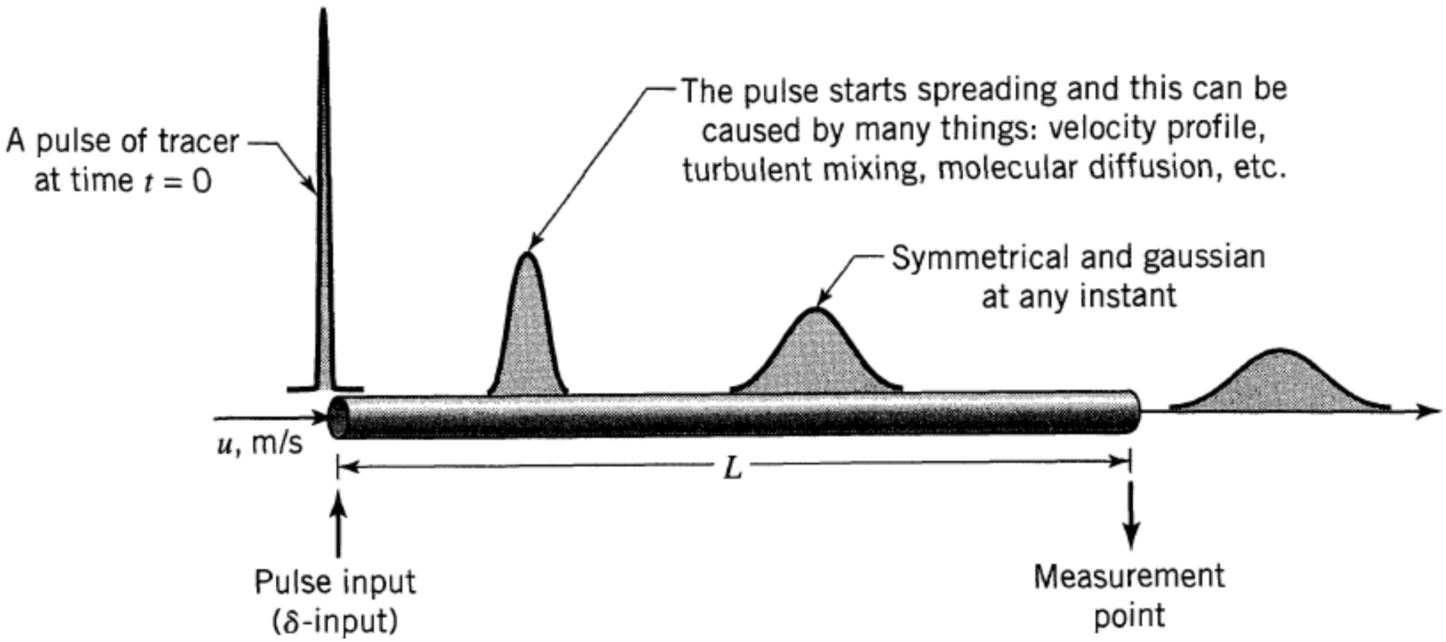
The Dispersion Model

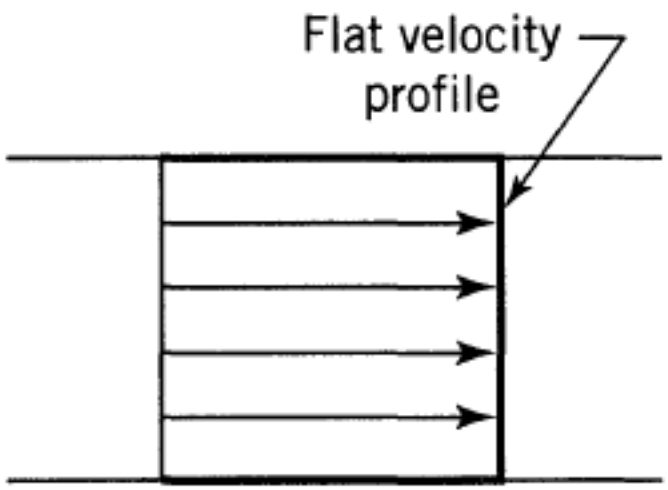


The dispersion coefficient **D** (m^2/s) represents this spreading process.

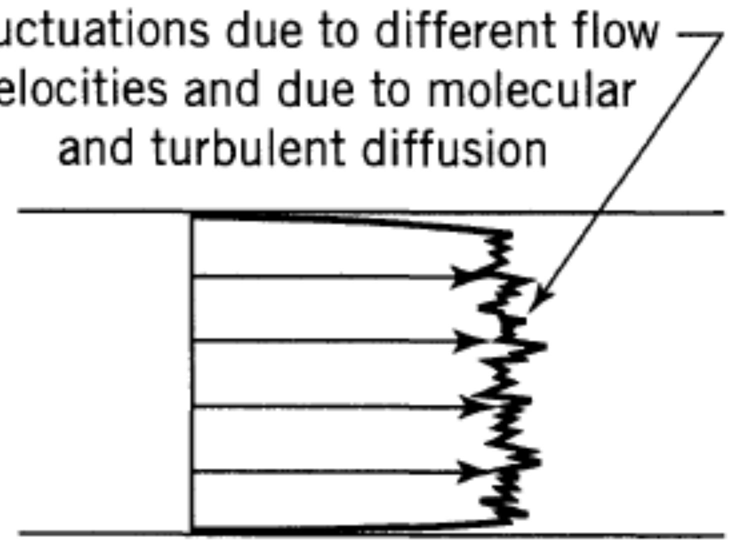
- large **D** means rapid spreading of the tracer curve
- small **D** means slow spreading
- **D** = 0 means no spreading, hence plug flow

Also

$\left(\frac{\mathbf{D}}{uL}\right)$ is the dimensionless group characterizing the spread in the whole vessel.



Plug flow



Dispersed plug flow

$$\frac{\partial C}{\partial t} = \mathbf{D}\,\frac{\partial^2 C}{\partial x^2}$$

Diffusion: Fick's law

where the parameter D is the axial dispersion coefficient

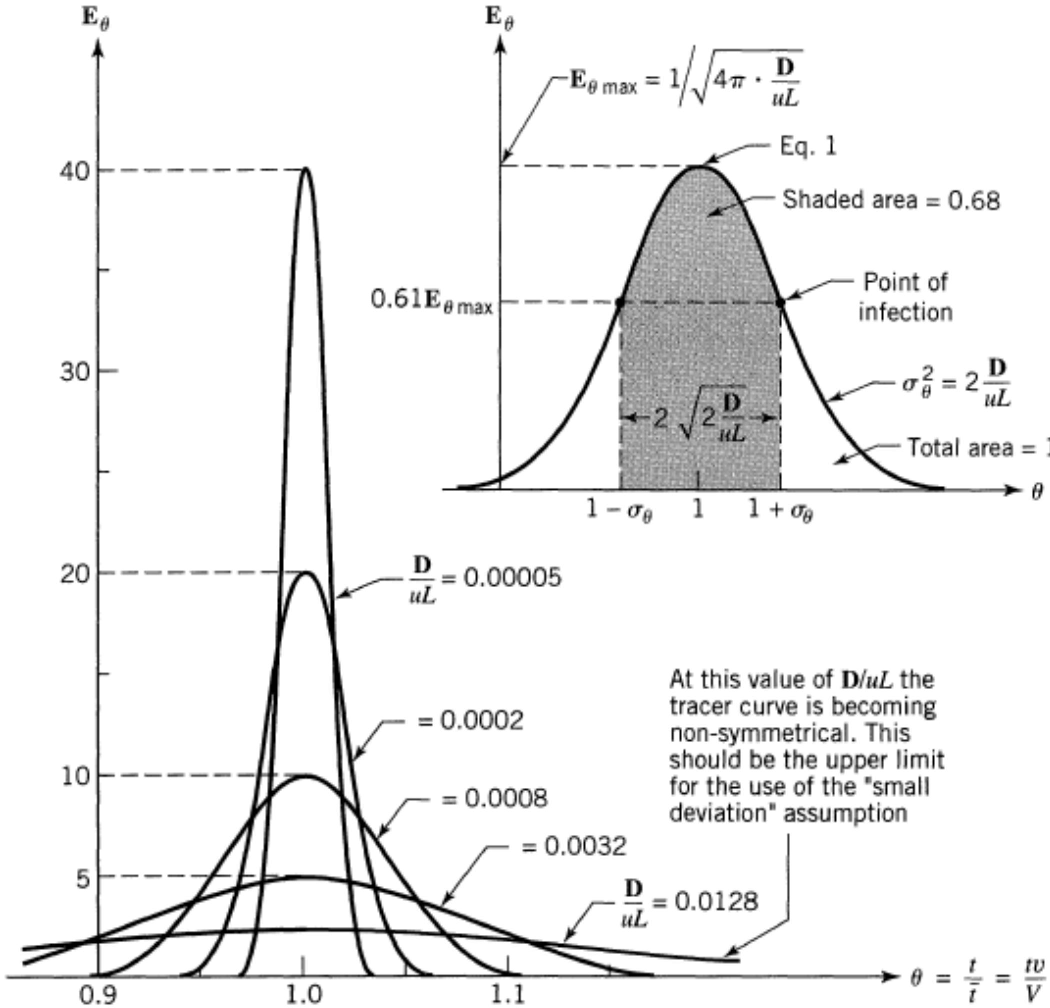


Figure 13.4 Relationship between **D**/uL and the dimensionless $\mathbf{E}_\theta$ curve for small extents of dispersion, Eq. 7.

$$\mathbf{E}_\theta = \bar{t} \cdot \mathbf{E} = \frac{1}{\sqrt{4\pi(\mathbf{D}/uL)}} \exp\left[-\frac{(1-\theta)^2}{4(\mathbf{D}/uL)}\right]$$

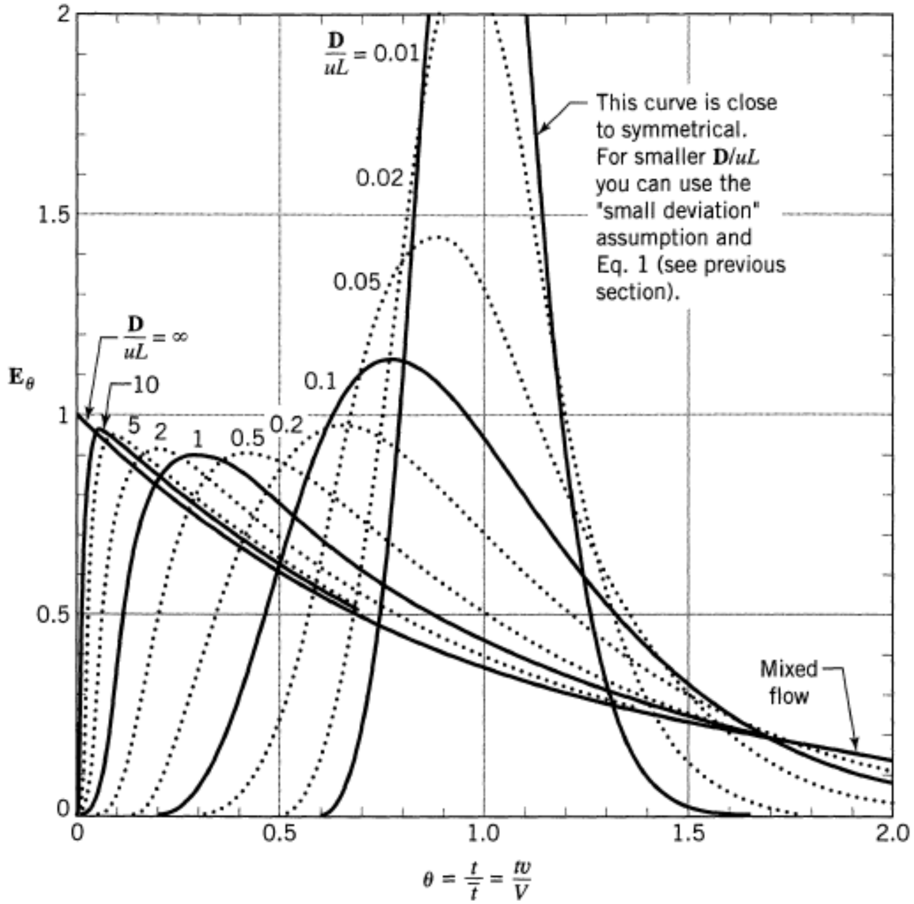
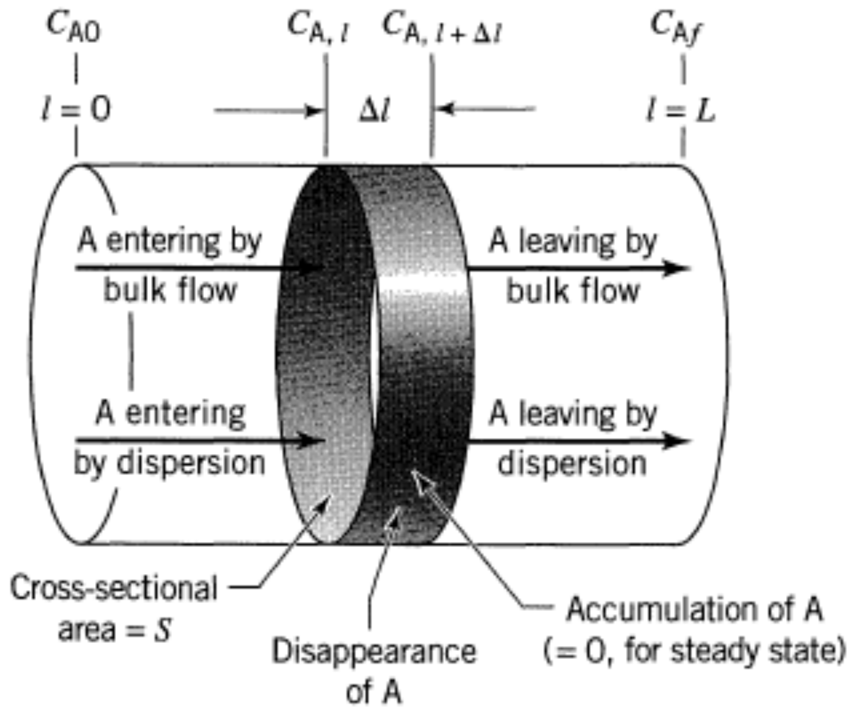


Figure 13.8 Tracer response curves for closed vessels and large deviations from plug flow.

Vessel dispersion number $\frac{\mathbf{D}}{uL} \to 0$ negligible dispersion, hence plug flow

$\frac{\mathbf{D}}{uL} \to \infty$ large dispersion, hence mixed flow



$$\text{input} = \text{output} + \text{disappearance by reaction} + \text{accumulation} \tag{4.1}$$

becomes for component A, at steady state,

$$(\text{out–in})_{\text{bulk flow}} + (\text{out–in})_{\text{axial dispersion}} + \begin{matrix}\text{disappearance}\\ \text{by reaction}\end{matrix} + \text{accumulation} = 0 \tag{17}$$

$$\text{entering by bulk flow} = \left(\frac{\text{moles A}}{\text{volume}}\right)\left(\begin{matrix}\text{flow}\\ \text{velocity}\end{matrix}\right)\left(\begin{matrix}\text{cross-sectional}\\ \text{area}\end{matrix}\right)$$

$$= C_{\mathrm{A},l}uS, \quad [\text{mol/s}]$$

$$\text{leaving by bulk flow} = C_{\mathrm{A},l+\Delta l}uS$$

$$\text{entering by axial dispersion} = \frac{dN_\mathrm{A}}{dt} = -\left(\mathbf{D}S\,\frac{dC_\mathrm{A}}{dl}\right)_l$$

$$\text{leaving by axial dispersion} = \frac{dN_\mathrm{A}}{dt} = -\left(\mathbf{D}S\,\frac{dC_\mathrm{A}}{dl}\right)_{l+\Delta l}$$

$$\text{disappearance by reaction} = (-r_\mathrm{A})\,V = (-r_\mathrm{A})S\,\Delta l, \quad [\text{mol/s}]$$

$$u\,\frac{(C_{\mathrm{A},l+\Delta l}-C_{\mathrm{A},l})}{\Delta l}-\mathbf{D}\,\frac{\left[\left(\frac{dC_{\mathrm{A}}}{dl}\right)_{l+\Delta l}-\left(\frac{dC_{\mathrm{A}}}{dl}\right)_{l}\right]}{\Delta l}+(-r_{\mathrm{A}})=0$$

Now the basic limiting process of calculus states that for any quantity Q which is a smooth continuous function of l

$$\lim_{l_2\to l_1}\frac{Q_2-Q_1}{l_2-l_1}=\lim_{\Delta l\to 0}\frac{\Delta Q}{\Delta l}=\frac{dQ}{dl}$$

So taking limits as $\Delta l \to 0$ we obtain

$$u \frac{dC_A}{dl} - \mathbf{D} \frac{d^2 C_A}{dl^2} + kC_A^n = 0 \tag{18a}$$

In dimensionless form where $z = l/L$ and $\tau = \bar{t} = L/u = V/v$, this expression becomes

$$\frac{\mathbf{D}}{uL} \frac{d^2 C_A}{dz^2} - \frac{dC_A}{dz} - k\tau C_A^n = 0 \tag{18b}$$

or in terms of fractional conversion

$$\frac{\mathbf{D}}{uL} \frac{d^2 X_A}{dz^2} - \frac{dX_A}{dz} + k\tau C_{A0}^{n-1} (1 - X_A)^n = 0 \tag{18c}$$

This expression shows that the fractional conversion of reactant A in its passage through the reactor is governed by three dimensionless groups: a reaction rate group $k\tau C_{A0}^{n-1}$, the dispersion group $\mathbf{D}/uL$, and the reaction order n.

First-order Reactions

$$\frac{C_A}{C_{A0}} = 1 - X_A = \frac{4a \exp\left(\frac{1}{2}\frac{uL}{\mathbf{D}}\right)}{(1+a)^2 \exp\left(\frac{a}{2}\frac{uL}{\mathbf{D}}\right) - (1-a)^2 \exp\left(-\frac{a}{2}\frac{uL}{\mathbf{D}}\right)}$$

$$a = \sqrt{1 + 4k\tau(\mathbf{D}/uL)}$$

For *small deviations from plug flow* $\mathbf{D}/uL$ becomes small, the **E** curve approaches gaussian; hence, on expanding the exponentials and dropping higher order terms Eq. 19 reduces to

$$\frac{C_A}{C_{A0}} = \exp\left[-k\tau + (k\tau)^2 \frac{\mathbf{D}}{uL}\right] \tag{20}$$

$$= \exp\left[-k\tau + \frac{k^2\sigma^2}{2}\right] \qquad \textbf{(21)*}$$

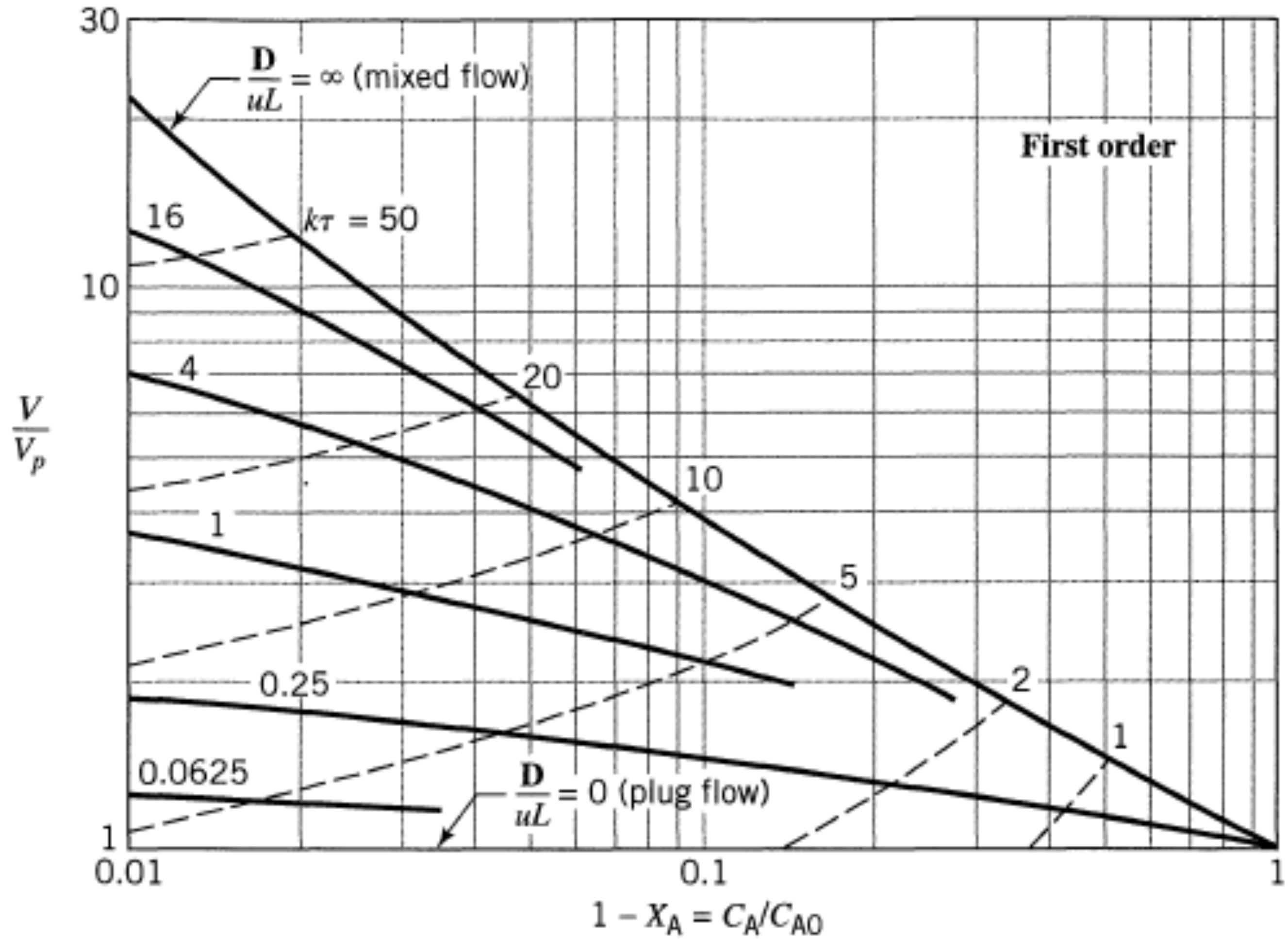


Figure 13.19 Comparison of real and plug flow reactors for the first-order A → products, assuming negligible expansion; from Levenspiel and Bischoff (1959, 1961).

1st order rxn

$K = 0.2/\text{min}$

$\bar{t} = 25 \text{ min}$

$D = 2 \text{ m}^2/\text{s}$

Calculate/estimate fractional conversion.

Second-order Reactions

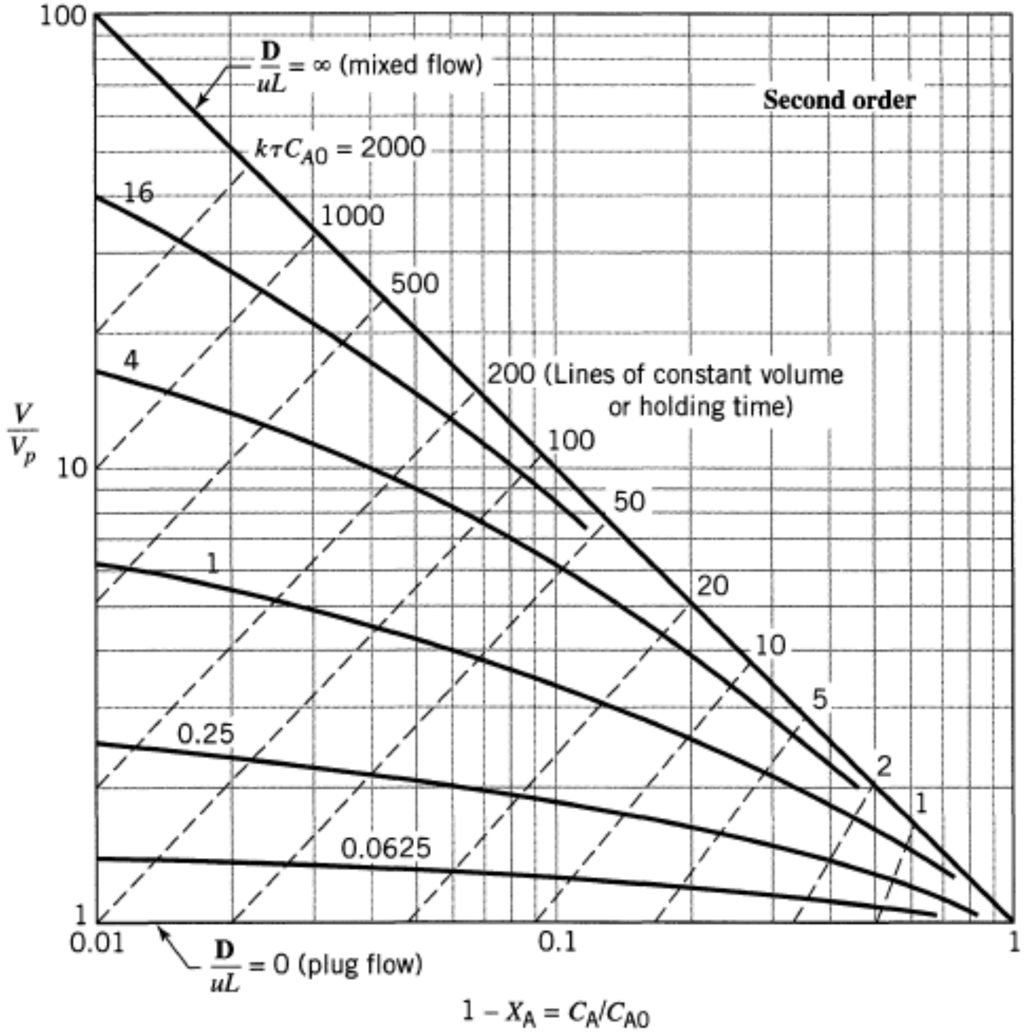


Figure 13.20 Comparison of real and plug flow reactors for the second-order reactions

2nd order rxn (cons't volume)

$K = 0.05 \ \frac{L}{mg\text{-}min}$ $\tau = 333.3\ min$

$C_0 = 1.2\ mg/L$

$\frac{D}{\nu L} = 4$ what is the conversion?