

## ***Applying Potential Theory Modeling to Solute Dispersion***

### **7.1 Introduction**

The fundamental goal in modeling solute dispersion, is to calculate the solute concentration as a function of position and time, given an initial concentration. Chapters 2, 4 and 5 laid the groundwork by describing the mathematics of models based on stochastic differential equations. It is now time to show how these ideas can be applied concretely to calculate the evolution of the solute concentration carried by porous flow. In this chapter, we will do this for two specific cases: a 1-dimensional flow in which the carrier fluid flow velocity is constant, and a generalization of this in which the flow velocity changes linearly with position. Our emphasis will be on obtaining analytical results which can lead to insights into the relationships between flow modeling at the microscopic level, where we describe the displacement of a fluid element as a stochastic process, and the effects that this has on the macroscopic concentration. For this, the potential theory approach is the obvious choice, rather than simulation of individual realizations that will be investigated in a later chapter.

We have already formulated the stochastic model for the 1-dimensional carrier fluid flow. It is given by equation (7.1) in a slightly modified notation:

$$dx = u(x) dt + \gamma^2 \sum_{n=0}^{\infty} \sqrt{\lambda_n} f_n(x) db_n(t, \omega). \quad (7.1)$$

Two changes have been made to the notation. First, the combination of materials constants that appears in Darcy's law has been replaced by the function  $u(x)$ . This is meant not only as an abbreviation, but also to signify that the work in this chapter is applicable to any situation where a fluid velocity field can be calculated from appropriate fluid dynamics equations,

not necessarily just Darcy's law. The significance of equation (7.1) is that a term has been added that models stochastic variations in this velocity field, whatever the origin of the field.

The second mainly cosmetic change is that the symbol  $\sigma$  that was used in equation (7.1) to indicate the variance of the covariance kernel, has been replaced by the symbol  $\gamma$ . This is to avoid confusion with the variance of the solute concentration, which plays an important role in the rest of this chapter. Also, it emphasizes that regardless of the way in which the factor now called  $\gamma$  was introduced, the role that it plays in equation (7.1) is essentially that of an amplitude characterizing the strength of the stochastic perturbation. All results of the stochastic model should reduce back to the corresponding deterministic ones in the limit  $\gamma \rightarrow 0$  which we will call the deterministic limit.

As we are here dealing with the application of an ID to an actual physical problem, it is also appropriate to remind the reader that the use in equation (7.1) of Wiener processes  $db_n(t, \omega)$  defined as in equations (2.5), implies that the position and time variables have been appropriately scaled to reflect the physical processes that cause the random displacements. This was discussed in detail just after equation (2.5). In other words,  $x$  and  $t$  in equation (7.1) should really be interpreted as  $x/\ell_x$  and  $t/\ell_t$  where  $\ell_x$  and  $\ell_t$  are scale constants to be determined below. For simplicity of notation, we will suppress the scale constants until we are in a position to determine their values later on.

Equation (7.1) is already in the standard form of equation (5.3) which defines an ID. But it only specifies the fluid flow problem; to describe solute transport we have to add additional equations and the first hurdle to overcome is to formulate these equations in ID form as well.

To discuss the problem, we revert to the deterministic formulation in 3 dimensions, as the form of the equations is most familiar in that case. Equation (7.1) in that case merely becomes

$$\frac{dx}{dt} = \underline{v} = \underline{u}(x) \quad (7.2)$$

where  $\underline{v}$  is the fluid velocity vector. The connection with solute transport is established by defining the solute flux vector  $\underline{J}$  by

$$\underline{J} = \underline{v}c - D_m \cdot \nabla c \quad (7.3)$$

where  $c$  is the solute concentration and  $D_m$  the diffusion coefficient, and the evolution of the concentration is determined by solute conservation as expressed by the equation of continuity:

$$\frac{\partial c}{\partial t} = -\nabla \cdot \underline{J} \quad (7.4)$$

If we eliminate  $\underline{J}$  from equations (7.3) and (7.4) we have

$$\frac{\partial c}{\partial t} = -c \nabla \cdot \underline{v} - \underline{v} \cdot \nabla c + \nabla D_m \cdot \nabla c + D_m \nabla^2 c. \quad (7.5)$$

This is the second equation needed in the deterministic description and for the stochastic description one would like to write this in a form that can be changed into an ID. There are a number of obstacles to this. For a start, we have to decide whether  $\underline{v}$  on the right hand side of equation (7.5) is also a stochastic variable, as would be expected if it is the derivative of the position. But as the time variation of the position of a fluid element is determined by a Wiener process, it does not have a derivative!

The root of the problem is the question whether  $\underline{v}$  represents the velocity of a fluid element which is at position  $\underline{x}$  at time  $t$  (i.e., a particle interpretation), or is it the fluid velocity field, which e.g. in the case of stationary flow is independent of  $t$ ? In changing from the deterministic equation (7.2) to the SDE (7.1) we have definitely taken the first view, but in the continuity equation we will argue below that it is the second view that is applicable.

In the case of deterministic stationary flow the distinction is unimportant. To show that, temporarily assign the superscripts “p” and “f” to distinguish between the particle and fluid interpretations. Starting with a particle interpretation of equation (7.2) we have

$$\frac{d\mathbf{x}^p}{dt} = \mathbf{u}(\mathbf{x}^p) \Rightarrow \mathbf{x}^p = \mathbf{x}^p(t). \quad (7.6)$$

i.e. a trajectory can be calculated for the fluid “particle”. Then  $\mathbf{x}^p$  can be differentiated to find  $\underline{v}^p(t)$  and by eliminating the common parameter  $t$  we can find  $\underline{v}^p(\mathbf{x}^p)$ . That gives the velocity of the particle when it arrives at the position  $\mathbf{x}^p$  irrespective of when it gets there and in stationary flow this is the same for all particles. Then it makes sense to associate  $\underline{v}^p(\mathbf{x}^p)$  with the flow rather than the particle, i.e.  $\underline{v}^p(\mathbf{x}^p) \equiv \underline{v}^f(\mathbf{x})$  which is independent of time because  $\mathbf{x}$  is now just a coordinate, independent of time. We may write

$$\frac{dv^f}{dt} = \frac{\partial v^f}{\partial t} = 0, \quad (7.7)$$

and together with the initial condition this is solved by  $v^f = u(x)$ , i.e we have shown that equation (7.2) applies to the flow velocity interpretation as well and there is no ambiguity about the meaning of  $v$  in equation (7.5) for the deterministic case.

However, this reasoning breaks down in the stochastic case, both because every fluid particle follows a different trajectory and because  $\underline{x}^p(t)$  cannot be differentiated any more. So we are forced to distinguish between the interpretations in the stochastic case.

Turning now to the continuity equation, it should be remembered that the underlying conservation law is an integral law, stating that the solute mass in a closed volume can only change as a result of the total flux across the surface. The continuity equation is merely a differential statement of this based on Taylor expansion of the flux, and assumes that the flux and hence also the velocity can be differentiated. So there is clearly a conceptual problem in applying the continuity equation to the particle velocity in stochastic flow. On the other hand, solute conservation as applied to a single fluid element holds trivially, at least in the absence of diffusion, which is the case we are mostly concerned with.

One way out of this difficulty is to conclude that the conservation law should be applied to the complete flow. By this we mean the superposition of individual realizations of the flow trajectory, just as the deterministic flow field is the superposition of trajectories of all fluid elements. Therefore  $\underline{v}(\underline{x})$  in equation (7.5) should be interpreted as the average velocity, averaged over all realizations that pass through position  $\underline{x}$ . We have seen in section 5.6.3 that when a stochastic population was averaged over all realizations the deterministic value was obtained; below it will be shown that the same holds for the stochastic flow velocity. So in the end we are justified to use the deterministic equation (7.2) to replace the unknown velocity  $\underline{v}$  in equation (7.5) by the known, non-stochastic function  $\underline{u}(\underline{x})$ .

Another way out is to recognize that the continuity equation is not really part of the stochastic problem, and that solute mass conservation should rather be applied in another way after solving the SDE equations. This will be further pursued below, but first we investigate where the use of  $\underline{u}(\underline{x})$  in equation (7.5) leads.

The next problem in obtaining an ID from equation (7.5), is that a total time derivative is needed on the left so that it can be written as  $dc = b(c) dt$ , to use the notation of equation (5.3). That is easily addressed by transferring the second term in equation (7.5) to the left and we are left with

$$\frac{dc}{dt} = -c\nabla \cdot u + \nabla D_m \cdot \nabla c + D_m \nabla^2 c. \quad (7.8)$$

The last two terms on the right still do not conform to the ID form, as they involve derivatives of the unknown  $c$ . That could be remedied by taking e.g.  $\nabla c$  and  $\nabla^2 c$  as new variables and adding more equations. This leads to an infinite hierarchy of equations, that would have to be truncated at some stage and does not look very promising. Another idea is to solve equation (7.8) iteratively; i.e., put an assumed form for  $c$  in the last two terms, solve the equations and put the resulting  $c$  back as the next iteration. In particular, we might take  $c = 0$  as the first guess; that seems appealing, since it is equivalent to taking  $D_m = 0$  and as discussed in chapter 1, microscopic diffusion is indeed found to be negligible in many experimental situations.

In what follows, we do make the simplifying assumption that diffusion can be neglected. However, equation (7.8) provides a clear way in which one could in principle move beyond this assumption and add diffusion effects at a later stage. Taking  $D_m = 0$  equation (7.8) reduces finally to the desired form. We could now proceed to combine it with equation (7.2) and set up the problem as a set of two ID equations. That would mean adding Wiener process terms to the right hand sides of both equations. However, the validity of this may be questioned.

From a physical perspective, it is clear that the random variations of the position increments represent the deflections suffered by a fluid element as it meanders thorough the porous medium; but there is no additional physical mechanism independent of this to randomize the concentration. Mathematically, one adds the Wiener terms to represent random variations in the driving coefficients of the original deterministic equation. But in equation (7.8) the driving coefficient is  $\nabla u$ , which is not independent of the driving coefficient  $u$  in equation (7.1). In fact the point of the eigenfunction sum in equation (7.1) was to explicitly introduce spatial correlation between random variations in  $u$  at neighboring points, and adding random variation to the spatial derivative would contradict this.

Therefore it is only appropriate to add the Wiener terms to equation (7.1) while (7.8) should remain as it is, a deterministic equation. Formally, it is

possible to carry such a deterministic equation along in a set of ID's, but as there is no coupling between the variables in the equations, this does not contribute anything and creates unnecessary baggage. So, once more, we are led to the conclusion that the continuity equation is not inherently part of the stochastic model and that solute mass conservation should be enforced in a different way.

## 7.2 Integral Formulation of Solute Mass Conservation

Consider, first, a deterministic flow of an incompressible carrier fluid specified by a stationary velocity field  $u(x) > 0$ , and transporting a solute with concentration  $c(x, t)$  without diffusion. We consider a 1-dimensional description, i.e.  $u$  and  $c$  have been averaged out over the other two dimensions and  $c$  represents the solute mass per unit length. Suppose that the solute is introduced into the flow at an initial time  $t_0$  with a localized distribution, e.g.  $c(x, t_0)$  may be a Gaussian peak. The problem is to find the concentration at a later time  $t$ , subject to solute mass conservation.

Because the fluid is incompressible, conservation of the fluid mass requires that the volume of fluid passing a point in an interval  $\Delta t$  is independent of position and time, i.e.

$$A(x)u(x)\Delta t = A(x')u(x')\Delta t, \quad \forall t \quad (7.9)$$

where  $A(x)$  is the cross-sectional area perpendicular to the flow.

The total amount of solute that passes  $x$  between  $t$  and  $t + \Delta t$  is given by  $c(x, t)u(x)\Delta t$ , but clearly a conservation equation of the type of equation (7.9) does not apply to this as the amount passing a given point changes with time. Nevertheless, as there is no diffusion, we can still make the statement that all the solute contained in the volume element  $A(x')u(x')\Delta t$  will pass a point  $x > x'$  in a time interval of the same length  $\Delta t$  at the later time  $t$  when that particular volume element reaches  $x$ .

Defining the kinematic time interval  $w(x|x')$  for traveling from  $x'$  to  $x$  by

$$w(x|x') = \int_{x'}^x \frac{dx}{u(x)} \quad (7.10)$$

that statement is expressed by

$$c(x, t)u(x)\Delta t = c(x', t - w(x|x'))u(x')\Delta t. \quad (7.11)$$

This is equivalent to the following equation, which appears more complicated but is formulated in a way that allows for later generalization:

$$c(x, t) = \frac{u(x_0)}{u(x)} \int_{-\infty}^t dt' c(x_0, t') \delta(t' - t + w(x|x_0)). \quad (7.12)$$

This form is appropriate for a boundary value problem, where the value of the concentration is known at the fixed boundary  $x_0$  for all times earlier than  $t$ . If instead, as originally stated above, we know the initial concentration at  $t = t_0$ , we have an initial value problem and to formulate the conservation law we need to first solve for  $x'$  from the equation

$$t_0 = t - w(x|x') \quad \Rightarrow \quad x' = \chi(x, t|t_0) \quad (7.13)$$

and then rewrite equation (7.11) as

$$\begin{aligned} c(x, t) &= \frac{1}{u(x)} [c(x', t_0)u(x')] \Big|_{x'=x}, \\ &= \frac{1}{u(x)} \int_{-\infty}^{\infty} dx' c(x', t_0)u(x') \delta(x' - \chi(x, t|t_0)). \end{aligned} \quad (7.14)$$

To illustrate the use of equations (7.12) and (7.14) as conservation laws, consider first the simple case where  $u(x)$  is constant; say  $u(x) = v_0$ . Then we have

$$w(x|x') = \frac{x - x'}{v_0}; \quad \chi(x, t|t_0) = x - v_0(t - t_0), \quad (7.15)$$

and this leads respectively for the boundary value and initial value problems to the results

$$\begin{aligned} c(x, t) &= c(x_0, t - \frac{x - x_0}{v_0}), \\ c(x, t) &= c(x - v_0(t - t_0), t_0). \end{aligned} \quad (7.16)$$

Both of these have the straightforward interpretation of simple plug flow, i.e. regardless of the shape of the input solute concentration, this is simply translated forward unchanged at the flow speed  $v_0$ .

The situation is a little more interesting when  $u$  changes with  $x$ . The simplest example of this is when we have a linear dependence, which we write as  $u(x) = v_0 + p(x - x_0)$ . In this case equation (7.10) yields

$$w(x | x') = \frac{1}{p} \ln \left( \frac{v_0 + p(x - x_0)}{v_0 + p(x' - x_0)} \right) \quad (7.17)$$

provided that the  $x$ -value at which  $u(x)$  becomes 0, is excluded from the interval  $[x', x]$ . If this  $x$ -value, referred to as a stagnation point of the flow, is inside the interval, the mathematical treatment might be salvaged by splitting the interval in two. More generally (for flow in the positive  $x$ -direction) we can say that the interval of applicability of the expressions to be derived, are limited from below by the stagnation point for accelerating flow, and from above for decelerating flow. The exclusion of stagnation points can also be justified on physical grounds, as is discussed further below.

Using equation (7.17) to calculate  $\chi$  leads to the expressions

$$\frac{u(x')}{u(x)} = \frac{v_0 + p(x' - x_0)}{v_0 + p(x - x_0)} = e^{-p(t-t')}, \text{ and} \quad (7.18)$$

$$\chi(x, t | t_0) = x_0 + \frac{v_0}{p} \left[ e^{-p(t-t_0)} - 1 \right] + (x - x_0) e^{-p(t-t_0)}. \quad (7.19)$$

It is instructive to take the concrete example where we have an initial value problem, specified by an initial Gaussian concentration peak centered at  $x = \xi$  and with a variance  $s^2$ :

$$c(x, t_0) = \frac{1}{\sqrt{2\pi s^2}} \exp \left[ -\frac{(x - \xi)^2}{2s^2} \right]. \quad (7.20)$$

The choice of a normalized Gaussian implies that we have for simplicity scaled the total solute mass to unity. Another useful simplification follows by noting that in the initial value problem there is no fixed boundary, i.e. the value of  $x_0$  just determines the value of  $v_0$  and we can just as well choose  $x_0 = \xi$ .

Equations (7.20) and (7.19) can now be substituted into (7.14). The resulting expression is simplified by noting that from (7.18)



$$\frac{u(\chi)}{u(x)} = e^{-p(t-t_0)} \quad (7.21)$$

and that with our choice of  $x_0$ , the expression  $(\chi - \xi)$  reduces to

$$\chi - \xi = e^{-p(t-t_0)}(x - X(t)), \text{ and} \quad (7.22)$$

$$X(t) = \xi + \frac{v_0}{p} \left[ e^{p(t-t_0)} - 1 \right]. \quad (7.23)$$

The expression  $X(t)$  has a straightforward physical interpretation. Going back to equation (7.13), note that the first equation merely represents the relationship between the initial position  $x'$  (at time  $t_0$ ) or *source point* of the fluid element that is found at the *target point*  $x$  at a later time  $t$ . So  $\chi$  is the function that calculates the source point, given a target point. Conversely,  $X(t)$  is the target point that originates from the particular source point  $x' = \xi$  (as is easily confirmed by putting  $\chi = \xi$  in equation (7.19)). In other words,  $X(t)$  represents the trajectory followed by the fluid element that contained the peak value of the concentration at the initial time.

We can now put together equations (7.14) and (7.20) to (7.23) to obtain the evolution of the concentration in a linearly accelerating flow, without diffusion or dispersion, as

$$c(x, t) = \frac{1}{\sqrt{2\pi\sigma(t)^2}} \exp \left[ -\frac{(x - X(t))^2}{2\sigma(t)^2} \right] \quad (7.24)$$

where

$$\sigma(t) = s \exp[p(t-t_0)]. \quad (7.25)$$

Equation (7.24) demonstrates some striking features:

- a concentration peak that starts off as a Gaussian, retains its Gaussian shape while propagating;
- the Gaussian remains normalized, i.e. the total solute mass is conserved;
- the peak of the Gaussian moves at the speed predicted by the kinematics of the fluid flow;

- the width of the Gaussian grows exponentially in an accelerating flow ( $p > 0$ ) and shrinks exponentially in a decelerating flow ( $p < 0$ ); and
- for  $p = 0$  the plug flow solution is regained.

The change in the extension of the concentration plume is easily understood qualitatively. In an accelerating flow, parts of the plume ahead of the peak value are always moving faster than those at the peak, and parts behind the peak move slower than the peak so that the plume is stretched out by the acceleration; and conversely it is compressed for deceleration. This effect appears superficially like dispersion, but is merely a result of the kinematics of the fluid motion. Unlike “real” dispersion, it is fully reversible in the sense that if, after propagating for a time  $\Delta t$  the acceleration is instantaneously reversed, equation (7.25) implies that the Gaussian plume will return to its original extension after a further time interval  $\Delta t$ . We will refer to this effect as *kinematical dispersion* in what follows.

However, the surprising thing is that this does not distort the peak shape. This property is a peculiarity of the linear acceleration; it depends on the fact that the factor  $u(\chi)/u(x)$  required by solute conservation turned out in equation (7.21) to depend on time only, and that is a consequence of the logarithm in the expression for  $w(x|x')$  in equation (7.17). For any other dependence of the velocity on position, distortions of the Gaussian shape are to be expected. That concludes our discussion of the integral form of the conservation law for deterministic solute transport, and we turn to the generalization of equations (7.12) and (7.14) to the stochastic transport model.

The latter case, that of an initial value problem, is quite straightforward. The input to this problem is a given initial spatial concentration profile,  $c(x, t_0)$ . Equation (7.14) can be interpreted in a physical way as saying that we divide up this concentration into fluid elements, one for each value of  $x'$ . For each of these, the position  $x$  at which it will end up at time  $t$ , is exactly determined from the flow velocity field. Conversely, to determine the concentration at  $x$  at time  $t$ , we merely need to identify the source point from which the target point fluid element originated, and that is exactly the effect of the Dirac  $\delta$ -function in the integral of equation (7.14). It picks out a single fluid element from the original concentration profile, and if there has been a velocity change while the fluid element moved from the source point to the target point, the concentration is corrected by the ratio of the velocities as required by solute conservation. Obviously, then, in a stochastic model we take into account that there is not a one-to-one correspondence between a source point and a target point any more, but rather for any fluid element in the original concentration there is a probability that it will reach the chosen target point. So we replace

the certainty of motion from the source point to the target point that the  $\delta$ -function expresses, by a probability density for such motion. Then the generalization of equation (7.14) is

$$c(x, t) = \frac{1}{u(x)} \int_{-\infty}^{\infty} dx' c(x', t_0) u(x') P_{t_0}(x' | x, t) \quad (7.26)$$

where we define  $P_{t'}(x' | x, t)$  as the probability density over the position variable  $x'$ , that a fluid element that is known to arrive at the target point  $(x, t)$ , has originated from  $x'$  at a time  $t'$ .

In a similar vein, the boundary value conservation equation might be written

$$c(x, t) = \frac{u(x_0)}{u(x)} \int_{-\infty}^t dt' c(x_0, t') P_{x_0}(t' | x, t) \quad (7.27)$$

where  $P_x(t' | x, t)$  is the probability density over time  $t'$ , that a fluid element that is known to arrive at the target point  $(x, t)$ , has originated from  $x'$  at a time  $t'$ . The two probability densities are not the same, but are related through an appropriate variable transformation.

While the initial value and boundary value formulations appear quite similar, as indeed they are in the deterministic case, there are subtle differences in how they can be applied in the stochastic situation. These differences are highlighted by considering how the input concentration might be prepared physically. In the case of the initial value problem, at least at the level of a gedanken experiment, there is no conceptual difficulty in dropping a previously prepared spatial concentration profile instantaneously into the carrier fluid flow at the instant  $t = t_0$ .

For a boundary value problem, the physical realization would be to inject solute into the flow at the point  $x = x_0$  with a predetermined time profile, say  $f(t)$ . However, the difficulty is that as a moment's consideration shows, the concentration profile in the actual flow at point  $x_0$ ,  $c(x_0, t)$ , will be different from  $f(t)$ . That is because the stochasticity implies that some of the solute concentration will be carried upstream of the injection point. For example, if  $f(t)$  is only a momentary pulse at  $t = 0$ , we would have  $c(x_0, 0+) = 1/2 f(0+)$  because over a short enough time interval the translation of the carrier fluid can be neglected and equal amounts of solute would be taken upstream and downstream by stochastic fluid displacements. Subsequently, some of the solute that was taken upstream by stochastic displacements will be carried past  $x_0$  by the flow, but a diminishing fraction will always remain upstream.

The net effect is that any abrupt change in the injection profile will be rounded off in the time profile at the injection point inside the flow.

The implication is that while a sharp edged spatial concentration profile (for example, a square pulse) can be introduced as an initial value, it is not possible to produce such a spatial profile by injection at a boundary point in the case of stochastic flow because of the inevitable rounding effect. That is in contrast to deterministic flow, where the initial value and boundary formulations are equivalent in the sense that any state specified in an initial value problem, could be prepared by an appropriate injection time profile at a suitably chosen boundary point.

A related remark stems from the observation that any initial value concentration of interest would be localized in space. That places limitations on the specification of a related boundary value problem, because of the fact that stochasticity leads to spreading. Consequently, an injection point cannot be put too far away upstream from the locality of the initial concentration, otherwise even the sharpest injection peak would have spread out too much by the time that it reaches that location. By the same token, for a chosen boundary point, there is an earliest possible time that the injection can start in order to produce a concentration with the appropriate degree of localization at the time  $t_0$  that specifies the initial value version of the problem. In other words, a cutoff time needs to be introduced into equation (7.27) instead of the  $-\infty$  integration limit, for a boundary value problem to represent a localized concentration in a related initial value formulation.

These somewhat vague remarks will have to be further explored and refined when we have obtained more quantitative information e.g. on the rate at which stochastic spreading takes place. For the moment, however, they serve as warning about the dangers of applying intuitive ideas based on deterministic models, directly to the stochastic model. To avoid such difficulties for now, we will base our analysis below on the conceptually simpler initial value formulation represented by equation (7.26) even though the boundary value version is closer to the physical situation in actual experiments.

The main conclusion reached here is that in order to calculate the concentration in an integral formulation of solute mass conservation, we need to find the probability distribution of fluid elements that result from the stochastic model. That task is addressed in the next section.

### 7.3 Stochastic Transport in a Constant Flow Velocity

After considerable preparation, we are now finally in a position to apply the SDE theory based on Dynkin's equation to solute transport modeling. Having disposed in the previous sections of the problem how to include solute mass conservation into the model, we are left with the single ID equation given by equation (7.1) to process further. This is already in the correct form according to equation (4.3) provided that we interpret  $dB_t$  in the latter as a vector, with components given by  $db_n(\omega, t)$ . To avoid complicating the argument by having to deal with a vector in an infinite dimensional space, we take the pragmatic view that the eigenfunction expansion can be truncated after  $M$  terms. In this case  $\sigma$  in equation (5.3) is also an  $M$ -dimensional vector, and by comparison with equation (7.1) it is given by

$$\sigma(x) = (\sqrt{\lambda_0} f_0(x), \sqrt{\lambda_1} f_1(x), \dots, \sqrt{\lambda_M} f_M(x)) \quad (7.28)$$

whereas the drift coefficient in equation (7.1) is simply the scalar function  $u(x)$ . The next step is to construct the generator of the ID according to equation (4.11). For this we need

$$\sigma \cdot \sigma^T = \sum_{n=0}^M \lambda_n f_n(x) f_n(x) = C(x, x) \quad (7.29)$$

which is also a scalar function, and for the second equality we have used equation (6.6). Note that in the final result  $M$  does not appear any more, so that the expansion can be truncated at any large finite  $M$  without needing to explicitly solve the eigenvalue problem.

In fact, we see from equation (6.11) that for the covariance kernel that was proposed in Chapter 6,  $C(x, x)$  reduces to a constant (1), if we assume that the amplitude factor in equation (6.11) has been absorbed into  $\gamma^2$  as explained in the introduction). This reflects the assumption that the covariance of realizations of the  $\alpha$ -processes of equation (6.4) at position  $x$ , is the same for all positions. This seems reasonable enough, although it is possible to construct a generalization where the time-dependent Wiener processes are not only generalized Wiener processes instead of standard ones, but in addition have different  $q$ -functions (in the notation of equation (2.10)) at different positions. In this case the spatial correlation kernel can be such that  $C(x, x)$  is a function of position. However, as there does not seem to be any physical reason to assume this more complicated behavior, we restrict ourselves to the case that  $C(x, x) = I$ . Then, we can write down the generator equation as

$$A f(x, t) = u(x) \frac{\partial f}{\partial x} + \frac{1}{2} \gamma^2 \frac{\partial^2 f}{\partial x^2}. \quad (7.30)$$

Bearing in mind that the generator is used to calculate expectation values and probabilities as detailed below, the fact that equation (7.30) does not contain any reference to the spatial correlation kernel any more, is very significant. It means that while individual realizations of the motion of a fluid element are affected by the functional form of the kernel, all such dependence is averaged out when taking expectation values over all representations. This is not obvious, and might be quite hard to determine from numerical simulations of individual realizations. The ease with which this conclusion follows from the potential theory approach is a striking illustration of its power.

As in the population growth example, different questions about the flow can be answered by solving the cases  $A f = 0$ ,  $A f = K$  and  $A f = \partial/\partial t$ . The first two of these relate respectively to questions about the probability that a fluid element starting from the origin reaches a predetermined position, and the expected time for it to do so. However, as the results agree with what would be expected from a deterministic model we do not dwell on them.

The third case on the other hand, is the one that eventually yields the probability distribution that is needed to implement solute mass conservation. In this section we limit ourselves to the case that  $u(x)$  is a constant, say  $v_0$ . That would for example apply in the case of a constant pressure gradient across a homogeneous porous medium described by the Darcy equation, where we would have  $v_0 = -(K/\phi)(d\phi/dx)$ . To facilitate solution, we transform the generator equation to a new position variable  $z$  and time variable  $T$  defined as

$$z = \frac{x v_0}{\gamma^2}; \quad T = \frac{t v_0^2}{\gamma^2}. \quad (7.31)$$

These are, in some sense, also scaling transformations to “dimensionless” parameters, but are distinct from the physical scaling that was mentioned in the introduction of this chapter. Here, we are merely dealing with a mathematical transformation that scales the various terms of the differential equation similarly, i.e. to a form in which all coefficients are simple numbers of order unity:

$$\frac{1}{2} \frac{\partial^2 f}{\partial z^2} + \frac{\partial f}{\partial z} = \frac{\partial f}{\partial T}. \quad (7.32)$$

In the standard way this partial differential equation is reduced to an ordinary one by separating variables in writing

$$f(z, T) = e^{-KT} f_K(z) \quad (7.33)$$

where  $K$  is introduced as a separation constant to be determined. It is easily seen that the resulting equation for  $f_K$  is solved by a simple exponential form,  $f_K(z) = \exp(-\alpha z)$ , provided that  $\alpha$  is related to the separation constant by

$$K = \alpha - \frac{1}{2} \alpha^2. \quad (7.34)$$

Finally, we revert back to the coordinate pair  $(x, t)$ . The resulting expression is cast in a particularly simple form by making use of the freedom allowed by the fact that  $K$  and therefore also  $\alpha$  are arbitrary constants. Hence we can as well write  $\alpha$  in terms of a new arbitrary constant  $a$  which we define by  $\alpha = a \gamma^2 / v_0$  to obtain the solution in the form:

$$f(x, t) = e^{-ax} e^{av_0 t - \frac{1}{2} a^2 \gamma^2 t}. \quad (7.35)$$

What we have achieved here, is to find a solution of equation (5.14) for the case of our solute transport model ID – in fact, due to the arbitrary nature of  $a$ , we have found not just one but a whole family of solutions. We can now invoke equations (5.13) and (5.15) to write down Kolmogorov's version of the Dynkin equation, just as was done for the population growth model:

$$E^0 \left[ e^{-aX_t} \right] = e^{av_0 t - \frac{1}{2} a^2 \gamma^2 t}. \quad (7.36)$$

To interpret this equation, it is useful to restate it in terms of an operational definition. We start with the position  $x$  of a fluid element at a time  $t$ . From this, we calculate the function  $e^{-ax}$ . Rather than  $x$  just being an ordinary function of  $t$ , we allow  $x$  to vary stochastically as represented by the stochastic process  $X_t$ . Then the expectation value at  $t > 0$  of the function, taken over all realizations of the process that start from the initial value  $x = 0$  at  $t = 0$ , is given by the right hand side of equation (7.36).

This expectation value can be expressed in an alternative way by using a probability density as introduced in the previous section. Let  $P_t(x|x',t')$  be the  $x$ -domain probability density that a fluid element known to start from  $x'$  at a time  $t'$ , arrives at the target point  $x$  at the time  $t > t'$ . Then we have

$$E^0 \left[ e^{-aX_t} \right] = \int_{-\infty}^{\infty} dx e^{-ax} P_t(x|0,0). \quad (7.37)$$

This equation is analogous to equation (5.21), except that in this case there is an infinity of possible values of  $e^{-ax}$  at the stopping time, instead of just two possible values as in the former case.

Combining equations (7.36) and (7.37) we now have an integral equation to solve for the probability density:

$$\int_{-\infty}^{\infty} dx e^{-ax} P_t(x|0,0) = e^{a v_0 t - \frac{1}{2} a^2 \gamma^2 t}. \quad (7.38)$$

As remarked at the end of Chapter 5, a formal approach might be taken to solve it. However, we present a more intuitive approach. The first step is to notice that if we make an expansion in powers of  $a$  on both sides of the integral equation, coefficients may be set equal because  $a$  is an arbitrary constant. This leads to expressions for all moments of the probability density and in particular to the following expressions for the mean and variance of the position:

$$\begin{aligned} \langle x \rangle &= v_0 t; \\ \text{Var}(x) &= \langle x^2 \rangle - \langle x \rangle^2 = \gamma^2 t. \end{aligned} \quad (7.39)$$

Also, by putting  $t = 0$  in equation (7.38) it is seen that as the equation holds for any value of  $a$ , we must have  $P_0(x|0,0) = \delta(x)$ . So the solution of the integral equation should be a function that starts at  $t = 0$  as a delta-function peak at the origin, then develops as a peak centered near  $v_0 t$  and with a variance increasing proportional to  $t$ . An obvious guess with these properties is a Gaussian peak of the form

$$P_t(x|0,0) = \frac{1}{\sqrt{2\pi\gamma^2 t}} \exp \left[ \frac{-(x - v_0 t)^2}{2\gamma^2 t} \right]. \quad (7.40)$$



Indeed, if we substitute equation (7.40) into (7.38), complete squares in the exponent and then perform the integration by use of the standard result

$$\int_{-\infty}^{\infty} e^{-y^2} dy = \sqrt{\pi} \quad , \quad (7.41)$$

it is seen that equation (7.40) is an exact solution. If the time and space origins are shifted to a different position, it is clear that the probability distribution can still only depend on the difference between the source and target point coordinates, i.e.

$$P_t(x|x',t') = \frac{1}{\sqrt{2\pi}\gamma^2(t-t')} \exp\left[\frac{-((x-x')-v_0(t-t'))^2}{2\gamma^2(t-t')}\right]. \quad (7.42)$$

The probability density required for calculating the solute concentration according to equation (7.26) is similar to that of equation (7.42), but not identical in principle. For the former, it is the target point  $(x,t)$  that is fixed and we specify the probability for a source point  $(x',t')$ ; but in equation (7.42) it is the other way around. In the case of a constant flow velocity that we discuss here, a symmetry argument could be made out to show that their functional forms are the same. However, as this result does not hold for more complicated situations, we prefer to derive the relation between the two by a more elaborate argument that can be generalized for example to the case of linearly accelerating flow treated in the next section. This based on noting that, since a fluid element known to be at the source point  $x'$  at  $t'$  must end up somewhere at a time  $t$ , we have

$$\int_{-\infty}^{\infty} dx P_t(x|x',t') = 1. \quad (7.43)$$

This equation states that when the function  $P$  of the four variables  $(x,t,x',t')$  is integrated out over only one of them, namely  $x$ , all three of the others also drop out of the result. That can only happen if the function is such that it is possible to find a transformation to a new variable  $y = y(x,t,x',t')$  in terms of which

$$\int_{y_{-\infty}}^{y_{\infty}} dy P(y) = 1 \quad (7.44)$$

where  $y_{\pm\infty} = f(\pm\infty, t, x', t')$ . In other words, the single variable  $y$  connects the point  $(x',t')$  with another point  $(x,t)$  with  $t > t'$ , and  $P(y)$  gives the probability that these points are related as source and target points respectively, as a

density in the combined variable. To retrieve  $P_t(x|x', t')$  one would transform the integration variable in equation (7.44) back to  $x$ , and by the same token  $P_t(x'|x, t)$  is obtained if we transform the integration variable to  $x'$ . So

$$\begin{aligned} P_t(x|x', t') &= P[y(x, t, x', t')] \frac{\partial y}{\partial x}, \\ P_t(x'|x, t) &= P[y(x, t, x', t')] \frac{\partial y}{\partial x'}. \end{aligned} \quad (7.45)$$

Time domain probability densities as needed for the boundary value formulation of solute conservation in equation (7.27), can obviously be obtained in a similar way. Applying these ideas to equation (7.42) we can identify

$$y(x, t, x', t') = \frac{(x - x') - v_0(t - t')}{\sqrt{2\gamma^2(t - t')}}. \quad (7.46)$$

Substituting equation (7.46) into (7.45), we only get a sign change in  $P_t(x'|x, t)$  compared to  $P_t(x|x', t')$ , but that is cancelled by the exchange of the integration limits needed in the former case. So in the end, the right hand side of equation (7.42) represents both of these probability densities for constant flow velocity. In the next section we will see that that is not true any more in accelerating flow.

We are now in a position to calculate the concentration from equation (7.26) given any initial concentration. The simplest case is when we only have a point source of solute that adds a unit mass of solute to the flow at the point  $x = \xi$ , i.e. we take  $c(x, t_0) = \delta(x - \xi)$ . As  $u(x) = u(x') = v_0$  it is trivial to see that this leads to

$$c(x, t) = \frac{1}{\sqrt{2\pi\gamma^2(t - t_0)}} \exp \left[ \frac{-((x - \xi) - v_0(t - t_0))^2}{2\gamma^2(t - t_0)} \right]. \quad (7.47)$$

In other words, the delta-function initial concentration peak develops into a Gaussian peak that moves at the constant speed  $v_0$ , and spreads, with a variance that increases linearly with time, as illustrated in Figure 7.1.

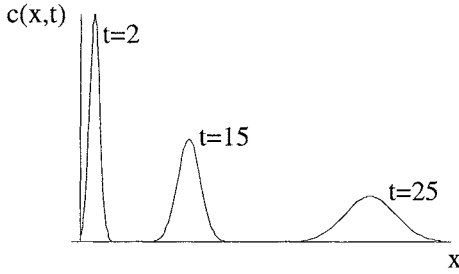


Figure 7.1 Development of concentration peaks.

The curves in the figure represent “snapshots” of the concentration profile at three consecutive times, with a positive value for  $v_0$ , i.e. the flow direction is to the right.

Moreover, we can conclude that if the initial concentration was a Gaussian peak rather than a delta function, it would also develop as a Gaussian that is simultaneously translated at the flow velocity and spreads proportional to time. This follows logically since if we divide the time interval  $(t_0, t)$  into two at an arbitrary intermediate point  $t_I$ , the concentration at  $t_I$  will be a Gaussian according to the result just derived; and its subsequent development cannot depend on whether the concentration at  $t_I$  was physically prepared by directly introducing a Gaussian distribution into the flow at  $t_I$  or by inserting a point source at the earlier time  $t_0$ . Of course, the same result can be proved in a more tedious fashion mathematically by inserting a Gaussian initial concentration into equation (7.26) and performing the integral by completing squares in the exponent.

Before proceeding to make direct connection to physical observations, we need to remember that the variables in equation (7.47) are still scaled variables. The scaling constants  $\ell_x$  and  $\ell_t$  are to be chosen to reflect the physical mechanisms that cause stochasticity. In our approach, stochasticity is used to model the deflections of fluid flow by pore walls. Individual displacements suffered by a fluid element when it hits a pore wall has to be on the scale of a pore diameter, and time intervals between deflections on the

scale of the time it needs to traverse a pore. Therefore, it is plausible that  $\ell_x$  should be of the order of a typical pore diameter, and that  $\ell_t$  is chosen as  $\ell_x/v_0$ . Having already introduced the correlation length  $b$  in equation (6.10) as a pore scale constant, it is consistent to use that also here for the length scale. That leads to the conclusion that if equation (7.47) is rewritten in terms of ordinary unscaled laboratory coordinates, it takes the form

$$c(x, t) = \frac{1}{\sqrt{2\pi\gamma^2 b v_0 (t - t_0)}} \exp \left[ -\frac{((x - \xi) - v_0(t - t_0))^2}{2\gamma^2 b v_0 (t - t_0)} \right]. \quad (7.48)$$

The variance of this concentration, about its uniformly translating peak value, is given by

$$\sigma^2(t) = \gamma^2 b v_0 (t - t_0). \quad (7.49)$$

The standard deviation,  $\sigma$ , is a natural measure of the extension of a concentration plume and we see that this increases proportional to the square root of the time. That is a well-known behavior usually associated with the advection-dispersion equation (ADE), and so it is useful to establish the connection. We write the ADE (1.9) in the following form, where the porosity has been absorbed into the concentration and a constant flow velocity is assumed:

$$\frac{\partial c}{\partial t} + v_0 \frac{\partial c}{\partial x} - D \frac{\partial^2 c}{\partial x^2} = 0. \quad (7.50)$$

Here,  $D$  represents the coefficient of hydrodynamic dispersion. The form of this equation closely resembles that of the time-dependent generator equation (7.32) but has a different sign for the spatial first derivative term. It may be confirmed by direct substitution that it is solved by a translating, dilating Gaussian of the form  $\exp\left(\frac{-(x-v_0 t)^2}{2\sigma^2}\right)$  provided that

$$\sigma^2(t) = (t - t_0) 2D. \quad (7.51)$$

In other words, the ADE equation also predicts that the variance of a Gaussian concentration peak will grow linearly with time and identifies the coefficient of this growth as twice the dispersion coefficient. Some interesting conclusions can be drawn from the comparison:

- the microscopic stochastic model agrees with the macroscopic ADE equation for the case of a constant flow velocity; and
- by comparing equations (7.49) and (7.51) we can write the macroscopic, empirically defined dispersion coefficient in terms of the parameters of the microscopic model:

$$D = \frac{1}{2} \gamma^2 b v_0. \quad (7.52)$$

The fact that the dispersion coefficient is proportional to the flow velocity follows in a natural way from the stochastic model. This is a crucial assumption in the commonly used definition of dispersivity as an intrinsic materials property of a porous medium – see section 1.3.3. Moreover, the dispersivity is also obtained in a natural way as a length on the scale of the pore diameter, again in agreement with work based on the ADE equation and shown in Table 1.1.

In the case of the ADE equation, the dispersion coefficient  $D$  is the fundamental empirical parameter and it is a consequence of the equation that a Gaussian concentration plume remains Gaussian but spreads in a way characterized by  $D$ . In the stochastic model, there is no dispersion coefficient as such but we can determine an effective value for it by reversing the argument. We start with a Gaussian plume, calculate its time evolution and then extract a coefficient for the linear growth of the variance with time.

That is only really plausible in a case like the one we discussed here where the variance of the Gaussian does grow in a linear fashion. Any other time dependence would reduce this procedure at best to an approximate one, where we might determine an effective  $D$  value, but which changes with time. At a more fundamental level, however, one could conclude from such a situation that the concept of dispersion as a phenomenon that is similar to diffusion, only on a larger scale, is flawed.

From this remark it is clear that although a study of the time evolution of a Gaussian plume may appear to be a very narrow focus on a special case, an understanding of it can contribute significantly to insights into the broader phenomenon.

The idea of replacing the definition of the dispersion constant as a Fickian coefficient, by one based on the variance of the concentration plume is one that is commonly used. In experimental work, the variance is a well-defined global property of the plume that is more easily measured than the local concentration gradient and flux needed for the Fickian definition. This idea is

applied for example in the work of Moroni and Cushman (2001), where the assumption of a linear time dependence is avoided by defining the dispersion coefficient as half the first time derivative of the variance.

If the Fickian description of dispersion contained in the ADE equation holds, the two definitions of the dispersion coefficient are consistent. The work in this section shows that the stochastic model supports such consistency in the case of a constant flow velocity.

However, more generally it does not necessarily follow that a dispersion coefficient obtained from variance measurements can consistently be used in the ADE equation. One would first have to show that the more detailed predictions of the ADE equation, such as the retention of an initially Gaussian concentration profile, but with a linear time dependence of the variance, also hold. For example, one might hypothetically picture a more complicated relation between the solute flux and the concentration gradient that causes the shape of the profile to change away from a Gaussian one but leaving the variance unchanged. Then the variance based or “global” value of the dispersion coefficient would be zero while on a local scale there is still dispersion manifested by solute flux in response to a concentration gradient.

The discussion above raises some interesting philosophical points about the relation of the stochastic dispersion model to diffusion. As explained after equation (7.8), in setting up the model that we solved above, ordinary physical (i.e. molecular scale) diffusion has been left out deliberately – but the final result, that a momentary point source develops into a spreading Gaussian, is in fact exactly what one expects from ordinary diffusion. From a mathematical perspective, this is not surprising; diffusion is after all the prototypical SDE phenomenon and the methods we used, based on ID’s and Dynkin’s equation, are in fact mathematical generalizations of diffusion theory. From a physical perspective, one might say that molecular diffusion results from stochastic displacements of individual solute molecules, as a result of molecular collisions (Brownian motion), and this is indeed very similar to our dispersion model where we have displacements of macroscopic fluid elements as a result of collisions with pore walls.

There are two striking differences, though. Firstly, the spatial scale is much larger, leading to a dispersion coefficient that can be orders of magnitude larger than the diffusion coefficient. And secondly, in dispersion the time scale (i.e., the interval between collisions) is determined by the average fluid flow velocity, while in diffusion the time scale is determined by the fluid density, temperature, etc.

For a constant flow velocity  $v$  the close connection between dispersion and the velocity only manifests in the fact that the dispersion constant is proportional to  $v$ , and we might describe this as a diffusion-like or “diffusive” dispersion behavior. There are more profound consequences for dispersion when  $v$  changes. That is the subject of the next section.

## 7.4 Stochastic Transport in a Flow with a Velocity Gradient

Applying the same model as before to study dispersion in a flow with a variable flow velocity, we need to go back to equation (7.30) and would ideally like to solve the generator equation for an undetermined  $u(x)$ . Unfortunately it is not possible to find an analytic solution to the generator equation in this general case. Of course, for any particular  $u(x)$  determined from some appropriate model of the fluid flow, it would in principle be possible to find a solution to the generator equation numerically. However, we saw in the previous section that the solution of the generator equation only yields an auxiliary function, from which the probability density needs to be extracted by solving an integral equation that is constructed using the auxiliary function. Following this route, the integral equation would also have to be solved numerically; and then finally, the concentration calculated by numerical integration of the solute conservation integral. Apart from possible numerical pitfalls along the way, this approach does not appear likely to yield any insight into the mechanisms of dispersion in a variable flow. For this reason, we restrict ourselves instead to a case where  $u(x)$  is simple enough to still allow all three of the listed steps to be done analytically, as was done for the constant flow. We assume that the flow velocity has a straight line dependence on position:

$$u(x) = v_0 + p(x - x_0) = v_0 \pm \mu^2(x - x_0) \quad (7.53)$$

where either  $p$  or  $\mu^2$  represents the velocity gradient, and the second form just facilitates some intermediate steps where it turns out that the algebra depends on whether the flow accelerates or decelerates.

The applicability of this simple assumption may be extended if one considers that any arbitrary variation of  $u$  may be approximated by a sequence of  $x$ -intervals with a different constant velocity gradient in each, i.e. a piecewise linear approximation for  $u(x)$ . While that strengthens the case for tackling the constant gradient case, a piecewise approximation is not as simple as it

sounds, because one needs to use the boundary value formulation of the conservation equation and as alluded to in the discussion of equation (7.27) complications arise from that. In fact, if one is prepared to deal with those complications, an even simpler model of a variable flow velocity would be a piecewise constant velocity.

Before turning to the mathematics of the solution, it may be helpful to find some concrete examples of a varying flow velocity to serve as mental pictures of the situations that we are trying to describe. A first example would be that of flow along a pipe with a constriction, pictured as a cross-section in Figure 7.2 below:

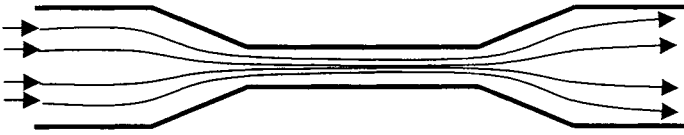


Figure 7.2      Flow along a pipe with a constriction.



The effective 1-dimensional flow velocity along the horizontal axis can be plotted schematically as follows:

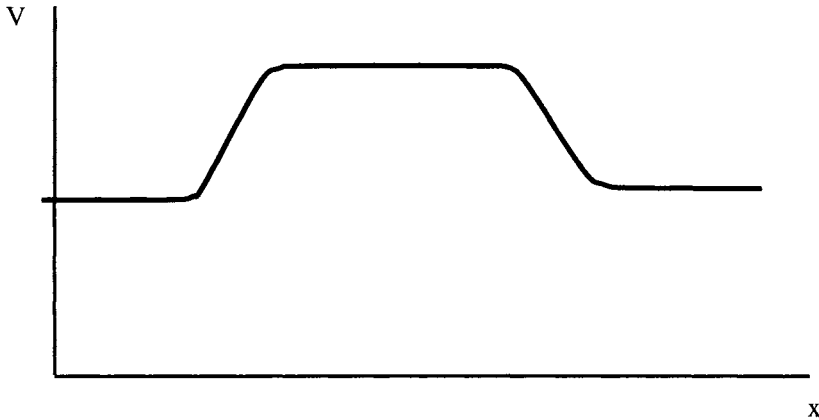


Figure 7.3 Flow velocity along the constricted pipe shown in Figure 7.2.

This velocity profile can obviously be modeled well as piecewise linear, with a constant velocity gradient over the interval representing the conical pipe section. Clearly, the drift velocity profile would be similar if the constricted pipe was filled with a homogeneous porous medium. If the constriction was formed not by the geometrical shape of the pipe, but by an equivalently shaped region of zero-conductivity porous medium inside it, the velocity profile would obviously be the same; and on the other hand, a similar drift velocity profile would also result if the pipe had a constant cross section but the porous medium filling it has a reduced porosity in the central region. These are just simple hypothetical examples but they demonstrate that variations in either the hydraulic conductivity or porosity of a porous medium, such as would be expected to be present in naturally occurring aquifers, are bound to cause local variations in the drift velocity, and that it is not unreasonable to model these as linear in the spatial coordinate (at least as a first approximation).

In a similar vein, we can consider the physical meaning of excluding stagnation points of the flow from our model. Figure 7.4 illustrates how stagnation points might arise physically. A decelerating and accelerating flow

velocity region that includes a stagnation point is shown at the top of the figure, and below that a 2-dimensional flow pattern that would give rise to such velocity profile when projected to 1-dimensional flow. The crucial point is that the sign change (i.e., direction change) of the flow at a stagnation point implies either a source or a sink of the 1-dimensional flow. Excluding these is quite plausible for describing the main problem of solute transport in an underground aquifer. The description of dispersion around a stagnation point is left as a special case that will have to be addressed separately.

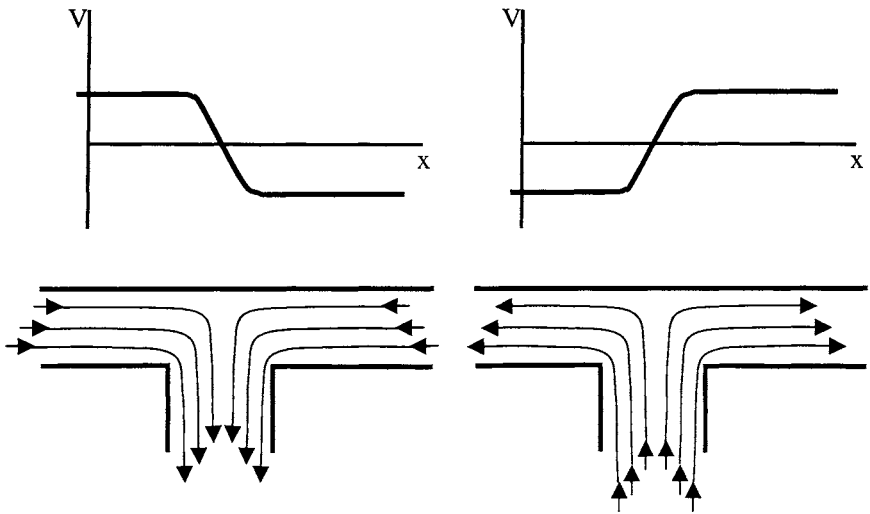


Figure 7.4 Physical stagnation points.

Returning to the mathematical problem, we put equation (7.53) into the generator equation (7.30) and once more transform to scaled position and time coordinates; this time the appropriate definitions are

$$z = \frac{1}{\mu\gamma}(\pm\mu^2(x-x_0)+v_0); \quad T = \mu^2 t. \quad (7.54)$$

and in terms of these the generator equation is

$$\frac{1}{2} \frac{\partial^2 f}{\partial z^2} \pm z \frac{\partial f}{\partial z} = \frac{\partial f}{\partial t}. \quad (7.55)$$

## 7.5 Standard Solution of the Generator Equation

The same substitution as before, equation (7.33), is used to separate variables and leads to the following equation for  $f_K$ , the spatial part of  $f$ :

$$\frac{1}{2} \frac{d^2 f_K}{dz^2} \pm z \frac{df_K}{dz} + K f_K(z) = 0. \quad (7.56)$$

Equation (7.56) may be recognized as an example of a standard differential equation, the hypergeometric equation (see Morse and Feshbach, 1953) and it has a pair of independent solutions that can be expressed in terms of confluent hypergeometric functions or Kummer functions,  $M(a, b, z)$  as follows :

$$f_K^\pm(z) = \begin{cases} M(\pm\frac{1}{2}K, \frac{1}{2}, \mp z^2), \\ z M(\frac{1}{2} \pm \frac{1}{2}K, \frac{3}{2}, \mp z^2). \end{cases} \quad (7.57)$$

From a compendium of special functions such as that by Abramowitz and Stegun (1965), Table 13.6, we find that Kummer functions with the special values  $1/2$  and  $3/2$  for the second argument in fact reduce to Hermite polynomials if the first argument is a negative integer. As  $K$  is still an arbitrary separation constant, we can choose values for it to satisfy this requirement.

Considering first the decelerating flow (lower sign) case, it is seen that any even positive integer value of  $K$  will be appropriate for the first solution in equation (7.57), and odd integers for the second. In this way both sets of solutions may be collected together and written as

$$f_n^-(z, T) = e^{-nT} e^{\frac{1}{2}z^2} h_n(z), \quad n = 0, 1, 2, 3, \dots \quad (7.58)$$

where we have introduced the orthonormal functions  $h_n(z)$  defined in terms of the Hermite polynomials  $H_n(z)$  by

$$h_n(z) = \left(2^n n! \sqrt{\pi}\right)^{-\frac{1}{2}} e^{-\frac{1}{2}z^2} H_n(z). \quad (7.59)$$

The  $h_n(z)$  are sometimes referred to as Weber or parabolic cylinder functions and are orthonormal on the  $z$ -interval  $[-\infty, \infty]$ . They form a complete basis, which is expressed mathematically by the closure relation

$$\sum_n h_n(z) h_n(y) = \delta(z - y). \quad (7.60)$$

For the case of accelerating flow (the upper sign in equation (7.57)) a similar set of manipulations can be done but in this case it is first necessary to extract a factor  $\exp(-z^2)$  by applying the Kummer transformation  $M(a, b, z) = e^z M(b - a, b, -z)$  in order to ensure that a real argument for the Hermite polynomials is obtained. The final result is

$$f_n^+(z, T) = e^{-(n+1)T} e^{-\frac{1}{2}z^2} h_n(z), \quad n = 0, 1, 2, 3, \dots \quad (7.61)$$

At this point we have solved the generator equation and arrived at the equivalent of equation (7.35) in the previous section. Following the same logic invoking Kolmogorov's version of the Dynkin equation, we are now led to the following integral equation corresponding to equation (7.38):

$$\int_{-\infty}^{\infty} dx f_n^+(z, 0) P_T^+(z | z', 0) = e^{-\frac{1}{2}z'^2} h_n(z') e^{-(n+1)T} \quad (7.62)$$

where  $z'$  is the scaled starting position of the fluid element. This integral equation is easy to solve by multiplying both sides by  $h_n(y)$ , summing over all  $n$  and applying equation (7.60). One finds that

$$\begin{aligned} P_T^+(z | z', 0) &= e^{\frac{1}{2}(z'^2 - z^2)} \sum_n e^{-(n+1)T} h_n(z') h_n(z), \\ P_T^-(z | z', 0) &= e^{-\frac{1}{2}(z'^2 - z^2)} \sum_n e^{-nT} h_n(z') h_n(z). \end{aligned} \quad (7.63)$$

Having found fully specified expressions for the probability density for both accelerating and decelerating flows, it might be expected that it is a routine

matter to use these in an equation like equation (7.26) to calculate the evolution of an input concentration profile. Unfortunately, it turns out that the solution found is not very useful for practical calculations. One problem with equation (7.63) is that it is hard to see any connection between either of those formulas and the Gaussian expression found for the constant flow probability density in equation (7.42); and after all, either of them must reduce to the constant flow case as  $\mu \rightarrow 0$ . More seriously, we run into convergence problems even for a simple calculation of the moments of the probability distribution. For the case of  $P^-$  i.e. deceleration, moments can be calculated, but for  $P^+$  the additional factor  $\exp(z^2)$  gives rise to a divergent integral inside the summation over  $n$ . Obviously the final result cannot diverge, so the problem is that the summation has to be carried out before the integration. Unfortunately however standard mathematical tables do not list a formula for a sum over products of Hermite polynomials as it appears in equation (7.63), nor are symbolic algebra computer packages of any help, suggesting that a calculation of this sum has not been performed before.

Finally, even if we abandon the idea of proceeding with analytical calculations, even for numerical work expansions in terms of Hermite polynomials, which is what equation (7.63) is, can be very slow to converge. This applies in particular to our case, since in the limit as  $T \rightarrow 0$  we know that the probability density must reduce to a Dirac delta function. The fact that it does so is manifestly clear from equation (7.63) by application of the closure equation (7.60), but numerically plotting the left hand side of the closure relation soon convinces one that truncation of the series at any reasonable value of  $n$  gives a very poor representation of the sharpness of a delta function peak.

## 7.6 Alternate Solution of the Generator Equation

We are faced with the situation that while the standard procedures for solving the differential equation and manipulating the resulting special functions gives a perfectly good formal solution, it is not of much practical use and something more creative is called for.

A key element in the alternative proposed here, is the generating function for Hermite polynomials, given by Abramowitz and Stegun (1965) as

$$e^{2rs-s^2} = \sum_n \frac{1}{n!} s^n H_n(r). \quad (7.64)$$

Consider first the decelerating flow case. Substituting equation (7.59) into (7.63) we may write  $P$  explicitly as a Hermite expansion

$$\begin{aligned} P_T^-(z|z', 0) &= e^{-z'^2} \sum_n p_n H_n(z), \\ p_n &= \left(2^n n! \sqrt{\pi}\right)^{-1} e^{-nT} H_n(z'). \end{aligned} \quad (7.65)$$

Now consider a power series in an indeterminate variable  $a$ , using the same coefficients  $p_n$ :

$$\begin{aligned} \sum_n p_n (-a)^n &= \frac{1}{\sqrt{\pi}} \sum_n \frac{1}{n!} \left(-\frac{1}{2} a e^{-T}\right)^n H_n(z'), \\ &= \frac{1}{\sqrt{\pi}} e^{-a z' e^{-T} - \frac{1}{4} a^2 e^{-2T}}. \end{aligned} \quad (7.66)$$

Here, the second step follows by application of equation (7.64). Now, we rewrite the left hand side of equation (7.66) as

$$\begin{aligned} \sum_n p_n (-a)^n &= \sum_n \sum_m p_n (-a)^n \delta_{nm}, \\ &= \sum_n \sum_m p_n (-a)^n \frac{1}{\sqrt{\pi} m! 2^m} \int_{-\infty}^{\infty} e^{-z^2} H_n(z) H_m(z) dz. \end{aligned} \quad (7.67)$$

where the second step follows from the orthogonality relation of the  $h_n(z)$ . Next, we apply first equation (7.65) to the  $n$ -summation and then equation (7.64) to the  $m$ -summation:

$$\begin{aligned} \sum_n p_n(-a)^n &= \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} dz P_T^-(z|z',0) \sum_m \frac{1}{m!} \left(-\frac{1}{2}a\right)^m H_m(z), \\ &= \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} dz P_T^-(z|z',0) e^{-a z - \frac{1}{4}a^2}. \end{aligned} \quad (7.68)$$

Finally, setting the right hand sides of equations (7.66) and (7.68) equal, we obtain

$$\int_{-\infty}^{\infty} dz e^{-az} P_T^-(z|z',0) = e^{-az' e^{-T} + \frac{1}{4}a^2(1-e^{-2T})}. \quad (7.69)$$

This is an integral equation that is very reminiscent of equation (7.38), and by comparison with how that equation arose from the Dynkin equation for constant flow we can conjecture that there should be a solution to the generator equation for decelerating flow of the form

$$f^-(z, T) = e^{-az e^{-T} + \frac{1}{4}a^2(1-e^{-2T})}. \quad (7.70)$$

Direct substitution of equation (7.70) into (7.55) confirms that is indeed a solution of the generator equation. Unlike the case of the Hermite polynomial solution, this solution does not allow the use of a closure relation to solve the integral equation; but instead, we model its solution on the one used for constant flow and that relied on completion of squares, by writing

$$P_T^-(z|z',0) = A e^{-(Bz+C)^2} \quad (7.71)$$

where  $A, B$  and  $C$  are terms independent of  $z$ . Substituting this expression in (7.69), completing squares and performing the integral by use of equation (7.41) leads to exponential expressions on both sides of the equation in which coefficients of powers of the arbitrary variable  $a$  can be set equal to fix the values of  $A, B$  and  $C$ . This results in a new expression for  $P^-$ :

$$P_T^-(z|z',0) = \frac{1}{\sqrt{\pi}\sqrt{1-e^{-2T}}} \exp\left(\frac{-(z-z'e^{-T})^2}{1-e^{-2T}}\right). \quad (7.72)$$

The same procedure applied to the case of accelerating flow leads to a somewhat different solution of the generator equation, but a rather similar expression for the probability density:

$$f^+(z, T) = e^{-[T + z^2 + uz e^{-T} + \frac{1}{4}a^2(1 - e^{-2T})]}, \quad (7.73)$$

and

$$P_T^+(z | z', 0) = \frac{1}{\sqrt{\pi} \sqrt{e^{2T} - 1}} \exp\left(\frac{-(z - z' e^T)^2}{e^{2T} - 1}\right). \quad (7.74)$$

In deriving equivalent expressions for the two probability densities, we have as a by-product also found a formula for performing the infinite sum over Hermite products contained in (7.63). Explicitly, the sum formula is

$$\sum_{n=0}^{\infty} \frac{e^{-nT}}{n! 2^n} H_n(z) H_n(z') = \frac{e^{T + z'^2}}{\sqrt{e^{2T} - 1}} e^{-\frac{(z - z' e^T)^2}{e^{2T} - 1}}. \quad (7.75)$$

It is directly evident that this formula holds by comparing the first equation in (7.63) with (7.74); it is less obvious that (7.75) also guarantees the equivalence of the second equation in (7.63) and (7.72), but that this true is a consequence of the following relationship between the probability densities for accelerating and decelerating flows:

$$P_T^-(z | z', 0) = e^{T - z^2 + z'^2} P_T^+(z | z', 0). \quad (7.76)$$

This relationship is in turn self-evident from equations (7.63) but to prove that it also holds for the exponential expressions in equations (7.72) and (7.74) requires some algebraic manipulation.

It is instructive to see how the limit in equation (7.75) is approached, i.e. when the series is truncated at consecutively larger index values  $N$ , how well the partial sums represent the limiting function on the right hand side of the equation. In Figure 7.5, we show some plots of this comparison where the exponential expression is drawn as a continuous line and the partial sum as dashed line. Both functions are plotted as functions of  $z$ , for the fixed values  $z' = 1$  and  $T = 2$ . From equation (7.75) it is clear that the limiting form is just a Gaussian peak if  $T$  is fixed, and the plots show that the partial sum represents the peak quite accurately for small values of  $|z|$ , but deviates



drastically outside the range. As more terms are added to the sum the usable range is extended, but clearly large values of  $N$  are needed to give an acceptable representation over the full extent of the peak. The situation becomes worse if  $T$  is increased, because as is clear from the exponential form the position of the peak value is at  $z = z'e^T$  which rapidly shifts to larger  $z$  values as  $T$  increases.

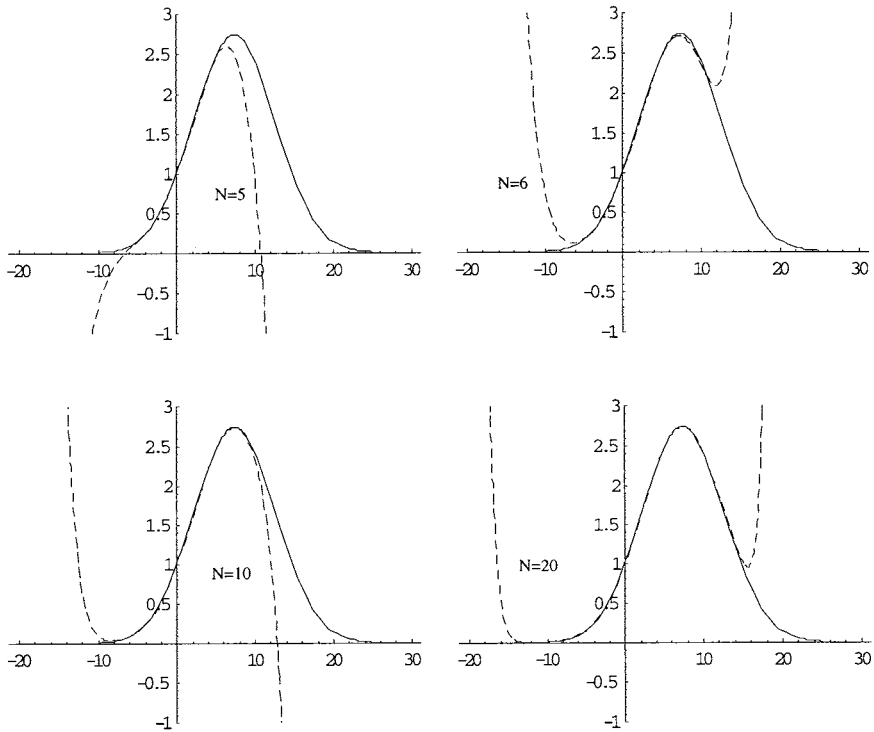


Figure 7.5 Comparisons of exponential expression and the partial sums.

This behavior demonstrates why the formally correct solution first found is not useful in practice, and may also boost the confidence of the skeptical reader about the correctness of the alternative solution in equations (7.72) and (7.74)!

For some purposes it is useful to collect the two probability expressions together by including the sign of the velocity gradient in the definition of the scaled time parameter  $T$ . In other words, also allowing for an arbitrary time origin, we may write

$$T = p(t - t') \quad (7.77)$$

in which case

$$P_T^\pm(z | z', 0) = \frac{1}{\sqrt{\pi} \sqrt{\pm(e^{2T} - 1)}} \exp\left(\frac{-(z - z' e^T)^2}{\pm(e^{2T} - 1)}\right). \quad (7.78)$$

As additional confirmation of this expression, one may check by straightforward algebra that as required by physical considerations, it is mathematically reduced to the appropriate limits:

- in the limit  $T \rightarrow 0$ , the probability density reduces to  $\delta(z - z')$ ;
- in the deterministic limit, substituting in equations (7.54) and letting  $\gamma \rightarrow 0$ , it reduces to  $\delta(x - X(t))$  where  $X(t)$  is given by equation (7.23) with the source point  $(\xi, 0)$  appropriately replaced by  $(x', 0)$ ; and
- in the constant flow velocity limit, once more reverting from  $z$  and  $T$  to  $x$  and  $t$ , and then taking the limit  $p \rightarrow 0$ , equation (7.42) is retrieved.

## 7.7 Evolution of a Gaussian Concentration Profile

Before the time dependent concentration can be calculated, we still need to transform the target-point probability density  $P(z|z_0, 0)$  found above, to the source-point density  $P(z_0|z, T)$ . The procedure is the same as was discussed for a constant flow velocity; the only difference is that now the variable  $y$  (given in that case by equation (7.46)) characterizing the joint source-target probability density, has the more complicated form as implied by equation (7.78) :

$$y = \frac{z - z' e^T}{\sqrt{\pm(e^{2T} - 1)}}. \quad (7.79)$$

From the form of equation (7.79) it is evident that when applying equations (7.45) the expression for  $P_T(z|z', 0)$  in (7.78) will be recovered but that  $P_0(z'|z, 0)$  differs from it by a factor  $e^T$ , allowing for the necessary exchange of integration limits:

$$P_0^\pm(z'|z, T) = \frac{e^T}{\sqrt{\pi} \sqrt{\pm(e^{2T} - 1)}} \exp\left(\frac{-(z - z' e^T)^2}{\pm(e^{2T} - 1)}\right). \quad (7.80)$$

The importance of this factor, and in fact the need to distinguish between the two closely related probabilities that in the constant flow case reduced to the same expression, can be well illustrated by considering integrals over the infinite  $z$ - and  $z'$ -domains. Using equation (7.79) as an integration substitution it is easy to see that

$$\int_{-\infty}^{\infty} dz P_T(z|z', 0) = 1; \quad \int_{-\infty}^{\infty} dz' P_T(z|z', 0) = e^{-T}. \quad (7.81)$$

Formulated verbally, the first of these equations expresses the fact that given the presence of a fluid element at the source point  $(z', 0)$  fluid mass conservation ensures that it must be found at some target point  $z$  at the later time  $T$ ; so summing the probabilities over all possible target points gives 1. On the other hand, if we select any target point  $z$  at random, there is no guarantee that there exists a source point from which a fluid element will proceed to  $z$  – it is logically conceivable that some points are unreachable, and in such a case summing probabilities over all source points will give 0. The second equation in equation (7.81) shows that indeed for accelerating flow this probability sum is not 1. But if we formulate the statement in terms

of the different conditional probability of equation (7.80), it reads: Given that a fluid element is found at the target point  $(z, T)$ , it must have come from somewhere at  $T=0$ ; so summing this probability over all possible source points must once again give 1. Obviously, the extra factor  $e^T$  in equation (7.80) is just what is needed to ensure that that happens.

Finally, we are in a position to calculate the evolution of an input concentration profile in an accelerating flow from equation (7.26) by substituting a Gaussian input peak from equation (7.20), the flow velocity from equation (7.53) and the probability density from (7.80) re-expressed in terms of  $x$  and  $t$ . The resulting integrand is complicated, but a moment's consideration shows that the terms in the exponent contributed by the concentration and the probability are both quadratic expressions in the integration variable  $x'$ , so we can write the integral as

$$c(x, t) = N \int_{-\infty}^{\infty} dx' u(x') \exp -[A x'^2 + B x' + C], \quad (7.82)$$

$$N = \frac{\mu / \gamma}{s \sqrt{2\pi^2} u(x) \sqrt{\pm(e^{2T} - 1)}}.$$

where  $A, B$  and  $C$  are complicated expressions but independent of  $x'$ . Squares in the exponent are completed by transforming to an integration variable  $Y = x' + B/2A$ , in terms of which

$$c(x, t) = N \exp\left[\frac{B^2}{4A} - C\right] \left\{ \left( v_0 - p \frac{B}{2A} \right) \int_{-\infty}^{\infty} dY \exp[-AY^2] + p \int_{-\infty}^{\infty} dY Y \exp[-AY^2] \right\} \quad (7.83)$$

By inspection of equations (7.20) and (7.80) it is seen that as the coefficients of the quadratic term in each is negative,  $A$  must be positive and therefore the second integral in the curly brackets vanishes while the first reduces to

$\sqrt{\pi/A}$ . All that remains at this point is to construct the detailed expressions for  $A, B$  and  $C$  and simplify the combinations of these terms that occur in (7.83), a task best accomplished by the use of symbolic algebra software. As in the deterministic case, we take  $x_0 = \xi$  to simplify the algebra. The result is as follows, expressed in terms of the auxiliary variable  $\phi = \gamma^2 / \mu^2$ :

$$c(x, t) = M(x, T) \mathcal{G}\left(x - X(T), s^2 e^{2T} \pm \frac{1}{2} \phi (e^{2T} - 1)\right) \quad (7.84)$$

where  $\mathcal{G}$  is the normalised Gaussian,  $X(T)$  is as given by equation (7.23) and  $M$  is a modulation factor:

$$\mathcal{G}(x, \sigma) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left[\frac{-x^2}{2\sigma^2}\right], \quad (7.85)$$

$$M(x, T) = \frac{2s^2 u(x) \pm \phi(e^{2T} - 1) e^T u(\xi)}{u(x) [2s^2 e^{2T} \pm \phi(e^{2T} - 1)]}. \quad (7.86)$$

Clearly, the propagation of a concentration plume is much more complex in an accelerating flow than in the constant flow velocity previously discussed. Even so, one can relate several of its features to those of constant velocity dispersion. Most striking is that as before there is a Gaussian peak and it also remains centered on the deterministic trajectory  $X(t)$ , as was the case for both equation (7.24) (accelerating flow, no dispersion) and equation (7.47) (constant velocity, with dispersion). The main difference is that here the variance of the Gaussian is given by

$$\sigma^2(T) = s^2 e^{2T} \pm \frac{1}{2} \phi(e^{2T} - 1). \quad (7.87)$$

In the deterministic limit,  $\gamma \rightarrow 0$ , so  $\phi \rightarrow 0$  and only the first term remains in agreement with equation (7.25). This means that the first term represents kinematical dispersion while the second one represents the intrinsic stochastic dispersion. Indeed, in the constant velocity limit  $p \rightarrow 0$  it is seen that the intrinsic dispersion term reduces to the diffusive dispersion expression (7.49) as it should.

We also need to consider the modulation factor by which the Gaussian is multiplied. Bearing in mind that with the choice made for  $x_0$  we have  $u(\xi) = v_0$ , it follows from equation (7.23) that

$$u(\xi) e^T = u(x) - p(x - X(T)) \quad (7.88)$$

and hence together with equation (7.87) we find

$$M(x, T) = 1 - \frac{\pm \phi(e^{2T} - 1) p(x - X(T))}{2\sigma^2(T) u(x)}. \quad (7.89)$$

Consider the behavior of  $M$  at a fixed time value. For  $x$  at the (moving) position of the peak we see from equation (7.89) that it has the value 1. Provided that there is no stagnation point (i.e.,  $u(x)=0$ ) in the  $x$ -interval under consideration, a case which is not generally of physical interest and was excluded from consideration already when discussing deterministic flow, both the numerator and denominator of the second term vary linearly as we move away from the peak and so the value of  $M$  will only change slowly with  $x$  – in particular compared to the Gaussian which falls away exponentially to either side of the peak. Also, note that deviations of  $M$  from 1 are proportional to the velocity gradient, so they fall away for a constant flow and a strictly Gaussian peak shape is recovered in that case. Generally it is reasonable to describe the concentration peak as still essentially Gaussian, but with a moderate time varying modulation. The explicit time variation in equation (7.89) will also largely cancel between the numerator and denominator. However, there is also an implicit time variation caused by the velocity factor that contributes mainly at the  $x$  position of the peak, and this increases with time. That will tend to extinguish the modulation with time for an accelerating flow, while for decelerating flow a slow increase will result.

The most striking qualitative feature of the modulation is that it is asymmetric, because the second term in equation (7.89) undergoes a sign change when  $x$  is taken through the peak value at  $X(T)$ . So flow acceleration causes the dispersion peak to become skewed, because values on one side of the peak is enhanced by the modulation and reduced on the other side; the direction of skewing will be backwards for acceleration and forwards for deceleration. Once more no drastic effect is expected because the numerator and denominator changes in a coordinated way.

In fact, on actual numeric plots the skewing is hard to recognize visually. Nevertheless the phenomenon is significant in principle, because it is an example of the fact that dispersion in the presence of a velocity gradient is different from merely superimposing stochastic variation on the deterministic evolution. We have seen in equations (7.24) and (7.47) that taken separately, the effects of flow acceleration and dispersion produce perfectly symmetric Gaussian concentration peaks; and yet we find here that together they give rise to a skewed, quasi-Gaussian peak. This is another demonstration of the essential difference between SDE's and the addition of random effects to a deterministic differential equation, that was discussed in some detail in Chapter 5 in connection with the population growth model.

The same point is made in a more dramatic fashion by considering in more detail the time behavior of the plume variance given in equation (7.87).

Separately, stochastic dispersion produces a variance that increases linearly with time (equation (7.48)) and flow acceleration gives an exponential increase (equation (7.25)). Together, this same exponential increase is present as the first term in equation (7.87), but in addition the stochastic term also acquires its own exponential time dependence. Once more, simple superposition fails and we might describe the result as an interaction between dispersion and the flow acceleration that is described by the full SDE treatment.

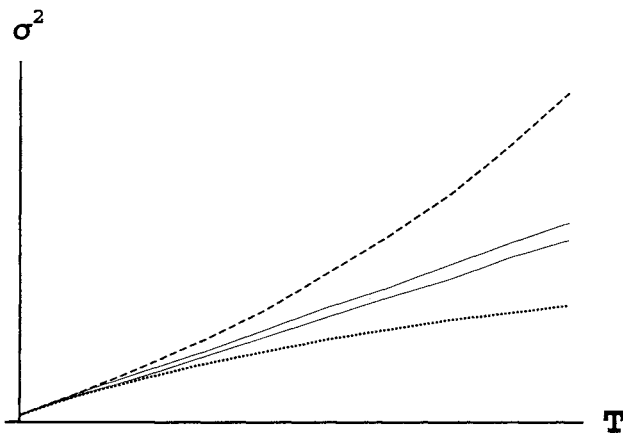


Figure 7.6 Plume variance in accelerating and decelerating flows.

The extent of the interaction may be judged by inspecting the plot in figure 7.6. It shows the calculated plume variance according to equation (7.87) in accelerating flow as a dashed line and in a decelerating flow as a dotted line. For comparison, the two solid lines show the result that would be obtained by superimposing a linear (diffusive) dispersion on two kinematical dispersion rates, for the same acceleration and deceleration rates respectively. The relatively small separation of the solid lines shows that for the parameters chosen for the plot, kinematical dispersion is quite small compared to the diffusive effect that would hold in a constant flow regime over the same time interval. Nevertheless, the interaction of this small kinematical effect and the dispersion produces a much larger final effect, enhancing dispersion for acceleration and suppressing it for deceleration.

The non-linear time dependence is also very significant from the point of view of traditional models of solute transport. In fact, the usefulness of the concept of dispersivity is called into question. One might formally extract a time dependent dispersivity expression by taking the time derivative of equation (7.87), but it does not reduce to a pure materials property that describes the porous medium any more, as it did for the constant flow expression discussed after equation (7.52). Instead, not only time, but also other variables such as the initial plume extension represented by  $s$  and the velocity gradient  $p$  that may at least partially be determined by the flow geometry, occur. It is more consistent to concede that when the flow velocity varies the Fickian model of dispersion is not adequate any more, and has to be replaced by a more complex model to describe the evolution of a contaminant plume, and that is exactly what equation (7.87) does for the case of linear acceleration.

On the other hand, if we do maintain the definition of dispersivity for the sake of comparison with the traditional description, the fact that it becomes time dependent opens the way to an explanation of the “scale dependence” observed in practical dispersivity measurements, as was discussed in Chapter 1. When the spatial scale of an experiment is increased, the time interval over which dispersion is observed also increases, and so scale- and time dependence are just different ways to describe the same phenomenon.

Having said that, the results derived here are still a long way from giving a detailed explanation of the observed scale effect. In fact, the mathematical treatment in this section would apply to a semi-infinite range of linearly increasing flow velocity, limited only on one side by the presence of a stagnation point. This is not a physically realistic situation. That is clear, for example, from the presence of exponential growth for a positive acceleration, which was found in both the deterministic and stochastic solutions. Obviously such exponential growth in any physical quantity is physically sustainable only over a limited spatial or time range. Indeed, the physical examples discussed at the beginning of this section show a linear velocity profile only over comparatively short spatial intervals. And in the physically realistic situation where there is a stable average flow velocity over larger scales, one would expect that intervals of velocity growth would alternate with intervals where the velocity decreases, i.e. velocity fluctuation rather than a sustained velocity growth is physically relevant.

If the results derived in this section are to be applied to such problems, it would thus have to be done by joining together solutions over discrete intervals in a piecewise linear model of the flow velocity. That leads to the



necessity of solving boundary problems at the points where intervals join, and that turns out to be a much more demanding problem mathematically than the initial value problem solved above.

The observation that one can make from Figure 7.6 that dispersion tends to be enhanced by acceleration and suppressed by deceleration, may lead one to speculate that a key issue in such a treatment will be whether these effects cancel over the extent of a fluctuation. If so, the ADE-type approach where it is assumed that dispersion may be described in terms of an average flow velocity should be in order; but if not, additional effects from fluctuations will change the dispersion behavior and might give rise to the observed scale effects.

In fact, it is easy to see from conservation of flux that kinematical dispersion is reversible and must cancel over the length of a fluctuation. In a simplified situation the form of equation (7.87) readily demonstrates this. A Gaussian peak that starts from an initial variance  $s^2$  and propagates for a time  $\tau$  in a flow with acceleration coefficient  $\mu^2$  in the absence of stochastic effects attains a variance value of  $s^2 e^{2\mu^2\tau}$  according to (7.87). If at that moment the acceleration is reversed, the variance after a further time interval  $\tau$  will by the same argument be given by  $(s^2 e^{2\mu^2\tau}) e^{-2\mu^2\tau} = s^2$ , i.e. the stretching of the peak during the first phase is exactly reversed in the second phase. On the other hand, the functional form of the intrinsic dispersion term does not allow the same manipulation, showing explicitly that that part is not reversible. Of course, a plume that consecutively penetrates an accelerating and a decelerating region is not quite the same as the hypothetical reversal of the acceleration at a given time, but if the intrinsic dispersion is not even reversible in the simpler situation it is plausible that it will also not cancel over the extent of a velocity fluctuation.

To summarize in conclusion, in addition to the detailed results on dispersion in constant and linearly accelerating flows, the study in this chapter also allows some observations of broader significance. Firstly, it demonstrates how an SDE-based model introduces interaction between the stochastic and deterministic aspect of a physical system. Secondly, the result in the contaminant dispersal problem is to modify the time dependence of dispersion, compared to the case where the interaction is neglected. Lastly, on a qualitative level at least, this modification has a bearing on explaining the observed scale dependent behavior of dispersivity. As conventional models do not explain this behavior, pursuit of the SDE approach is a promising avenue for further research.