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Theory for Dynamic Longitudinal Dispersion in Fractures and Rivers with Poiseuille Flow

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Theory for dynamic longitudinal dispersion in fractures and rivers with Poiseuille flow

Lichun Wang,[1] M. Bayani Cardenas,[1] Wen Deng,[1] and Philip C. Bennett[1]

[1]   We present a theory for dynamic longitudinal dispersion coefficient (D) for transport by Poiseuille flow, the foundation for models of many natural systems, such as in fractures or rivers. Our theory describes the mixing and spreading process from molecular diffusion, through anomalous transport, and until Taylor dispersion. D is a sixth order function of fracture aperture (b) or river width (W). The time (T) and length (L) scales that separate preasymptotic and asymptotic dispersive transport behavior are $T = b^2/(4D_m)$, where D_m is the molecular diffusion coefficient, and $L = \frac{b^4}{48\mu D_m}\frac{\partial p}{\partial x}$, where p is pressure and μ is viscosity. In the case of some major rivers, we found that L is $\sim 150W$. Therefore, transport has to occur over a relatively long domain or long time for the classical advection-dispersion equation to be valid. **Citation:** Wang, L., M. B. Cardenas, W. Deng, and P. C. Bennett (2012), Theory for dynamic longitudinal dispersion in fractures and rivers with Poiseuille flow, *Geophys. Res. Lett.*, *39*, L05401, doi:10.1029/2011GL050831.

1.   Introduction

[2]   Scalar mixing and spreading processes, which are typically represented by some diffusion or dispersion coefficient in transport equations, are fundamental to many geophysical systems and engineering applications. Mass transport driven by a concentration gradient is conventionally assumed to obey a diffusive process or is at least described by a diffusion-type equation. In a stratified flow field, the velocity profile due to shear stress enhances the mixing/spreading process resulting in so-called Fickian dispersion which is encapsulated in an effective dispersion coefficient. *Taylor* [1953] first showed that at some long enough time scale the mixing/spreading process through a tube follows Fickian behavior with a longitudinal dispersion coefficient. Later, *Fischer et al.* [1979] derived a corresponding longitudinal dispersion coefficient for a river also at a large time scale. *Güven et al.* [1984] analyzed horizontal transport through aquifers and showed that differences in stratified groundwater flow velocity caused by vertically-varying hydraulic conductivity would also lead to a Fickian dispersive process at some large enough scale. In such circumstances, the classical advection-dispersion (or diffusion) equation (ADE) is valid. However, at preasymptotic time scales, the classical ADE is invalid due to anomalous early arrival and persistent tails in breakthrough curves both in fractured and porous media [*Berkowitz*, 2002]. This phenomenon is referred to as non-Fickian behavior.

[3]   Non-Fickian transport can be mathematically represented in many ways but one simple approach is to define a dynamic longitudinal dispersion coefficient (D) for the ADE. Several researchers have studied and quantified dynamic D using various approaches including spatial moment analysis [*Dentz and Carrera*, 2007], series expansion methods [*Gill and Sankarasubramanian*, 1970], center manifold description [*Mercer and Roberts*, 1990], and Lagrangian approach [*Haber and Mauri*, 1988]. These studies showed that D increases monotonically from its value at preasymptotic time scale to the value according to *Taylor*'s theory. Yet, the theoretical analysis by *Taylor* [1953] for a tube and *Fischer et al.* [1979] for a river at asymptotic time scales is not sufficiently complete.

[4]   There are three key assumptions adopted by both *Taylor* [1953] and *Fischer et al.* [1979]: (1) the Peclet number is sufficiently large (i.e., advection dominated transport) so as to ignore longitudinal diffusion; (2) the longitudinal advective mass flux is balanced by transverse diffusive mass flux, and the gradient of the cross-sectional averaged concentration in the longitudinal direction is at steady-state; and (3) the gradient of the cross-sectional averaged concentration in the longitudinal direction is much greater than the gradient of concentration fluctuations. The validity of the above assumptions has since been ignored and subsequent studies have either retained these assumptions or circumvented them by following approaches that are not directly based on the complete transport equations. Here, we develop a more general theory that does not require the first two assumptions, and using this theory we derive a closed-form expression for the dynamic longitudinal dispersion coefficient. Afterwards, we analyze the time and length scales for distinguishing Fickian (asymptotic) and non-Fickian (preasymptotic) transport regimes.

2.   Theoretical Development

2.1.   Two-Dimensional Transport Model

[5]   *Fischer et al.* [1979] investigated the longitudinal dispersion coefficient for two-dimensional, steady-state, fully-developed, laminar flow between parallel plates. In this case, the advection-diffusion equation with appropriate boundary conditions is:

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = D_m\frac{\partial^2 C}{\partial x^2} + D_m\frac{\partial^2 C}{\partial y^2} \tag{1}$$

$$C = 0, \quad 0 \le x < \infty, \quad t = 0 \tag{2}$$

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$$\frac{\partial C}{\partial y} = 0, \quad y = b/2 \quad \text{or} - b/2 \tag{3}$$

$$C = C_0, \quad x = 0, \quad t > 0 \tag{4}$$

$$C = 0, \quad x = \infty, \quad t > 0 \tag{5}$$

where C is the concentration, x is the longitudinal direction, y is the transverse direction, u is the x-direction velocity that is only a function of y (uniform in x), D_m is molecular diffusion coefficient, t is time, b is the aperture of parallel plates (or the river width W), and C_0 is the constant inlet concentration.

2.2. One-Dimensional Macroscopic Transport Model With Dynamic Dispersion Coefficient

[6] Concentration and velocity in (1) can be decomposed into cross-sectional mean and fluctuation components:

$$C = \bar{C} + C' \quad \text{and} \quad u = \bar{u} + u' \tag{6}$$

where $\bar{C}$ and $\bar{u}$ are cross-sectional mean components, and C' and u' are fluctuations about the mean. According to *Taylor* [1953], $\bar{C}$ can be described by a one-dimensional macroscopic transport model written as:

$$\frac{\partial \bar{C}}{\partial t} + \bar{u}\frac{\partial \bar{C}}{\partial x} = D\frac{\partial^2 \bar{C}}{\partial x^2} \tag{7}$$

To obtain an explicit expression for D, we start from the basic ADE (1). Substituting (6) into (1) yields:

$$\frac{\partial \bar{C}}{\partial t} + \frac{\partial C'}{\partial t} + \bar{u}\frac{\partial \bar{C}}{\partial x} + \bar{u}\frac{\partial C'}{\partial x} + u'\frac{\partial \bar{C}}{\partial x} + u'\frac{\partial C'}{\partial x}$$
$$= D_m\left(\frac{\partial^2 \bar{C}}{\partial x^2} + \frac{\partial^2 C'}{\partial x^2} + \frac{\partial^2 C'}{\partial y^2}\right) \tag{8}$$

Taking a coordinate transformation (9) and applying the chain rule (10) (see equations (S1)–(S3) in the auxiliary material)[1]

$$\xi = x - \bar{u}t \quad \text{and} \quad \tau = t \tag{9}$$

$$\frac{\partial}{\partial x} = \frac{\partial}{\partial \xi}; \quad \frac{\partial}{\partial t} = -\bar{u}\frac{\partial}{\partial \xi} + \frac{\partial}{\partial \tau} \tag{10}$$

lead to:

$$\frac{\partial \bar{C}}{\partial \tau} + \frac{\partial C'}{\partial \tau} + u'\frac{\partial \bar{C}}{\partial \xi} + u'\frac{\partial C'}{\partial \xi} = D_m\left(\frac{\partial^2 \bar{C}}{\partial \xi^2} + \frac{\partial^2 C'}{\partial \xi^2} + \frac{\partial^2 C'}{\partial y^2}\right) \tag{11}$$

Instead of neglecting longitudinal molecular diffusion, we retain it and apply the averaging $\frac{1}{b}\int_{-b/2}^{b/2}$ (equation (11)) dy, and note that:

$$\frac{1}{b}\int_{-b/2}^{b/2} u'dy = 0; \quad \frac{1}{b}\int_{-b/2}^{b/2} C'dy = 0 \tag{12}$$

The cross-sectional averaging translates (11) into:

$$\frac{\partial \bar{C}}{\partial \tau} + \overline{u'\frac{\partial C'}{\partial \xi}} = D_m\frac{\partial^2 \bar{C}}{\partial \xi^2} \tag{13}$$

where $\overline{u'\frac{\partial C'}{\partial \xi}}$ is the cross-sectional averaged value of $u'\frac{\partial C'}{\partial \xi}$. The second term in (13) needs to be further analyzed as it is unknown and ideally it should be expressed in terms of $\frac{\partial^2 \bar{C}}{\partial \xi^2}$. To this end, we subtract (13) from (11), which gives the transport equation for C':

$$\frac{\partial C'}{\partial \tau} + u'\frac{\partial \bar{C}}{\partial \xi} + u'\frac{\partial C'}{\partial \xi} - \overline{u'\frac{\partial C'}{\partial \xi}} = D_m\left(\frac{\partial^2 C'}{\partial \xi^2} + \frac{\partial^2 C'}{\partial y^2}\right) \tag{14}$$

Since the longitudinal diffusion of C' is much less than transverse diffusion, i.e., $\frac{\partial^2 C'}{\partial \xi^2} \ll \frac{\partial^2 C'}{\partial y^2}$, and since $u'\frac{\partial C'}{\partial \xi}$ and $\overline{u'\frac{\partial C'}{\partial \xi}}$ are the products of two typically relatively small fluctuation-related terms therefore making them much smaller than the other terms in (14), and that we take the difference of these small terms, we can effectively ignore them. Then (14) simplifies to:

$$\frac{\partial C'}{\partial \tau} + u'\frac{\partial \bar{C}}{\partial \xi} = D_m\frac{\partial^2 C'}{\partial y^2} \tag{15}$$

At the asymptotic time scale, when longitudinal advection is balanced by transverse diffusion, equilibrium can be assumed resulting in:

$$u'\frac{\partial \bar{C}}{\partial \xi} = D_m\frac{\partial^2 C'}{\partial y^2} \tag{16}$$

The solution to (16) with boundary conditions (similar to (3)):

$$\frac{\partial C'}{\partial y} = 0, \quad y = b/2 \quad \text{and} - b/2 \tag{17}$$

is:

$$C' = \int_{-b/2}^{y}\int_{-b/2}^{y} \frac{u'}{D_m}\frac{\partial \bar{C}}{\partial \xi}dydy + C'(-b/2) \tag{18}$$

By definition, and allowing for the extra term $\int_{-b/2}^{b/2} u'C'(-b/2)dy = 0$, the unknown second term in (13) is therefore (see equations (S4)–(S6) in the auxiliary material):

$$\overline{u'\frac{\partial C'}{\partial \xi}} = \frac{1}{bD_m}\frac{\partial^2 \bar{C}}{\partial \xi^2}\int_{-b/2}^{b/2} u'\int_{-b/2}^{y}\int_{-b/2}^{y} u'dydydy \tag{19}$$

Substituting (19) into (13) and expressing the result back in the ordinary coordinate system results in:

$$\frac{\partial \bar{C}}{\partial t} + \bar{u}\frac{\partial \bar{C}}{\partial x} = \left(D_m - \frac{1}{bD_m}\int_{-b/2}^{b/2} u'\int_{-b/2}^{y}\int_{-b/2}^{y} u'dydydy\right)\frac{\partial^2 \bar{C}}{\partial x^2} \tag{20}$$
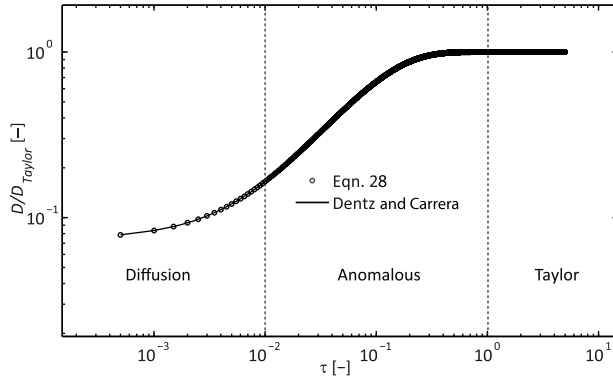
Figure 1. D/D_{Taylor} as a function of dimensionless time $\tau = 4tD_m/b^2$ following (28) and *Dentz and Carrera* [2007].

Therefore, the D in (7) at asymptotic time scale (D_{Taylor}) is:

$$D = D_m - \frac{1}{bD_m} \int_{-b/2}^{b/2} u' \int_{-b/2}^{y} \int_{-b/2}^{y} u' dy dy dy \qquad (21)$$

However, (21) is only valid assuming longitudinal advection is balanced by transverse diffusion. Simplification of (15) into (16) is not valid if the goal is to describe the transient dispersive processes. Therefore, in accordance with initial condition (2) and the no-flux boundary condition (17), we solved (15) directly through a unique Green function [*Polyanin*, 2002]:

$$G(y, \eta, t) = \frac{1}{b} + \frac{2}{b} \sum_{n=1}^{\infty} \cos \left[\frac{n\pi(y + b/2)}{b} \right] \cos \left[\frac{n\pi(\eta + b/2)}{b} \right]$$
$$\cdot \exp \left[-\frac{D_m n^2 \pi^2 (\tau - t)}{b^2} \right] \qquad (22)$$

The unknown second term in (13) is now expressed as:

$$\overline{u' \frac{\partial C'}{\partial \xi}} = -\frac{1}{b} \int_{-b/2}^{b/2} u' \frac{\partial}{\partial \xi} \left\{ \int_{0}^{\tau} \int_{-b/2}^{b/2} u' \frac{\partial \bar{C}}{\partial \xi} G(y, \eta, t) d\eta dt \right\} dy \qquad (23)$$

Assuming that the term $\frac{\partial \bar{C}}{\partial \xi}$ is constant with time, we are able to extract it from the integral operation and then do the manipulation as we did to obtain (21). Finally, we get the expression for the dynamic D in the ordinary coordinate system:

$$D = D_m + \frac{1}{b} \int_{-b/2}^{b/2} u' \int_{0}^{t} \int_{-b/2}^{b/2} u' G(y, \eta, \tau) d\eta d\tau dy \qquad (24)$$

2.3. Parabolic Flow Model

[7] The closed form expressions of (21) and (24) require the solution for the flow field which is well-known for Poiseuille flow. The velocity field for fully-developed pressure-gradient driven flow in between two parallel no-slip walls, e.g., fracture surfaces or river banks, is described by:

$$u = \frac{b^2}{8\mu} \frac{\partial p}{\partial x} \left(1 - \frac{4y^2}{b^2} \right) \qquad (25)$$

where $\frac{\partial p}{\partial x}$ is the pressure gradient. (25) is widely-known as Cubic Law for flow through fractures [*Ge*, 1997]. From (25), the cross-sectional mean and fluctuation velocity components are calculated as:

$$\bar{u} = \frac{b^2}{12\mu} \frac{\partial p}{\partial x} \quad \text{and} \quad u' = \frac{b^2}{\mu} \frac{\partial p}{\partial x} \left(\frac{1}{24} - \frac{y^2}{2b^2} \right) \qquad (26)$$

Therefore, in a parabolic (Poiseuille) velocity field (25), (26), the asymptotic (21) and dynamic (24) D can be respectively expressed as:

$$D = D_m + \frac{(\bar{u}b)^2}{210 D_m} \qquad (27)$$

$$D = D_m + \frac{72(\bar{u}b)^2}{\pi^6 D_m} \sum_{n=1}^{\infty} \frac{1}{n^6} \left[\cos(n\pi) + 1 \right]^2 \left[1 - \exp \left(-\frac{D_m n^2 \pi^2 t}{b^2} \right) \right] \qquad (28)$$

3. Results and Discussion of Threshold Scales

[8] Our exact expression for dynamic D is valid across all transport regimes (Figure 1) – diffusive, anomalous, and Taylor dispersion – and our theory agrees conceptually and qualitatively with results of scaling relationships for dynamic D derived via spatial moment analysis of numerical simulation results [*Latini and Bernoff*, 2001]. *Dentz and Carrera* [2007] presented a theory, also derived through spatial moment analysis, for apparent dynamic D. Our results are equivalent to *Dentz and Carrera* [2007] despite the very different approaches (Figure 1). Beyond the diffusion regime, the dynamic D would increase asymptotically towards the value predicted by (27), which has been shown through less direct methods [*Gill and Sankarasubramanian*, 1970; *Güven et al.*, 1984; *Haber and Mauri*, 1988; *Mercer and Roberts*, 1990; *Dentz and Carrera*, 2007]. In contrast to previous studies, we developed an exact and complete expression for dynamic D by direct solution of the general transport equations.

[9] Within the anomalous preasymptotic regime, the dynamic D is found to increase rapidly at small time scale $\tau < 0.1$ ($\tau = 4tD_m/b^2$), and it then varies slowly at a relatively large time scale $\tau > 0.5$ and gets close to its maximum when $\tau = 1$ which corresponds to the time it takes a particle to travel from the center to the side boundary. By $\tau = 1$, the initial concentration would be completely smeared out, and the dynamics of the cross-sectional averaged concentration follows a macroscopic transport model with constant D (27).

[10] The time scale for Taylor dispersion is therefore $\tau = 1$ or:

$$T = b^2/(4D_m) \qquad (29)$$

whereas the counterpart length scale is:

$$L = \bar{u} \, b^2/(4D_m) \qquad (30)$$

Below T and L, the classical ADE with constant D is invalid and transport is anomalous. While this behavior is well studied theoretically and experimentally for other systems such as in heterogeneous porous media [*Güven*
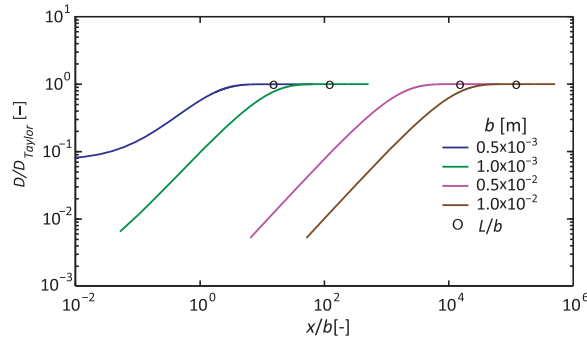
Figure 2. D/D_{Taylor} as a function of dimensionless length x/b (following equation (28)) showing the different length scales L for fractures with different apertures b (following equation (31)).

Figure 3. D/D_{Taylor} as a function of dimensionless length x/W (following equation (28)) showing the different length scales L for rivers with different widths W (following equation (31)).

et al., 1984; *Koch and Brady*, 1987; *Gelhar*, 1993], to our knowledge, our work is the first direct solution of the problem for classic Poiseuille flow with few assumptions in the general transport theory and without resorting to spatial moment analysis.

[11] Non-Fickian transport through fractures has been extensively studied at preasymptotic time scales, but few have highlighted the significance of length scales. To this end, we investigate the effect of aperture (b) and pressure gradient on L in straight fractures. Substitution of $\bar{u}$ in (26) into (30) gives:

$$L = \frac{b^4}{48 \mu D_m} \frac{\partial p}{\partial x} \quad (31)$$

which shows strong sensitivity (fourth order) to b. To further emphasize the importance of b, we calculated L for different b using typical values of subsurface pressure gradients and $D_m = 2.03 \times 10^{-9}$ m²/s (typical for salt) (Figure 2). Additionally and perhaps more importantly, since $\bar{u}$ is a second order function of b, the dynamic D depends on b via a sixth order function. Moreover, L is only linearly related to the pressure gradient. Both observations highlight b as a critical parameter.

[12] Our theory for predicting dynamic D is also applicable to rivers. Since transverse velocity variation is typically 100 or more times more effective compared to vertical velocity variation in causing longitudinal dispersion [*Fischer et al.*, 1979], it is reasonable to simplify the stream into a planform 2D transport problem, not different from a fracture. For a stream with uniform water depth, *Fischer*
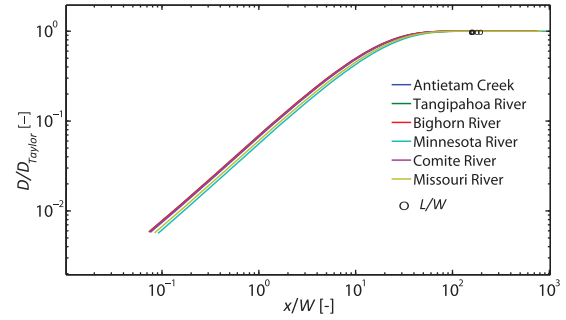
et al. [1979] showed that (21) is still valid but with the transverse mixing coefficient ε_t in the place of D_m. The transverse mixing coefficient for natural rivers is given by [*Deng et al.*, 2001]:

$$\varepsilon_t = \left[0.145 + \frac{\bar{u}}{3520 u_*} \left(\frac{W}{H} \right)^{1.38} \right] u_* H \quad (32)$$

where u_* is the shear velocity describing shear stress-related motion, W is the width, and H is the depth. In the same sense, (24) can be modified by using ε_t in the place of D_m for rivers.

[13] Our theory works well for predicting D of natural straight rivers (Table 1) by using reported u_*, W, and H to calculate ε_t. ε_t is further applied by replacing D_m in (31) to estimate L. But unlike the significant effect of b on L (which is analogous to W for rivers), L for the rivers we analyzed only varies over 1–2 orders of magnitude (Figure 3 and Table 1) since the pressure gradient in wide streams is generally less than that in narrow streams, and the pressure gradient also corresponds to a relatively small range (~1–2 orders of magnitude) in mean velocity (Table 1). Nonetheless, our calculations show that L varies around 150–200 times the stream width. This is much larger than the rule of thumb of 25 stream widths suggested as a mixing length when conducting stream tracer studies [*Day*, 1977]. Alternatively, *Rutherford* [1994] proposed a semi-empirical method for L:

$$L = \beta \frac{\bar{u} b^2}{0.23 H u_*} \quad (33)$$

where β is a coefficient which varies from 1–10 for rough channels and where the denominator is an approximation for

Table 1. Comparison of Measured and Theoretical Dispersion Coefficients (D) Calculated Using Equation (28) at Asymptotic Time Scale and From *Deng et al.* [2001], and Comparison of Theoretical Length Scales (L) Calculated With Equation (31)[a]

| | | | | | D (m²/s) | | | | | L (Equation (31)) | L (Equation (33)) |
River	W (m)	H (m)	$\bar{u}$ (m/s)	u_* (m/s)	Measured Value	Equation (28)	Deng et al.	T (hr)	L/W (−)	(km)	(km)
Antietam Creek, MD	12.8	0.30	0.42	0.057	17.5	15.6	17.6	1.3	152	1.9	17.5–175
Tangipahoa River, LA	31.4	0.81	0.48	0.072	45.1	42.2	49.1	2.7	147	4.6	35.2–352
Bighorn River, WY	44.2	1.37	0.99	0.142	184.6	121.1	150.9	1.8	146	6.5	43.2–432
Minnesota River	80.0	2.74	0.03	0.002	22.3	9.5	12.1	118.7	182	14.6	143.4–1434
Comite River	13.0	0.26	0.31	0.044	7.0	11.5	12.3	1.7	146	1.9	19.9–199
Missouri River	197.0	3.11	1.53	0.078	892.0	964.2	950.8	6.0	167	33.1	1064–10640

[a]The normalized L/W is calculated using L from equation (31).

the transverse mixing coefficient. Calculations with (33) resulted in scales that are larger, and may in fact be several orders of magnitude larger, than those calculated using (31) (Table 1). Therefore, anomalous transport with a dynamic D in rivers can be relevant at scales much larger than what (31) predicts.

[14] We present a closed-form expression for dynamic dispersion coefficient by direct solution of the general transport equations. Using this, we analyzed the time and length scales for typical fractures and some large rivers when transport has completely transitioned from non-Fickian to Fickian. Our theoretical approach can also be applied to transport of other scalars such as heat, or other related problems such as cases with mass transfer across fracture walls. Future work should focus on non-trivial boundary conditions to provide further insight on dynamic dispersive transport.

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