

## Chapter 2 Dispersion of Concentration (Saturation) Waves

Earlier we calculated how concentration and saturation waves propagated in the absence of dispersion. Here we will examine the effect of dispersion on the transport through porous media. **Dispersion** is the process of distributing or spreading out of concentration (or saturation) profiles due to mechanisms in which the flux is proportional to the concentration (saturation) gradient. **Diffusion** is a special case of dispersion when the velocity of the fluid is zero. The spreading of waves due to the dependence on the fractional flow curve, partitioning between phases, and/or the adsorption on the solid are **not** dispersion phenomena because in these phenomena the flux depends on the concentration, not on the gradient of the concentration. The species mass conservation equation includes a term with the divergence of the flux of the species. If the flux depends on the concentration gradient, then the conservation equation will have second order spatial derivatives of concentration. Thus, dispersion will add second order spatial derivatives of concentration (or saturation) to the conservative equation. Some people refer to dispersion as a special case of dissipation. We will not use that definition because dissipation is defined as the act of disappearing, wasting away, or vanishing; e.g., viscous dissipation refers to the irreversible conversion of mechanical energy to thermal energy. Dispersion is a process in which the mass of the species is conserved. The definition of dissipation suggests that some quantity is not being conserved.

Dispersion flux in porous media is described by an anisotropic dispersion tensor,  $\mathbf{K}$ . The equation for dispersion flux that is analogous to Fick's law for diffusion is as follows (Perkins and Johnston 1963).

$$\mathbf{J}_i = -\phi \mathbf{K} \nabla C_i$$

### Mechanisms of Dispersion

#### Molecular diffusion

The most fundamental process for dispersion is molecular diffusion. Molecules in the liquid or vapor states are not stationary even if the bulk fluid velocity is zero because the molecules are in continuous motion. The trajectory of a molecule during a time interval  $\tau$  may appear as in Fig. 2.1 as a result of collisions with surrounding molecules. If the direction after each collision is random, then the mean square distance traveled is proportional to time and the proportionality constant is the molecular diffusivity (Haile 1992).

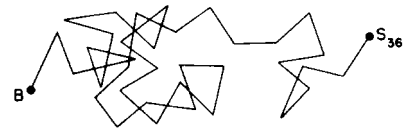


Fig. 41-6. A random walk of 36 steps of length  $l$ . How far is  $S_{36}$  from  $B$ ?  
Ans: about  $6l$  on the average.

Fig. 2.1 Random walk trajectory of a molecule (Feynman 1963)

$$\langle |\mathbf{x} - \mathbf{x}_B|^2 \rangle = 6D\tau$$

or

$$D \equiv \frac{\langle |\mathbf{x} - \mathbf{x}_B|^2 \rangle}{6\tau}$$

Einstein reasoned that if the specie is a spherical solute molecule in a solvent that is made up of much smaller molecules, then the molecular diffusivity can be modeled by the Stokes-Einstein model (Einstein 1905).

$$D_o = \frac{kT}{6\pi\mu R}$$

where  $k$  is the Boltzmann constant,  $T$  is the absolute temperature,  $\mu$  is the viscosity of the solvent, and  $R$  is the radius of the solute.

Fig. 2.2 illustrates a transport zone along which the concentration of component  $i$  changes. To the left of reference plane  $AB$  (unit area), the concentration of component  $i$  is  $C_{i1}$ , and similarly  $C_{i2}$  on the right hand side. During the time,  $\tau$ , all particles will move a distance,  $\bar{x}$ , due to thermal motions of the molecules

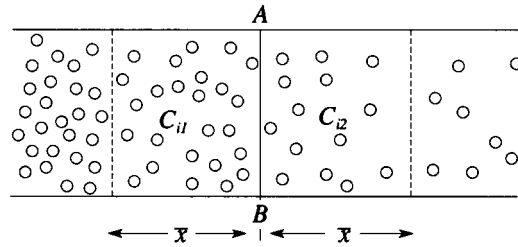


Fig. 2.2 Model for diffusion with a concentration gradient (T. Holt 1992)

(average displacement due to Brownian motion during  $\tau$ ). As the probability of the molecule to move in either direction is the same, the amount of component  $i$ ,  $n_i$ , crossing  $AB$  from the left during the time  $\tau$  is

$$\bar{n}(C_{i1}) = \frac{1}{2} C_{i1} \bar{x}$$

and a corresponding amount of component  $i$  moving from the right, crossing  $AB$  is

$$\bar{n}(C_{i2}) = \frac{1}{2} C_{i2} \bar{x}$$

The net flux,  $J_i$ , across  $AB$  then becomes

$$\begin{aligned}
J_i &= \frac{\bar{n}(C_{i1}) - \bar{n}(C_{i2})}{\tau} \\
&= \frac{\bar{x}^2 (C_{i1} - C_{i2})}{2\tau \bar{x}} \\
&= -\frac{\bar{x}^2}{2\tau} \frac{dC_i}{dx} \\
&= -D_{oi} \frac{dC_i}{dx}
\end{aligned}$$

(Note: The above equation defined D as 1/2 mean squared distance divided by time whereas we earlier defined D as 1/6 mean squared distance divided by time. However, the above equation considered displacement in only one dimension. The projection of the mean squared distance onto one coordinate axis is 1/3 of the mean squared distance, i.e.,  $\langle |\mathbf{x} - \mathbf{x}_o|^2 \rangle = \langle |x - x_o|^2 \rangle + \langle |y - y_o|^2 \rangle + \langle |z - z_o|^2 \rangle$ .)

In three dimensions the flux is expressed in vector form.

$$\mathbf{J}_i = -D_{oi} \nabla C_i$$

The last equation is Fick's law for diffusion (Bird, Stewart, Lightfoot 1960). We showed earlier that the mean squared distance divided by time was a constant equal to the molecular diffusivity.

### Diffusion through porous media

Consider the case a single fluid phase and zero velocity. The dispersion will be due to only molecular diffusion. If the porosity is unity then the equation for the dispersion flux reduces to Fick's law. However, the porous media reduces the cross-sectional area available for diffusion. This is taken into account by the porosity multiplying the dispersion coefficient (Perkins and Johnston 1963).

$$\mathbf{J}_i = -\phi \mathbf{K} \nabla C_i$$

Consider diffusion through a porous medium such as illustrated in Fig. 2.3. Not only is the cross-sectional area reduced but the path length for diffusion is increased because of the tortuous path through the medium. A factor is needed to quantify the tortuosity of the medium in addition to the reduction in the cross-sectional area. The factor that is commonly used is the **formation factor**,  $F$ , which is also used for the quantification of electrical conductivity through porous media. It is interpreted as the tortuosity divided by the porosity.

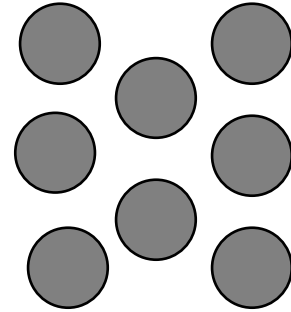


Fig. 2.3 Diffusion through porous media

$$\mathbf{J}_i = -\frac{D_{oi}}{F} \nabla C_i$$

Thus the dispersion coefficient due to molecular diffusion through porous media is as follows.

$$K_i = \frac{D_{oi}}{\phi F} = \frac{D_{oi}}{\tau}, \quad \text{zero fluid velocity}$$

where  $\tau$  is the tortuosity in the above equation. If the medium is anisotropic then the above equation will be a tensor equation with a different value of  $F$  in each principal direction of the formation factor tensor.

### Flow in a straight capillary tube

Next consider the case of laminar flow in a straight capillary tube. We now have convection in addition to diffusion. We will consider fluid  $B$  displacing fluid  $A$  with identical properties but yet distinguishable, e.g., containing a tracer. First assume that the molecular diffusivity is zero. If the velocity profile in the capillary is plug flow (constant velocity), then the displacement will just be steady translation and the concentration wave will be a step indifferent wave. The velocity profile of a Newtonian (constant viscosity) fluid is parabolic with the maximum velocity at the centerline equal to twice the average velocity. If the molecular diffusivity is zero then the interface between fluids  $A$  and  $B$  will be parabolic as in Fig. 2.4 and the displacement front will have a velocity that is twice the average velocity and the last traces of  $A$  next to the capillary wall will have a zero velocity. Therefore, in the absence of diffusion in a capillary, the displacement will be a spreading wave in which the profile spreads in proportion to throughput. Suppose now that diffusion smears out the sharp interface illustrated in Fig. 2.4. If the product of the dispersivity,  $D_0$ , and the capillary length,  $L$ , is large compared to the product of the average velocity,  $v$ , and the square of the capillary radius,  $a$ , then the mixing zone will travel with the mean speed of the injected fluid and would be dispersed as if there were a constant longitudinal dispersion coefficient given by the following equation.

$$K_{\ell} = D_o + \frac{v^2 a^2}{48D_o}$$

This dispersion in a capillary tube is called

**Taylor's dispersion** (Taylor 1953). It is a formula that can be used to experimentally determine the molecular diffusivity. It is important to note that Taylor's dispersion has a dependence on the **square** of the velocity.

### Ideal porous media

Fig. 2.5 illustrates a part of an idealized porous medium which may be viewed as an array of pore bodies connected by pore throats. The fluid stream enters a body from one or more throats and exits through one or more throats. The fluid streams mix in the body before exiting through the exit throats. Even if there were no branching, longitudinal mixing will still occur because the exit stream is a mixture of the incoming stream and the current content of the body (Aris and Admundson 1957). The mixing in grid blocks of finite difference methods is analogous to this mixing.

The dispersion in this system can be modeled by estimating the mean squared displacement in one dimension during a time interval  $\tau$ .

$$K = \frac{\bar{x}^2}{2\tau}$$

The **longitudinal** dispersion can be estimated by approximating the distance  $\bar{x}$  over which the fluid travels before mixing, is on the average,  $d_p$ , and the corresponding time  $\tau$  is equal to  $d_p/v$ , where  $v$  is the interstitial velocity. Substituting into the above equation yields an expression for the longitudinal dispersion coefficient.

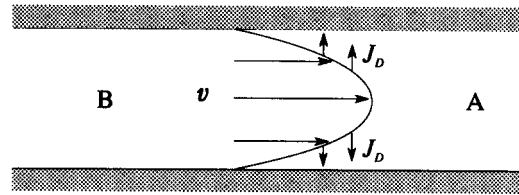
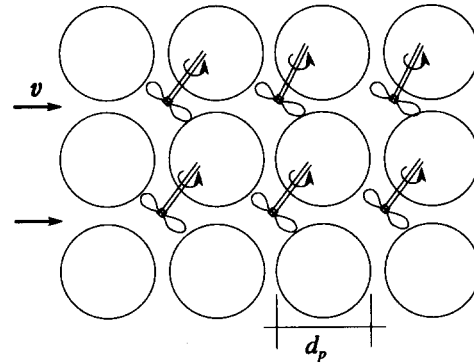
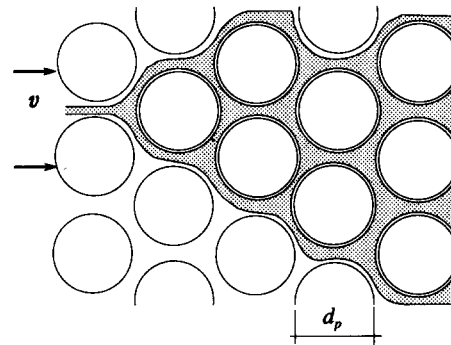


Fig. 2.4 Velocity and concentration profile in capillary (Holt 1992)



(a) Idealization of longitudinal mechanical mixing.



(b) Idealization of transversal dispersion by stream splitting.

Fig. 2.5 Mixing in ideal porous media (Holt 1992)

$$K_\ell = \frac{d_p v}{2}$$

The **transversal** dispersion can be viewed as caused by the streams splitting as it flows through a staggered array of particles as in Fig. 2.5b. Upon splitting, the stream moves in the transversal direction  $\bar{x}$  by  $d_p/2$ . The time for this split to occur is equal to the time elapsed while the fluid moved longitudinally one particle diameter, or  $\tau = \frac{d_p}{v}$ .

$$K_t = \frac{d_p v}{8}$$

Assuming that the effects of molecular diffusion and mechanical mixing are additive, the total dispersion may be expressed as follows.

$$K_\ell = \frac{D_o}{\phi F} + \frac{d_p v}{2}$$

$$K_t = \frac{D_o}{\phi F} + \frac{d_p v}{8}$$

The relative importance of diffusion and mixing can be examined if the above equations are made dimensionless by dividing by the diffusivity.

$$\frac{K_\ell}{D_o} = \frac{1}{\phi F} + \frac{d_p v}{2D_o}$$

$$\frac{K_t}{D_o} = \frac{1}{\phi F} + \frac{d_p v}{8D_o}$$

The dimensionless group on the right side of the equation is called the microscopic Peclet number. It is the ratio of convective mixing and molecular diffusion.

$$N_{Pe} = \frac{d_p v}{D_o}$$

Molecular diffusion dominates when the Peclet number is small compared to unity and convective mixing dominates when the Peclet number is large compared to unity. The upper limit of Peclet numbers where the dispersion remains linear with velocity is about 50. Above this value the correlated exponent on velocity is greater than unity, e.g. 1.2. Apparently there is insufficient time for diffusion to completely mix the fluids in the pore body and the

dispersion has some of the characteristics of Taylor's diffusion which has a velocity exponent of 2.0.

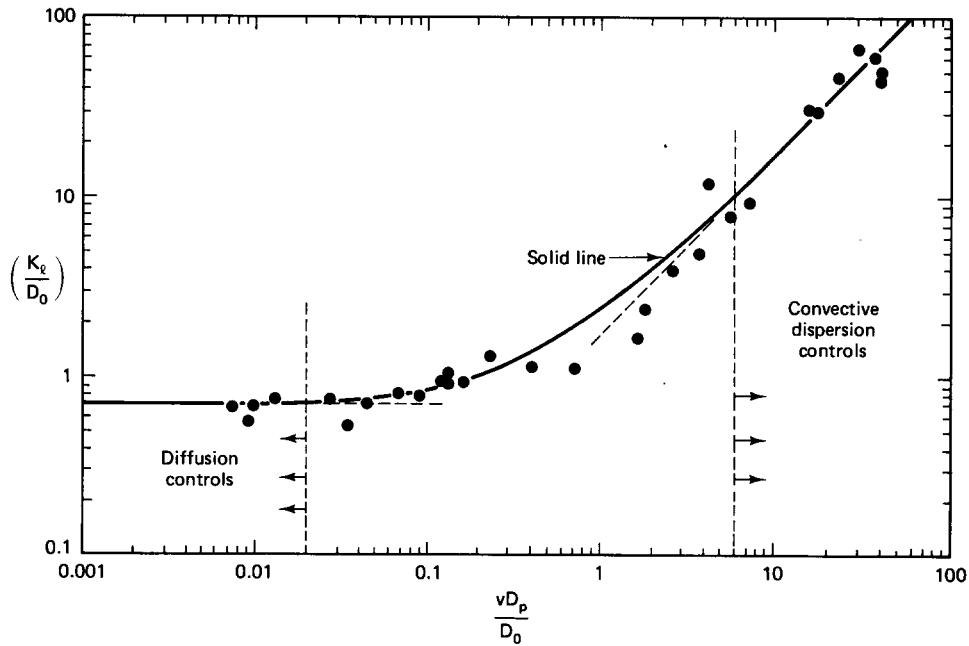


Fig. 2.6 Longitudinal dispersion coefficient of unconsolidated, random packs of uniform size sand or beads (Perkins and Johnston, 1963)

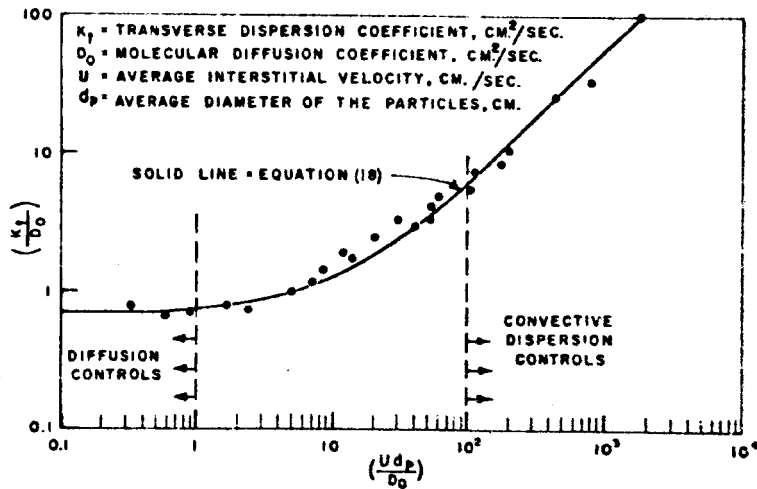


Fig. 2.7 Transverse dispersion coefficients of unconsolidated, random packs of uniform sand or beads (Perkins and Johnston, 1963)

The correlation of the longitudinal and transverse dispersion in the previous two figures are given as follows.

$$\frac{K_l}{D_o} = \frac{1}{\phi F} + 1.75 \frac{d_p v}{D_o}, \quad \frac{d_p v}{D_o} < 50$$

$$\frac{K_t}{D_o} = \frac{1}{\phi F} + 0.055 \frac{d_p v}{D_o}$$

The above model assumed that the porous medium was of uniform size and packing. Studies have shown that an inhomogeneity parameter is required to correlate with measurements. This parameter increases with decreasing bead size and has been measured to be as large as a factor of 8 for 0.1 mm beads (Perkins and Johnston 1963). The fit of the longitudinal dispersion data in Fig. 2.6 has a coefficient of 1.75 rather than the coefficient of 1/2 in the simple derivation. The fit of the transverse dispersion data in Fig. 2.7 has a coefficient of 0.055 rather than the coefficient of 1/8 in the simple derivation. Thus we see that the experimentally measured dispersion coefficients have longitudinal coefficients that are a factor of 32 larger than the transverse dispersion coefficient.

Real porous media are more complex than a bed of uniform spheres. Besides having a distribution of pore or particle sizes, some other mechanisms are illustrated in Fig. 2.7. These mechanisms will cause the longitudinal dispersion to be larger than the model given above.

Other factors affect dispersion. These include the presence of more than one phase, unequal viscosities and densities, and turbulent flow. These mechanisms are beyond the scope of this class (Perkins and Johnston, 1963).

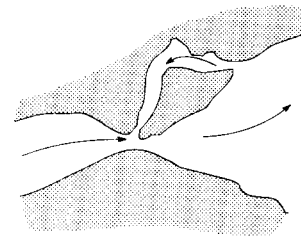
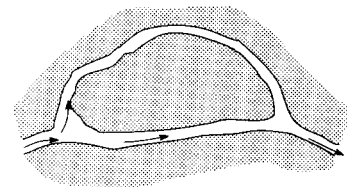
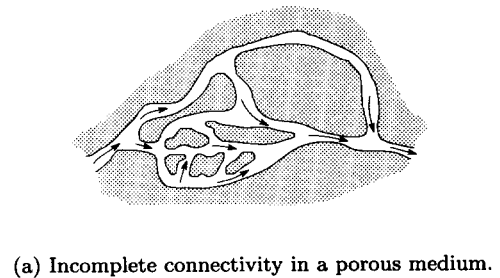


Fig. 2.7 Additional mechanisms for convective mixing (Holt 1992)



## Longitudinal and Transverse Dispersivity of Medium

We saw above that the dispersion coefficient,  $\mathbf{K}$ , is not just a function of the medium but is a function of the molecular dispersivity, fluid velocity, and the properties of the medium. However, if the microscopic Peclet number is large compared to unity, then the dispersion coefficient is proportional to velocity. From here on we will assume that the microscopic Peclet number is large compared to unity and the dispersion coefficient depends linearly on the mean fluid interstitial velocity.

$$K_\ell = \alpha_\ell |v|, \quad \frac{d_p v}{D_o} > 6$$
$$K_t = \alpha_t |v|, \quad \frac{d_p v}{D_o} > 100$$

The coefficients,  $\alpha_\ell$  and  $\alpha_t$ , are the longitudinal and transverse dispersivity of the medium. They are a property of the porous medium and are independent of the fluid and velocity if the Peclet number is large enough.

We see that the dispersion coefficient depends on the direction of the flow. Thus it must be a tensor. Bear suggested the following expression for the dispersion tensor for an isotropic medium and Cartesian coordinates (Bear 1972).

$$K_{ij} = \alpha_t |v| \delta_{ij} + (\alpha_\ell - \alpha_t) \frac{v_i v_j}{|v|}$$

It is easy to see that this expression gives the correct dispersivity for a concentration gradient that is parallel or perpendicular to the velocity.

So far we have considered porous media that may be heterogeneous on a microscopic scale but is homogeneous on a macroscopic scale. Geological formations are heterogeneous at all length scales. We will see later that macroscopic heterogeneities result in increased dispersion for displacement over macroscopic length scales.

## Equation for One Dimensional Adsorption, Convection, and Dispersion

We will derive an analytical solution for one dimensional, miscible displacement with adsorption, convection, and dispersion. The miscible components will either be a tracer solute (e.g. radio-isotope, dye, electrolyte) or similar material (octane - decane) such that effects of buoyancy and viscosity ratio can be neglected. It is assumed that the concentration range is small enough that the adsorption isotherm can be approximated with a constant slope over the range of concentrations. The dispersion coefficient is assumed to be proportional to velocity and the velocity is constant. The medium is homogeneous. The mass conservation equation with these phenomena is as follows.

$$\phi \frac{\partial (C + C_s)}{\partial t} + u \frac{\partial C}{\partial x} = \phi K_t \frac{\partial^2 C}{\partial x^2}, \quad x > 0, \quad t > 0$$

$$C(x, 0) = C^{IC}, \quad x > 0$$

$$C(0, t) = C^{BC}, \quad t > 0$$

The concentration is transformed to a reduced concentration which has a range between 0 and 1.

$$C_r = \frac{(C - C^{IC})}{(C^{BC} - C^{IC})}$$

Hereafter, the subscript r will be dropped.

The slope of the adsorption isotherm with respect to the reduced concentration is denoted by  $\beta$ . The interstitial velocity is denoted by  $v = u/\phi$ . The differential equation then reduces to the following.

$$\frac{\partial C}{\partial t} + \frac{v}{(1 + \beta)} \frac{\partial C}{\partial x} = \frac{K_t}{(1 + \beta)} \frac{\partial^2 C}{\partial x^2}$$

In the absence of dispersion, the solution to this differential equation is an indifferent step wave with a velocity equal to  $\frac{v}{(1 + \beta)}$ . Thus the slope of the

adsorption isotherm describes the **retardation** of the concentration wave. The independent variables will be transformed from  $(x, t)$  to a spatial coordinate that translates with the velocity of the wave in the absence of dispersion,  $(y, t)$ .

$$y = x - \frac{vt}{(1+\beta)}$$

$$\frac{\partial y}{\partial t} = -\frac{v}{(1+\beta)}$$

$$\frac{\partial y}{\partial x} = 1$$

The total differential expressed as a function of  $(x,t)$  or  $(y,t)$  are equal to each other.

$$dC = \left(\frac{\partial C}{\partial t}\right)_x dt + \left(\frac{\partial C}{\partial x}\right)_t dx$$

$$dC = \left(\frac{\partial C}{\partial t}\right)_y dt + \left(\frac{\partial C}{\partial y}\right)_t dy$$

The total differential expressed each way are equal. The partial derivatives in  $t$  and  $x$  can be expressed in terms of partial derivatives in  $t$  and  $y$  by equating the total differential with either  $dt$  or  $dx$  equal to zero and dividing by the nonzero differential.

$$\begin{aligned} \left(\frac{\partial C}{\partial t}\right)_x &= \left(\frac{\partial C}{\partial t}\right)_y + \left(\frac{\partial C}{\partial y}\right)_t \left(\frac{\partial y}{\partial t}\right)_x \\ &= \left(\frac{\partial C}{\partial t}\right)_y - \frac{v}{(1+\beta)} \left(\frac{\partial C}{\partial y}\right)_t \end{aligned}$$

$$\begin{aligned} \left(\frac{\partial C}{\partial x}\right)_t &= \left(\frac{\partial C}{\partial y}\right)_t \left(\frac{\partial y}{\partial x}\right)_t \\ &= \left(\frac{\partial C}{\partial y}\right)_t \end{aligned}$$

$$\left(\frac{\partial^2 C}{\partial x^2}\right)_t = \left(\frac{\partial^2 C}{\partial y^2}\right)_t$$

Substituting into the original PDE, we have the PDE in the transformed coordinates.

$$\left(\frac{\partial C}{\partial t}\right)_y = \frac{K_\ell}{(1+\beta)} \left(\frac{\partial^2 C}{\partial y^2}\right)_t$$

This equation is the classic diffusion equation. However, the boundary condition that we specified for  $x=0$  is now at changing values of  $y$ . We will seek an approximate solution that has the boundary condition,  $C(y \rightarrow -\infty, t) = 1$ .

$$\begin{aligned} C(y, 0) &= 1, & y < 0 \\ &= 1/2, & y = 0 \\ &= 0, & y > 0 \end{aligned}$$

$$C(y \rightarrow -\infty, t) = 1$$

$$C(y \rightarrow +\infty, t) = 0$$

This system is a step wave in a doubly infinite domain with no dispersion at  $t=0$ . Dispersion occurs for  $t>0$  as the wave propagates through the system.

A similarity transformation is possible because the system does not have a characteristic length. Let

$$C(y, t) = C(\eta)$$

$$\eta = \frac{y}{2\sqrt{\frac{K_\ell}{(1+\beta)}t}}$$

$$\frac{\partial \eta}{\partial y} = \frac{1}{2\sqrt{\frac{K_\ell}{(1+\beta)}t}}$$

$$\frac{\partial \eta}{\partial t} = -\frac{1}{2t}\eta$$

$$\frac{\partial C}{\partial t} = \frac{dC}{d\eta} \frac{\partial \eta}{\partial t} = -\frac{\eta}{2t} \frac{dC}{d\eta}$$

$$\frac{\partial C}{\partial y} = \frac{1}{2\sqrt{\frac{K_\ell t}{(1+\beta)}}} \frac{dC}{d\eta}$$

$$\frac{\partial^2 C}{\partial y^2} = \frac{1}{4\frac{K_\ell t}{(1+\beta)}} \frac{d^2 C}{d\eta^2}$$

Substitute into PDE and factor out common terms.

$$\frac{d^2 C}{d\eta^2} + 2\eta \frac{dC}{d\eta} = 0$$

$$C(\eta \rightarrow -\infty) = 1$$

$$C(\eta = 0) = 1/2$$

$$C(\eta \rightarrow +\infty) = 0$$

Let  $\psi = \frac{dC}{d\eta}$

$$\frac{d\psi}{d\eta} + 2\eta \psi = 0$$

$$\frac{d\psi}{\psi} = -2\eta d\eta$$

$$\psi = C_1 e^{-\eta^2}$$

$$C = C_1 \int_0^\eta e^{-\eta^2} d\eta + C_2$$

$$C(0) = 1/2 = 0 + C_2$$

$$C(\eta \rightarrow +\infty) = 0 = C_1 \int_0^\infty e^{-\eta^2} d\eta + 1/2$$

$$C_1 = \frac{-1/2}{\int_0^\infty e^{-\eta^2} d\eta} = \frac{-1}{\sqrt{\pi}}$$

$$C = \frac{1}{2} \left[ 1 - \frac{2}{\sqrt{\pi}} \int_0^\eta e^{-\eta^2} d\eta \right]$$

$$= \frac{1}{2} \operatorname{erfc}(\eta)$$

This solution was derived for a system that has a doubly infinite domain, i.e., it does not have a characteristic length. However, we will be using this solution to analyze problems that have a characteristic system length,  $L$ . Thus the distance variable will be made dimensionless with respect to  $L$ .

$$\eta = \frac{x - \frac{vt}{(1+\beta)}}{2 \sqrt{\frac{K_\ell}{(1+\beta)} t}} = \frac{\frac{x}{L} - \frac{\phi Avt}{\phi AL(1+\beta)}}{2 \sqrt{\frac{uA\phi K_\ell}{uA\phi L^2(1+\beta)} t}}$$

Let

$$x_D = \frac{x}{L}, \quad t_D = \frac{uAt}{\phi AL}, \quad N_{Pe} = \frac{Lv}{K_\ell}$$

The dimensionless time is the throughput made dimensionless with respect to the system pore volume. The Peclet number defined here is different than that used earlier for correlating experimental dispersion data. The definition used here may be considered as the relative importance of convection to dispersion during transport across the length of the system. The independent variable,  $\eta$ , can now be expressed in terms of these dimensionless variables.

$$\eta = \frac{x_D - \frac{t_D}{(1+\beta)}}{2 \sqrt{\frac{t_D}{N_{Pe}(1+\beta)}}}$$

The concentration profiles are shown on Fig. 8 for the case of zero retardation,  $\beta=0$ . The upper part of the figure shows the profile as a function of throughput for a Peclet number of 100. The lower part of the figure shows the profiles at  $t_D=0.5$  for different values of the Peclet number. If the mixing zone is defined as the distance over which the profile changes from 10% to 90% of the concentration change, then the mixing zone length will appear as in the upper part of the figure. Notice that the mixing zone is growing as the wave propagates through the system. The lower figure shows that with low Peclet numbers and/or low throughput, the concentration at  $x=0$  is not equal to unity. A solution that satisfies this boundary condition exactly is available.

When the microscopic Peclet number is large enough for the dispersion coefficient to be proportional to velocity, the Peclet number reduces to a form with particular physical significance.

$$N_{Pe} = \frac{L}{\alpha_l}, \quad \frac{vd_p}{D_o} > 6$$

The velocity cancels from the Peclet number and the solution no longer has an explicit dependence on the velocity if the time is expressed as pore volumes of throughput. Also, the macroscopic Peclet number is the ratio of the system length and the longitudinal dispersivity. This result tells us that if the system length is increased for the same medium (i.e.  $\alpha_l$  constant), the Peclet number increases and the relative effect of dispersion on the effluent history will decrease. This conclusion is valid provided the medium is homogeneous. Geological formations have heterogeneities of all length scales and thus mixing at all length scales. The net result is that the measured longitudinal dispersivity increases with the system length. Fig. 9 illustrates this dependence. Later we will show why this occurs (Lake and Hirasaki, 1981).

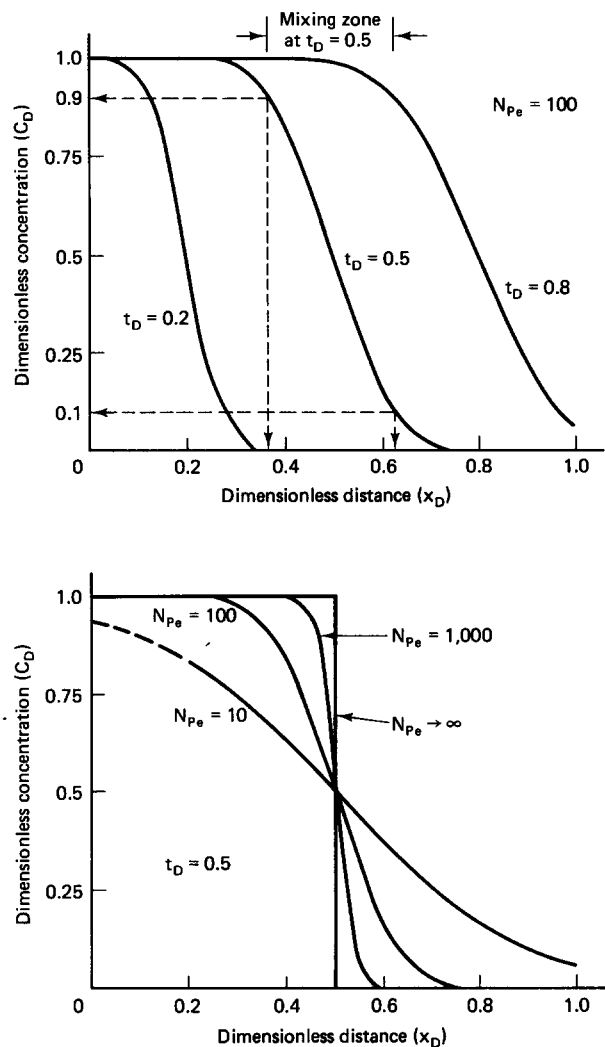


Fig. 8 Concentration profiles (Lake 1989)

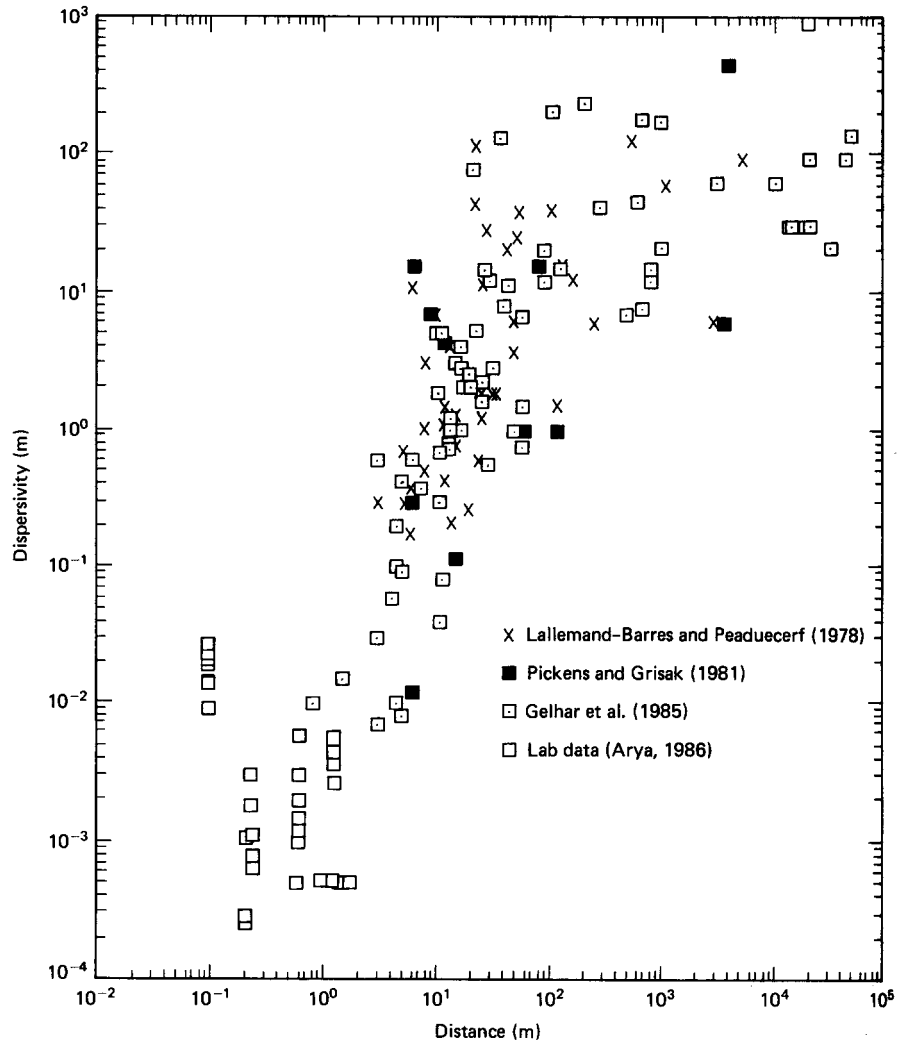


Fig. 8 Field and laboratory measured dispersivities [Lake 1989 (from Arya et al, 1988)]



## Estimation of Dispersion Coefficient from Displacement Data

The dispersion coefficient can be estimated from the effect of dispersion on the effluent history. We will consider the case of no adsorption, i.e.,  $\beta=0$ . The effluent history is evaluated as a function of time with  $x_D=1.0$ .

$$\eta(x_D=1) = \frac{1-t_D}{2\sqrt{N_{Pe}^{-1} t_D}}$$

Denote as  $\eta_{10}$  and  $\eta_{90}$  the value of  $\eta$  at which  $C$  is equal to 0.10 and 0.90, respectively.

$$\begin{aligned} C(\eta) &= \frac{1}{2} \operatorname{erfc}(\eta) \\ &= \frac{1}{2} [1 - \operatorname{erf}(\eta)] \end{aligned}$$

$$\operatorname{erf}(\eta_{10}) = 0.8$$

$$\eta_{10} = 0.906$$

$$0.9 = \frac{1}{2} [1 - \operatorname{erf}(\eta_{90})]$$

$$-\operatorname{erf}(\eta_{90}) = \operatorname{erf}(-\eta_{90}) = 0.8 = \operatorname{erf}(\eta_{10})$$

$$-\eta_{90} = \eta_{10} = 0.906$$

$$\eta_{10} - \eta_{90} = 1.812$$

$$\frac{\sqrt{N_{Pe}}}{2} \left[ \frac{1-t_{D,10}}{\sqrt{t_{D,10}}} - \frac{1-t_{D,90}}{\sqrt{t_{D,90}}} \right] = 1.812$$

$$\frac{K_\ell}{vL} = \left\{ \frac{1}{3.625} \left[ \frac{1-t_{D,10}}{\sqrt{t_{D,10}}} - \frac{1-t_{D,90}}{\sqrt{t_{D,90}}} \right] \right\}^2$$

The interpolation may be aided by plotting the data on probability paper such that the data can be fitted with a straight line.

An alternative approach to estimate the Peclet number is to recognize the relation of the complementary error function solution to the cumulative Gaussian probability distribution. We used linear regression to estimate the mean and standard deviation of a Gaussian distribution in assignment 3 of CENG 571. We will show how linear regression can be used to estimate the Peclet number. The cumulative Gaussian probability distribution is given by the following formula.

$$P\{y\} = \frac{1}{2} \left[ 1 + \operatorname{erf} \left( \frac{u}{\sqrt{2}} \right) \right]$$

$$u = \frac{y - \mu}{\sigma}$$

$$y = \mu + \sigma u$$

where  $\mu$  and  $\sigma$  are the mean and standard deviation of the Gaussian distribution.

Recall that the effluent concentration is given by the following equations.

$$C(\eta) = \frac{1}{2} [1 - \operatorname{erf}(\eta)]$$

$$\eta(x_D = 1) = \frac{1 - t_D}{2\sqrt{N_{Pe}^{-1} t_D}}$$

What we need to do is to transform the variables such that the transformed variables is a cumulative Gaussian distribution. First, transform  $C$  such that it has the same dependence on the error function as the Gaussian distribution.

$$\begin{aligned} \frac{1}{2} [1 + \operatorname{erf}(\eta)] &= 1 - C \\ &\Rightarrow P \end{aligned}$$

The argument of the error function should map the independent variables.

$$\begin{aligned} \eta(x_D = 1) &\Rightarrow \frac{u}{\sqrt{2}} \\ \frac{1 - t_D}{2\sqrt{N_{Pe}^{-1} t_D}} &\Rightarrow \frac{y - \mu}{\sqrt{2} \sigma} \\ \frac{1 - t_D}{\sqrt{t_D}} &\Rightarrow y \end{aligned}$$

$$\mu = 0$$

$$\sigma = \sqrt{2} \sqrt{N_{Pe}^{-1}}$$

$$N_{Pe} = \frac{2}{\sigma^2}$$

The mean  $\mu$  being equal to zero implies that the median concentration (which is equal to the mean of a Gaussian distribution) should occur at  $t_D = 1$ . If the adsorption was non zero, then the slope of the isotherm,  $\beta$ , can be determined from the mean of the Gaussian distribution.

$$\eta(x_D = 1) = \frac{1 - t_D + \beta}{2 \sqrt{\frac{(1 + \beta) t_D}{N_{Pe}}}}$$

$$\mu = \beta$$

$$\sigma = \sqrt{2} \sqrt{\frac{1 + \beta}{N_{Pe}}}$$

The steps is estimating the Peclet number (and slope of adsorption isotherm) is as follows: (1) determine the initial and injected concentration to normalize the concentration between these values, (2) determine which data should be fit by the linear regression (do not fit data in which the response is less than the noise), (3) transform the variables, (4) view fit of regression line with data and repeat step 2 if necessary, (5) estimate the mean and standard deviation with the program *gaussf.m* used in assignment 3 of CENG571 (owlnet userID: *gjh*, directory: *class*), (6) calculate the Peclet number from the standard deviation.

### Assignment 2.1 Measurement of Dispersion Coefficient

Porous material: Kern River sand  
 Pack diameter: 1.0 inch  
 Pack length: 12.25 inch  
 Porosity: 36%  
 Permeability: 4 darcy  
 Injected NaCl: 1% (nominal) NaCl  
 Initial condition: synthetic Kern River formation connate water  
 Flow rate: 0.072 cm<sup>3</sup>/minute

#### Tracer Effluent Data for Kern River Sand

Q, PV	Chloride, meq/gm	Q, PV	Chloride, meq/gm
0.112	0.022	1.593	0.178

0.271	0.022	1.695	0.176
0.422	0.022	1.801	0.179
0.572	0.025	2.033	0.179
0.731	0.029	2.089	0.179
0.871	0.053	2.136	0.174
1.037	0.105	2.234	0.182
1.211	0.143	2.396	0.177
1.286	0.155	2.558	0.179
1.377	0.166	3.387	0.176
1.4787	0.173	4.030	0.176

Determine the Peclet number, longitudinal dispersion coefficient,  $K_L$  (cm<sup>2</sup>/sec), and longitudinal dispersivity of medium,  $\alpha_L$ , (cm). Estimate the parameters by: (1) using interpolated 10% and 90% values and the formula, and (2) using linear regression to determine the slope of the data on a Gaussian cumulative probability plot.

### Assignment 2.2 Numerical Dispersion of Finite Difference Formulation

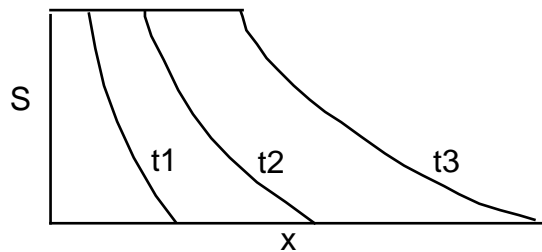
Do the same as the previous assignment but for the finite difference problem with  $M=1$ ,  $n=1$ ,  $\Delta t/\Delta x=0.1$ . Let  $NX = 10$  and  $100$ . Compare with the calculated dispersion coefficient from the truncation error analysis.

### Mixing Zone Length with Distance Traveled

Consider for the moment a system with no dispersion but with a spreading wave for a system described by a first order PDE, e.g. water-oil displacement with unfavorable mobility ratio.

$$x_D(S=0.1) = t_D \frac{df}{dS}(S=0.1)$$

$$x_D(S=0.9) = t_D \frac{df}{dS}(S=0.9)$$



mixing zone length:

$$\Delta x_D = x_D(S=0.1) - x_D(S=0.9)$$

average distance traveled:

$$x_D^f = t_D$$

$$\frac{\Delta x_D}{x_D^f} = \frac{df}{dS}(S=0.1) - \frac{df}{dS}(S=0.9)$$

The length of the spreading wave (analogous to mixing zone length) is proportional to the distance traveled or the normalized (with respect to average distance traveled) length of the spreading wave is independent of the distance traveled.

Now consider a system with dispersion.

$$C = \frac{1}{2} [1 - \text{erf}(\eta)]$$

$$\eta = \frac{x_D - t_D}{2\sqrt{N_{Pe}^{-1} t_D}}$$

$$\eta_{10} - \eta_{90} = 1.812$$

distance traveled:  $x_D^f = t_D$

mixing zone length:  $\Delta x_D = x_{D,10} - x_{D,90}$

$$\frac{(x_{D,10} - x_D^f) - (x_{D,90} - x_D^f)}{2\sqrt{N_{Pe}^{-1} x_D^f}} = 1.812$$

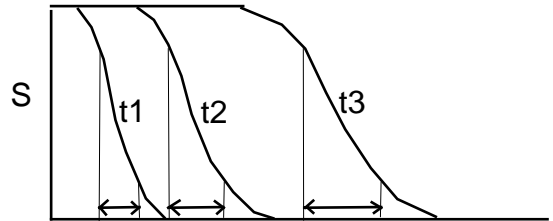
$$\Delta x_D = 3.625\sqrt{N_{Pe}^{-1} x_D^f}$$

$$\frac{\Delta x_D}{x_D^f} = 3.625 \frac{1}{\sqrt{N_{Pe} x_D^f}}$$

The length of the dispersive mixing zone increases proportional to the square root of the distance traveled. The length of the dispersive mixing zone normalized with the distance traveled decreases inversely proportional with the square root of the distance traveled.

Suppose that the Peclet number is proportional to velocity. Recall that in this case the Peclet number is equal to the ratio of the system length and longitudinal formation dispersivity. The system length cancels out of the previous equation for the normalized dispersive mixing zone length.

$$\frac{\Delta x}{x^f} = 3.625 \sqrt{\frac{\alpha_L}{x^f}}$$



The dispersive mixing zone length normalized with the distance traveled decreases inversely with the square root of the distance traveled and is independent of the system length and velocity.

$$\Delta x = 3.625\sqrt{\alpha_L x^f}$$

The length of the dispersive mixing zone increases proportional to the square root of the distance traveled.

## Finite or Pulse Slug

The proceeding analysis was for continuous injection of the same composition. Tracer and displacement experiments are often conducted with a finite size slug or a pulse injection sequence and the injected concentration is returned to that of the initial condition. If the slug size is small enough, the mixing zone from the front and back of the slug will overlap and the maximum concentration will fall below the injected concentration. An example of a tracer is the pulse response of a gas chromatograph. An example of a finite slug is the surfactant slug in enhanced oil recovery.

Since we have assumed that the dispersion coefficient and the slope of the adsorption isotherm are independent of concentration, the response is a linear function of concentration and we can apply the principle of superposition to calculate the response of a finite slug. Pulse injection will be a special case of a finite slug in the limit of zero injection time but with a specified cumulative injection. The expression for continuous injection was derived earlier as follows.

$$C(\eta) = \frac{1}{2} [1 - \text{erf}(\eta)]$$

where

$$\eta = \frac{x_D - \frac{t_D}{(1+\beta)}}{2\sqrt{\frac{t_D}{N_{Pe}(1+\beta)}}}$$

Let  $t_D$  be the time from the start of the slug injection. If the slug is injected for a time interval  $\Delta t_D$  and then returned to zero concentration then the time since the slug injection was discontinued is  $t_{D\Delta}$ , where  $t_{D\Delta} = t_D - \Delta t_D$ . The concentration is

$$C(\eta) = \frac{1}{2} [1 - \text{erf}(\eta)] - \frac{1}{2} [1 - \text{erf}(\eta_\Delta)], \quad t_D > t_{D\Delta}$$

$$= -\frac{1}{2} [\text{erf}(\eta) - \text{erf}(\eta_\Delta)], \quad t_D > t_{D\Delta}$$

where

$$\eta_\Delta = \frac{x_D - \frac{t_D - \Delta t}{(1 + \beta)}}{2 \sqrt{\frac{t_D - \Delta t}{N_{Pe}(1 + \beta)}}}$$

If  $t_D \gg \Delta t_D$ , then the difference of the error functions can be approximated by the differential.

$$C(\eta) \approx \frac{1}{2} \frac{d \text{erf}(\eta)}{d\eta} (\eta - \eta_\Delta), \quad \Delta t_D \ll t_D$$

$$\frac{d \text{erf}(\eta)}{d\eta} = \frac{2}{\sqrt{\pi}} e^{-\eta^2}$$

$$\eta - \eta_\Delta \approx \frac{-\frac{\Delta t_D}{(1 + \beta)}}{2 \sqrt{\frac{t_D}{N_{Pe}(1 + \beta)}}}, \quad \Delta t_D \ll t_D$$

$$C \approx \frac{\Delta t_D \sqrt{\frac{N_{Pe}}{(1 + \beta)}} e^{-\eta^2}}{2\sqrt{\pi} \sqrt{t_D}}, \quad \Delta t_D \ll t_D$$

This equation is the pulse response function of a source with a strength (cumulative injection) equal to  $\Delta t_D$ . The peak value occurs at  $\eta=0$ . Notice that the peak value decreases inversely with the square root of time. This concentration profile is a Gaussian distribution. The equation can be rearranged as follows.

$$C \approx \frac{\Delta t_D}{(1+\beta)} \frac{1}{\sqrt{2\pi} \sqrt{\frac{2t_D}{N_{pe}(1+\beta)}}} \exp \left[ \frac{-\left(x_D - \frac{t_D}{(1+\beta)}\right)^2}{2 \frac{2t_D}{N_{pe}(1+\beta)}} \right]$$

$$= \frac{\Delta t_D}{(1+\beta)} \frac{1}{\sqrt{2\pi} \sigma} \exp \left[ \frac{-(x_D - \mu)^2}{2\sigma^2} \right]$$

$$\mu = \frac{t_D}{(1+\beta)}$$

$$\sigma = \sqrt{\frac{2t_D}{N_{pe}(1+\beta)}}$$

From this equation we can see that the concentration profile (function of x at constant t) is a Gaussian distribution with area equal to  $\frac{\Delta t_D}{(1+\beta)}$ , mean and median given by the concentration velocity multiplied by time, and the standard deviation that is proportional to the square root of time divided by the Peclet number.

The effect of formation dispersivity and system length can be examined in the case when the dispersion coefficient is proportional to velocity so that the Peclet number is the ratio of system length and formation dispersivity. In this case the pulse response can be expressed as follows.

$$C \approx \frac{\Delta t_D \sqrt{\frac{L}{\alpha_l(1+\beta)}}}{2\sqrt{\pi}} \frac{e^{-\eta^2}}{\sqrt{t_D}}, \quad \Delta t_D \ll t_D$$

Consider the effect of dispersion on a finite slug with increasing system length. If the slug size expressed as a fraction of a pore volume,  $\Delta t_D$ , is held fixed, then the peak concentration will increase proportional to the square root of the system length. i.e., dispersion has less effect on a slug of the same pore volume size when the system length is increased if  $\alpha_l$  is constant. However,  $\alpha_l$  can increase with distance traveled in a stratified porous media (Lake and Hirasaki, 1981).

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