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Modelling of the Dispersion-Advection Equation with Spatially Varying Mechanical Dispersion

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Summary Mechanical dispersion is the term used to describe the spreading of a contaminant as it is transported through a porous medium by advection. In the dispersion-advection equation, mechanical dispersion is taken into account by treating it in a way that is analogous to molecular diffusion, so that the effective diffusion coefficient and the mechanical dispersion coefficient are added together, the sum being referred to as the hydrodynamic dispersion coefficient. Typically, the hydrodynamic dispersion is taken as a constant. In this paper it is shown that this maybe misleading, particularly at an inlet boundary. A more accurate method is to vary the mechanical dispersion spatially so that it is zero at the inlet boundary. The resulting difference can be very large (over 1000%) and cause incorrect contaminant profiles, mass flow rates, and breakthrough times.

1. INTRODUCTION

There are three primary modes of contaminant transport in a porous medium. These are advection, mechanical dispersion, and molecular diffusion. Mechanical dispersion is only present if advection is present. The mathematical description of these three processes is quite often taken for granted and for the purposes of this paper it is worthwhile to consider how they arise. See Bear (1972) for a detailed description.

The mass flux of contaminant per unit time per unit area, f, due to advection is given by

$$f = nvc \tag{1}$$

where n is the porosity of the medium, v is the pore water velocity, and c is the concentration of the contaminant. The velocity and concentration can be expressed as a mean value plus fluctuations about the mean. The resulting flux can be expressed as

$$f = n(c + c_f)(v + v_f) \tag{2}$$

where v and c are the mean pore water velocity and the mean concentration, respectively, and v_f and c_f are the fluctuations from the mean. By taking the time average of (2) and noting that given a long enough time that the average fluctuations in velocity and concentration will be zero, then (2) may be rewritten as

$$f = ncv + nc_fv_f \tag{3}$$

where ncv represents the average advective flux and nc_fv_f represents the combined effects of the fluctuations in velocity and concentration. In a porous medium the fluctuations arise from the tortuous path the fluid particles must travel and velocity changes due to the presence of grains. This phenomena is referred to as mechanical dispersion. In the absence of any mechanical dispersion the mass flux due to advection may be described as "plug flow".

Experimental results for contaminant transport along a column of porous media with a flux controlled inlet boundary illustrate the analogy between mechanical dispersion and diffusion, Figure 1. Mechanical dispersion causes a spreading of the plug flow as time increases, Figure 1a). The degree of spreading increases with time. It is worthwhile to consider the derivative of this contaminant profile, Figure 1b). It is evident by observation of the derivatives that mechanical dispersion resembles diffusion of a point source, Figure 1c). This is analogous to molecular diffusion, Cussler (1984). This analogy leads to a diffusive equation describing mechanical dispersion (Bear, 1972), viz.,

$$nc_fv_f = -nD_{md}\frac{\partial c}{\partial z} \tag{4}$$

where D_{md} is the coefficient of mechanical dispersion. D_{md} is velocity dependent and for 1-D transport is usually defined as $D_{md} = \alpha v$, where α is called the dispersivity. It is found experimentally that the dispersivity is scale dependent, $\alpha = \alpha(L)$ (Gelhar *et al.*, 1985).

Equation (4) describes mechanical dispersion adequately on a laboratory scale. However, in the field (4) is less accurate since mechanical dispersion is effected by macroscopic structures comprising the medium (Pickens and Grisak, 1981; Sudicky *et al.*, 1983; Gelhar *et al.*, 1985). On the laboratory scale mechanical dispersion is dominated by the tortuous paths caused by the grains in the porous medium.

Diffusive transport in a porous medium results from concentration gradients. In an aqueous solution this is governed by Fick's Law,

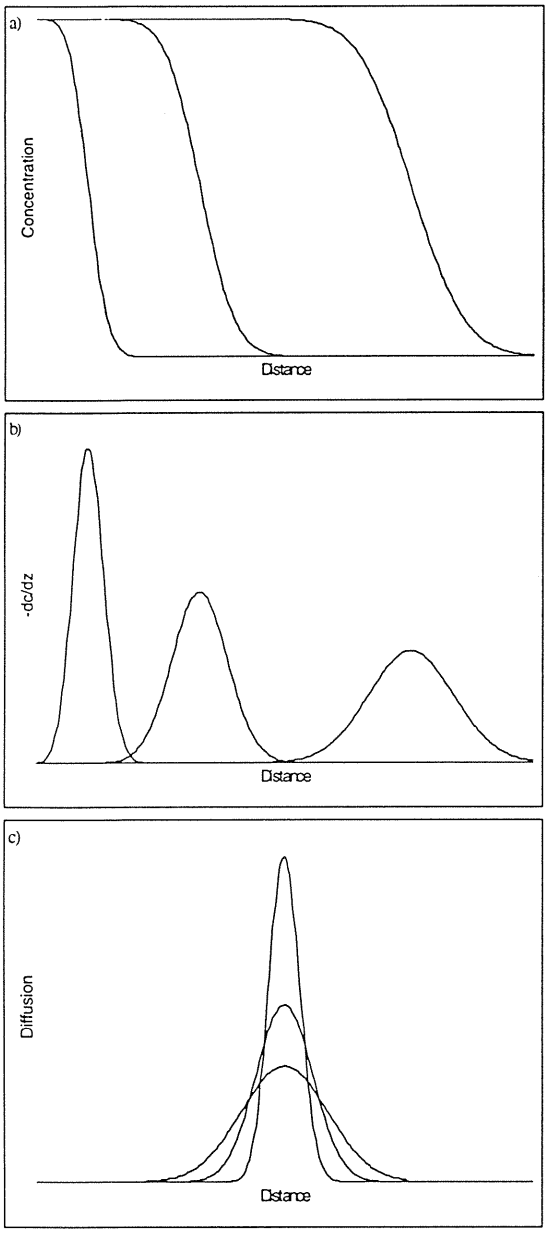

Figure 1. Flow of contaminant in a column of porous media with a flux controlled inlet boundary showing the analogy between mechanical dispersion and diffusion. a) Three concentration profiles at three different times; b) The negative of the derivative of the concentration profiles shown in a); c) When the curves in b) are centred, they are analogous to the solution of the transient diffusion equation with a delta function initial condition.

$$f = -D_d\frac{\partial c}{\partial z} \qquad (5)$$

where D_d is the coefficient of molecular diffusion. In a porous medium the tortuous paths followed by the contaminant particles modifies D_d. The effective coefficient of molecular diffusion is defined as $D_e = \tau D_d$, where τ is primarily a geometry depended quantity called the tortuosity. The mass flux due to diffusion is then given by

$$f = -nD_e\frac{\partial c}{\partial z} \qquad (6)$$

The total mass flux in a porous medium is obtained by adding the contributions of advection, mechanical dispersion, and diffusion, viz.,

$$f = nvc - nD\frac{\partial c}{\partial z} \qquad (7)$$

where $D = D_e + D_{md} = D_e + \alpha v$, is the coefficient of hydrodynamic dispersion.

By considering conservation of contaminant mass in a representative volume element and using (7), the equation describing time-dependent contaminant transport through a porous medium with constant flow conditions is given by (ignoring chemical reactions and decay),

$$D\frac{\partial^2 c}{\partial z^2} - v\frac{\partial c}{\partial z} = R\frac{\partial c}{\partial t} \qquad (8)$$

where R is the retardation coefficient. (8) is referred to as the dispersion-advection equation and is commonly employed to describe contaminant transport through a porous medium.

To solve the dispersion-advection equation appropriate initial and boundary conditions are required. The initial condition is $c(z,0) = f(z)$; here $f(z)$ is taken to be zero. The boundary conditions are more complicated. If the porous medium is bounded by another porous medium then the concentrations and normal components of the mass fluxes (given by (7)) are matched across the boundary. Models that consider a single porous medium can not apply these boundary conditions and so the boundary conditions need to be approximated in an appropriate manner. The typical choices are Dirichlet boundary conditions (constant concentration), Neumann boundary conditions (constant gradient), or a linear combination of the two leading to flux, finite mass, etc. boundary conditions (Bear, 1972; Rowe et al., 1995).

Even though mechanical dispersion is represented by a diffusion equation it still arises from a different physical mechanism. For instance, at the inlet boundary it is not expected that mechanical dispersion will draw mass across the boundary as is the case for diffusion. Mechanical dispersion causes a redistribution of contaminant mass. It does *not* bring extra mass across the boundary. To stop this mass flow across the boundary the dispersivity must be zero at the inlet boundary. For this to occur the dispersivity must vary smoothly with the spatial coordinate in order to obtain a non zero value throughout the porous medium.

In this paper the dispersivity is allowed to vary spatially in the dispersion-advection equation. Keeping the dispersivity zero at the inlet boundary stops mass flow across the boundary due to mechanical dispersion. The results are compared to the standard and commonly used approach of using a constant dispersivity.

2. MATHEMATICAL MODEL

Consider a porous medium of length L. The boundary at $z = 0$ is the inlet boundary and the boundary at $z = L$ is the outlet or exit boundary. As required by continuity of fluid flow, in the absence of any fluid sources or sinks, the pore water has a constant velocity v from the inlet boundary to the outlet boundary. Contaminant transport through such a medium is governed by (8). Initially the medium is free from contaminant, $c(z,t) = 0$. Dirichlet boundary conditions are used, $c(0,t) = c_0$ and $c(L,t) = 0$. Although these boundary conditions are comparatively simple they are adequate for the demonstrative purposes of this paper.

Given that the dispersivity varies spatially, $\alpha = \alpha(z)$, the contaminant mass flux, (7), becomes

$$f = nvc - n(De + \alpha(z)v)\frac{\partial c}{\partial z} \qquad (9)$$

By considering conservation of mass the following dispersion-advection equation is obtained

$$D(z)\frac{\partial^2 c}{\partial z^2} - v(1 - \frac{d\alpha}{dz})\frac{\partial c}{\partial z} = R\frac{\partial c}{\partial t} \qquad (10)$$

where

$$D(z) = D_e + \alpha(z)v \qquad (11)$$

This is a more general form of the dispersion-advection equation, (8).

A functional form for the dispersivity needs to be selected in order to solve (10). To stop the flow of mass across the inlet boundary due to mechanical dispersion the dispersivity must be zero at the inlet boundary, $\alpha(z{=}0) = 0$. Numerical experiments have shown that α can not vary too rapidly, particularly near z=0. This is due to both numerical problems (the concentration gradient at the inlet boundary depends on the first few grid points) and the development of an unrealistically large negative velocity in (10) (due to the gradient of the dispersivity in the advective term of (10)). It is found that a gradually changing dispersivity is most appropriate.

In natural soils it is known empirically that the dispersivity is scale dependent, $\alpha = \alpha(L)$, see Figure 2 (Gelhar *et al.*, 1985). A contaminant particle moving across the inlet boundary does not know the scale of the porous medium it is entering. For example, if a contaminant particle had travelled 100 m into a porous medium it would behave as though it had a dispersivity of around 100 m (Figure 2). However, a contaminant particle that had travelled 1 m would behave as though it had a dispersivity of 0.01 m (Figure 2). This reinforces that the dispersivity should be scale dependent. It may be postulated that the contaminant particle behaves as though it is in a porous medium of length z, where z is the contaminant particle location. The dispersivity would vary as in Figure 2, that is, instead of $\alpha = \alpha(L)$ the dispersivity varies as $\alpha = \alpha(z)$, that is, L is replaced by z. The function form of α being,

$$\alpha(z) = \frac{z^2}{100} \qquad (12)$$

This gives a smooth variation of α with z (Rowe et al., 1995). Note that Tompson and Gray (1986) have modelled the dispersive flux as both spatially and temporally varying, however, they derive this by the use of volumetric averaging techniques.

For comparative reasons the solution of (10) using a constant dispersivity will be called the Standard Method. It is called the Standard Method because it is the usual assumption made by numerical analysts. The use of the spatially varying dispersivity, (12), in (10) will be called the New Method. In order to compare the two methods the dispersion-advection equation, (10), will be non-dimensionalised. Defining

$$Z = \frac{z}{L} \qquad T = \frac{D_{max}t}{RL^2}$$
$$P = \frac{vL}{D_{max}} \qquad C \rightarrow \frac{c}{c_0} \qquad (13)$$

where $D_{max} = D_e + \alpha(L)v$. For the Standard Method (10), becomes

$$\frac{\partial^2 C}{\partial Z^2} - P\frac{\partial C}{\partial Z} = \frac{\partial C}{\partial T} \qquad (14)$$

which is the non-dimensional equivalent of (8). For the New Method, (10) becomes

$$\frac{P}{P(Z)}\frac{\partial^2 C}{\partial Z^2} - P(1 - \frac{1}{L}\frac{d\alpha}{dZ})\frac{\partial C}{\partial Z} = \frac{\partial C}{\partial T} \qquad (15)$$

where

$$P(Z) = \frac{vL}{D_e + \alpha(Z)v} \qquad (16)$$

is a spatially varying Peclet number. Given this definition the Peclet number in (13) is defined equivalently as $P = P(L)$. It is clearly evident that the advective and diffusive terms in (15) vary spatially. In non-dimensional form (12) becomes

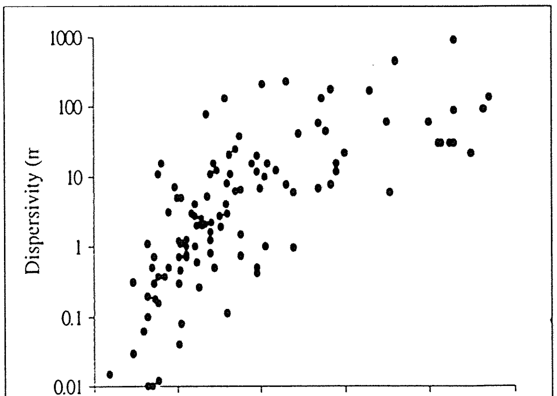

Figure 2. The longitudinal dispersivity as a function of scale (Gelhar *et al.*, 1985).

$$\alpha(Z) = \frac{L^2Z^2}{100} \qquad (17)$$

The dispersivity is defined as an increasing function of Z. Therefore, the coefficient of the diffusive term in (15) is a minimum at Z=0 and increases to a maximum at Z=1. The diffusive component (the P/P(Z) term in (15)) decreases with L and v. Figure 3 shows the coefficient of the diffusive component as a function of L for D_e=0.01 m^2/a and v=0.05 m/a. It can be seen that for small L the diffusive component is close to unity, as in the Standard Method. As L increases the diffusive component is significantly reduced.

The coefficient of the advective term can decrease from a maximum of P to negative values as the value of L increases. The relative magnitude of the advective term compared with the Standard Method, viz.,

$$1 - \frac{1}{L}\frac{d\alpha}{dZ} \qquad (18)$$

is governed solely by L and is shown in Figure 4. The difference from the Standard Method is small for small L, however, there is the unusual phenomena of the advective term becoming negative when $L > 50$. However, in this case $P < 2$ and as L increases, P decreases and so the advective term is quite small. For contaminant transport a negative Peclet number is unusual and it may suggest the wrong choice of dispersivity, (12), or it may require more understanding of the physical processes to interpret it correctly in relation to mechanical dispersion.

To compare the differences between the Standard Method and the New Method, the total mass entering and leaving the porous medium is compared. The non-dimensional mass passing a given point Z up to time T is given by,

$$M(Z,T) = \int_0^T F(Z,\tau)d\tau \qquad (19)$$

where the non-dimensional mass fluxes, F, are

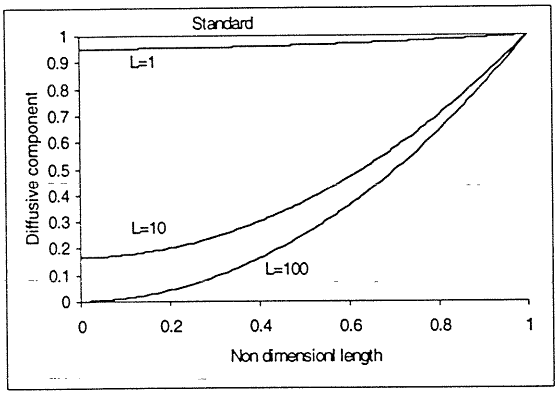

Figure 3. The coefficient of the diffusive component plotted as a function of non-dimensional length for the case D_e = 0.01m^2/a, v=0.05 m/a.

$$F = Pc - \frac{\partial c}{\partial z} \qquad (20)$$

for the Standard Method, and

$$F = Pc - \frac{P}{P(Z)}\frac{\partial c}{\partial z} \qquad (21)$$

for the New Method.

3. NUMERICAL METHOD

An explicit finite difference scheme is used to solve the governing equations ((14) and (15)). Great care is required when calculating the mass fluxes at the boundaries. Numerically, the mass flux is calculated as

$$M(Z,T) = \sum_{j=1}^{N} F(Z, j\Delta T)\Delta T \qquad (22)$$

where N is the number of time steps (c.f. (19)). The mass flux, obtained from (20) or (21), requires a knowledge of the concentration gradient. Initially, the boundary condition $c(0,T) = 1$ represents a sharp concentration front. For early time steps the value of the concentration gradient is inaccurate and so the calculation of the contaminant mass flux will be inaccurate. This can be overcome by use of the identity

$$M(0,T) - M(1,T) = \int_0^1 c(\xi,T)d\xi \qquad (23)$$

which is a statement of the conservation of contaminant mass, viz., the mass entering the porous medium minus the mass leaving must be equal to the contaminant mass in the porous medium. For early time steps the mass leaving the outlet boundary is zero. When this reaches a predetermined minimum value the total mass entering the porous medium is equal to the area under the concentration profile

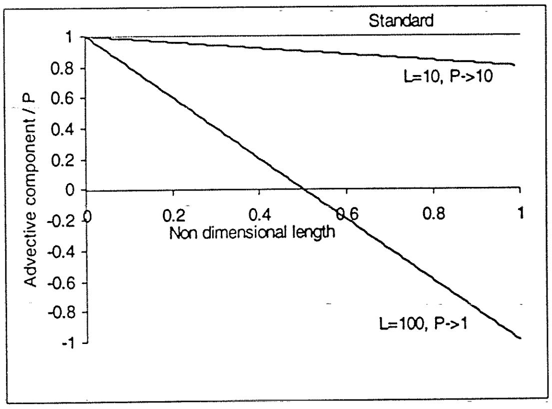

Figure 4. The coefficient of the advective component, (18), plotted as a function of non-dimensional length. The L=1 case is not shown as it closely approximates the Standard case. The Peclet number shown is the limit as the velocity increases to infinity.

(given by the right hand side of (23)). After this time the concentration profile has smoothed at the inlet boundary and (22) can then be used to calculate the remaining mass to flow across the inlet boundary.

4. RESULTS

To compare the differences between the Standard and New Methods, the ratio of the mass transported across the inlet boundary is plotted as a function of velocity, Figure 5. These plots are repeated for different lengths of porous media. Although similar plots may be obtained for the outlet boundary the data is less accurate since the flow rates are quite often low. However, it is found that the mass at the outlet boundary follows similar trends to the mass at the inlet boundary. Note that the time in Figure 5 is non-dimensional. The velocity has been plotted in place of the Peclet number as the Peclet number is non-uniform due to the definition (16) and causes a bunching of points at high velocities.

To put the differences between the two methods more practically, consider a porous medium of length 10m, Figure 5b). If the parameters are v=1 m/a, D_e = 0.01 m^2/a, and R=10, which gives P~10. For a non-dimensional time of 0.01, that is, a real time of 100 years, the error in the computed mass entering the boundary is around 70%. In this case the error is very significant.

From the definition of D(Z), (11), it is evident that changing the magnitude D_e will only shift the curves in Figure 5 along the horizontal axis, since D(Z) is a linear function of v. So without loss generality, a value of D_e can be selected for all calculations. The results for other choices of D_e are the same, except that the curves are translated along the horizontal axis. A value of D_e= 0.01 m^2/a was used for all plots in Figure 5. A typical range of values for D_e is between 0.005 and 0.05 m^2/a (Rowe et al., 1995).

Most evident in Figure 5 is the large overestimate of mass across the inlet boundary for the L=100m case. This can be understood by considering the definition of D(Z), (11), and analysis of the concentration profiles. Figure 6 shows a contaminant concentration profile comparing the two methods for the particular case L=100 m, v=1 m/a, D_e=0.01 m^2/a, and T=0.1, which gives P~1. As can be seen from Figure 6, the two methods result in completely different solutions. Given the above parameters the problem is dominated by mechanical dispersion. For both methods, D_e = 0.01 m^2/a, however, D_{md} = 100 m^2/a for the Standard Method. The large D_{md} at the inlet boundary for the Standard Method will cause a large amount of mass to be drawn into the porous medium. This clearly does not happen for the New Method as seen in Figure 6.

To explain the difference between the two methods consider the mass that enters the porous medium. It is apparent that the problem is dominated by mechanical dispersion, the major component of mass flux will be from advection. A total of P*T=1*0.1=0.1 mass units (non-dimensional) will enter the porous medium. By (23) this must be equal to the area under the curve minus the mass out, which for the New Method is approximately 0.1-0=0.1. Thus (23) holds for the New Method. However, for the Standard Method the mass flux entering was calculated to be approximately 0.4, four times greater than the mass that physically flowed across the boundary due to advection! The extra mass is caused by the mechanical dispersion term drawing mass across the boundary down an apparent chemical concentration gradient, this does not happen physically. This example clearly illustrates the problems associated with a constant dispersivity, that is, the Standard Method.

This method of comparing the contaminant mass fluxes in advection dominated problems was used to test various functional forms for the dispersivity. It was found that correct mass flows were predicted only when the dispersivity varied in a smooth and gradual fashion, similar to the functional form given by (12) and shown in Figure 3. Further work needs to be done to identify the most realistic functional form

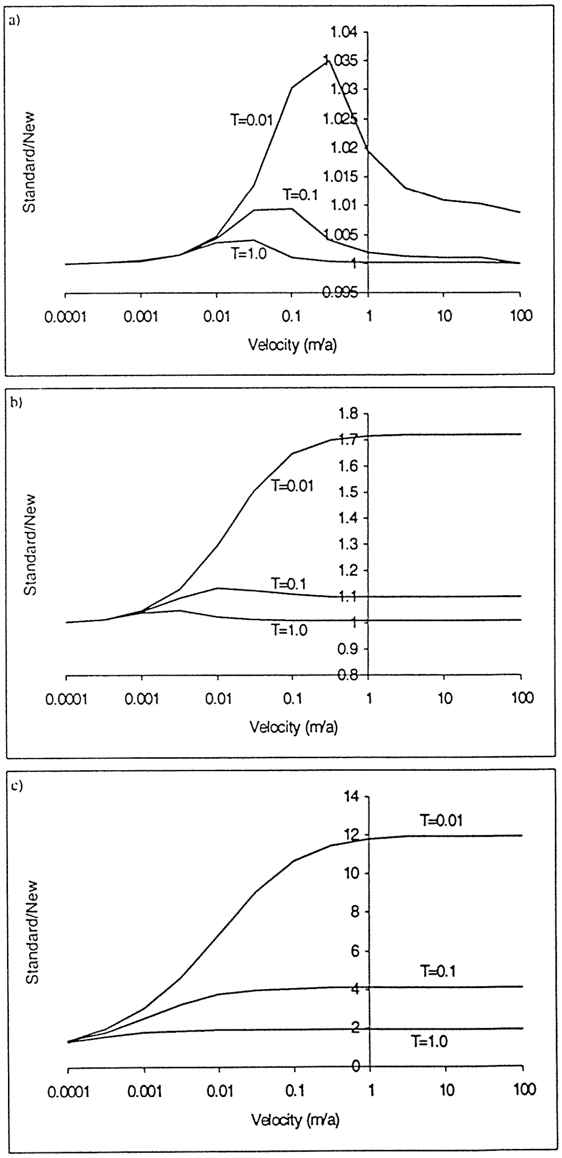

Figure 5. Plots of the ratio between the Standard Method and the New Method against velocity for a) L=1m, b) L=10m, and c) L=100m. Note that the time is non-dimensional, however, instead of plotting the Peclet number the dimensional velocity has been used since it gives a uniform scale as the velocity increases (see (13)).

for dispersivity. Although, for the demonstrative purposes of this paper (12) is satisfactory.

At small velocities the Peclet number will become small and be dominated by diffusion. Under these conditions it would be expected that the two methods would predict similar results. This is shown in Figure 5 at small velocities. In other words, the use of a constant dispersivity is satisfactory for low velocities and large molecular diffusion coefficients.

At high velocities the contaminant is quickly swept away from the boundary, and so the concentration gradient at the boundary will be zero, that is, it becomes flux controlled. The only mass entering the porous medium will be due to advection. However, Figure 5 shows that the two methods are not equivalent at high velocities, instead they converge to a constant difference. This is because at small times the concentration gradient at the inlet boundary will be non-zero and the Standard Method will draw in additional mass. Since the mass crossing the inlet boundary is a cumulative total over time, the effect at small times will be carried over to larger times. For this reason it is not unexpected that there is a difference between the two methods, even at high velocities.

Given the arguments made for the behaviour at the inlet boundary it could be suggested that a similar situation will arise at the outlet boundary. The influence of the mechanical dispersion on the outlet boundary will be investigated in a future paper.

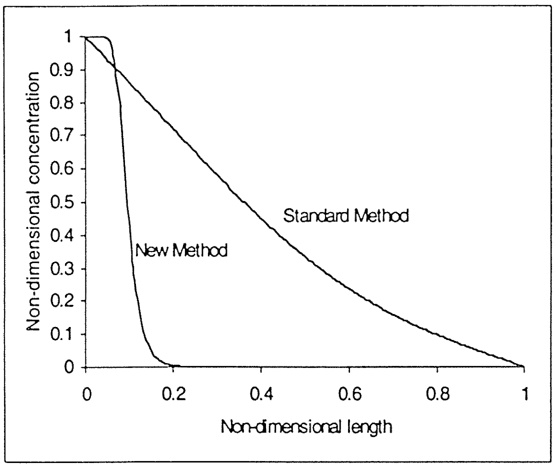

Figure 6. A comparison of the Standard Method and the New Method for L=100 m, D_e=0.01 m^2/a, v=1 m/a, and T=0.1.

6. CONCLUSION

For a mechanical dispersion coefficient that varies spatially, solutions of the dispersion-advection equation deviate greatly compared to the standard approach, which assumes a constant value for the mechanical dispersion coefficient along the porous medium. The difference between the two methods is greatest for small times and long lengths of porous media where the effects at the boundary are greatest. The standard implementation of dispersion-advection equation with constant mechanical dispersion is clearly inadequate under certain conditions. The conditions where a significant difference will be expected have been partially clarified in this paper, Figure 5. The use of a constant dispersivity is very conservative in many cases and will greatly alter contaminant profiles and breakthrough times estimated numerically.

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