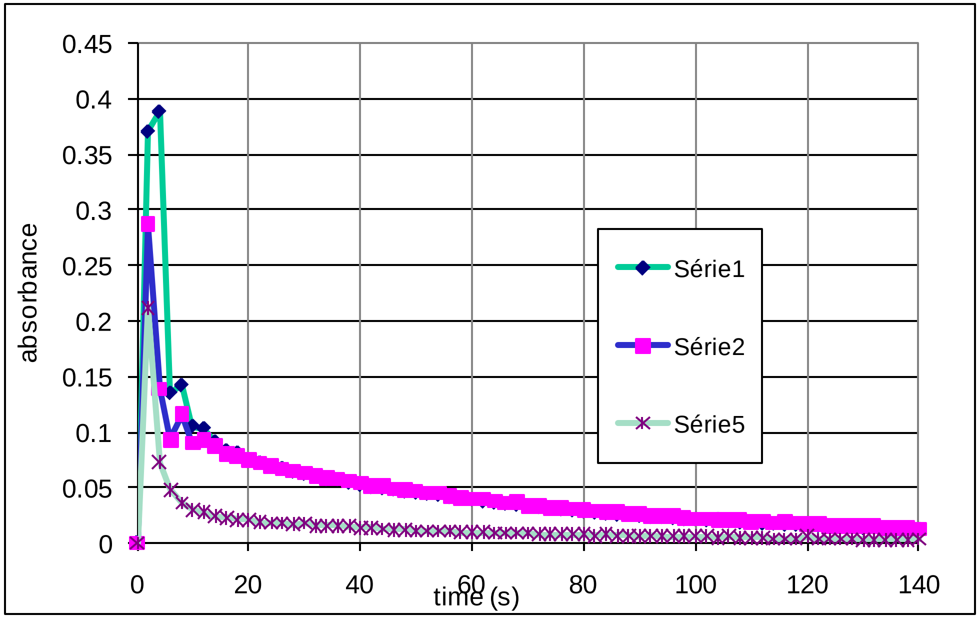


Assignment #4: Given the experimental data (absorbance versus time) of a pulse RTD experiment in a real tank reactor (fluid = water), fit the compartment model considering a dead volume and a by-pass, and determine the fraction of by-pass $\beta = v_b/v$ and the fraction of active volume $\alpha = V_s/V$

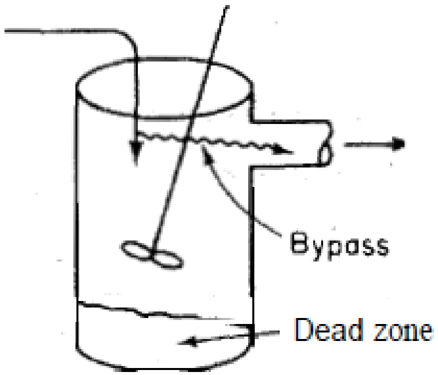


$$E(t) = \left(\frac{v_b}{v_0}\right)\delta(t) + \left(\frac{v_a^2}{V_s v_0}\right)\exp\left(-\frac{v_a}{V_s}t\right) = \beta.\delta(t) + \frac{(1-\beta)^2}{\alpha\tau}\exp\left(-\frac{(1-\beta)}{\alpha\tau}t\right)$$

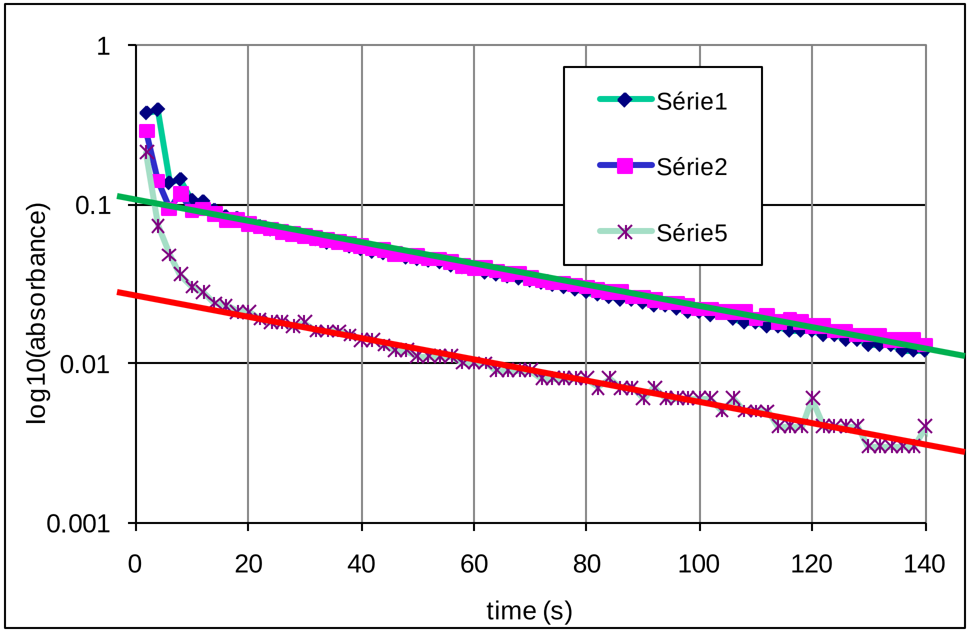
$$F(t) = 1 - \left(\frac{v_a}{v_0}\right)\exp\left(-\frac{v_a}{V_s}t\right) = 1-(1-\beta)\exp\left(-\frac{(1-\beta)}{\alpha\tau}t\right)$$



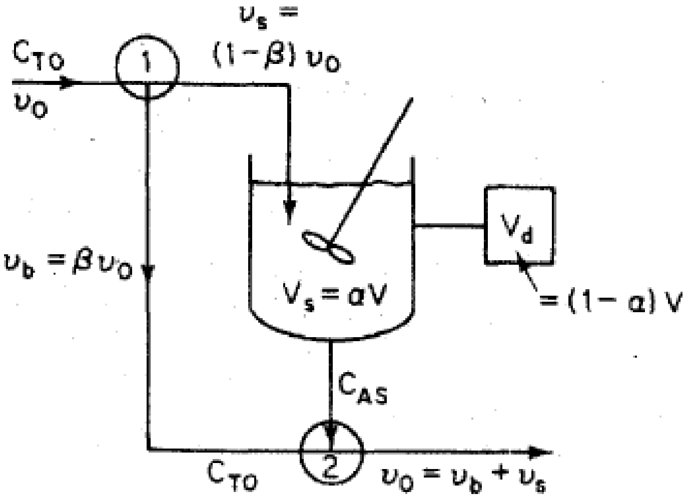
0.45
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
absorbance
0
20
40
60
80
100
120
140
time (s)
Série1
Série2
Série5



Bypass
Dead zone



1
0.1
0.01
0.001
log10(absorbance)
0
20
40
60
80
100
120
140
time (s)
Série1
Série2
Série5



C_{TO}
υ_0
1
$\upsilon_s = (1-\beta)\,\upsilon_0$
$\upsilon_b = \beta\,\upsilon_0$
$V_s = \alpha V$
V_d
$= (1-\alpha)\,V$
C_{AS}
C_{TO}
2
$\upsilon_0 = \upsilon_b + \upsilon_s$