



CHAPTER 2

CONCEPTS , MODELS , BOUNDARY CONDITIONS AND TRANSIENT SOLUTIONS FOR AXIAL DISPERSION FLOW IN PACKED BED

The present chapter will present the concepts of axial dispersion , a derivation of the dispersion model with a discussion of boundary conditions , then a transient solution for the model will be obtained under a selected set of boundary conditions .

2.1 Concepts of axial dispersion in packed beds

In general , when a fluid passes through the interstices of a packed bed , small amounts of fluid will be subjected to splitting , acceleration , deceleration and trapping . If these individual modes of mixing are repeated several times in a random order , then it results in a phenomena called axial mixing .

2.1.1 The axial dispersion mechanism

Langer et al (19) introduced the additive effect of two main mechanisms which contribute to axial dispersion ; molecular diffusion and turbulent mixing arising from the splitting and recombination of flow around the adsorbent particle , by ignoring the

influence from nonuniformity of packing¹ ,

Under extremely low flow rates and assuming that all flow has ceased , molecular diffusion would be the only operating mechanism in the bed which is considered as an assemblage of randomly oriented cylindrical pores formed by any given shape of packing . Diffusion in the axial direction will occur along the dormant fluid within the interstitial channels created by the packing as shown in figure 2.1 .

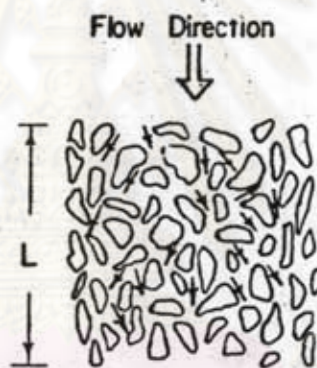


Fig. 2.1 Schematic Diagram of Packed Bed Illustrating the Nature of Tortuous and Constricted Paths

 1/ The uniformity of packing can give rise to significant addition dispersion from wall effects if the ratio of bed to particle diameter is not sufficiently large , usually a value larger than 10 should be appropriate (20) .

The molecular diffusion may be slowed down by two vital characteristics of the bed . One factor is the constriction or enlargement or branching of channels . Any of these constricted points will form traffic bottle necks , and thus obstruct diffusion . Another effect relates to the tortuous zigzag path of channels that prevent the diffusion from taking place along the shortest and direct path . Hence the combined tortuosity and constriction of channels provide the hindrance effect for molecular diffusion by a tortuosity factor . Many experimental results , derived from dispersion measurements for gases at low Reynolds number , confirm an approximate value of $1/\sqrt{2}$ or 0.707 for tortuosity . Carberry and Bretton (4) obtained a value of 0.67 while Evan and Kenney (7) had a value of 0.69 for spherical particles , and Edwards and Richardson (6) obtained a value of 0.73 . Therefore molecular diffusion mechanism is pertinent to axial dispersion by the relationship shown in equation 2.1 (2) .

$$E_z = \tau D_m \quad 2.1$$

At very high flow rates , the above expression cannot be used as turbulent mixing develops . Aris and Amundson (21) explained this phenomena using a simple model based on a series of mixing chambers , separated on the average by the mean particle diameter . They recommended a relationship between Peclet number and particle

diameter which was shown experimentally by Mc Henry and Wilhelm (8) to yield Peclet numbers in the region of 2 for high Reynolds numbers . Thus , for very high flow rates the following equation has been proposed ²

$$E_z = 1/2*(u*d_p) \quad 2.2$$

Combination of these two effects represents an axial dispersion coefficient expression as follows (24) :

$$E_z = \tau D_m + 1/2*(u*d_p) \quad 2.3$$

or

$$E_z/(u*d_p) = \tau D_m/(u*d_p) + 1/2 \quad 2.4$$

This ultimate representation fits the prospects of axial dispersion data in the fully turbulent region quite well , but at intermediate Reynolds numbers , dispersion is commonly somewhat greater than predicted by equation 2.3 . This is due to the effect of radial dispersion on the concentration gradient caused by axial dispersion (2) . Edward and Richardson (6) eventually suggested a particular term , which accounts for such effect , into the second

2/ See appendix A for the derivation of this relationship (23)

term on the right - hand side of equation 2.3 , and it becomes (2)

$$E_z/(u*d_p) = \gamma D_m/(u*d_p) + 1/\{2*[1 + \gamma D_m/(u*d_p)]\}$$

or

$$1/Pe = \gamma \epsilon / (Re * Sc) + 1/\{2*[1 + \beta \gamma / (Re * Sc)]\} \quad 2.4$$

The previous discussion in this section provides a global outlook of causes and effects for axial dispersion to arise . Now the concise definition of longitudinal dispersion will be cited and followed by two ideal flow models .

2.1.2 Definitions of axial dispersion

Carberry (23) defined the axial dispersion of a fluid flowing through a vessel , pipe , or packed bed as " a phenomenon which results in a distribution of residence times for a differential element of fluid entering the apparatus " . This infers that all species of fluid entering the device together must leave together if there exists a complete absence of forward and /or backward dispersion , termed axial dispersion and characterized by an axial dispersion coefficient (E_z) .

2.2 Models for axial dispersion in packed beds

2.2.1 The ideal plug flow model and the perfect mixing model

From the definitions given in the previous section , two extremes will be envisaged here (24,25) . At one extreme , a plug - flow or piston flow pattern shown in figure 2.2 is encountered with no longitudinal mixing but with complete radial mixing . This is characterized by an identical velocity and residence time of all elements of fluid within the reactor . For example , the flow pattern in a fixed bed reactor with very small ratios of the tube and particle diameter to length can be closely approximated by a plug - flow model .

The other extreme , referring to figure 2.3 , is a complete mixing flow characterized by a well - defined residence - time distribution of exponential form , and the identical composition of the exit stream and the fluid within the reactor . The behavior of many vigorously stirred - tanks closely approximates this flow pattern .

In the case of packed beds , neither of the two mentioned extremes describes the flow behavior within it properly (22) ; nevertheless the actual pattern deviates from these limiting conditions . Such deviations may arise from the velocity fluctuations due to molecular or turbulent diffusion (2) , channeling of fluid (26) , nonuniform velocity profiles caused by nonuniformity of packing (9) . The complexity of these phenomena leads to the investigation of a suitable model as discussed in the next section .

2.2.2 The Axial dispersed plug flow model

Various models have been proposed by previous investigators to describe the complicated flow behavior in packed beds (22) . However one of the most widely used models is the dispersion model in which the diffusion is superimposed on plug - flow and , thus , it is sometimes called the axial dispersed plug flow model or dispersion model . The general expression for this model is (27)

$$\frac{\partial c}{\partial t} + u \cdot \nabla c = (\tilde{D} \nabla^2 c) + S' + r_c \quad 2.5$$

For isothermal non - reactive compressible gas systems , a usual assumption is indicated as follows :



- Radial dispersion is negligible .
- Velocity profiles are uniform .
- Axial dispersion coefficients remain constant .
- No variations for all properties of the gas

With the above restrictions and omission of the source term (S'), equation (2.5) may be simplified to an ultimate model as :-

$$\frac{\partial c}{\partial t} + u \left(\frac{\partial c}{\partial z} \right) - E_z \left(\frac{\partial^2 c}{\partial z^2} \right) = 0 \quad 2.6$$

HOLD UP	CONVECTION	DISPERSION
TERM	TERM	TERM

In the last model the effects of all mechanisms which contribute to axial mixing are lumped together into a single effective axial dispersion coefficient (E_z) .

2.2.3 The relationship between the dispersion model and the compartments in series model

In the next section the derivation of the boundary conditions will be given . These matters relate to the dispersion model by some mathematical representation in the form of a compartments-in-series model. First , let us consider N equal sized , completely mixed

compartments arranged in series with back - flow characteristics as shown in figure 2.4

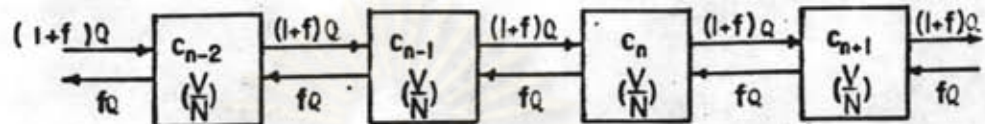


Fig. 2.4 Compartments-in-Series with Back-Flow Model

The material balance around the n-th compartment can be expressed as

$$(V/N) \frac{\partial c_n}{\partial t} = fQ(c_{n+1} - 2c_n + c_{n-1}) + Q(c_{n-1} - c_n) \quad 2.7$$

If we let $\Delta z = L/N$ then $QN/V = u/\Delta z$ and the above equation eventually becomes

$$\frac{\partial c_n}{\partial t} = (f \cdot u / \Delta z) (c_{n+1} - 2c_n + c_{n-1}) - (u / \Delta z) (c_n - c_{n-1}) \quad 2.8$$

By means of the Taylor expansion, the dispersion model represented by equation 2.6 can be approximated by the following difference equation

$$\partial c_n / \partial t = E_z / (\Delta z)^2 (c_{n+1} - 2c_n + c_{n-1}) - (u/\Delta z)(c_n - c_{n-1}) \quad 2.9$$

Comparing equation 2.8 and 2.9 , an approximation of these two models is

$$fu/\Delta z = E_z / (\Delta z)^2 \quad \text{or} \quad f = E_z / (u\Delta z) = (L/\Delta z)/M \quad 2.10$$

where $M = uL/(2E_z)$

This gives rise to a replacement of the dispersion model by the compartment - in - series with back flow model when a first order approximation is used . Or vice versa , if the number of compartments approaches infinity , the compartment - in - series with back - flow model approaches the dispersion model .

Now consider another compartment - in - series without back - flow model depicted in figure 2.5

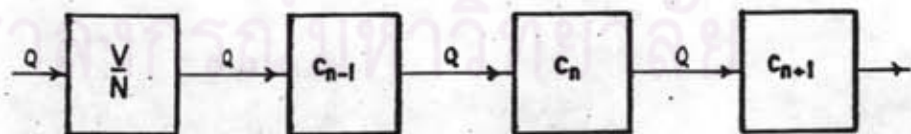


Fig. 2.5 Compartments-in-Series without Back-Flow Model

The material balance around the n - th compartment gives

$$(V/N) * (\partial c_n / \partial t) = -Q * (c_n - c_{n-1})$$

or

$$\begin{aligned} \partial c_n / \partial t &= u \Delta z / 2 (\Delta z)^2 * (c_{n+1} - 2c_n + c_{n-1}) \\ &\quad - u / 2 \Delta z (c_{n+1} - c_{n-1}) \end{aligned} \quad 2.11$$

Again comparing equation 2.17 with 2.9 , of which the third term can also be written as $(u/2\Delta z) * (c_{n+1} - c_{n-1})$, thus the equivalence of the two models yields

$$u * \Delta z / 2 = E_z \quad \text{or} \quad u * L / 2E_z = N \quad 2.12$$

Therefore , for a large N , $M = N$; for a small N , $M = N - 1$ or $N \rightarrow 1$ as $M \rightarrow 0$

Both suggested models lead to the two limiting cases of ideal flow models as mentioned earlier , i.e. , the plug - flow model when $N \rightarrow \infty$ then $E_z \rightarrow 0$ and the complete mixing model when $N \rightarrow 1$ and $E_z \rightarrow \infty$

2.3 General boundary conditions for axial dispersion in packed beds

2.3.1 General boundary conditions formulation

Usually , the proper boundary conditions at the entrance region and / or the exit region must be assigned . Therefore the focus on a general specification of appropriate boundary conditions will contribute to satisfy the continuity imposed on the system concentration field , $c(z,t)$.

In a tube of finite length , the dispersion is presumed to persist in the upstream section and / or the downstream section with dispersion coefficients that may or may not be identical to that in the tube . The practical lengths of the appended sections depend on the magnitudes of the dispersion coefficients in these portions , virtually vanishing when negligible dispersion occurs there . For the present , let us consider the appended sections to be infinitely long if finite dispersion exists there . On the other hand , it is feasible to conceive of pre- or post- tube sections in which the dispersion coefficient may be regarded as being assigned to an infinite length . Finally the case of zero dispersion , that dispenses with the need for ascribing a definite length to the appended sections , will also be observed .

Figure 2.6 depicts the system with the tube length between $z = -L$ and $z = L$, the dispersion coefficients are assumed to be uniform in the tube , fore section and aft section with symbols given by E_z , E_z^- , E_z^+ .

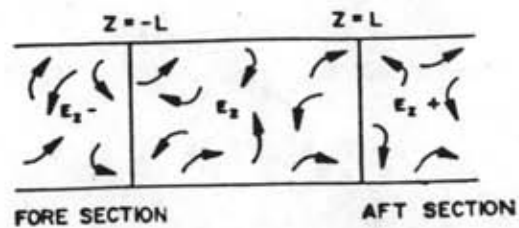


Fig 2.6 Column showing dispersion in fore-, packed- and aft-sections of flow system

Based on the continuity conditions of the concentration field, the following two equations are obtained :

$$\lim_{Z \rightarrow -L-0} c = \lim_{Z \rightarrow -L+0} c \quad ; \quad \lim_{Z \rightarrow -L-0} (E_z(\partial c / \partial z)) = \lim_{Z \rightarrow -L+0} E_z(\partial c / \partial z) \quad 2.13$$

$$\lim_{Z \rightarrow L-0} c = \lim_{Z \rightarrow L+0} c \quad ; \quad \lim_{Z \rightarrow L-0} E_z(\partial c / \partial z) = \lim_{Z \rightarrow L+0} E_z(\partial c / \partial z) \quad 2.14$$

equation 2.13 implies a finite non - zero dispersion coefficient in the infinitely long fore section ; while equation 2.8 holds when the aft section is infinitely long with a finite non - zero dispersion coefficient , if the pre - tube section can be represented by equation 2.15 . Similarly , a well - mixed aft section of volume V_+ yields a condition as represented by equation 2.16

$$\lim_{Z \rightarrow L+0} c = c_- \quad ; \quad \lim_{Z \rightarrow L+0} (E_z(\partial c / \partial z) - vc) + vc_f = V_- / A (dc / dt) \quad 2.15$$

$$\lim_{z \rightarrow L-0} c = c_+ \quad ; \quad \lim_{z \rightarrow L-0} (-E_z(\partial c / \partial z)) = V_+ / A (dc/dt) \quad 2.16$$

In the case where either volume , V_- or V_+ ,at the end of the tube is allowed to vanish , the foregoing boundary conditions appear :

$$\lim_{z \rightarrow -\infty} c = c_f \quad 2.17$$

$$\lim_{z \rightarrow -\infty} c < \infty \quad 2.18$$

Upon the nature of the appended section , Parulekar and Ramkishna (17) gave a complete list of nine possible boundary conditions corresponding to those of Yano and Aratani (28) . Table 2.1 lists these various possibilities obtained from equation 2.13 - 2.18 .

2.3.2. Boundary conditions at the tracer input point

Let us pictorially represent the nature of nine cases with different boundary conditions . Based on the two models suggested in section 2.2.3 , boundary conditions at tracer input point are first derived , then followed by those at the tracer output point . To deal with the former case , let us introduce a tracer with a very small volumetric flow rate , Q , be introduced at $z = 0$ into the

TABLE 2.1 VARIOUS POSSIBILITIES OF BOUNDARY CONDITIONS

Case	E_z^-	E_z^+	Volume of fore section	Volume of aft section	Boundary condition at tube outlet	Boundary condition at tube inlet
1	finite, non-zero	finite, non-zero	infinite	infinite	Eq. 2.13	Eq. 2.14
2	finite, non-zero	0	infinite	-	Eq. 2.13	D.B.C.*
3	0	finite, non-zero	-	infinite	D.B.C.	Eq. 2.14
4	0	0	-	-	D.B.C.	D.B.C.
5	∞	finite, non-zero	finite	infinite	Eq. 2.15	Eq. 2.14
6	∞	0	finite	-	Eq. 2.15	D.B.C.
7	0	∞	-	finite	D.B.C.	Eq. 2.16
8	finite, non-zero	∞	infinite	finite	Eq. 2.13	Eq. 2.16
9	∞	∞	finite	finite	Eq. 2.15	Eq. 2.16

*D.B.C. is Danckwerts boundary condition

tube , to using a flow that could possibly be described by both dispersion model and the compartment - in - series with back - flow model as shown in figure 2.7

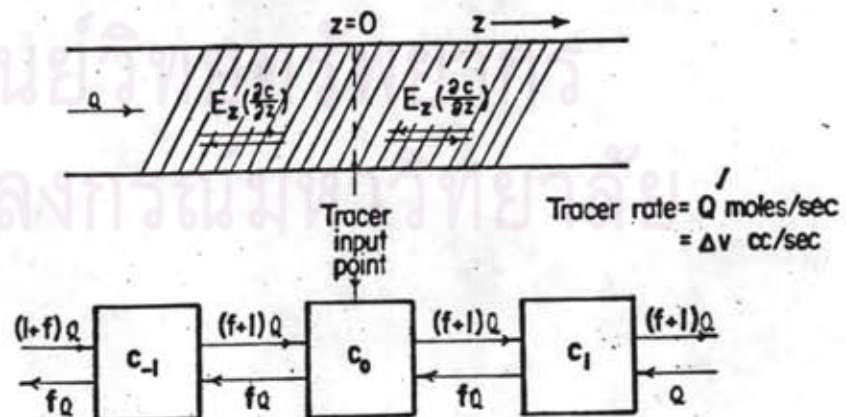


Fig. 2.7 Tracer Input to the Dispersion Model with an Open Entrance and to the Compartment-in-Series with Back-flow Model

As $\Delta Q \ll Q$ and if no dispersion occurs, tracer concentration c_{in} downstream from the injection point can be given as

$$c_{in} = Q' / (Q + \Delta Q) = Q' / Q$$

However, the tracer concentration in the main stream, c , should differ from c_{in} since the dispersion of the tracer does take place

$$(V/N)(dc_0/dt) = Q(c_{-1} - c_0) + Qc_{in} + fQ(c_{-1} - 2c_0 + c_{+1}) \quad 2.19$$

By applying the equivalent relation as in equation 2.10, equation 2.19 becomes

$$\Delta z(dc_0/dt) = u(c_{-1} - c_0 + c_{in}) + E_z((c_{+1} - c_0)/\Delta z - (c_0 - c_{-1})/\Delta z)$$

when $\Delta z \rightarrow 0$

$$uc_{z \rightarrow 0^+} - uc_{z \rightarrow 0^-} - uc_{in} = E_z(\partial c / \partial z)_{z \rightarrow 0^+} - E_z(\partial c / \partial z)_{z \rightarrow 0^-}$$

with regards to continuity of concentration at the tracer input point, we have $c_{z \rightarrow 0^+} = c_{z \rightarrow 0^-}$. Therefore for the non-constricted or open entrance region of the tube as shown in figure 2.7, the ultimate boundary condition can be obtained as



$$uc_{in} = E_z(\partial c/\partial z)_{z \rightarrow 0^-} - E_z(\partial c/\partial z)_{z \rightarrow 0^+} \quad 2.20$$

Similarly the boundary condition for close - entrance region of the dispersion model in figure 2.8 may be obtained as follows :

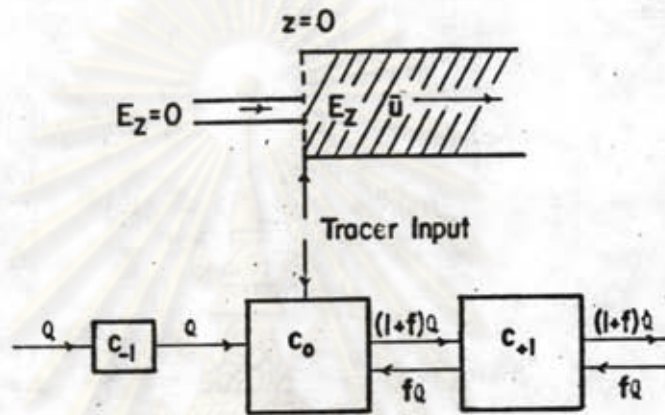


Fig. 2.8 Tracer Input to the Dispersion Model with a Closed Entrance and to the Compartments-in-Series Model

a material balance around compartment zero gives

$$(V/N)(dc_0/dt) = Q(c_{-1} - c_0) + Qc_{in} + fQ(c_{+1} - c_0)$$

or

$$\Delta z(dc_0/dt) = u(c_{-1} - c_0 + c_{in}) + E_z\{(c_{+1} - c_0)/\Delta z\}$$

as $\Delta z \rightarrow 0$ and $c_{-1} = 0$

$$uc_{in} = uc_{z \rightarrow 0^+} - E_z (\partial c / \partial z)_{z \rightarrow 0^+}$$

This condition shows that once the material enters the tube, none diffuses out from it.

2.3.3 Boundary conditions at the tracer detection point

At the exit region, the boundary conditions may be derived by the same procedure as the previous illustration. Referring to figure 2.9, the material balance for the n -th compartment in the case of open exit can be written as

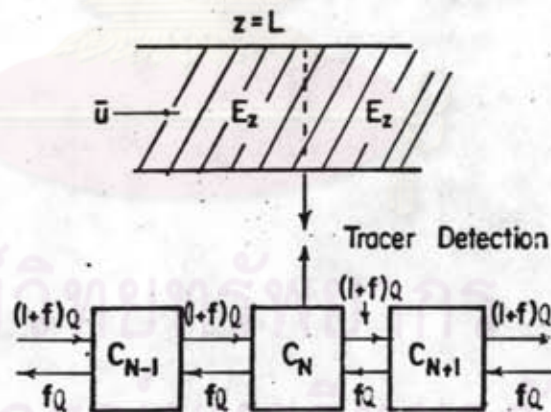


Fig. 2.9 Tracer Detection at an Open Exit Point for the Dispersion Model and the Compartments-in-Series Model

$$(V/N)(dC_N/dt) = Q(C_{N-1} - C_N) + fQ(C_{N-1} - 2C_N + C_{N+1})$$

or

$$\Delta z(dC_N/dt) = u(C_{N-1} - C_N) + E_z [\{ (C_{N-1} - C_N) / \Delta z \} - \{ (C_N - C_{N+1}) / \Delta z \}]$$

letting $\Delta z \rightarrow 0$ and $C_{N-1} \rightarrow C_N \rightarrow C_{N+1}$, thus

$$C_{out} = C_{z=L} \quad 2.22$$

For the close - exit region depicted in figure 2.10 , the material balance around the N - th compartment is

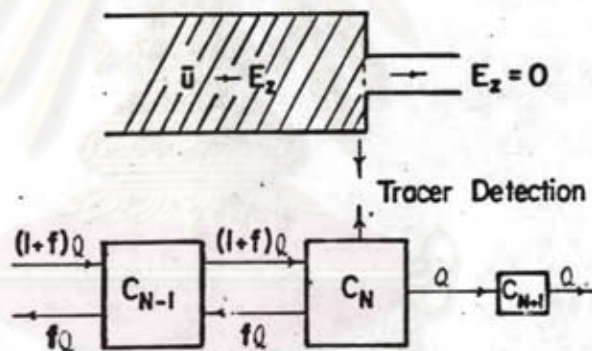


Fig.2.10 Tracer Detection at a Closed Exit Point for the Dispersion Model and the Compartments-in-Series Model

$$(V/N)(dC_N/dt) = Q(C_{N-1} - C_N) + fQ(C_{N-1} - C_N)$$

or

$$z(dC_N/dt) = u(C_{N-1} - C_N) + E_z [\{ (C_{N-1} - C_N) / \Delta z \}]$$

As $\Delta z \rightarrow 0$, $C_{N-1} \rightarrow C_N$ and $C_{out} = C_{z=L}$, the final results can be expressed as

$$(ec/\partial z)_{z=L} = 0 \quad 2.23$$

Once again equation 2.23 represents the case where no material diffuses back to the system when it leaves the tube .

In many cases , the fluid mixing at the exit and entrance region is often very close to perfect mixing condition . Therefore a dispersion model coupled with complete mixing tanks at either ends may be employed (28) .

In order to summarize the forementioned cases pictorially , table 2.2 presents all nine cases with their boundary conditions corresponding to those defined in table 2.1 (29) .

Since assigning a particular boundary condition to the system of interest leads to a specific solution of which result can be used to predict total system flow patterns , thus for measurement of tracer output signals made outside the boundaries of the packing in the packed bed , it necessitates the use of a closed-closed system .

Table 2.2 Transfer Function and Boundary Conditions for Axial-Dispersion Model

Type of Vessel	Boundary Conditions	Transfer Function	Mean	Variance
<p>Open - Open</p>	$\left. \begin{aligned} \bar{u}c_{in} - E_z \left(\frac{\partial c}{\partial z} \right)_{z=0^-} \\ - E_z \left(\frac{\partial c}{\partial z} \right)_{z=0^+} \\ c_{z=0^-} = c_{z=0^+} \end{aligned} \right\} \text{ at } z=0$ $\left. \begin{aligned} c_{z=L} = c_{out} \end{aligned} \right\} \text{ at } z=L$	$\frac{\exp[M(1-\beta)]}{\beta}$ <p>where $\beta = \sqrt{1+250/M}$ $M = \bar{u}L/2E_z$, $\beta = L/\bar{u}$</p>	$1 + \frac{1}{M}$	$\frac{(M+2)}{M^2}$
<p>Open - Closed</p>	$\left. \begin{aligned} \bar{u}c_{in} - E_z \left(\frac{\partial c}{\partial z} \right)_{z=0^-} \\ - E_z \left(\frac{\partial c}{\partial z} \right)_{z=0^+} \\ c_{z=0^-} = c_{z=0^+} \end{aligned} \right\} \text{ at } z=0$ $\left. \begin{aligned} \left(\frac{\partial c}{\partial z} \right)_{z=L} = 0 \\ c_{z=L} = c_{out} \end{aligned} \right\} \text{ at } z=L$	$\frac{2\exp[M(1-\beta)]}{(1+\beta)}$	$1 + \frac{1}{2M}$	$\frac{(4M+3)}{(2M)^2}$
<p>Closed - Open</p>	$\left. \begin{aligned} \bar{u}c_{z=0^+} - \bar{u}c_{in} \\ - E_z \left(\frac{\partial c}{\partial z} \right)_{z=0^+} \\ c_{z=0^-} = 0, c = 0 \text{ for } z < 0 \end{aligned} \right\} \text{ at } z=0$ $\left. \begin{aligned} c_{z=L} = c_{out} \end{aligned} \right\} \text{ at } z=L$	$\frac{2\exp[M(1-\beta)]}{(1+\beta)}$	$1 + \frac{1}{2M}$	$\frac{(4M+3)}{(2M)^2}$
<p>Closed - Closed</p>	$\left. \begin{aligned} \bar{u}c_{z=0^+} - \bar{u}c_{in} \\ - E_z \left(\frac{\partial c}{\partial z} \right)_{z=0^+} \\ c_{z=0^-} = 0, c = 0 \text{ for } z < 0 \end{aligned} \right\} \text{ at } z=0$ $\left. \begin{aligned} \left(\frac{\partial c}{\partial z} \right)_{z=L} = 0 \\ c_{z=L} = c_{out} \end{aligned} \right\} \text{ at } z=L$	$\frac{48\exp[M(1-\beta)]}{(1+\beta)^2 - (1-\beta)^2 \exp(-2M\beta)}$	1.0	$\frac{2M-1+e^{-2M}}{2M^2}$

2.4 Transient equation for the axial dispersed plug - flow model with a delta function input

Referring to equation 2.6^a, if the following closed - closed boundary condition equation

$$c_{in}(t) = c|_{z=0} - (1/Pe)(\partial c/\partial z)|_{z=0} \quad 2.24$$

$$(\partial c/\partial z)|_{z=1} = 0 \quad 2.25$$

is applied in its dimensionless form

$$(1/Pe)(\partial^2 c/\partial z^2) - (\partial c/\partial z) = \tau(\partial c/\partial z) \quad 2.26$$

with the following initial condition

$$c(z,t=0) = 0 \quad 2.27$$

3/ The derivation of equations 2.6 and 2.24 - 2.28 is shown in appendix B

2.4 Transient equation for the axial dispersed plug - flow model with a delta function input

Referring to equation 2.6³, if the following closed - closed boundary condition equation

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with the following initial condition

$$c(z,t=0) = 0 \quad 2.27$$

3/ The derivation of equations 2.6 and 2.24 - 2.28 is shown in appendix B

point $z=0$ in the column) is the dirac function defined as follows
(29)

$$\delta(t) = \lim_{A \rightarrow 0} \delta_A(t)$$

$$\text{where } \delta_A(t) = \begin{cases} 0 & \text{for } t < 0 \\ 1/A & \text{for } 0 < t < A \\ 0 & \text{for } t > 0 \end{cases}$$

and its Laplace transform is

$$\begin{aligned} \mathcal{L}[\delta(t)] &= \mathcal{L}[\lim_{A \rightarrow 0} \delta_A(t)] = \int_0^{\infty} \lim_{A \rightarrow 0} [\delta_A(t) e^{-st}] dt \\ &= \lim_{A \rightarrow 0} \int_0^{\infty} [\delta_A(t) e^{-st}] dt = \lim_{A \rightarrow 0} [(1/A)s(1-e^{-sA})] \end{aligned}$$

Using l'Hospital's rule ,

$$\lim_{A \rightarrow 0} [(1/A)s(1-e^{-sA})] = \lim_{A \rightarrow 0} [se^{-sA}/s] = 1$$

Therefore the ultimate exit concentration in the Laplace domain is equivalent to equation 2.28 multiplied by one or

$$\bar{c}(z=1,s) = H(s) = Pe[(\lambda_1 - \lambda_2) / (\lambda_1^2 e^{-\lambda_2} - \lambda_2^2 e^{-\lambda_1})] \quad 2.29$$

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$$\begin{aligned} \mathcal{L}[\delta(t)] &= \mathcal{L}[\lim_{A \rightarrow 0} \delta_A(t)] = \lim_{A \rightarrow 0} \int_0^{\infty} \delta_A(t) e^{-st} dt \\ &= \lim_{A \rightarrow 0} \int_0^A [\delta_A(t) e^{-st}] dt = \lim_{A \rightarrow 0} [(1/As)(1-e^{-sA})] \end{aligned}$$

Using l'Hospital's rule ,

$$\lim_{A \rightarrow 0} [(1/As)(1-e^{-sA})] = \lim_{A \rightarrow 0} [se^{-sA}/s] = 1$$

Therefore the ultimate exit concentration in the Laplace domain is equivalent to equation 2.28 multiplied by one or

$$\bar{c}(z=1,s) = H(s) = Pe[(\lambda_1 - \lambda_2) / (\lambda_1^2 e^{-\lambda_2} - \lambda_2^2 e^{-\lambda_1})] \quad 2.29$$

If equation 2.29 can be transformed into the time domain , the result obtained is also the effluent concentration at any point of time .

Since the analytical inversion of equation 2.29 is not possible , it requires the transformation of this expression from the Laplace domain to the frequency domain by replacing s by i . The ultimate expression yields ⁴

$$H(i\omega) = \text{Re}(\omega) + i\text{Im}(\omega) \quad 2.30$$

where $\text{Re}(\omega)$ represents the real part of the complex number
 $\text{Im}(\omega)$ is the imaginary part of the complex number

In this study , this Fourier function is completely inverted into the time domain by using MathCad , a commonly used PC package programe .⁵

4/ See Appendix C for the derivation of this complex form

5/ The concept of Fast Fourier Transform is presented in appendix D