Fractal Travel Time Estimates for Dispersive Contaminants

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Abstract

Alternative fractional models of contaminant transport lead to a new travel time formula for arbitrary concentration levels. For an evolving contaminant plume in a highly heterogeneous aquifer, the new formula predicts much earlier arrival at low concentrations. Travel times of contaminant fronts and plumes are often obtained from Darcy's law calculations using estimates of average pore velocities. These estimates only provide information about the travel time of the average concentration (or peak, for contaminant pulses). Recently, it has been shown that finding the travel times of arbitrary concentration levels is a straightforward process, and equations were developed for other portions of the breakthrough curve for a nonreactive contaminant. In this paper, we generalize those equations to include alternative fractional models of contaminant transport.

Introduction

Travel time estimates for contaminants are typically found from Darcy's law calculations using the average velocity. Such estimates will represent the arrival time of the average concentration for a contaminant front or the peak arrival time for a well-defined pulse. In a recent paper, Wheatcraft (2000) discussed this process and pointed out the drawbacks. Since migrating contaminants experience a variety of velocities due to dispersive processes, smaller concentrations will arrive at a downgradient location significantly before the average. For better estimates of travel times, Wheatcraft used the traditional advection-dispersion (ADE) model to develop equations for travel times for arbitrary concentration levels that only require two pieces of information: (1) the dispersivity and (2) the average pore velocity. However, there may be times when a fractional ADE model is more appropriate. Here, we take the ideas from Wheatcraft

(2000) and extend them to include the fractional ADE model.

The first part of this paper lays out a step-by-step approach to estimate the travel times for a contaminant front and for a pulse/plume. Equations, tables, graphs, and examples are provided so that the reader can make quick and easy estimates. Later in the paper, we discuss the reasoning behind our methods and describe in detail how we developed the travel time equations.

Classical ADE Model

We will first consider a contaminant front where dispersion is modeled by the standard ADE equation. The breakthrough curve of a front expands as the contaminant disperses, as shown in Figure 1. The relative concentration, C, is plotted against the distance traveled by the contaminant, x. In a front model, the contaminant will eventually reach a constant maximum level, and the relative concentration refers to a percentage of the contaminant at its maximum level. We will start with the traditional ADE for a contaminant front (Bear 1979)

$$C(x, t) = \frac{1}{2} \operatorname{erfc} \left[\frac{x - vt}{2\sqrt{avt}} \right] \quad (1)$$

where C = normalized concentration, $0 \leq C \leq 1$; a = dispersivity; and v = average velocity. At this time, it is helpful to introduce the following notation in this analysis. x_C

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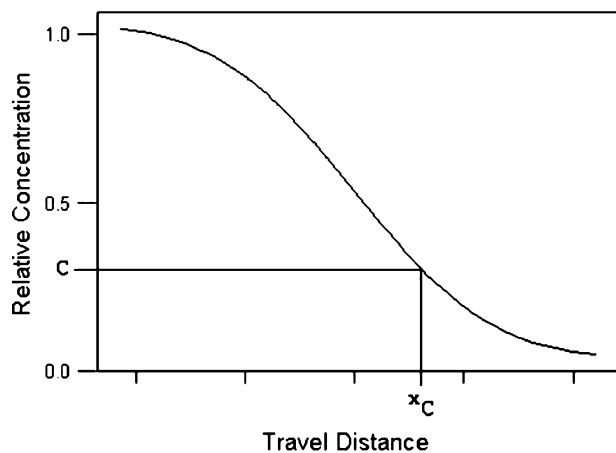
Figure 1. ADE solution for a contaminant front.

is the distance traveled by the point on the breakthrough curve with concentration C. For example, x_{50} would represent the distance traveled by the 50% point on the breakthrough curve. In the Appendix, we show that Equation 1 leads to the following travel time equation

$$x_C = vt + \beta\sqrt{2avt} \qquad (2)$$

where β is the $1 - C$ quantile of the standard normal distribution, defined by

$$1 - C = P(Z \leq \beta) \qquad (3)$$

and Z is a standard normal variable with mean = 0 and standard deviation = 1. Table 1 provides typical values of concentration and the corresponding quantiles for a standard normal.

To obtain the travel time t from Equation 2, input the distance downstream x_C, the advective velocity v, the dispersivity a, and the quantile β for the desired relative concentration level C from Table 1, then solve for t. As an illustration, we will use a bromide tracer test conducted by Garabedian et al. (1991) at Cape Code in 1985 to 1986. They estimated that $v = 0.43$ m/d for the average velocity and $a = 0.96$ m for the dispersivity. Using these estimates and $C = 0.5$, we substitute $\beta = 0$, found from Table 1, into Equation 2 and solve for t, when $x_C = 100$ m. Solving this equation, we find that $t = 232.558$ d. This means that the average concentration traveled 100 m from the injection point in ~233 d. In comparison, we also calculated the travel time for the 10% concentration ($C = 0.10$, so that $\beta = 1.282$) and arrived at a travel time of 194.95 d. This is ~38 d earlier than the time that would

have been predicted using the average concentration. The travel time for the 1% concentration ($C = 0.01$, so that $\beta = 2.326$) was 168.7 d.

If we were to solve Equation 2 for t, we would arrive at the same result of Wheatcraft (2000)

$$t = \frac{x_C + a\beta^2 - \sqrt{a^2\beta^4 + 2ax_C\beta^2}}{v} \qquad (4)$$

However, for reasons that will become clear in the next section, we choose not to solve for t in this presentation. Notice that the distance traveled by the contaminant is related to the square root of time. We plotted Equation 2 in Figure 2, and the graph shows the distance traveled x_C vs. travel time t, with varying concentration levels. One can see evidence that concentration spreads like the square root of time, especially when the concentration is small. Another interesting observation is that the lower levels of concentration travel much faster than the average concentration, $C = 0.5$ on the graph. Therefore, using Darcy's law calculations and the average pore velocity for all concentration levels can result in longer and inaccurate travel times.

Next, we consider relative concentration using the ADE solution for a contaminant pulse/plume (Bear 1972)

$$C(x,t) = \frac{1}{2\sqrt{\pi avt}} \exp\left[\frac{-(x-vt)^2}{4avt}\right] \qquad (5)$$

With a slightly different interpretation than the front model, we get the same equation for the travel time. Recall, in the front model the relative concentration is the percentage of what the maximum level of contaminant will be. With a pulse/plume contaminant, the relative concentration refers to the percentage of the total contaminant mass that has passed point x_C.

Looking at the curve of the ADE for a contaminant pulse/plume in Figure 3, it is easy to see that the relative concentration C is the area under the curve past x_C, for the total area under the curve would have to equal 1 (100% of the contaminant). In order to find the travel time, we should evaluate the following equation for x_C

$$C = \int_{x_C}^{\infty} \frac{1}{2\sqrt{\pi avt}} \exp\left[\frac{-(x-vt)^2}{4avt}\right] dx \qquad (6)$$

In the Appendix, we show that derivation of this equation results in the same travel time equation as Equation 2. The equation can be used in the same manner as before, except that now t represents the time until a fraction C of the total mass passes point x_C.

Table 1
Quantiles, β, for a Standard Normal Distribution

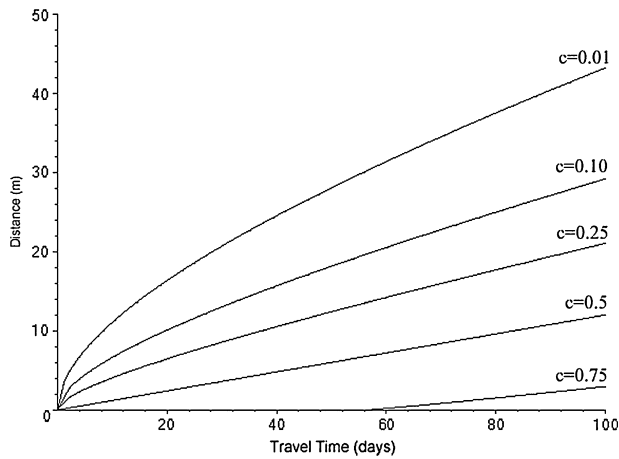|	$C = 0.99$	0.95	0.90	0.75	0.50	0.25	0.10	0.05	0.01
β	-2.326	-1.645	-1.282	-0.674	0.000	0.674	1.282	1.645	2.326

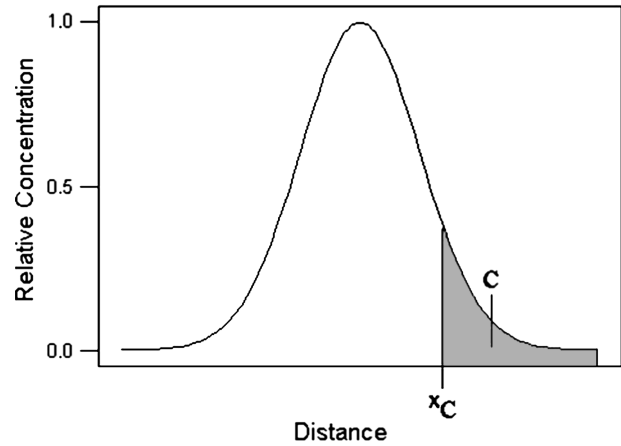Figure 2. Travel time vs. distance for an ADE front.

Figure 3. The ADE solution for a contaminant pulse/plume.

Fractal ADE Model

Wheatcraft (2000) considered two cases: plume growth by traditional dispersion (his Case 1) and plume growth by Mercado-type macrodispersion, where hydraulic conductivity in a perfectly stratified aquifer varies by layer according to a specific probability distribution (his Case 2). For Case 1, plume growth is proportional to the square root of time, whereas in Case 2, plume growth is proportional to time. The two cases cannot be directly compared because their parameters are not the same (dispersivity for Case 1; mean and variance of the hydraulic conductivity distribution for Case 2), but travel times for Case 2 would generally be faster than for Case 1 because the aquifer is considered to be perfectly layered, and therefore the horizontal autocorrelation of hydraulic conductivity is effectively infinite. The Mercado model is a very simple way of accounting for macrodispersive effects, but recent work has led to a completely new way of accounting for macrodispersive transport.

Benson et al. (2000) developed the fractional ADE theory, which models contaminant migration based on a generalization of the normal distribution called the α-stable distribution. The parameter α in this distribution has the range $1 \leq \alpha \leq 2$. The normal distribution is contained within the family of α-stable distributions and is recovered in the case where $\alpha = 2$. For values of $\alpha < 2$, the distribution looks similar to the normal, but there is considerably more probability of finding extreme values. Because of the relatively larger probabilities in the distribution tails for smaller values of α, stable distributions are also known as heavy-tailed distributions (Meerschaert and Scheffler 2001).

Fractional ADE models based on α-stable distributions have been used successfully to model the migration of contaminant plumes for a number of laboratory experiments and field tracer tests (Benson et al. 2000, 2001). They are based on fractional derivatives (Samko et al. 1993) that model enhanced dispersion in a heterogeneous medium due to high-velocity contrasts (Schumer et al. 2001), leading to fractal particle traces (Taylor 1986). Ground water transport is a complex

phenomenon, and many sophisticated models are available that allow prediction of travel times. Most of these models require either a detailed site characterization or a number of additional assumptions about the stochastic nature of aquifer descriptors, such as hydraulic conductivity, as well as significant numerical computation.

There remains a great deal of controversy about the broader applicability (Lu and Molz 2001; Lu et al. 2002) and physical meaning (Molz et al. 2002) of heavy-tailed models in ground water hydrology. However, the fractional ADE provides a simple way to account for scale-dependent dispersivity in the classical ADE as well as the power-law tailing typically seen in ground water plumes and in our opinion provides the most useful basis for a quick and effective estimation of travel time at the field scale. Benson et al. (2000) showed that the 1-D solution to the fractional ADE equation is

$$C = \frac{1}{2}\left[1 - \mathrm{serf}_\alpha\left(\frac{x - vt}{(avt)^{1/\alpha}}\right)\right] \qquad (7)$$

where C = normalized concentration, $0 \leq C \leq 1$; a = fractional dispersivity; v = average velocity, and serf_α is the analogue of the error function erf, with a normal density replaced by an α-stable density (see Appendix Equation 22). The value of α is related to the degree of heterogeneity. A value of $\alpha = 2$ would be equivalent to a perfectly homogeneous aquifer, and values of $\alpha < 1.5$ corresponding to very heterogeneous aquifers. For instance, the well-known tracer test at Columbus Air Force Base, Mississippi, has been shown to have a value of $\alpha = 1.1$ and variance of the logarithm of hydraulic conductivity, log $K = 4.6$ (Benson et al. 2001). For the more homogeneous tracer test at the Cape Cod site, it was found that $\alpha = 1.8$ (Benson et al. 2000) and the variance of log $K = 0.24$ (Garabedian 1991). The parameter α can also be estimated by determining how fast the plume variance is growing (Benson et al. 2001), which shows that α is related to the fractal dimension of Wheatcraft and Tyler (1988). With this information, we can consider the fractional ADE (Equation 7) in the same manner as we did the classical ADE (see Appendix for details). This comparison leads to the fractional travel time equation

$$x_C = vt + \beta_\alpha (avt)^{1/\alpha} \qquad (8)$$

where β_α is the $1 - C$ quantile of the standard, symmetric α-stable distribution. Table 2 provides some common concentration levels and the corresponding β_α values. Note that Equation 8 reduces to Equation 2 if $\alpha = 2$. This happens because the normal distribution is simply a special case of an α-stable distribution when $\alpha = 2$. However, due to the definition of the stable density, there is a factor of $\sqrt{2}$ within the calculations. Notice that when $\alpha = 2$ in Table 2 for β_α, the values must be divided by $\sqrt{2}$ in order to obtain the same values as the normal β in Table 1. Also, when $\alpha = 2$ the concentration, which spreads like $t^{1/\alpha}$, will now disperse at a rate of $t^{1/2}$, as in the classical model. Using $C = 0.01$, we show the relationship between x_C, the location of the C concentration at time t for different α, in Figure 4. As before, to obtain the travel time t from Equation 8, input the distance downstream x_C, the advective velocity v, the dispersivity a, and the stable quantile β_α for the desired relative concentration level C from Table 2, then solve for t.

We will illustrate use of the fractal travel time equation by using the same data as before, collected by the USGS during a 511-d tracer test within a relatively uniform sand and gravel aquifer on Cape Cod. These data were analyzed by Benson et al. (2000), and they estimated $\alpha = 1.8$, $v = 0.43$ m/d for the average velocity, and $a = 0.58$ for the fractional dispersivity. Solving Equation 8 with these values along with $x_C = 100$ m, we obtain $t = 232.558$ d. This means that the average concentration traveled 100 m from the injection point in ~233 d. In comparison, we also calculated the travel time for the 10% concentration ($C = 0.10$, so that $\beta_\alpha = 1.880$) and found that it traveled 100 m downstream from the injection point in 194.75 d. This is about 38 d earlier than the time that would have been predicted using the average concentration. The travel time for the 1% concentration ($C = 0.01$, so that $\beta_\alpha = 4.227$) was 157.1 d.

Since this paper illustrates two different models for travel time, it is useful to compare them now. The travel time for the 50% concentration or plume center of mass

is the same for both models, 100 m in 233 d, since this travel time only depends on the advective velocity. For the 10% concentration level, 100-m travel time is around 195 d for both models, perhaps because the dispersivity parameters were chosen to fit the plume spread at about this level. The 100-m travel time for the 1% concentration level is 169 d for the classical ADE and 157 d for the fractional ADE. The fractional model predicts significantly earlier arrival at very low concentrations. Hence, if low levels of contamination are of concern, we advise use of the fractional model.

Comparison of Travel Distances

It is very interesting to compare the travel distances for values of $\alpha < 2$ with those for the traditional ADE ($\alpha = 2$). Their ratio is

$$\frac{vt + \beta_\alpha (avt)^{1/\alpha}}{vt + \beta (avt)^{1/2}} \qquad (9)$$

This equation is plotted in Figure 5 for a concentration of $C = 0.01$. This plot illustrates the fact that, especially for low concentrations, travel distances for low values of α are much farther than what would be predicted by the traditional ADE ($\alpha = 2$). For example, for $\alpha = 1.1$ (a very heterogeneous aquifer such as the MADE site) after 100 d, the contaminant has traveled nearly 10 times farther than the traditional ADE prediction. This may help explain why at the MADE site, mass was continually "lost" at each sampling period (Garabedian et al. 1991). In other words, the sampling points used at a given sampling period were chosen based on predictions of the traditional ADE and stochastic theories. However, it has been shown that the plume can be well modeled by the fractional ADE (Benson et al. 2001), which means that travel distances for low concentrations would be much larger than those predicted by traditional theories. The "lost mass" may be just the heavy plume tail traveling much faster than traditional predictions, as shown in Figure 5.

Table 2
Quantiles, β_α, for a Standard Symmetric α-Stable Distribution. When $\alpha = 2$ the Values Are the Same as the Standard Normal Distribution Multiplied by a Factor of $\sqrt{2}$. The Factor of $\sqrt{2}$ is Due to a Change in Parameterization

|	C = 0.99	0.95	0.90	0.75	0.50	0.25	0.10	0.05	0.01
$\alpha = 1.1$	−22.071	−5.165	−2.729	−0.989	0.000	0.989	2.729	5.165	22.071
1.2	−16.160	−4.369	−2.480	−0.982	0.000	0.982	2.480	4.369	16.160
1.3	−12.313	−3.795	−2.297	−0.976	0.000	0.976	2.297	3.795	12.313
1.4	−9.659	−3.370	−2.162	−0.972	0.000	0.972	2.162	3.370	9.659
1.5	−7.736	−3.052	−2.061	−0.969	0.000	0.969	2.061	3.052	7.736
1.6	−6.284	−2.814	−1.985	−0.966	0.000	0.966	1.985	2.814	6.284
1.7	−5.152	−2.637	−1.927	−0.963	0.000	0.963	1.927	2.637	5.152
1.8	−4.277	−2.505	−1.880	−0.960	0.000	0.960	1.880	2.505	4.277
1.9	−3.669	−2.404	−1.843	−0.957	0.000	0.957	1.843	2.404	3.669
2.0	−3.290	−2.326	−1.812	−0.954	0.000	0.954	1.812	2.326	3.290
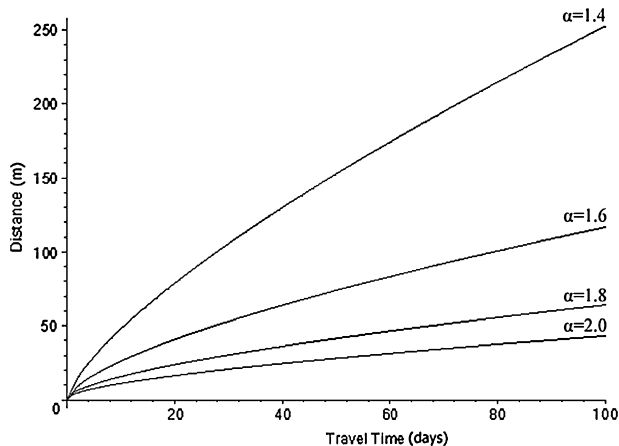
Figure 4. Travel time vs. location for a fractional ADE front with C = 0.01 or 1% of the eventual maximum. Here, _v_ = 0.12 m/d and _a_ = 7.5 m.

Conclusions

A fractional travel distance/time relationship (Equation 8) has been developed in a manner similar to the method developed by Wheatcraft (2000) for the traditional ADE. Equation 8 depends on two parameters in addition to the advective velocity and dispersivity:

1. The concentration C that one wishes to know the travel distance or time for
2. The value of α chosen based on the degree of heterogeneity of the aquifer.

As a guideline

1. Relatively homogeneous aquifers would be expected to have $1.7 \leq \alpha \leq 2.0$
2. Aquifers of "average heterogeneity" would be expected to have $1.3 \leq \alpha \leq 1.7$
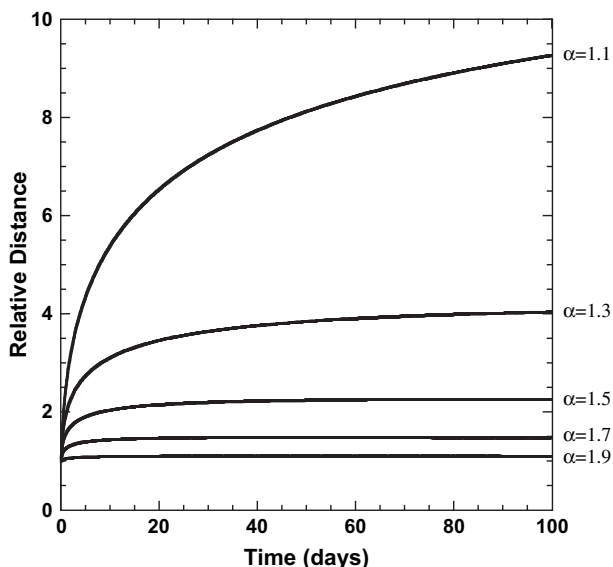3. Relatively heterogeneous aquifers would be expected to have $1.0 \leq \alpha \leq 1.3$.

Figure 5. Travel time ratio (fractional/classical) vs. location for an ADE front with C = 0.01, a = 1 m, and v = 0.1 m/d.

Once values of concentration and α have been selected, β_α is obtained from Table 2 and Equation 8 can be solved directly for travel time. Because α is a fraction, one cannot solve Equation 8 directly, so solver routines must be employed (e.g., the solver in Excel). For low concentrations in a highly heterogeneous aquifer, travel distances can be far in excess (more than a factor of 10 in ~100 d) for a contaminant that is following the fractional ADE, as compared to a contaminant that is following the traditional ADE.

The travel distance/time Equation 8 developed here can be used to provide better estimates of travel distance or time than Darcy's law calculations that are only valid for the mean concentration or for the center of mass of a plume.

Appendix: Derivation of Travel Time Equations

In this section, our approach to developing the travel time equations is a probabilistic one. We will start with the ADE solution for a contaminant front (Equation 1). With a contaminant front, the level of concentration continues to increase with time. As time approaches infinity, the contaminant will approach a level of 100% (Figure 1). This means that the relative concentration C (x,t) for a contaminant front refers to the contaminant level at location x at time t as a percentage of the highest level that will ultimately be observed. Equation 1 contains the complementary error function, which is defined as

$$\mathrm{erfc}(a) = \frac{2}{\sqrt{\pi}} \int_a^\infty e^{-y^2} \, \mathrm{d}y \tag{10}$$

The complementary error function can also be written as

$$\mathrm{erfc}(a) = 2P(Y > a) \tag{11}$$

where Y is a normal random variable with mean = 0 and standard deviation = $1/\sqrt{2}$. Therefore, Equation 1 simplifies to

$$C = P\left(Y > \frac{x_C - vt}{2\sqrt{avt}}\right) \tag{12}$$

If we standardize this normal probability by subtracting the mean and dividing by the standard deviation, we get

$$C = P\left(\frac{Y - 0}{1/\sqrt{2}} > \frac{x_C - vt}{2\sqrt{avt}/\sqrt{2}}\right) = P\left(Z > \frac{x_C - vt}{\sqrt{2avt}}\right) \tag{13}$$

where Z is a standard normal variable with mean = 0 and standard deviation = 1. Then

$$1 - C = P\left(Z \leq \frac{x_C - vt}{\sqrt{2avt}}\right) \tag{14}$$

and comparing with Equation 3 implies that

$$\frac{x_C - vt}{\sqrt{2avt}} = \beta \tag{15}$$

where β is the $1 - C$ quantile of the standard normal distribution, as discussed earlier. Solving for x_C, we arrive at the travel time Equation 2.

Next, we will consider the pulse/plume contaminant model. Even though we ended up with an equivalent equation to the front model, the approach differs slightly due to the definition of relative concentration in the pulse/plume. With a pulse/plume model, the contaminant concentration passing point x_C will increase with time until the peak of the plume. After the peak, the concentration will decrease with time. In order to find the travel time for a particular concentration, we must consider how much of the pulse/plume has traveled past point x_C. From Figure 3, we can see that in order to find the relative concentration we should integrate the ADE solution (Equation 5) from x_C to infinity

$$C = \int_{x_C}^{\infty} \frac{1}{2\sqrt{\pi avt}} \exp\left[\frac{-(x-vt)^2}{4avt}\right] dx \quad (16)$$

Again, we compare this equation to that of a normal probability density to get

$$C = P(Y > x_C) \quad (17)$$

However, this time the normal random variable Y has mean = vt and standard deviation = $\sqrt{2avt}$. If we standardize Y by subtracting the mean and dividing by the standard deviation, we get

$$C = P\left(\frac{Y-vt}{\sqrt{2avt}} > \frac{x_C-vt}{2\sqrt{avt}}\right) \quad (18)$$

This simplifies to

$$C = P\left(Z > \frac{x_C-vt}{2\sqrt{avt}}\right) \quad (19)$$

where Z is again a standard normal random variable with mean = 0 and standard deviation = 1. This implies that

$$1-C = P\left(Z \leq \frac{x_C-vt}{2\sqrt{avt}}\right) \quad (20)$$

and again we apply Equation 3 to arrive at Equation 2. As mentioned earlier, the concentration is spreading away from the center of mass at a rate of $t^{1/2}$.

Our approach to finding the travel time equations for dispersion modeled by the fractional ADE is identical to the classical case. The only difference is that we reference a symmetric α-stable probability density instead of a normal probability density. We will start with the solution to the fractional ADE for a contaminant front

$$C = \frac{1}{2}\left[1 - \text{serf}_\alpha\left(\frac{x_C-vt}{(avt)^{1/\alpha}}\right)\right] \quad (21)$$

We define the α-stable error function (serf_α) similarly to the error function, i.e., twice the integral of a symmetric α-stable density from 0 to a

$$\text{serf}_\alpha(a) = 2\int_0^a f_\alpha(x)dx \quad (22)$$

where $f_\alpha(x)$ is the standard, symmetric α-stable density characterized by its Fourier transform

$$f_\alpha(k) = \int_{-\infty}^{\infty} e^{ikx} f_\alpha(x)dx = \exp\left(-|k|^\alpha\right) \quad (23)$$

Note the similarity between Equation 23 and that of the Fourier transform of a standard normal, $\exp(-k^2/2)$. The slight difference accounts for the $\sqrt{2}$ factor between the standard normal (values in Table 1) and the standard, symmetric stable when $\alpha = 2$ (values in Table 2).

When we combine Equation 21 with the definition of $\text{serf}_\alpha(x)$ from Equation 22, we get

$$C = \frac{1}{2}\left[1 - 2\int_0^{\frac{x_C-vt}{(avt)^{1/\alpha}}} f_\alpha(x)dx\right] \quad (24)$$

Using the definition of a probability density, we arrive at

$$C = \frac{1}{2}\left[1 - 2P\left(0 \leq Z_\alpha \leq \frac{x_C-vt}{(avt)^{1/\alpha}}\right)\right] \quad (25)$$

where Z_α is a standard, symmetric α-stable random variable. Then

$$C = \frac{1}{2}\left[1 - P\left(|Z_\alpha| \leq \frac{x_C-vt}{(avt)^{1/\alpha}}\right)\right] =$$
$$\frac{1}{2}P\left(|Z_\alpha| > \frac{x_C-vt}{(avt)^{1/\alpha}}\right) = P\left(Z_\alpha > \frac{x_C-vt}{(avt)^{1/\alpha}}\right)$$

so that

$$1-C = P\left(Z_\alpha \leq \frac{x_C-vt}{(avt)^{1/\alpha}}\right) \quad (26)$$

Since the $1 - C$ quantile β_α of the standard, symmetric α-stable distribution is defined by

$$1-C = P(Z_\alpha \leq \beta_\alpha) \quad (27)$$

it follows that

$$\beta_\alpha = \frac{x_C-vt}{(avt)^{1/\alpha}} \quad (28)$$

This equation can be solved for x_C to obtain the fractional travel time Equation 8. Equation 8 shows that the contaminant is dispersing at the rate of $t^{1/\alpha}$. For $0 < \alpha < 2$, the dispersion rate is faster than the classical ADE, resulting in faster travel times for contaminant concentrations in the fractional ADE model.

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