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(Skill Based Project- Chemical Reaction Engineering-1)

REPORT ON-

"FLOW MODELS"

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Table of Contents;-

1- ***Abstract ;-***

One way of approaching the study of no ideal reactors is to consider them, in a first approximation, as if the flow model were the one corresponding to a continuously stirred tank reactor (CSTR) or a plug flow reactor. However, in real reactors, the no ideal flow model implies a minor conversion, so a method that allows for this conversion loss to be considered must be available. Therefore, a higher level of approximation implies the use of information about the residence time distribution.[1] There is a need to model the real reactor with some type of combination of ideal reactors or introduce new models. In the case of tubular reactors, there are two models that usually represent the flow: the tanks-in-series model and the dispersion model. In one case, the real reactor is modelled as a series of CSTRs of the same size. In the other (dispersion model), an axial dispersion is superimposed on the piston flow.[2]

Not all tank reactors are perfectly mixed nor do all tubular reactors exhibit plug-flow behaviour. In these situations, some means must be used to allow for deviations from ideal behaviour. We use the segregation and maximum mixedness models to bound the conversion when no adjustable parameters are used. For non-first-order reactions in a fluid with good micro mixing, more than just the RTD is needed. These situations compose a great majority of reactor analysis problems and cannot be ignored. For example, we may have an existing reactor and want to carry out a new reaction in that reactor. To predict conversions and product distributions for such systems, a model of reactor flow patterns is necessary. To model these patterns, we use combinations and/or modifications of ideal reactors to represent real reactors. With this technique, we classify a model as being either a one-parameter model (e.g., tanks-in-series model or dispersion model) or a two-parameter model (e.g., reactor with bypassing and dead volume).[2]

Keywords- **Reactor, CSTR, RTD, Dispersion Segregation, Adjustable parameters, Conversion, Bypassing.**

2- Introduction ;-

The overall goal is to use the following equation RTD Data + Kinetics + Model = Prediction The choice of the particular model to be used depends largely on the engineering judgment of the person carrying out the analysis. It is this person's job to choose the model that best combines the conflicting goals of mathematical simplicity and physical realism. There is a certain amount of art in the development of a model for a particular reactor, and the examples presented here can only point toward a direction that an engineer's thinking might follow. For a given real reactor, it is not uncommon to use all the models discussed previously to predict conversion and then make a comparison. Usually, the real conversion will be bounded by the model calculations.[1] The following guidelines are suggested when developing models for non ideal reactors: 1.The model must be mathematically tractable. The equations used to describe a chemical reactor should be able to be solved without an inordinate expenditure of human or computer time. 2.The model must realistically describe the characteristics of the non ideal reactor. The phenomena occurring in the non ideal reactor must be reasonably described physically, chemically, and mathematically. 3.The model must not have more than two adjustable parameters. This constraint is used because an expression with more than two adjustable parameters can be fitted to a great variety of experimental data, and the modeling process in this circumstance is nothing more than an exercise in curve fitting. The statement "Give me four adjustable parameters and I can fit an elephant; give me five and I can include his tail!" is one that I have heard from many colleagues.[2] Unless one is into modern art, a substantially larger number of adjustable parameters is necessary to draw a reasonable-looking elephant.1 A one-parameter model is, of course, superior to a two-parameter model if the one-parameter model is sufficiently realistic. To be fair, however, in complex systems (e.g., internal diffusion and conduction, mass transfer limitations) where other parameters may be measured independently, then more than two parameters are quite acceptable.

2.1- Some guidelines that will help your analysis and model building of nonideal reaction systems.

1. Look at the reactor.

a. Where are the inlet and outlet streams to and from the reactors? (Is by-passing a possibility?)

b. Look at the mixing system. How many impellers are there? (Could there be multiple mixing zones in the reactor?)

c .Look at the configuration. (Is internal recirculation possible? Is the packing of the catalyst particles loose so channeling could occur?)

2. Look at the tracer data.

a. Plot the E(t) and F(t) curves.

b. Plot and analyze the shapes of the E(Θ) and F(Θ) curves. Is the shape of the curve such that the curve or parts of the curve can be fit by an ideal reactor model? Does the curve have a long tail suggesting a stagnant zone? Does the curve have an early spike indicating bypassing? [3]

c. Calculate the mean residence time, t m , and variance, σ 2 . How does the t m determined from the RTD data compare with τ as measured with a yardstick and flow meter? How large is the variance; is it larger or smaller than τ 2 ?

3. Choose a model or perhaps two or three models.

4. Use the tracer data to determine the model parameters (e.g., n, D a , v b).

5. Use the CRE algorithm Calculate the exit concentrations and conversion for the model system you have selected.

2.2 - One-Parameter Models

Here we use a single parameter to account for the nonideality of our reactor. This parameter is most always evaluated by analyzing the RTD determined from a tracer test. Examples of one-parameter models for non ideal CSTRs include a reactor dead volume V D , where no reaction takes place, or a fraction f of fluid bypassing the reactor, thereby exiting unreacted. Examples of one-parameter models for tubular reactors include the tanks-in-series model and the dispersion model. For the tanks-in-series model, the parameter is the number of tanks, n , and for the dispersion model, it is the dispersion coefficient, D a . Knowing the parameter values, we then proceed to determine the conversion and/or effluent concentrations for the reactor. We first consider non ideal tubular reactors.[4] Tubular reactors may be empty, or they may be packed with some material that acts as a catalyst, heat-transfer medium, or means of promoting interphase contact. Until now when analyzing ideal tubular reactors, it usually has been assumed that the fluid moved through the reactor in piston-like flow (PFR), and every atom spends an identical length of time in the reaction environment. Here, the velocity profile is flat, and there is no axial mixing. Both of these assumptions are false to some extent in every tubular reactor; frequently, they are sufficiently false to warrant some modification. Most popular tubular reactor models need to have means to allow for failure of the plug-flow model and insignificant axial mixing assumptions; examples include the unpacked laminar flow tubular reactor, the unpacked turbulent flow, and packed-bed reactors. One of two approaches is usually taken to compensate for failure of either or both of the ideal assumptions. One approach involves modeling the non ideal tubular reactor as a series of identically sized CSTRs. The other approach (the dispersion model) involves a modification of the ideal reactor by imposing axial dispersion on plug flow.

2.3- Two-Parameter Models

The premise for the two-parameter model is that we can use a combination of ideal reactors to model the real reactor. For example, consider a packed bed reactor with channeling. Here the response to a pulse tracer input would show two dispersed pulses in the output as shown

Here we could model the real reactor as two ideal PBRs in parallel with the two parameters being the fluid that channels, v_b, and the reactor dead volume, V_D. The real reactor volume is $V = V_D + V_S$ with $v_0 = v_b + v_S$.

3- The Residence Time Distribution, RTD

Deviation from the two ideal flow patterns can be caused by channeling of fluid, by recycling of fluid, or by creation of stagnant regions in the vessel. In all types of process equipment, such as heat exchangers, packed columns, and reactors, this type of flow should be avoided since it always lowers the performance of the unit. If we know precisely what is happening within the vessel, thus if we have a complete velocity distribution map for the fluid in the vessel, then we should, in principle, be able to predict the behavior of a vessel as a reactor. Unfortunately, this approach is impractical, even in today's computer age.[5]

The residence time of a fluid parcel is the total time that the parcel has spent inside a control volume (e.g.: a chemical reactor, a lake, a human body). The residence time of a set of parcels is quantified in terms of the frequency distribution of the residence time in the set, which is known as residence time distribution (RTD), or in terms of its average, known as mean residence time.

Residence time plays an important role in chemistry and especially in environmental science and pharmacology. Under the name lead time or waiting time it plays a central role respectively in supply chain management and queuing theory, where the material that flows is usually discrete instead of continuous.

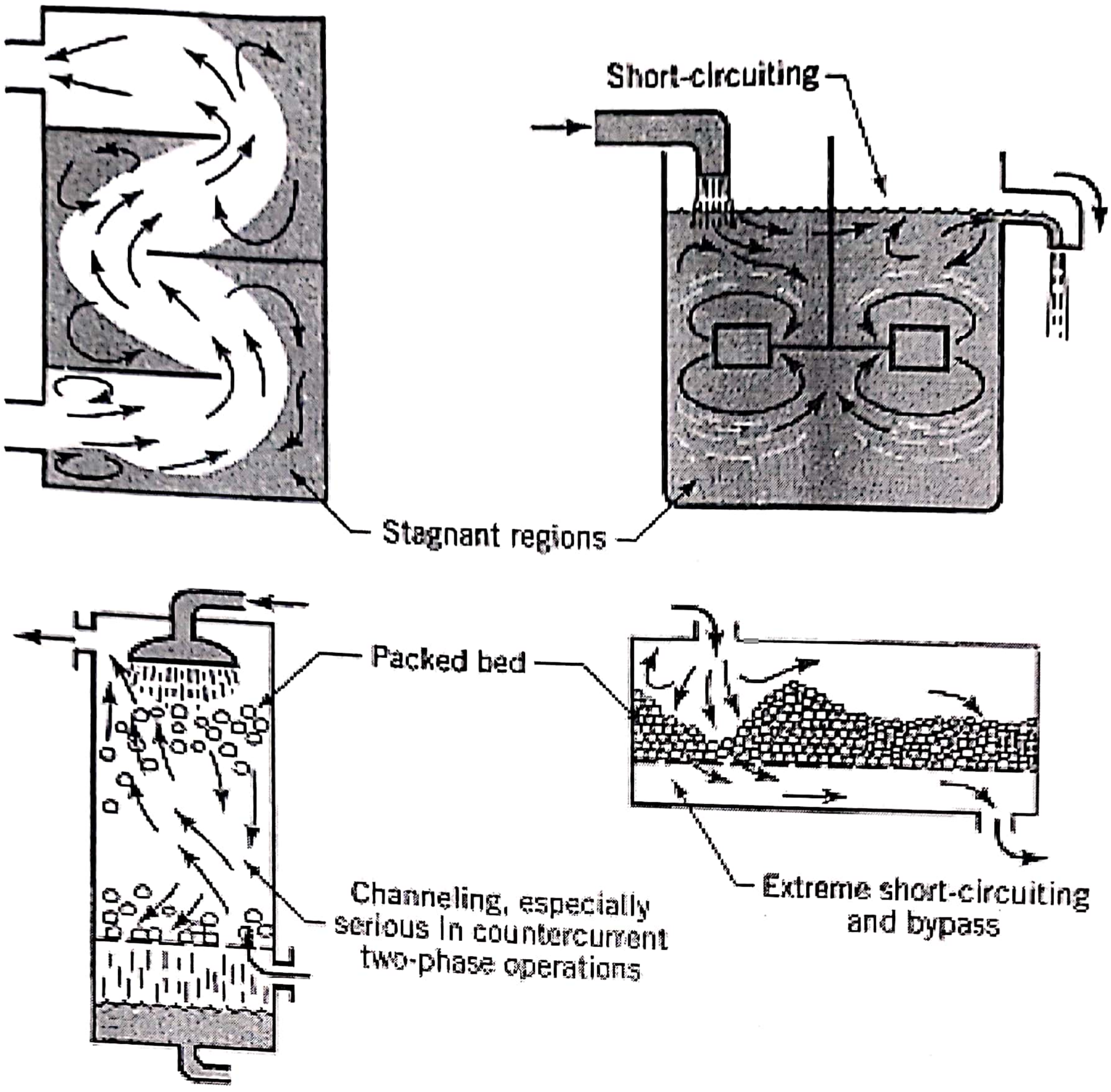


Figure 3- Non ideal flow patterns which may exist in process equipment

Image Source- Levenspiel, Octave. Chemical Reaction Engineering. Wiley, 1999.

Setting aside this goal of complete knowledge about the flow, let us be less ambitious and see what it is that we actually need to know. In many cases we really do not need to know very much, simply how long the individual molecules stay in the vessel, or more precisely, the distribution of residence times of the flowing fluid. This information can be determined easily and directly by a widely used method of inquiry, the stimulus-response experiment. This report deals in large part with the residence time distribution (or RTD) approach to non ideal flow. We show when it may legitimately be used, how to use it, and when it is not applicable what alternatives to turn to. In developing the "language" for this treatment of nonideal flow (see Danckwerts, 1953), we will only consider the steady-state flow, without reaction and without density change, of a single fluid through a vessel.[1]

3.1- THE AGE DISTRIBUTION OF FLUID

It is evident that elements of fluid taking different routes through the reactor may take different lengths of time to pass through the vessel. The distribution of these times for the stream of fluid leaving the vessel is called the exit age distribution E, or the residence time distribution RTD of fluid. E has the units of time-l.

$$\int_0^\infty \mathbf{E}\, dt = 1$$

We find it convenient to represent the RTD in such a way that the area under the curve is unity, or This procedure is called normalizing the distribution, and Fig. 11.6 shows this. We should note one restriction on the E curve-that the fluid only enters and only leaves the vessel one time. This means that there should be no flow or diffusion or up flow eddies at the entrance or at the vessèl exit. We call this the closed vessel boundary condition. Where elements of fluid can cross the vessel boundary more than one time we call this the open vessel boundary condition.[1]

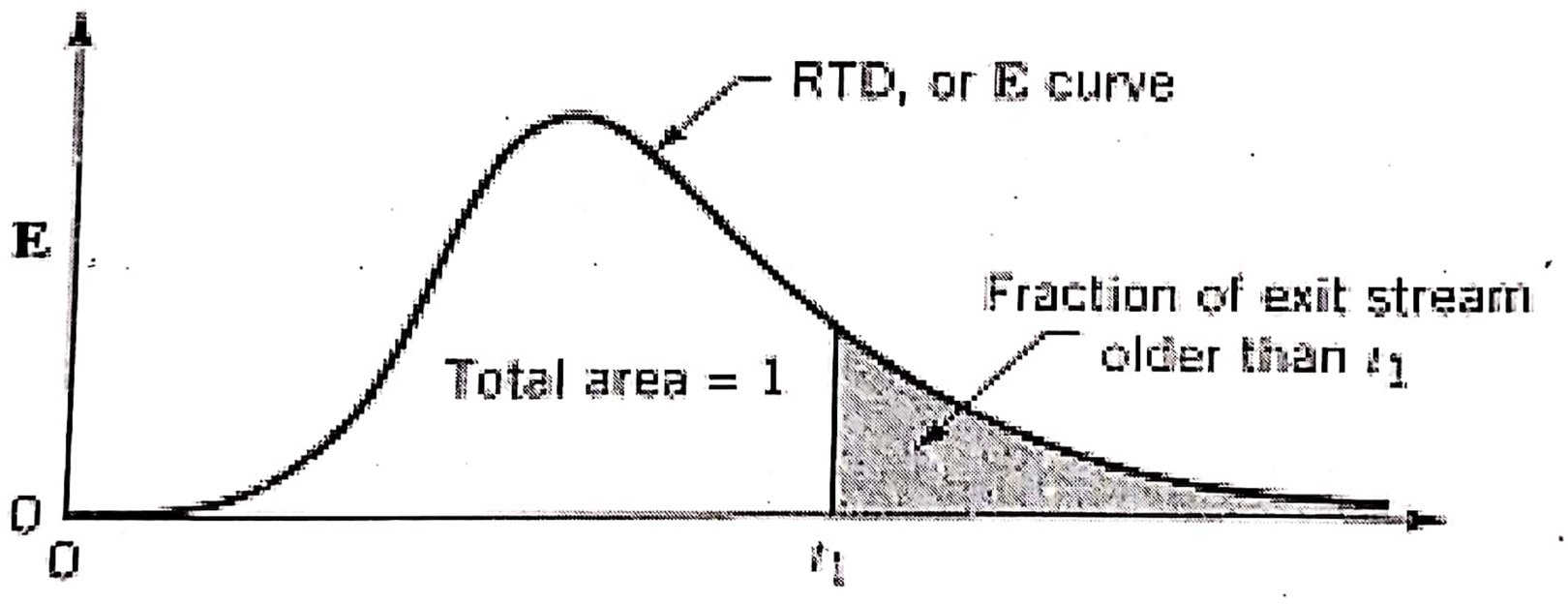


Figure 3.1 The exit age distribution curve E for fluid flowing through a vessel

Image Source- Levenspiel, Octave. Chemical Reaction Engineering. Wiley, 1999.

4- Compartment Model

Flow models can be of different levels of sophistication and the compartment models assumes the extremes of plug flow and mixed flow. By comparing the E curve for the real vessel with the theoretical curves for various combinations of compartments and through flow, we can find which model best best fits the real vessel. Of course, the fit will not be perfect; however, models of this kind are often a reasonable approximation to the real vessel.

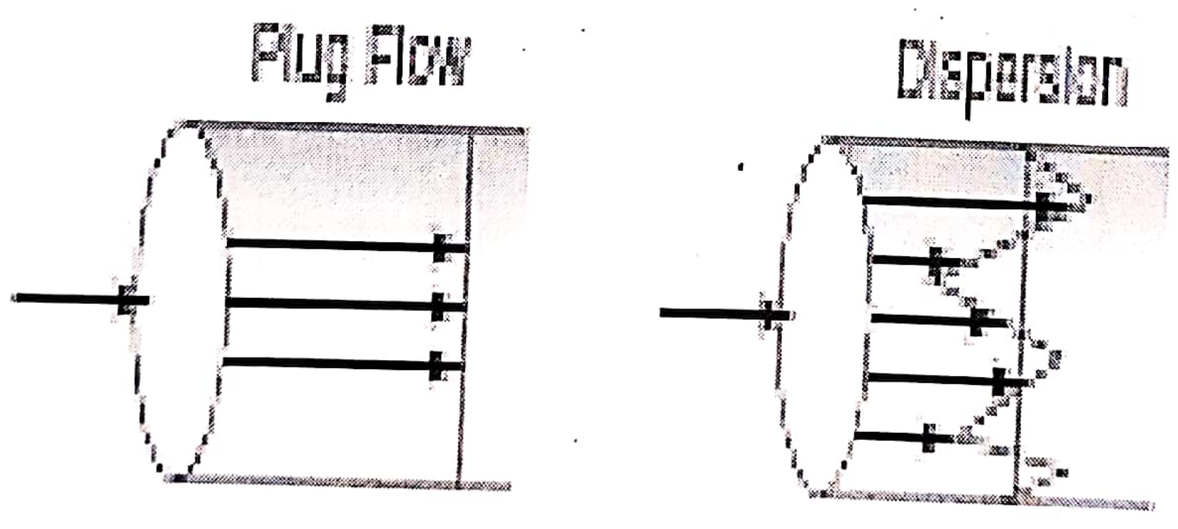
If we know M (kilograms of tracer introduced in the pulse) we can make a material balance check. Remember that M = v (area of curve). However, if we only measure the output C on an arbitrary scale, we cannot find M or make this material balance check[1]

We must know both V and v if we want to properly evaluate all the elements of a model, including dead spaces. If we only measure jobs, we cannot find the size of these stagnant regions and must ignore them in our model building.

The semilog plot is a convenient tool for evaluating the flow parameters of a mixed flow compartment. Just draw the tracer response curve on this plot, find the slope and intercept and this gives the quantities A, B, and C

5- The Dispersion Model

The one parameter to be determined in the dispersion model is the dispersion coefficient, Da. The dispersion model is used most often for non-ideal tubular reactors. The dispersion coefficient can be found by a pulse tracer experiment. The dispersion model is also used to describe nonideal tubular reactors. In this model, there is an axial dispersion of the material, which is governed by an analogy to Fick's law of diffusion, superimposed on the flow as shown in Figure. So in addition to transport by bulk flow, every component in the mixture is transported through any cross section of the reactor at a rate equal to [–DaAc(dC/dz)] resulting from molecular and convective diffusion. By convective diffusion (i.e., dispersion) we mean either Aris-Taylor dispersion in laminar flow reactors or turbulent diffusion resulting from turbulent eddies. Radial concentration profiles for plug flow (a) and a representative axial and radial profile for dispersive flow (b) are shown in Figure Some molecules will diffuse forward ahead of the molar average velocity while others will lag behind.[3]



(a) (b)

Figure 5 Concentration profiles (a) without and (b) with dispersion.

Image Source- Levenspiel, Octave. Chemical Reaction Engineering. Wiley, 1999.

Models are useful for representing flow in real vessels, for scale up, and for diagnosing poor flow. We have different kinds of models depending on whether flow is close to plug, mixed, or somewhere in between.. There are two models for this: the dispersion model and the tanks-in-series model. Use the one that is comfortable for you. They are roughly equivalent. These models apply to turbulent flow in pipes, laminar flow in very long tubes, flow in packed beds, shaft kilns, long channels, screw conveyers, etc. For laminar flow in short tubes or laminar flow of viscous materials these models may not apply, and it may be that the parabolic velocity profile is the main cause of deviation from plug flow. We treat this situation, called the pure convection model. [3]

Suppose an ideal pulse of tracer is introduced into the fluid entering a vessel. The pulse spreads as it passes through the vessel, and to characterize the spreading according to this model, we assume a diffusion-like process superimposed on plug flow. We call this dispersion or longitudinal dispersion to distinguish it from molecular diffusion. The dispersion coefficient D (m2/s) represents this spreading process. Thus large D means rapid spreading of the tracer curve small D means slow spreading D = 0 means no spreading, hence plug flow

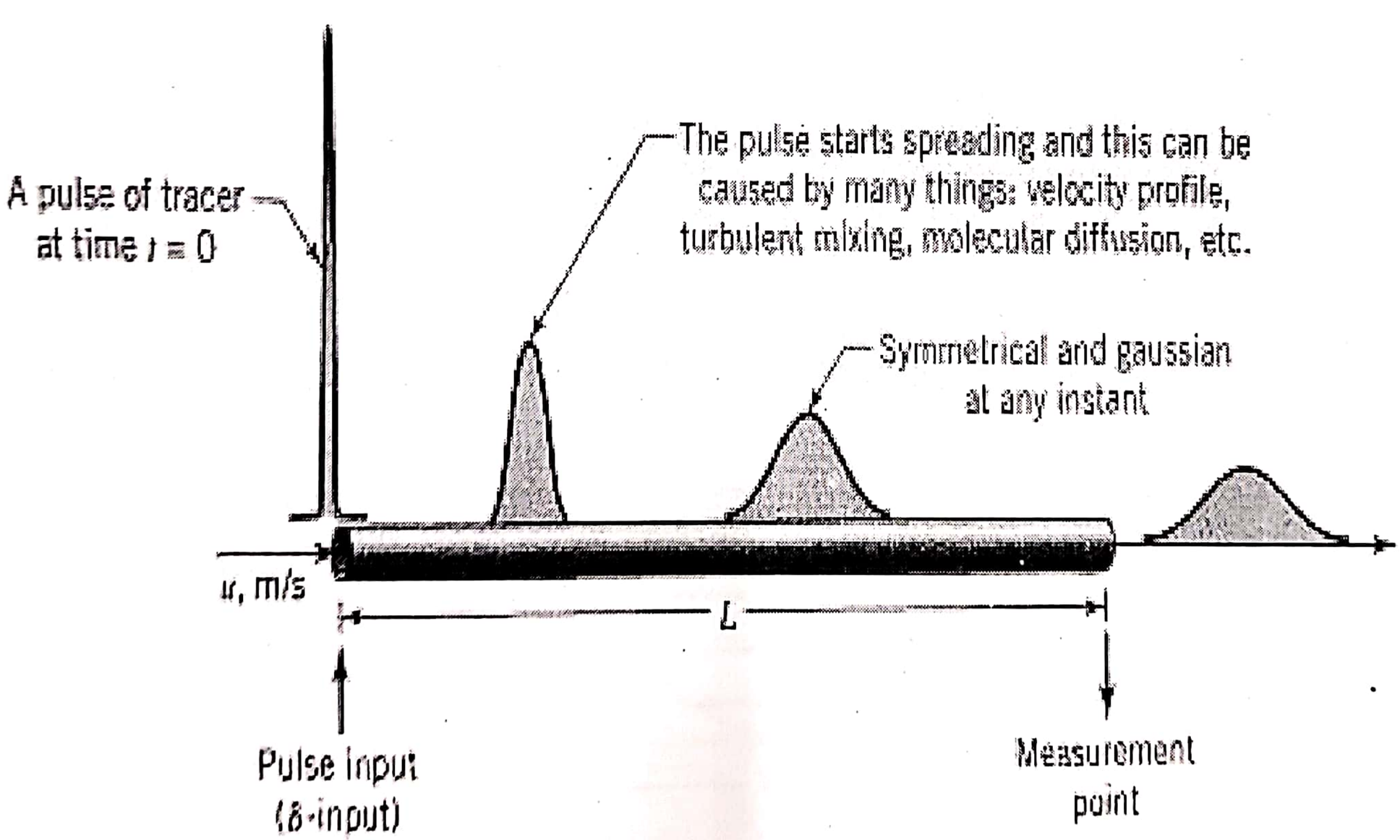


Figure5..1 The spreading of tracer according to the dispersion model.

Image Source- Levenspiel, Octave. Chemical Reaction Engineering. Wiley, 1999.

The one parameter to be determined in the dispersion model is the *dispersion coefficient*, D_a. The dispersion model is used most often for non-ideal tubular reactors. The dispersion coefficient can be found by a pulse tracer experiment.

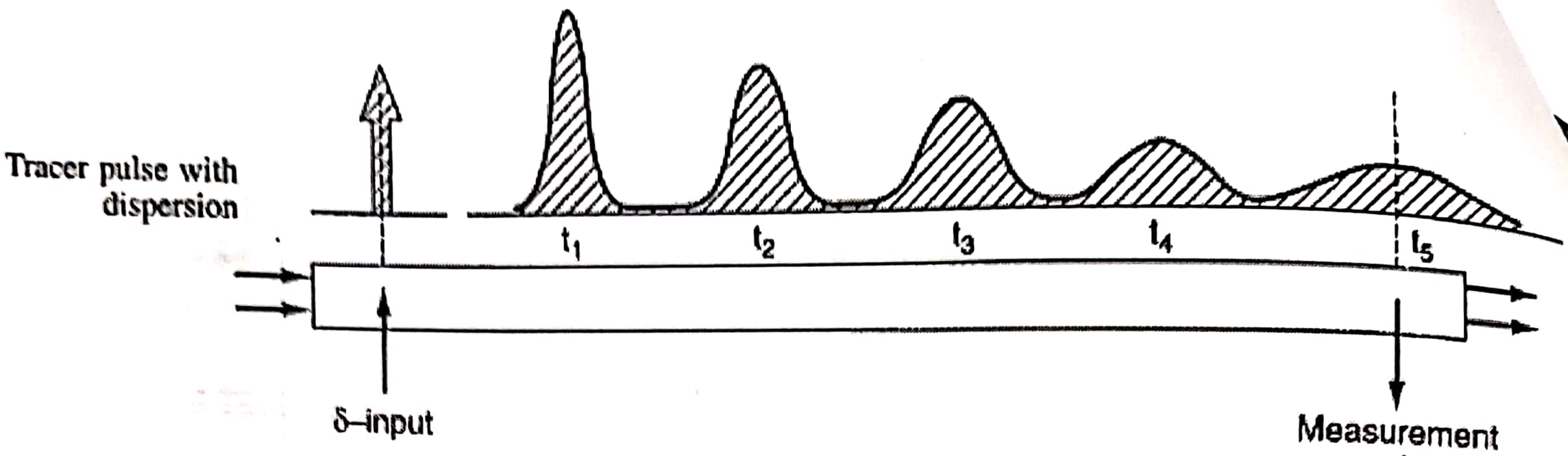


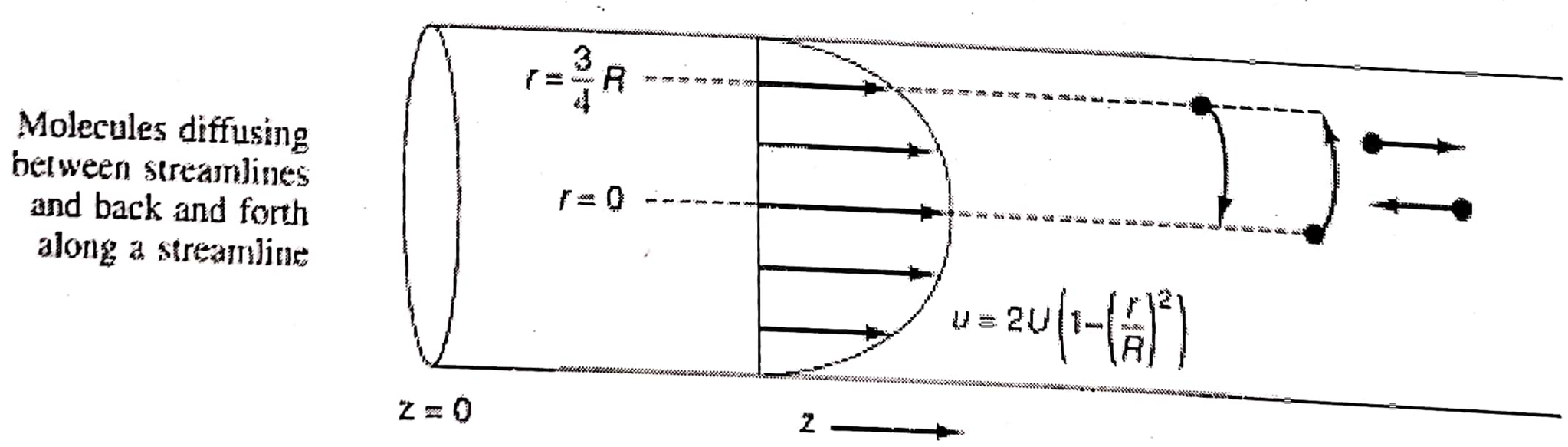
Image Source- Levenspiel, Octave. Chemical Reaction Engineering. Wiley, 1999.

After a very, very narrow pulse of tracer is injected, molecular diffusion (and eddy diffusion in turbulent flow) cause to pulse to widen as the tracer molecules diffuse randomly in all directions. The convective transport equation is:

$$D_a \frac{\partial C_T}{\partial Z^2} - U \frac{\partial C_T}{\partial Z} = \frac{\partial C_T}{\partial t}$$

Finding the Dispersion Coefficient

1) For laminar flow Taylor-Aris Dispersion, the molecules diffuse across radial streamlines as well as axially to disperse the fluid.



$$D_a = D_{AB} + \frac{UR^2}{D_{AB}}$$

Image Source- Levenspiel, Octave. Chemical Reaction Engineering. Wiley, 1999.

6- Tanks-In-Series Model

This model can be used whenever the dispersion model is used; and for not too large a deviation from plug flow both models give identical results, for all practical purposes. Which model you use depends on your mood and taste. The dispersion model has the advantage in that all correlations for flow in real reactors invariably use that model. On the other hand the tanks-in-series model is simple, can be used with any kinetics, and it can be extended without too much difficulty to any arrangement of compartments, with or without recycle. [4]

A real reactor will be modeled as a number of equally sized tanks-in-series. Each tank behaves as an ideal CSTR. The number of tanks necessary, n (our one parameter), is determined from the E(t) curve.

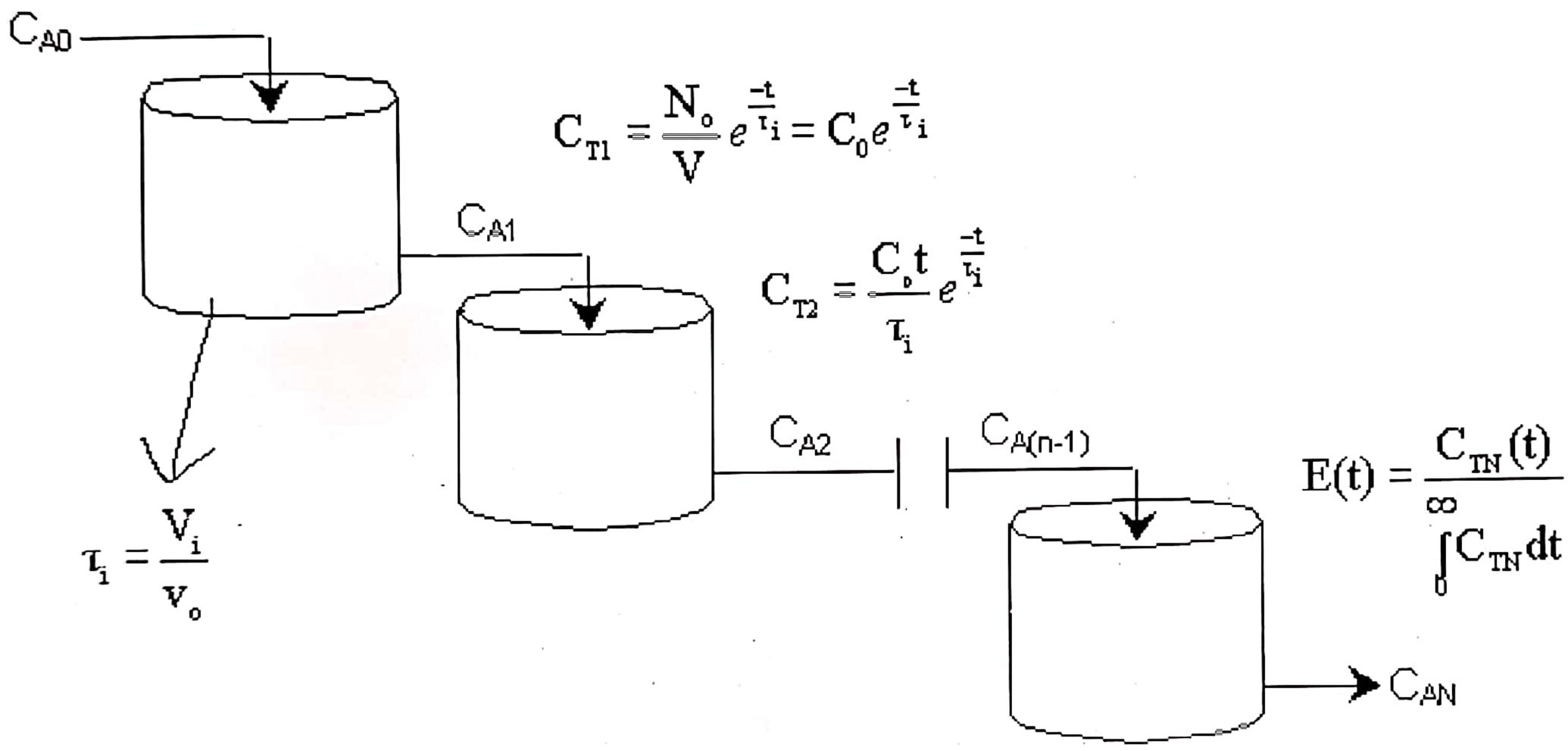


Image Source- Levenspiel, Octave. Chemical Reaction Engineering. Wiley, 1999.

For n tanks in series, E(t) is

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

where $\tau_i = \frac{\tau}{n}$

It can be shown that

$$t_m = \tau = n\tau_i$$

In dimensionless form $\theta = t/\tau = t/n\tau_i$

$$n\theta = t/\tau_i$$

$$E(\theta) = \tau E(t) = \frac{n(n\theta)^{n-1} e^{-n\theta}}{(n-1)!}$$

$$\sigma_\theta^2 = \frac{\sigma^2}{\tau^2} = \frac{\int_0^\infty (t-\tau)^2 E(t)dt\tau}{\tau^2}$$

$$\sigma_\theta^2 = \frac{\sigma^2}{\tau^2} = \int_0^\infty (\theta-1)^2 E(\theta)d\theta$$

Carrying out the integration for the n tanks-in-series $E(t)$

$$\boxed{\sigma_\theta^2 = \frac{\sigma^2}{\tau^2} = \frac{1}{n}}$$

$$\boxed{n = \frac{\tau^2}{\sigma^2}}$$

For a first order reaction

$$\boxed{X = 1 - \frac{1}{(1+\tau_i k)^n}}, \quad \tau_i = \frac{\tau}{n}$$

For reactions other than first order and for multiple reactions the sequential equations must be solved

$$V_i = V/n$$

$$V_i = v_o \frac{(C_{A0} - C_{A1})}{-r_{A1}}$$

$$V_i = v_o \frac{(C_{A1} - C_{A2})}{-r_{A2}}$$

$$\vdots$$

$$V_i = v_o \frac{(C_{An-1} - C_{An})}{-r_{An}}$$

Example

For a second order reaction with n = 3 $\left(V_1 = V_2 = V_3 = \frac{V}{3}\right)$

$$V_3 = \frac{(C_{A0} - C_A)V_0}{kC_A^2}$$

$\left(\tau_1 = \tau_2 = \tau_3\right)$ $\qquad \tau_3 k C_A^2 + C_A - C_{A0} = 0$

$$C_{A1} = \frac{-1 + \sqrt{1 + 4\tau_3 k C_{A0}}}{2\tau_3 k}$$

Similarly

$$C_{A2} = \frac{-1 + \sqrt{1 + 4\tau_3 k C_{A1}}}{2\tau_3 k}$$

$$C_{A3} = \frac{-1 + \sqrt{1 + 4\tau_3 k C_{A2}}}{2\tau_3 k}$$

$$X = 1 - \frac{C_{A3}}{C_{A0}} \,,\ \tau_3 = \frac{\tau}{3}$$

Image Source- Levenspiel, Octave. Chemical Reaction Engineering. Wiley, 1999.

7- Convection Model

When a tube or pipe is long enough and the fluid is not very viscous, then the dispersion or tanks-in-series model can be used to represent the flow in these vessels. For a viscous fluid, one has laminar flow with its characteristic parabolic velocity profile. Also, because of the high viscosity there is but slight radial diffusion between faster and slower fluid elements. In the extreme we have the pure convection model. This assumes that each element of fluid slides past its neighbour with no interaction by molecular diffusion. Thus the spread in residence times is caused only by velocity variations.[1][2]

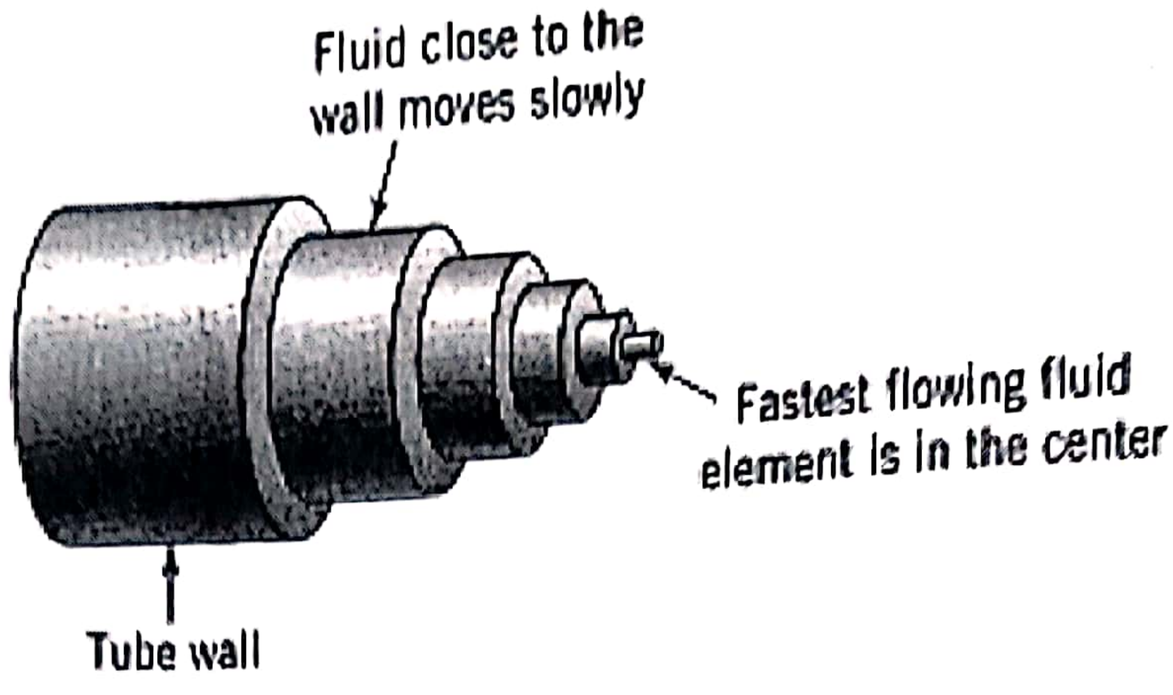


Figure 7 Flow of fluid according to the convection model.

Image Source- Levenspiel, Octave. Chemical Reaction Engineering. Wiley, 1999.

How to Tell from Theory Which Model to Use The first question to ask is, "Which model should be used in a given situation?" The following chart, adapted from Ananthakrishnan et al. (1965), tells what regime you are in and which model to use. Just locate the point on Fig. which corresponds to the fluid being used (Schmidt number), the flow conditions (Reynolds number), and vessel geometry (LldJ. But be sure to check that your system is not in turbulent flow. Remember that this chart only has meaning if you have laminar flow. In this chart !3lud, is the reciprocal of the Bodenstein number. It measures the flow contribution made by molecular diffusion. It is NOT the axial dispersion number, Dlud, except in the pure diffusion regime. The pure diffusion regime is not a very interesting regime because it represents very very slow flow. Gases are likely to be in the dispersion regime, not the pure convection regime. Liquids can well be in one regime or another. Very viscous liquids such as polymers are likely to be in the pure convection regime. If your system falls in the no-man's-land between regimes, calculate the reactor behavior based on he two bounding regimes and then try averaging. The numerical solution is impractically complex to use. Finally, it is very important to use the correct type of model because the RTD curves are completely different for the different regimes.[1]

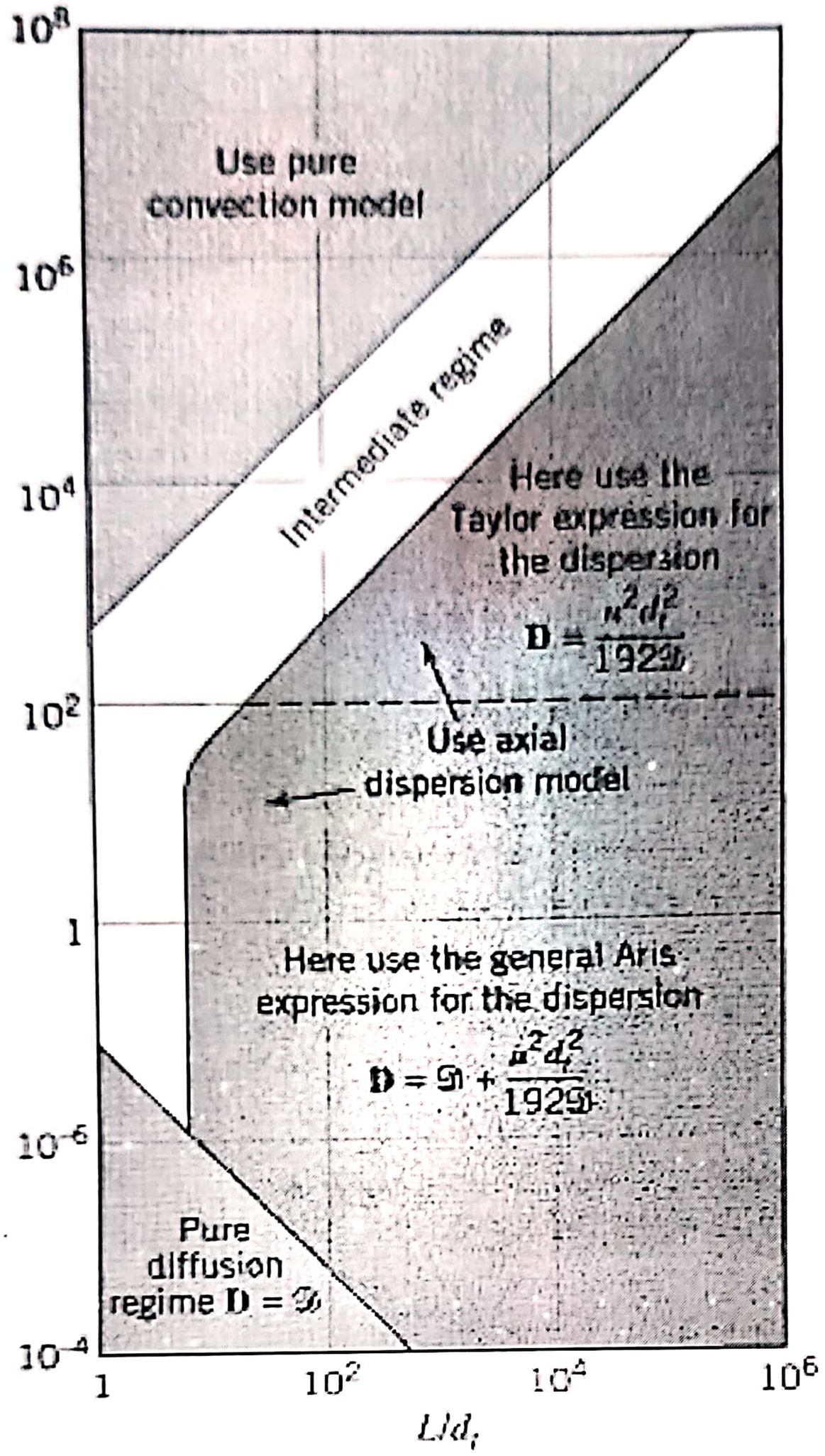


Figure 7.1 Map showing which flow models should be used in any situation

Image Source- Levenspiel, Octave. Chemical Reaction Engineering. Wiley, 1999.

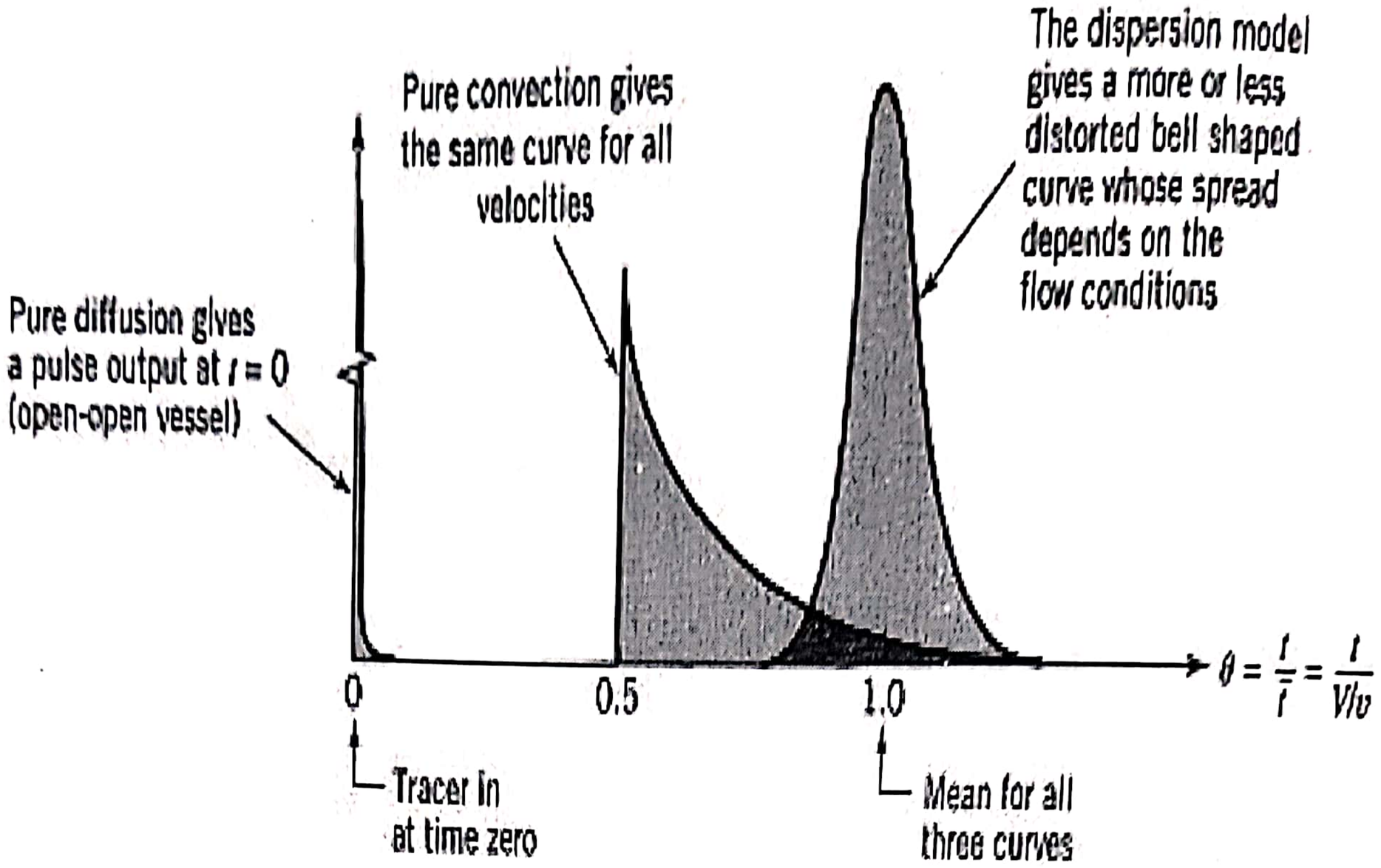


Figure 7.2 Comparison of the RTD of the three models

Image Source- Levenspiel, Octave. Chemical Reaction Engineering. Wiley, 1999.

8- Conclusion

The sharpest way of experimentally distinguishing between models comes by noting how a pulse or sloppy input pulse of tracer spreads as it moves downstream in a flow channel. For example,. The dispersion or tanks-in-series models are both stochastic models; 3 we see that the variance grows linearly with distance or The convective model is a deterministic model; thus, the spread of tracer grows linearly with distance, or Whenever you have measurements of a at 3 points use this test to tell which model to use.

The shape of the response curve is strongly influenced by the way tracer is introduced into the flowing fluid, and how it is measured. You may inject or measure the tracer in two main ways, as shown in. We therefore have four combinations of boundary conditions,, each with its own particular E curve. [5]

The application of the RTD to the prediction of reactor behaviour is based on the assumption that each fluid element (assume constant density) behaves as a batch reactor, and that the total reactor conversion is then the average conversion of all the fluid elements. Steady-state, isothermal ideal reactors were described in the context of their use to acquire kinetic data. In practice, conditions in a reactor can be quite different than the ideal requirements used for defining reaction rates. For example, a real reactor may have non uniform flow patterns that do not conform to the ideal PFR or CSTR mixing patterns because of comers, baffles, non uniform catalyst packing's, etc. Additionally, few real reactors are operated at isothermal conditions; rather they may be adiabatic or non isothermal. In this Techniques to handle non ideal mixing patterns are outlined. Although most of the discussion was centre around common reactor types found in the petrochemicals industries, the analyses presented can be employed to reacting systems in general (e.g., atmospheric chemistry, metabolic processes in living organisms, and chemical vapour deposition for microelectronics fabrication)

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3) Lecture 32 Chemical Reaction Engineering (CRE) is the field that studies the rates and mechanisms of chemical reactions and the design of the reactors. Published by Angelica Bell| SlidePlayer

4) Chapter 14 Models of Non Ideal Reactors ,Summary Notes, University Of Michigan

5) Non Ideal Flow in Reactors CalTech Authors, The California Institute of Technology by M.E Davis