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## MODELLING CONTAMINANT DISPERSION IN SATURATED SAND

### MODELISATION DE DISPERSION CONTAMINEES DANS DES SABLES SATURES

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**SYNOPSIS:** The paper describes traditional techniques for the laboratory measurement of dispersion, and presents centrifugation as a new experimental technique for modelling dispersive processes. Comparisons between centrifuge test data and laboratory data are given: these comparisons serve to illustrate the validity of using centrifugation to model dispersion. Furthermore, the feasibility of using centrifuge test data to predict field scale concentration profiles is investigated, by comparing centrifuge test data with a prototype concentration profile. In order to overcome limitations in the scaling of dispersion, due to incorrect scaling of the particle size, a separate scaling law for pollutant spread is introduced. The new scaling law is shown to give good agreement in the spread of pollutant concentration between centrifuge and prototype data.

#### INTRODUCTION

When a fluid placed in a porous medium is displaced by another, both fluids being miscible, the development of a transition zone between the fluids with time can be observed. In a stationary fluid, the evolution of the transition zone is interpreted as a diffusion process. In a moving fluid, the evolution of the transition zone is attributed to the mechanism of dispersion. The dispersion of fluids moving through porous media is of interest in many practical environmental engineering problems, including problems concerning pollutant behaviour in soils. For this reason, the study of dispersive processes has contributed much of the research work carried out in the field of environmental geotechnology.

The bulk of experimental data on pollutant behaviour in soil has traditionally been supplied by controlled field experiments and/or laboratory column data. However, researchers have recently come to recognise that a geotechnical centrifuge can provide a powerful experimental tool for investigation of many environmental engineering problems (Savvidou, 1988; Hensley and Schofield; 1991, Cooke and Mitchell, 1991). A geotechnical centrifuge has the ability to model complex two and three dimensional problems, under repeatable and controlled boundary conditions. The research presented in this paper investigated the feasibility of using centrifuge testing to model dispersive processes in saturated, uniform sand.

#### THE DISPERSION MECHANISM

Dispersion results from the simultaneous actions of two mechanisms: mechanical dispersion and molecular diffusion. The combined action of these mechanisms is termed hydrodynamic dispersion (Bear, 1972). Spreading by mechanical dispersion occurs due to velocity variations in both magnitude and direction within a pore domain. Spreading by molecular diffusion occurs as a result of gradients in chemical potential within the liquid phase.

The best representation of the dispersion mechanism has proved to be the macroscopic equation of dispersion. Much experimental work in uniform porous media is based upon verification of this equation and computation of its coefficients, which are termed dispersion coefficients. For the dispersion of a conservative pollutant species (tracer) in uniform one dimensional flow, the macroscopic dispersion equation is (Fried, 1975)

$$\frac{\partial c}{\partial t} = D_h \frac{\partial^2 c}{\partial x'^2} \quad (1)$$

where:

- $c$  = pollutant concentration in pore fluid phase ( $M/L^3$ ),
- $t$  = time (T)
- $D_h$  = coefficient of hydrodynamic dispersion ( $L^2/T$ )
- $x'$  =  $x - ut$  (L)
- $u$  = one-dimensional pore fluid velocity (L/T).

For continuous injection of a pollutant of concentration  $c_0$  at  $x = 0$ , the solution to equation (1) can be approximated by a normal distribution function with mean,  $m = ut$  and standard deviation  $\sigma = (2D_h t)^{0.5}$ . A classic property of the normal distribution function is that 2/3 of all variables lie between  $m - \sigma$  and  $m + \sigma$ . The magnitude of  $D_h$  can thus be determined from a profile of pollutant concentration at time  $t$ , viz:

$$D_h = \frac{(x_{0.16} - x_{0.84})^2}{8t} \quad (2)$$

where  $x_{0.16}$  and  $x_{0.84}$  refer to the distance,  $x$ , at concentrations of  $0.16c_0$  and  $0.84c_0$ .

An alternative means of determining  $D_h$  is to observe the evolution of concentration at a fixed distance ( $x$ ) with time. When this method is undertaken, the magnitude of  $D_h$  may be computed from:

$$D_h = \frac{1}{8} \left[ \frac{(x - ut_{0.16})}{(t_{0.16})^{0.5}} - \frac{(x - ut_{0.84})}{(t_{0.84})^{0.5}} \right]^2 \quad (3)$$

where  $t_{0.16}$  and  $t_{0.84}$  are the times to achieve concentrations of  $0.16c_0$  and  $0.84c_0$ .

The magnitude of  $D_h$  is a function of both the characteristic microscopic length of the system  $d$ , the pore fluid velocity  $u$ , and the free molecular diffusion coefficient of the pollutant species in solution,  $D_d$ . Much experimental and laboratory work has shown the relationship between dispersion and the dimensionless Peclet number,  $P_e = ud/D_d$ , given in Figure 1. For  $P_e \leq 0.4$ , the dispersion mechanism is dominated by the process of molecular diffusion, and the value of  $D_h$  is independent of velocity. For  $P_e \geq 5$ , the dispersion mechanism is dominated by

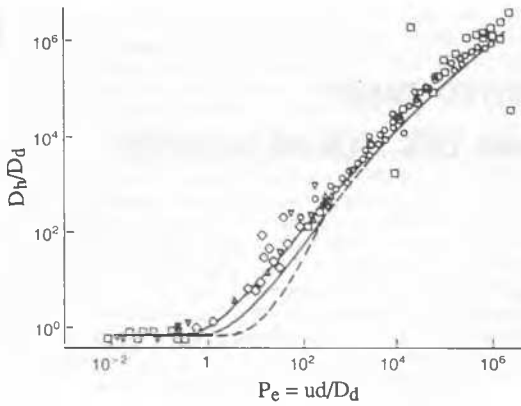


Fig. 1. Dependence of dispersion on  $P_e$  (after Bear and Verruijt, 1987)

mechanical dispersion, and there is an approximately linear relationship between  $D_h$  and the pore fluid velocity,  $u$ , provided that the validity of Darcy's law is maintained. For intermediate values of the Peclet number ( $0.4 < P_e < 5$ ), a transition zone exists, where dispersion is governed simultaneously by the mechanisms of molecular diffusion and mechanical dispersion (Bear, 1979).

For one-dimensional flow it is common to describe  $D_h$  in the form (Freeze and Cherry, 1979):

$$D_h = TD_d + \alpha u \quad (4)$$

where  $T$  is the tortuosity of the porous medium (a scalar) and  $\alpha$  is the longitudinal dispersivity of the medium (dimensions of  $L$ ). The first term on the right hand side of equation (4) characterises that contribution made to contaminant dispersion by molecular diffusion, whereas the second term characterises that contribution made by mechanical dispersion.

Experimental observation has shown that, for uniform, unconsolidated media such as sand, equation (4) is well described by (Perkins and Johnston, 1963):

$$\frac{D_h}{D_d} = 0.7 + 1.75P_e \quad (5)$$

## LABORATORY MEASUREMENT OF DISPERSION

In order to allow a comparison between dispersion coefficients measured using centrifuge modelling techniques, and those identified by traditional laboratory testing techniques, a series of one-dimensional laboratory column tests was performed over a range of seepage velocities in two uniform silica sands. Throughout the test series, a 0.2 Molar sodium chloride (NaCl) solution, having a free molecular diffusion coefficient  $D_d = 1.5 \times 10^{-9} \text{ m}^2/\text{s}$ , was used as the pollutant species.

The column apparatus employed during the laboratory tests was designed and built at the University of Western Australia, and is described in detail by Campbell (1991). Two grades of sand were used during the investigation, a 'coarse' sand, having an average particle diameter of 0.85 mm, and a 'fine' sand, having an average particle diameter of 0.3 mm. All tests were conducted on saturated sand samples uniformly packed to a height of 150 mm, and with an average volume porosity,  $n = 0.36$ .

Figure 2 gives a schematic diagram of the test set-up. A displacement pump was used to supply a constant flux of salt solution to the base of the soil column. The evolution of concentration with time at the top of the column was determined by collecting the column effluent in fractions, and analysing the chloride content of each fraction. The resulting 'break-through' curve was then used to determine the coefficient of hydrodynamic dispersion for chloride through the sample (see equation (3)).

For each grade of sand, the coefficient of hydrodynamic dispersion was determined over a range of average pore fluid velocities. The results of the test series are summarised in Table 1.

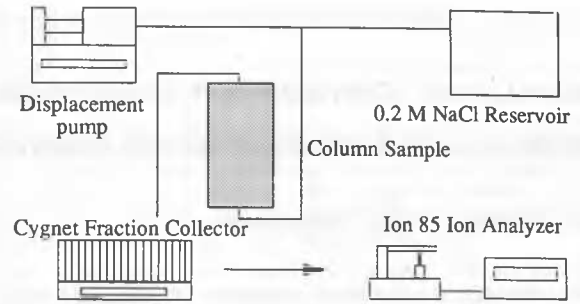


Fig. 2. Laboratory measurement of dispersion (after Campbell, 1991)

Table 1. Summary of Laboratory Dispersion Tests (from Campbell, 1991)

Sample	$u$ (m/s)	$P_e$	$D_h$ ( $\text{m}^2/\text{s}$ )
Coarse	$1 \times 10^{-6}$	0.57	$2.72 \times 10^{-9}$
	$3 \times 10^{-6}$	1.7	$5.79 \times 10^{-9}$
	$10 \times 10^{-6}$	5.67	$7.65 \times 10^{-9}$
Fine	$1 \times 10^{-6}$	0.2	$1.53 \times 10^{-9}$
	$3 \times 10^{-6}$	0.6	$1.14 \times 10^{-9}$
	$10 \times 10^{-6}$	2.0	$5.96 \times 10^{-9}$

## GEOTECHNICAL CENTRIFUGE MODELLING

It is now widely accepted that centrifuge modelling provides the most versatile technique for obtaining stress conditions that are homologous in model and prototype (Fahey et al, 1990). This is achieved by accelerating a scale model, where all linear dimensions are reduced by a factor  $N$ , to a centrifugal acceleration of  $N$  gravities ( $g$ ) (Schofield, 1980).

General scaling factors for the centrifuge modelling of environmental engineering problems are summarised in Table 2. These relationships have been derived assuming similitude of the dispersion mechanism between model and prototype (Hensley, 1988; Arulanandan et al, 1988).

Table 2. Scaling Factors for Centrifuge Modelling

Parameter	Prototype-model ratio
Gravity	$1/N$
Length	$N$
Pressure	1
Concentration	1
Velocity	$1/N$
Time	$N^2$

## Centrifuge Modelling of Dispersion

An experimental programme was undertaken to model contaminant dispersion in saturated sand using centrifugation. The programme was initiated to investigate the feasibility of using centrifuge modelling techniques to identify dispersion coefficients in situations where self-weight effects, such as soil compressibility or gradients in ambient stress and fluid density, may influence the dispersion mechanism. The work reported in this paper formed the first stage of the programme, and aimed to demonstrate that centrifuge testing techniques could be used to obtain dispersion coefficients in soil systems. As for the laboratory test series, a 0.2 Molar sodium chloride (NaCl) solution was used as the pollutant species. The arrangement of the centrifuge model is shown in Figure 3.

A saturated coarse sand layer with an average volume porosity of 0.36 and a height of 158 mm was constructed over a 53 mm thick silt layer underlain by a permeable base drain. The layers of sand and silt were separated by a sheet of filter paper, 0.15 mm thick. The upward hydraulic gradient through the sample was controlled by water levels within standpipes connected to the model. A fluid head difference of 7.5 mm was imposed during all tests. Pore fluid velocities were varied between each test, by altering the centrifugal force acting on the model.

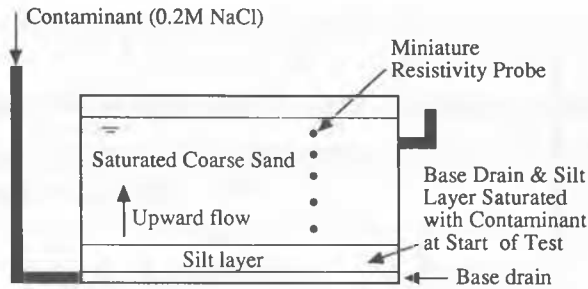


Fig. 3. Arrangement of centrifuge model

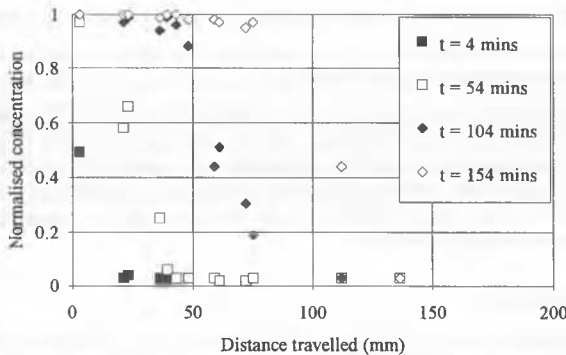


Fig. 4. Typical normalised concentration profiles from centrifuge tests

At the start of each test, the base drain and silt layer were saturated with the 0.2 M NaCl solution. Subsequent progress of the pollutant species as it was driven upwards through the sand was mapped by an array of miniature resistivity probes, that were designed and developed at The University of Western Australia. The coefficient of hydrodynamic dispersion for chloride through each centrifuge sample was determined from an observed profile of pollutant concentration at a fixed time,  $t$  (see equation (2)).

A total of three centrifuge tests were conducted using a 'coarse' sand having an average particle diameter of 0.85 mm. A range of  $g$ -levels, and hence seepage velocities, were investigated during the test series. Figure 4 presents typical normalised concentration profiles observed during the first test in the series. A summary of the test series is given in Table 3.

Table 3. Summary of Centrifuge Test Series

Test	$g$ -level	$u$ (m/s)	$Pe$	$D_h$ ( $m^2/s$ )
1	150g	$9.66 \times 10^{-6}$	5.41	$1.84 \times 10^{-8}$
2	53g	$3.55 \times 10^{-6}$	2.01	$0.99 \times 10^{-8}$
3	100g	$6.33 \times 10^{-6}$	3.59	$1.48 \times 10^{-8}$
Prototype	1g	$0.06 \times 10^{-6}$	0.03	$0.11 \times 10^{-8}$

### COMPARISON OF DISPERSION COEFFICIENTS

Figure 5 presents a comparison of the dispersion coefficients measured in the laboratory with those deduced from the centrifuge tests, and compares the experimental data with the theoretical relationship described by equation (5). In all cases, the average particle diameter was selected as the microscopic characteristic length,  $d$ , of the system.

It is clear from Figure 5, that the dispersion coefficients obtained using centrifuge modelling techniques are in accord with those obtained using traditional laboratory methods. Thus centrifuge modelling offers a viable means of obtaining hydrodynamic dispersion coefficients through soils. In addition, the data presented in Figure 5 verify that dispersion coefficients in uniform, saturated sands are adequately described by the theoretical relationship presented in equation (5). This suggests that we can predict, with reasonable accuracy, the coefficient of hydrodynamic dispersion through uniform sand samples at any velocity within the range of validity of equation (5) ( $Pe < 50$ , Perkins and Johnston (1963)).

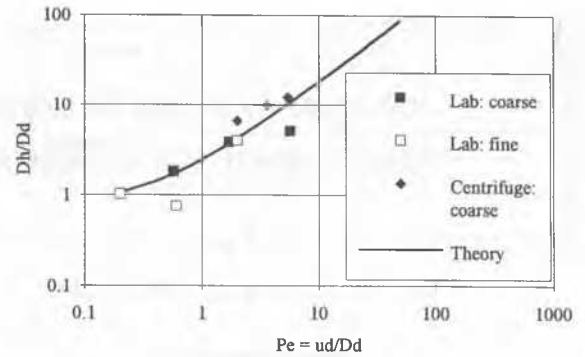


Fig. 5. Comparison of dispersion coefficients

### PREDICTING DISPERSION IN A PROTOTYPE

The centrifuge test series summarised in Table 3 modelled pollutant transport through a uniform, coarse sand prototype having an upward seepage velocity  $u_p = u_m/N \approx 0.064 \times 10^{-6}$  m/s, and an average characteristic microscopic length  $d_p = 0.85$  mm. The prototype system was thus characterised by a Peclet Number  $Pe_p \approx 0.036$ , and a hydrodynamic dispersion coefficient  $D_{hp} = 0.11 \times 10^{-8}$   $m^2/s$  (using equation (5)).

Theoretically, the pollutant concentration profiles observed during each centrifuge test (see for example Figure 4) may be transformed into predicted prototype concentration profiles by means of the scaling laws presented in Table 2. Figure 6 presents prototype concentration profiles at  $t = 2.4$  years predicted using centrifuge test data, together with the prototype concentration profile obtained from a solution to the macroscopic dispersion equation.

It is clear from Figure 6 that there is agreement between all profiles at the 'mean' concentration  $c/c_0 = 0.5$ . However, there is obvious disagreement between the predicted 'spread' of each profile about the mean.

This disagreement can be explained by the variation in the dispersion coefficients presented in Table 3. The scaling laws given in Table 2 assume similarity of dispersion between model and prototype, which has clearly not been observed. We note that the higher the dispersion coefficient characterising the centrifuge model, the wider the 'spread' of the predicted profile, and the greater the disparity between the predicted profile and the prototype. These observations are consistent with our understanding that the dispersion coefficient characterises the development of a transition zone between two fluids of different concentration. Thus, at any given time, a system described by a 'high' dispersion coefficient will manifest a wider transition zone between two marked fluids than a comparable system described by a lower dispersion coefficient.

Due to the  $N$ -fold increase in flow velocity within a centrifuge model ( $u_m = Nu_p$ ), strict similarity of dispersion between a centrifuge model and the prototype can only be achieved if the characteristic length governing the mechanical dispersion process (the average soil particle size) is reduced by a factor  $N$  in the centrifuge model (Hensley and Savvidou, 1992). In reality, this criterion is often not met, as in the tests reported here. Thus, much centrifuge research work concerning pollutant transport involves a scaling error in modelling dispersion, that needs to be addressed.

### A Scaling Law for Pollutant Spread

The data offered above demonstrate that the scaling factors presented in Table 2 can not be used directly to predict the behaviour of a prototype if there is a scaling error in modelling dispersion ( $D_{hm} \neq D_{hp}$ ). Instead, it is necessary to develop a separate scaling law for pollutant spread.

The microscopic equation of dispersion (equation (1)) can be written for the prototype ( $p$ ) and the model ( $m$ ) as

$$\frac{\partial c_p}{\partial t_p} = D_{hp} \frac{\partial^2 c_p}{\partial x_p^2}, \quad \frac{\partial c_m}{\partial t_m} = D_{hm} \frac{\partial^2 c_m}{\partial x_m^2} \quad (6)$$

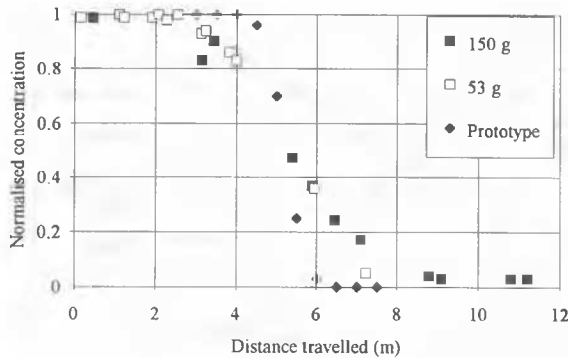


Fig. 6. Predicted prototype concentration profiles

If we define the following ratios ( $r$ ) between a value in the prototype to that in the model

$$c_r = \frac{c_p}{c_m}; D_r = \frac{D_{hp}}{D_{hm}}; x'_r = \frac{x'_p}{x'_m} \quad (7)$$

we may re-write equation (6) for the prototype as

$$\frac{c_r}{t_r} \frac{\partial c_m}{\partial t_m} = D_r D_{hm} \frac{c_r}{x'_r{}^2} \frac{\partial^2 c_m}{\partial x'_m{}^2} \quad (8)$$

Comparing equation (8) with equation (6) for the model, and using the scaling relationship in Table 2 of  $t_r = N^2$ , we find that for correct scaling

$$\frac{1}{t_r} = \frac{D_r}{x'_r{}^2} = \frac{1}{N^2} \quad (9)$$

The co-ordinate  $x'$  characterises the spread of a pollutant profile about the mean concentration  $c/c_0 = 0.5$ . Thus, if we know the ratio  $D_r$ , we can establish, through equation (9), the appropriate scaling ratio for transcribing the observed spread of concentration in a centrifuge model to the prototype situation.

For centrifuge model tests carried out using prototype soil, we can use equation (4) to estimate that

$$D_r = \frac{D_{hp}}{D_{hm}} = \frac{TD_d + \alpha \nu_p}{TD_d + \alpha (N \nu_p)} \quad (10)$$

Thus, for tests dominated by molecular diffusion, where  $TD_d \gg \alpha (N \nu_p)$ ,  $D_r = 1$  and  $x'_r = N$ . This will give no scaling error in modelling dispersion, and the scaling factor for the spread of pollutant ( $x'_r$ ) will be identical to that for scaling length ( $x_r$ ). However, for tests conducted outside this region, the value of  $x'_r$  will lie between  $N$  and  $N^{0.5}$ , and the scaling factor for the spread of pollutant will be less than that for scaling length.

The data presented in Figure 6 were plotted assuming, incorrectly, that the same scaling factor applies to pollutant spread and length. Figure 7 presents the same centrifuge test data 'corrected' to account for the proper scaling of pollutant spread; for each test, the appropriate scaling factor for  $x'_r$  was determined using equation (9). This Figure demonstrates the validity of the scaling law derived for pollutant spread, and suggests that, even if a scaling error is introduced when modelling dispersion on a centrifuge, we can still relate model concentration profiles to a prototype.

## CONCLUSIONS

This paper has presented centrifuge testing as a new experimental technique for modelling dispersive processes. Comparisons between centrifuge test data and laboratory data served to illustrate the validity of using centrifugation to obtain hydrodynamic dispersion coefficients in soil systems. This suggests that a geotechnical centrifuge is a potentially useful tool with which to identify dispersion coefficients in situations where, for

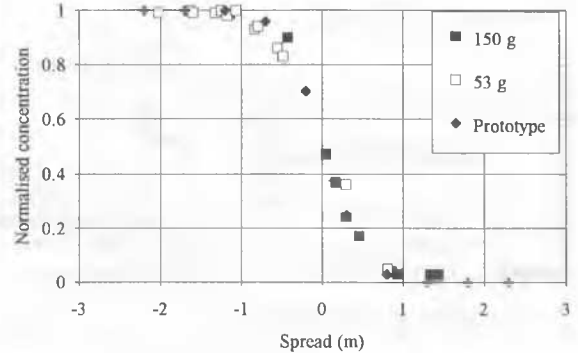


Fig. 7. Corrected concentration profiles

example, soil compressibility and gradients in ambient stress and fluid density influence system characteristics.

Comparison between predictions using centrifuge test data and a prototype concentration profile demonstrates that we can account for the scaling error introduced when modelling dispersion on a geotechnical centrifuge. This suggests that centrifuge test data can be used to predict prototype behaviour, even when similitude of dispersion processes is not achieved between model and prototype.

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