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Using a physical model to determine the hydrodynamic dispersion coefficient of a solution through a horizontal sand column

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Abstract:

Miscible displacement can be understood as a physical process in a porous medium whereby two or more fluids fully dissolve into each other when a fluid mixes and goes into the pore space occupied by other fluids without the existence of an interface. A physical model was made in Can Tho University, which included an electrical current system connecting nine groups of four-electrode probes for measuring the electrical conductivity of a potassium chloride solution flowing through a horizontal sand column placed in a firm frame. The experiments were performed with different volumetric flow rates and three types of sand (fine, medium and coarse). The breakthrough curves were analysed, and then the hydrodynamic dispersion coefficients were calculated. The hydrodynamic dispersion coefficient was one of the hydraulic and solute transport parameters used to design a constructed subsurface flow wetland. The research proves that the flows were laminar, and that mechanical dispersions dominated over molecular diffusions and that the dispersions were large enough to cause combined mixing and flowing processes.

Keywords: **breakthrough curves, electrical conductivity, four-electrode probes, hydrodynamic dispersion coefficients, physical model.**

Classification number: **2.3**

Theory

The main mechanisms governing transport in porous media are convection (advection), diffusion, and mechanical dispersion [1]. Partitioning processes and decaying processes also affected to transport mechanisms. Miscible pollutant transport processes are shown in more detail in Fig. 1.

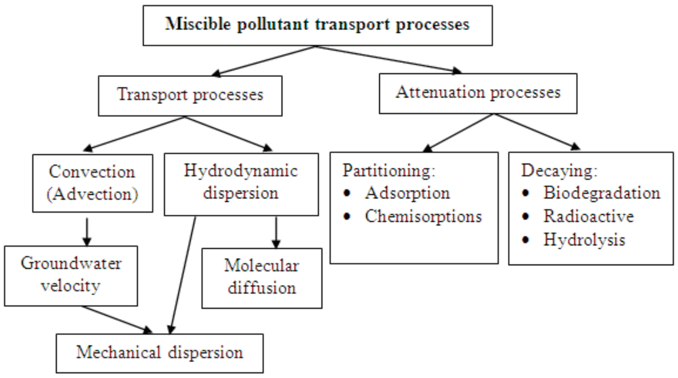

Fig. 1. Flowchart of pollutant transport processes.

The convection-dispersion equation (CDE) describes the transport of solutes through porous media, as in a constructed wetland. Breakthrough experiments with tracers in a horizontal sand column can be used to determine the solute transport parameters for the CDE. The important underlying assumptions for the mathematical analysis are that the sand in the experimental column is homogeneous and that the transport parameters remain constant during the experiment and that, therefore, the solute transport is a linear process. It is necessary to know the transport parameters and the relationship between dispersion and velocity in the solution. The transfer function method is proposed to determine the transport parameters from the solute breakthrough data [2, 3].

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The phenomenon of a solute spreading and occupying an ever-increasing portion of the flow domain in a porous media is called hydrodynamic dispersion. It causes dilution of the solute and is composed of two different processes: mechanical dispersion (or hydraulic dispersion) and molecular diffusion. Hydraulic dispersion refers to the spreading of a tracer due to microscopic velocity variations within individual pores. Molecular diffusion is the net transfer of mass (of a chemical species) by random molecular motion. While these two processes are different in nature, they are in fact completely inseparable because they occur simultaneously. The process of hydrodynamic dispersion is illustrated in Fig. 2.

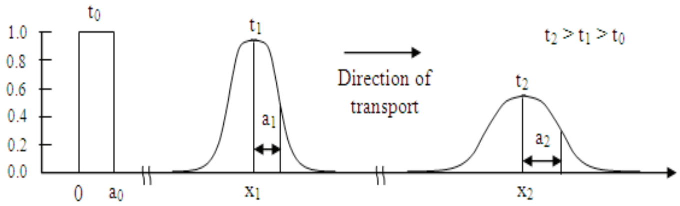

Fig. 2. Spreading of a solute slug with time due to convection and dispersion [4].

The CDE was developed to predict the average concentration of a tracer solute transported in a porous media [5]. It can include adsorption, degradation, and chemical transformation. The CDE for a conservative solute can be expressed in mathematical form as:

$$R\frac{\partial C}{\partial t} = D_h\frac{\partial^2 C}{\partial^2 x} - V_{pore}\frac{\partial C}{\partial x} \quad (1)$$

where the variables t and x represent time and the spatial direction coordinates of the flow, respectively. R is the retardation factor (R = 1 means no interaction between the solute and the solid matrix in porous media), C is the solute concentration (mg/l), V_{pore} is the pore water velocity (m/s), and D_h is the coefficient of hydrodynamic dispersion (m^2/s) in the longitudinal direction (i.e. along the x-flow direction). Analytical solutions to the CDE have been developed for a number of specific initial and boundary conditions. Solute transport parameters are estimated by matching analytical solutions to the CDE or alternative models with measured breakthrough curves (BTC) from miscible displacement experiments [6].

By analysing the solution under steady-state flow conditions in the soil column, the initial and boundary conditions for the solute concentration distribution are obtained as follows:

$$\begin{cases} C(x,0) = C_i \\ C(0,t) = C_0 \\ \frac{\partial C}{\partial t}(\infty,t) = 0 \end{cases} \quad (2)$$

Mojid, et al. [2, 3], following Wakao and Kaguei's [7] use of the Laplace transform of convolution, calculated the estimated response concentration [$C_{r.est(t)}$] at time t as:

$$C_{r.est(t)} = \int_0^\infty C_{i(\alpha)} f(t-\alpha)d\alpha \quad (3)$$

where $C_{i(\alpha)}$ is the time-dependent input concentration of the solute in the soil column, α is the time interval between two consecutive measurements of the input concentration, and f(t), the Laplace inversion of the transfer function, is the impulse response to a Dirac delta input (at t = 0) of tracer into the soil column. Equation (2) estimates a set of response concentrations from a set of input concentrations. For a reactive solute, the transfer function f(t) governed by the CDE is calculated as [7]:

$$f(t) = \frac{\left[\pi N\left(\frac{t}{\tau R}\right)^3\right]^{-1/2}}{2\tau R}\exp\left[-\left(1-\frac{t}{\tau R}\right)^2\left(4N\frac{t}{\tau R}\right)^{-1}\right] \quad (4)$$

where N is the mass-dispersion number (= D_{disp}/LV_p), which is the reciprocal of the column Peclet number P (= LV_p/D_{disp}), τ is the mean travel time or the mean residence time of the solute, and L is the distance between the positions where the input and response concentrations were measured.

$$\tau = \frac{L}{V_p} \quad (5)$$

A BTC is a graphical representation of the outflow concentration versus time during an experiment. It shows the concentration of the solute when it breaks through the outflow end [8]. The BTCs should be normalized to identify differences in the areas beneath the peak input and response positions. The mean travel time, the optimal pore velocity V_{opt}, and the optimal hydrodynamic dispersion coefficients D_{opt} are determined for each case. Then, the mean residence time τ is calculated using equation (5) and the dispersivity values λ using the equation $D_{disp} = \lambda_{disp} V_{pore}$. Finally, the column Peclet number is obtained using the equation $Pe_{col} = V_{pore}.L/D_{disp}$, and the mass-dispersion number N is estimated as $N = 1/Pe_{col}$.

Equations (4) and (5) can be used to calculate the estimated response BTCs at any time from the measured BTCs in the input time domain to determine the solute transport parameters. The root-mean-square error (RMSE) between the measured and estimated BTCs is calculated to evaluate the accuracy of fit of the transfer function method. The RMSE is obtained as follows:

$$RMSE = \sqrt{\frac{\int_0^{\infty} \left[C_{r(t)} - C_{r.est(t)}\right]^2 dt}{\int_0^{\infty} \left[C_{r(t)}\right]^2 dt}} \qquad (6)$$

where $C_{r(t)}$ is the time-dependent measured response concentration of the solute.

Method and materials

Method

The objective of this research is to investigate the hydrodynamic characteristics and transport of solutes in a porous media using a physical sand column model. A four-electrode salinity sensor was used to measure the electrical conductivity (EC) of the soil with the purpose of determining the hydraulic characteristics of water movement by conducting tracer tests on a laboratory model of a subsurface wetland. In situ, EC sensors and salinity tracers reduce the amount of time and effort required for sampling and laboratory analysis. They also prevent destructive sampling in experimental column studies. In this last setup, the measurements were taken manually. Breakthrough experiments can take days, so a low-cost data-logging system that measures continuously and automatically throughout the day and night was required. Three grain sizes of sand (coarse, medium and fine) collected from the bottom of the Mekong river in Vietnam were used in the experiments. They are useful materials for domestic wastewater treatment since they can be used to construct a subsurface flow wetland.

Materials

A physical model was made locally in Can Tho University. The model included an electrical multiplexer system connecting nine groups of four-electrode probes. This was fitted into a horizontal sand column placed in a firm stainless steel frame (Fig. 3). The framework consisted of enclosed transparent Perspex plates of 3 mm thickness covered by a removable lid. The experimental sand column was a long rectangular box with outer dimensions of 2.050 x 0.180 x 0.183 m. A 1 cm-thick polystyrene plate was placed between the lid and the sand column to ensure minimal bypass flow on top of the horizontal column. The whole system was closed watertight.

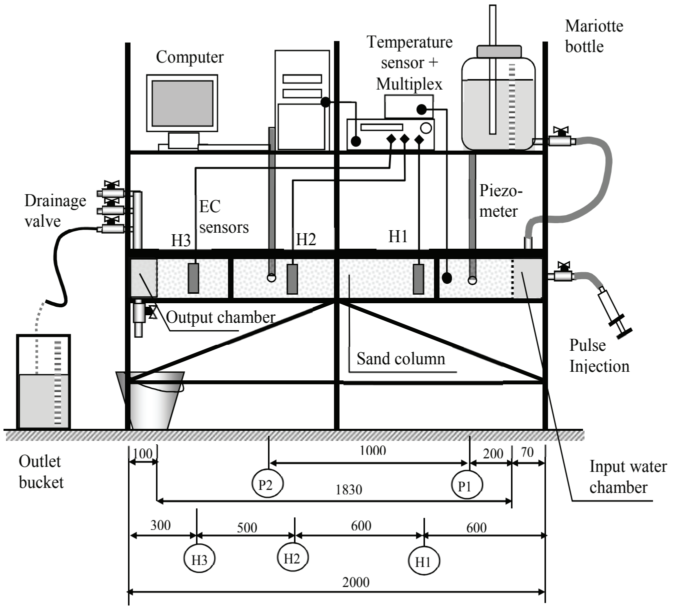

Fig. 3. Sand column system layout (H1, H2 and H3 are groups of three sensors each).

There were three chambers in the rectangular sand column: the input water chamber measuring 0.170 x 0.145 x 0.070 m; the sand column (0.170 x 0.145 x 1.830 m); and the outlet water chamber (0.170 x 0.145 x 0.100 m). The cross-section area of the sand column was 0.02465 m^2. The input water chamber received water from a 20 l Mariotte bottle. The Mariotte bottle had the function of maintaining constant water pressure and, therefore, constant flux during the experiment. The input chamber was also where the tracer solution was injected. Three groups of three four-electrode sensors were installed and connected to the multiplexer, as shown in Fig. 4. The sensors were 140 mm-long stainless steel rods with an outside diameter of 3 mm. The rods were inserted perpendicularly into the plastic block leaving 8 mm between each rod. The plastic blocks were fastened firmly outside the sand column, and the rods were submerged in the sand to a depth of 137 mm, seen through the Perspex frame.

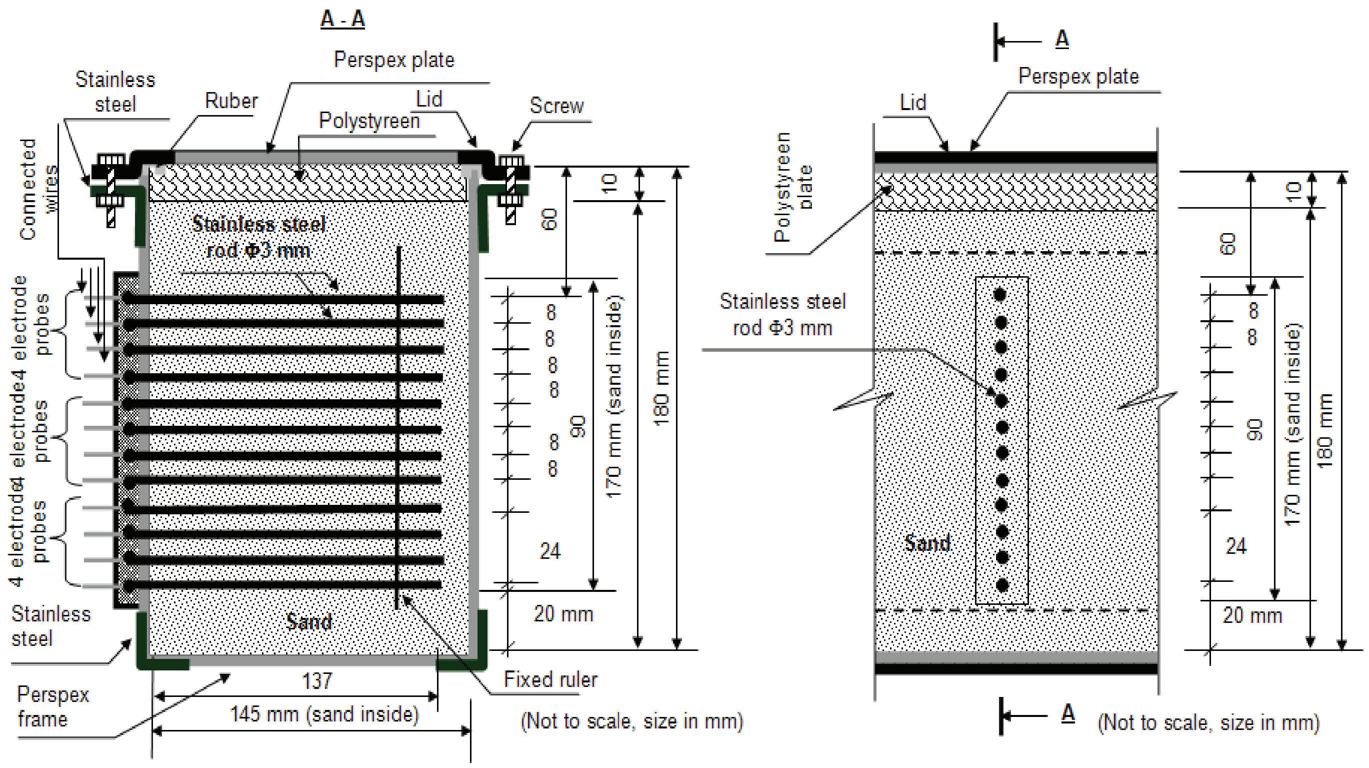

Fig. 4. One vertical group (H1, H2 or H3) of three four-electrode probes each.

The three groups of three four-rod sensors were used to monitor BTCs in the porous horizontal sand column using a saline trace. All sensors were connected to a locally made multiplexing system and a computer. The nine sensors were coded as follows: H1V1, H1V2, H1V3 for group H1; H2V1, H2V2, H2V3 for group H2; and H3V1, H3V2, H3V3 for group H3. H1, H2, and H3 were at a horizontal distance of 53 cm, 113 cm, and 613 cm, respectively, from the start of the sand column. V1, V2 and V3 were 5.6 cm, 4.4 cm, and 3.2 cm, respectively, from the bottom of the sand column. In addition, a thermal sensor was installed and connected to the computer. The codes and distances between the sensor groups are presented in Fig. 5.

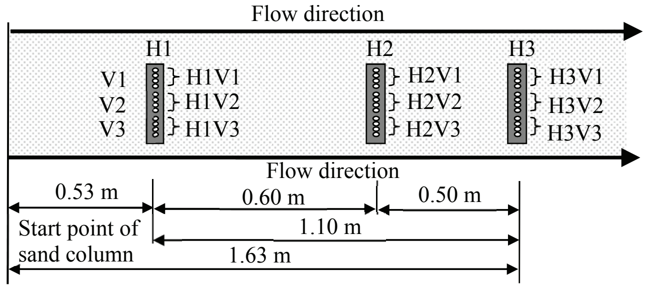

Fig. 5. Distances and coding for groups of sensors.

For each sensor measurement, three values were measured: the current was measured through electrodes 1 and 4; the voltage was measured between electrode 2 and 3, and the temperature was taken. The current through electrodes 1 and 4 was measured by reading the voltage drop over a known resistance R_{cs}. An alternating current (AC) was used, which required amplification and conversion to a direct current (DC), as most data acquisition cards require DC. A type K thermocouple was inserted to measure the temperature.

In order to collect and store data automatically, a measuring system was designed using a commercial personal computer with a data acquisition card. The graphical user interface was developed using the computational language MATLAB and the SIMULINK tool. A cost-effective data acquisition card, HUMUSOFT AD512, with a driver for extended real-time tool box software [9] was installed in a personal computer. The card had eight analogue input channels, two analogue output channels with 12-bit resolution and up to 100 Ks per second data access velocity, which is sufficient for this measurement. In addition, there were eight digital outputs and eight digital inputs which were useful for logical control, as shown Fig. 6.

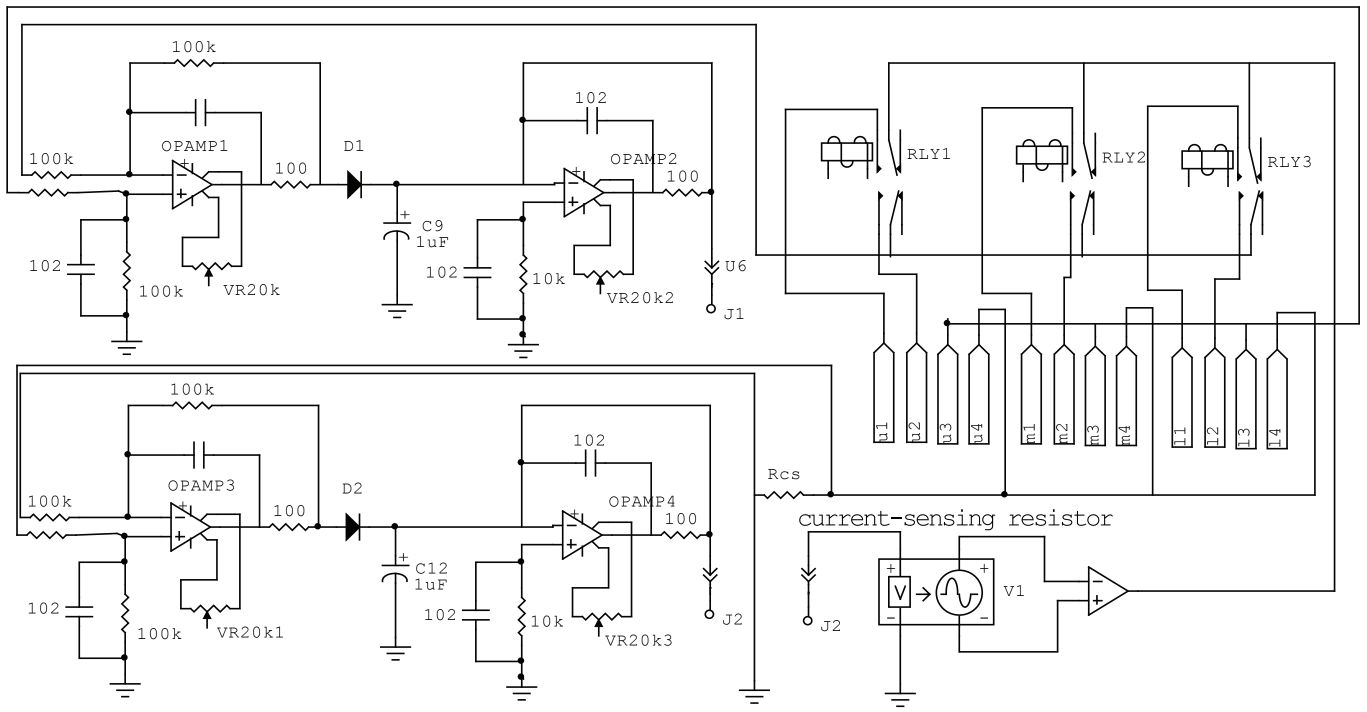

Fig. 6. The signal conditioning circuit for measuring V_{drop} and V_{2-3}.

At a set time interval, the measurement system collected the data at each of the 4-electrode sensors and stored them on the hard drive. Since only one sensor was operated at a time, the multiplexer switched between sensors. The switching circuit was crucial in this design. The ratio of the electric current (I) between the outer electrodes to the voltage difference (V_{drop}) between the two inner electrodes was calculated. The ratio I/V_{drop} was defined as the voltage drop F. First, the different AC frequencies were tested, and it was confirmed that any frequency between 100 and 1,000 Hz was suitable. A constant frequency of 220 Hz was selected. In these experiments, the R_{cs} was 15.8 Ohm. The voltage difference V/V_{drop} was automatically measured using a digital voltmeter. The geometrical factor K_e between the output value V/V_{drop} and the bulk EC depends on the shape and construction of the sensor. The value was calibrated based on the measurements of a laboratory EC meter in water solutions with a prepared concentration and at a known reference temperature, and the F values were measured by the sensor system. The multiplexer recorded EC values in sequence. It began with the sensor H1V1 and switched after 60 seconds to the next sensor, continuing to H1V2, H1V3… until H3V3, after which it returned to H1V1 (Fig. 7). With nine sensor groups, the entire cycle required 540 seconds. The electrical system was designed to record EC values in sequence and display them on a computer monitor.

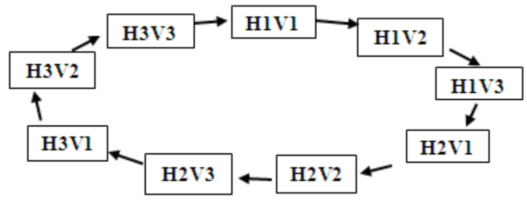

Fig. 7. Sensor group measurement turnover.

A program developed in the R programming language was used to calculate the solute transport parameters, and the Monte Carlo method was used for the analysis. In the R program, the user can define the random sampling number of the set of transport parameters, i.e. V_{pore} and D_{opt}. The optimised V_{pore} and D_{disp} are expressed as V_{opt} and D_{opt}, respectively. They are determined by searching for the minimal RMSE value in equation (6). In this case, 10,000 sets of (V_{pore}, D_{disp}) were generated randomly within a sample range of $\left(V_{opt}/5, V_{opt}\times 5\right)$ for V_{opt} and $\left(D_{opt}/5, D_{opt}\times 5\right)$ for D_{opt}. The squared correlation coefficient R^2 was determined for each set. Values of $R^2 > 0.5$ were plotted, and the highest R^2 value was identified as the optimized (V_{pore}, D_{disp}).

Results and discussion

The regression equations and the correlation coefficients (R-square) between the ratios of the measured current to the measured voltage drop (F) over the sensor with the EC measured using an Orion EC-meter (σ_M) are presented in Table 1.

Table 1. Regression equations and R^2 values of F (mA/mV) and σ_M (dS/m).

Sensor groups	Regression equations	R^2
H1V1	$\sigma_M = 13.015F + 0.1557$	0.9930
H1V2	$\sigma_M = 11.453F + 0.2004$	0.9985
H1V3	$\sigma_M = 12.258F + 0.2175$	0.9942
H2V1	$\sigma_M = 12.179F + 0.2116$	0.9970
H2V2	$\sigma_M = 14.400F + 0.0533$	0.9724
H2V3	$\sigma_M = 12.047F + 0.2140$	0.9915
H3V1	$\sigma_M = 11.917F + 0.1799$	0.9940
H3V2	$\sigma_M = 13.010F + 0.2071$	0.9928
H3V3	$\sigma_M = 13.521F + 0.2025$	0.9982

Three kinds of sand, coded as S1, S2 and S3, were used for the sand column experiments. Table 2 shows the sand sieve results and their average porosity. The values of 50% and 10% smaller (d_{50} and d_{10}) were determined by interpolation.

Table 2. Sand sieve analysis.

Sieve size (mm)	% smaller		
	Sand S1	*Sand S2*	*Sand S3*
4.000	99.290	98.096	100.000
2.000	98.300	93.205	99.975
1.000	95.662	75.896	99.873
0.500	74.967	40.873	88.005
0.250	7.895	9.716	53.003
0.125	1.039	1.955	0.923
0.075	0.409	0.662	0.840
Pan	0.079	0.000	0.000
d_{50} (mm)	0.407	0.573	0.242
Sand classification	Medium	Coarse	Fine
d_{10} (mm)	0.258	0.252	0.147
d_{60} (mm)	0.444	0.773	0.299
d_{60}/d_{10}	1.723	3.060	2.074
Uniformity	Uniform	Uniform	Uniform
Average porosity n (%)	46.3	49.7	45.7

For each tracer experiment using a particular sand class, the volumetric flow rate was changed. Each experiment was coded with the general identifier QiSj, with i (i = 1, 2, 3, 4) representing the flow rates which varies across sand classes j (j = 1 for medium sand, j = 2 for coarse sand, and j = 3 for fine sand). Table 3 summarises the flow rates corresponding to the three different sand types.

Table 3. Flow rates (m^3/s) in the sand column experiments.

	S1 (Medium)	S2 (Coarse)	S3 (Fine)
Q1	2.383×10^{-7}	4.383×10^{-7}	3.933×10^{-7}
Q2	3.400×10^{-7}	6.900×10^{-7}	4.483×10^{-7}
Q3	4.383×10^{-7}	7.250×10^{-7}	4.933×10^{-7}
Q4		7.933×10^{-7}	

Considering that the flows are through a finite area, the soil fluxes in sand column experiments are calculated. When the flow is laminar, Darcy's law is valid. Therefore, the Reynolds number is calculated using the mean grain diameter d_{50}. The water temperatures in the experiments are between 25 and 27°C and the density of the solute varies a little with the tracer concentration. However, to simplify the calculation of the Re number, it is assumed that the density of the solute is approximately that of clean water. If $Re < 10$, the saturated hydraulic conductivity K_s for each experiment is determined. Table 4 summarises the results for Re and K_s.

Table 4. Reynolds number and the saturated hydraulic conductivity.

QiSj	Q (m^3/s)	J_w (m/s)	Re	$-(\Delta h/l)$	K_s (m/s)
Q1S1	2.383E-07	9.649E-06	4.408E-03	0.018	5.371E-04
Q2S1	3.400E-07	1.377E-05	6.288E-03	0.021	6.568E-04
Q3S1	4.383E-07	1.775E-05	8.107E-03	0.025	7.113E-04
Q1S2	4.383E-07	1.775E-05	1.142E-02	0.014	1.270E-03
Q2S2	6.900E-07	2.794E-05	1.798E-02	0.021	1.333E-03
Q3S2	7.250E-07	2.935E-05	1.889E-02	0.022	1.337E-03
Q4S2	7.933E-07	3.212E-05	2.067E-02	0.023	1.399E-03
Q1S3	3.933E-07	1.592E-05	4.337E-03	0.021	7.598E-04
Q2S3	4.483E-07	1.856E-05	5.054E-03	0.023	8.084E-04
Q3S3	4.933E-07	1.997E-05	5.440E-03	0.024	8.339E-04

The results in Table 4 show that the Reynolds numbers are below 10, so all the flows in the experiments were laminar, and Darcy's law can be applied to calculate the saturated hydraulic conductivity K_s. If there is no flow ($Q = 0$ m^3/s) in the sand column, the ($\Delta h/l$) should be zero. The trend lines of water flux versus hydraulic gradient have to go through the zero point, as shown in Fig. 8.

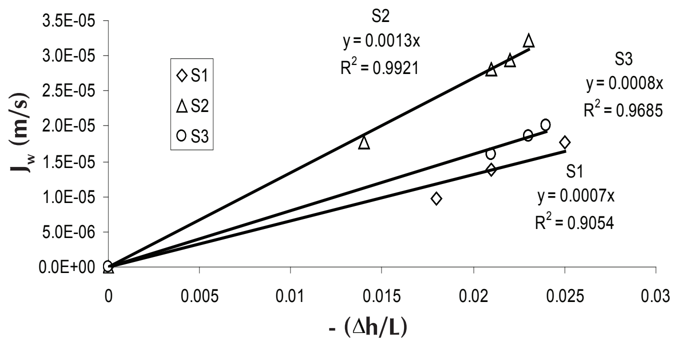

Fig. 8. Water flux versus hydraulic gradient.

The saturated hydraulic conductivity K_s should be constant for each sand class. The standard deviations of the calculated K_s were very small, lower than 5%. Fig. 9 shows the trend lines of the water flux versus the saturated hydraulic conductivity. The slopes of these lines are very small, so the values of K_s can be accepted as having the same order of magnitude.

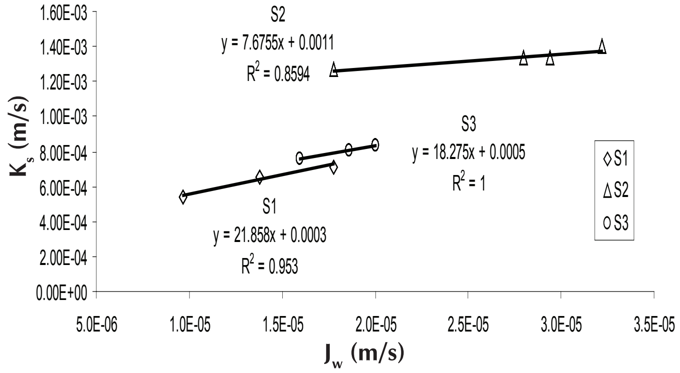

Fig. 9. Water flux versus the saturated hydraulic conductivity.

Figure 10 shows two examples of BTCs measured in the experiments and the normalised BTCs. Based on the results of the transfer function method, the solute transport parameters, which are average residence time (or breakthrough time) τ, dispersivity λ, the column Peclet number Pe_{col} and mass dispersion number N, were estimated for each transport case. The average residence time decreased with as the water pore velocity increased. This can be seen in Fig. 11, which shows results of the transport from sensor H1V3 to sensor H3V3 for each sand type.

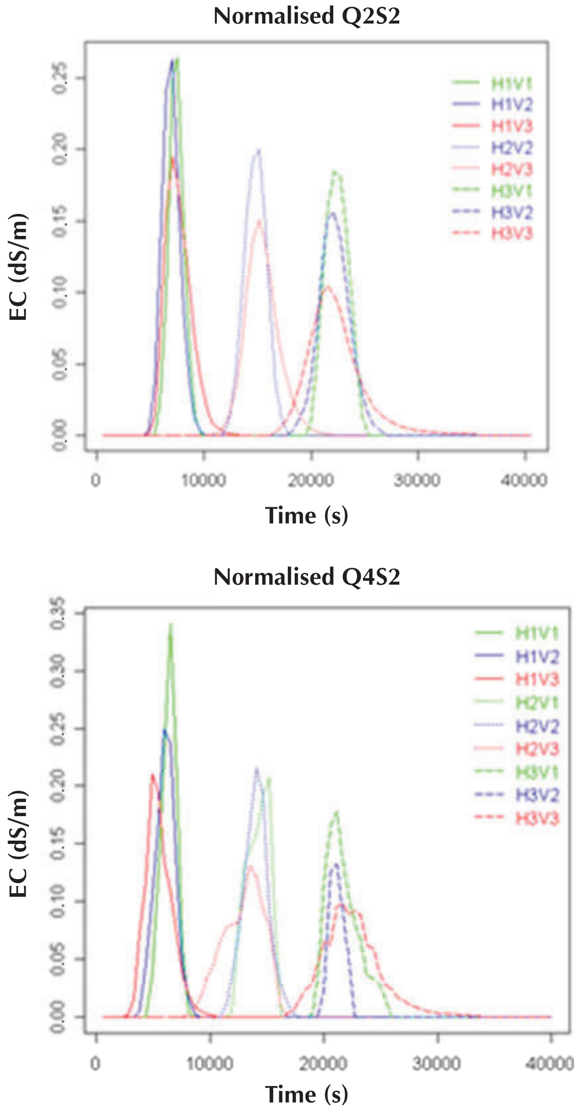

Fig. 10. Normalised BTCs plotted at location Q2S2 and Q4S2.

Based on the results of the transfer function method, the solute transport parameters, i.e. the average residence time (or breakthrough time) τ, dispersivity λ, the column Peclet number Pe_{col}, and the mass dispersion number N were estimated for each transport cases of the transport. Table 5 shows the estimated solution transport parameters.

The Monte Carlo method is used to identify the sensitivity of the parameters. The sensitivity analysis evaluates the interactions between the model parameters, i.e. the impact of changes in inputs on the outputs. The dotty plots show clearly the optimal point for the (V_{pore}, D_{disp}) set of estimated

Table 5. Estimated solution transport parameters.

Sand type	Flow rate	Optimal pore velocity	Optimal dispers coefficient	Residence time	Dispersivity	Column Pe number	Mass disp. number
	Q (m³/s)	V_{opt} (m/s)	D_{opt} (m²/s)	τ (hr)	λ (m)	Pe	N
S1	2.383E-07	2.434E-05	1.217E-07	12.554	5.000E-03	2.200E+02	4.545E-03
	3.400E-07	3.779E-05	1.868E-07	8.086	4.943E-03	2.225E+02	4.494E-03
	4.383E-07	3.430E-05	1.362E-07	8.908	3.971E-03	2.770E+02	3.610E-03
S2	4.383E-07	4.202E-05	5.543E-07	7.272	1.319E-02	8.339E+01	1.199E-02
	6.900E-07	6.542E-05	4.750E-07	4.671	7.261E-03	1.515E+02	6.601E-03
	7.250E-07	7.753E-05	6.569E-07	3.941	8.473E-03	1.298E+02	7.703E-03
	7.933E-07	7.633E-05	6.373E-07	4.003	8.349E-03	1.317E+02	7.590E-03
S3	3.933E-07	4.123E-05	1.005E-07	7.411	2.438E-03	4.513E+02	2.216E-03
	4.583E-07	5.705E-05	1.487E-07	5.356	2.606E-03	4.220E+02	2.370E-03
	4.933E-07	5.185E-05	8.608E-08	5.893	1.660E-03	6.626E+02	1.509E-03

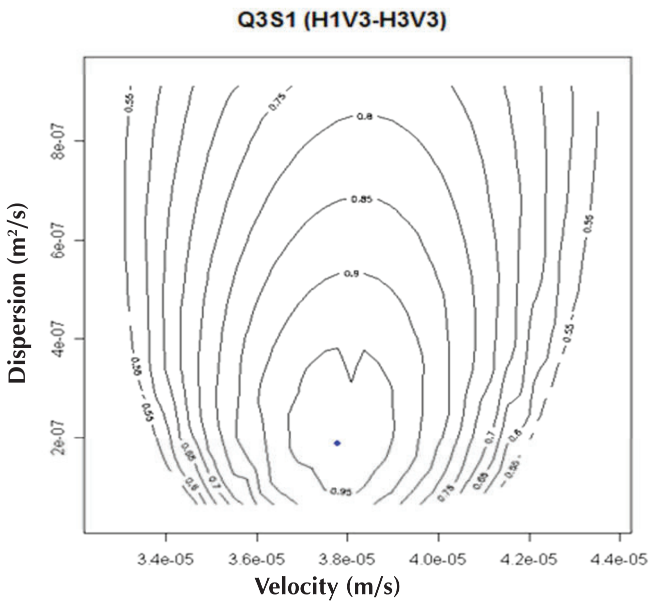

Fig. 11. Contour lines for optimal (V_{pore}, D_{disp}).

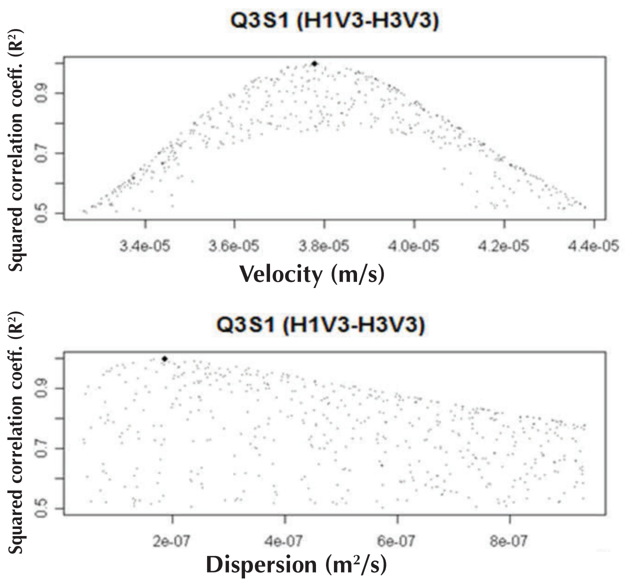

Fig. 12. Dotty plots (.) and highest values (•) of R^2 for optimal V_{pore} and D_{disp}.

transport parameters for the CDE. As an example, Fig. 11 and Fig. 12 illustrates the sensitivity analysis for the case Q3S1 (H1V3 - H3V3) with medium sand and water flux of 1.778E-05 m/s. These two plots represent the response surface between the two parameters V_{pore} and D_{disp}.

Conclusions

This research uses theories on the transport mechanism of a solute in a porous medium. The experiments were performed using sand from the Mekong river. The results were the optimal water pore velocities and the optimal dispersion for three types of sand.

Four-electrode probes were successfully constructed, calibrated and operated using a multiplexing system. The multiplexing system enabled the EC at different locations in the sand column to be continuously monitored. The system was made locally at a low cost and worked well for testing a tracer flowing through a saturated horizontal sand column.

The concentration values of the tracer flowing through the horizontal sand column were measured using a series of sensors and were plotted in the form of BTCs. In each experiment, laminar flow was concluded from the calculated Reynolds number. Laminar flow is necessary for Darcy's law, from which the saturated hydraulic conductivity was calculated. For the experiments within the same sand class, the values of the saturated hydraulic conductivity had the same order of magnitude. From these curves, the pore water velocity and the mechanical dispersion coefficient were determined using the transfer function method. From these variables, the average residence time, the dispersivity, the column Peclet number and the mass-dispersion number were calculated.

It is possible to conclude that the continuous movement of a solute through sand is governed by the CDE, which is a second-order differential equation. The convection-dispersion equation for inert and non-adsorbing solutes is estimated using measured BTCs and normalised BTCs. The solute transports are identified as mixed-flow processes rather than plug-flow processes. The sensitivity analysis shows that the CDE is highly sensitive to the dispersion parameter.

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The authors declare that there is no conflict of interest regarding the publication of this article.

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