13th Mediterranean Congress of Chemical Engineering
Barcelona, Spain, September 30-October 3, 2014
13MCCE
Universitat d'Alacant
Universidad de Alicante

APPLICATION OF THE DISPERSION MODEL AND COMPARISON WITH HYDRODYNAMIC PARAMETERS IN POROUS MEDIA COLUMN

Boluda-Botella, N., García Cortés, A.N., Cenador Marín, I., Hernández Teruel, M.J. and Acevedo Sempere, M.
Chemical Engineering Department, University of Alicante, Apdo. 99, E-03080 Alicante, Spain. Tel.+34 965903400. Fax:+34 965903826.
E-mail: nuria.boluda@ua.es, Angela.Garcia@ua.es, mjht1@alu.ua.es, icm30@alu.ua.es, mcas3@alu.ua.es

INTRODUCTION

Reactive transport experiments carried out in columns filled with different porous media (aquifer sediment and soil-sea sand mixtures) and injection of seawater or calcium chloride showed differences between tracer breakthrough curves (BTC) used to calculate the column hydrodynamic parameters[1] [2].

These research experiments in columns filled with glass beads were carried out with the main goal to study transport and dispersion processes in inert homogeneous media.

The column hydrodynamic characteristics were determined with the program ACUAINTRUSION TRANSPORT[3], designed by the Chemical Engineering Department of the University of Alicante.

On the other hand, the estimation of the dispersion module was performed using different approximations, depending on the dispersion degree and the tracer injection mode (pulse or step) in the column, as shown in Levenspiel[4]. Different results are obtained in this research to obtain the best approximation to ACUAINTRUSION TRANSPORT parameters.

MATERIALS AND METHODS

The experimental set-up consisted of a column connected to a pump injecting continuously a tracer that displaced resident deionized water. A conductivity detector recorded changes in outlet flow conductivity (Figure 1).

Column: Cylindrical stainless steel column (22.4 cm in length and 2.5 cm internal diameter).
Column fill: glass beads (2mm).
Pump: HPLC pump (Shimadzu LC 9A).
Conductivity detector: LS-3300, connected to PC for data acquisition every minute.
Fraction collector: Frac-100 Pharmacia Biotech.
Flow (upward): 0.5 mL/min
Tracer concentration: 0.04 M $CaCl_2$

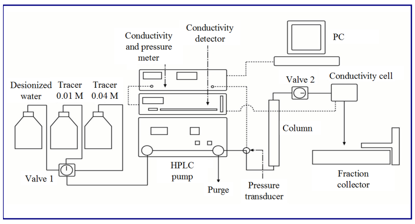

Figure 1. General scheme of the experimental set-up.

The experimental data used to obtain the tracer breakthrough curve (BTC) were dimensionless conductivity versus time, as shown in the next section. These data as well as flow, length and column diameter were introduced into ACUAINTRUSION TRANSPORT in order to calculate the parameters: Darcy velocity (u), interstitial water velocity (v), mean residence time (t_m= L/v), column Péclet number (Pe=vL/D_L), effective porosity (ε), longitudinal dispersion coefficient (D_L) and dispersivity (α=L/Pe).

The software fits the experimental data using the analytical solution of the convection-dispersion equation[5] and minimizes the mean square deviation between the experimental and calculated projections. Calculated hydrodynamic column parameters are shown in the following section.

The dispersion model[4] in the case of an ideal pulse with a low dispersion degree (D/uL <0.01) produces a symmetric curve represented by the following equation:

$$C = \frac{1}{2\sqrt{\pi\left(\frac{D}{uL}\right)}}\exp\left[-\frac{(1-\theta)^2}{4\left(\frac{D}{uL}\right)}\right]$$

Equation (1)

Where C is concentration and θ is dimensionless time (t/t_m). Dispersion module of the recipient is (D/uL).

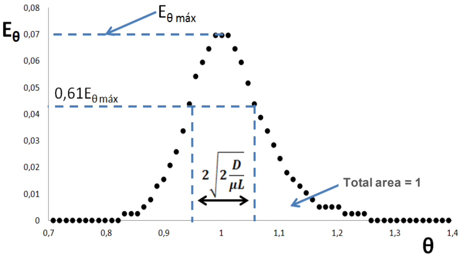

Figure 2. Relation between dimensionless conductivity change and dimensionless time (t/t_m).

The curve in Figure 2 was directly calculated from experimental step BTC, through the partial derivative of the dimensionless conductivity (E_θ) with respect to the dimensionless time (θ).

$$E_\theta = \frac{\Delta(C - C_0)}{\sum\Delta(C - C_0)}$$

Equation (2)

$$\theta = \frac{t}{t_m}$$

Equation (3)

According to Levenspiel[4], two different approximations can be used to determine the dispersion module from the calculated curve in Figure 2:

(1) Maximal E_θ height
(2) Variance (σ), half width of the pulse at an height of 0.61 $E_{\theta max}$

Experimental step BTC was obtained from the experimental cumulative dimensionless conductivity data. The theoretical one was calculated by obtaining the cumulative dimensionless conductivity data from Equation (1). A worksheet was developed to obtain conductivity data (equivalent to concentration) vs dimensionless time according to Equation 1.

The cumulative conductivity data were obtained by addition of values:

$$C_{cumulative,\,\theta} = C_{cumulative,\theta-\Delta\theta} + C_\theta$$

These data were normalized to obtain the theoretical step BTC:

$$C_{cumulative\ dimensionless,\,\theta} = C_{cumulative,\theta} / (C_{cumulative,\theta})_{max}$$

The values of t_m and D/vL were optimized by minimizing differences between experimental and calculated dimensionless conductivity using the Solver function.

RESULTS

Table 1. Hydrodynamic column parameters obtained by ACUAINTRUSION TRANSPORT software.

u (cm/h)	t_m (h)	Pe= vL/D	ε	v (cm/h)	D_L (cm²/h)	α (mm)
6.11	1.51	428	0.41	14.9	0.78	0.52

The dispersion module obtained following Levenspiel approximations are: 1.53x10^{-3} for variance calculations and 1.09x10^{-4} for maximal E_θ height. In the case of the optimization method explained in previous section, the results are according with ACUAINTRUSION TRANSPORT parameters, as shown in Table 2.

It must be taken into account that dispersion module using the software was obtained considering interstitial water velocity (v) and longitudinal dispersion (D_L).

Table 2. Comparison of the parameters obtained from ACUAINTRUSION and optimization

	ACUAINTRUSION T.	Optimization
D_L/v·L	2.34 x10^{-3}	2.34 x10^{-3}
t_m (s)	5420	5452

The error between parameter values obtained from both methods is very low (nil in the case of dispersion module and 0.6% for the mean residence time). The good agreement between BTCs can be seen in Figure 3.

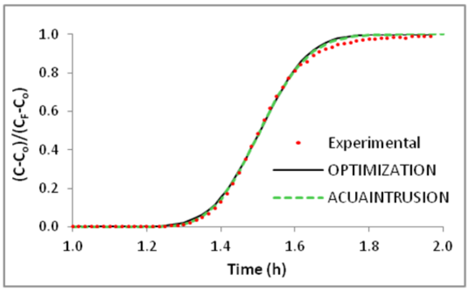

Figure 3. Experimental BTC and modelled by optimization of equation (1) and calculated with ACUAINTRUSION TRANSPORT.

CONCLUSIONS

The program ACUAINTRUSION TRANSPORT exhibited a good fit to data (BTCs) acquired in column experiments in glass beads media. The calculated column hydrodynamic parameters are completely reliable, as it was demonstrated in previous papers.

The conversion of step curve to pulse allows to calculate the dispersion module from Levenspiel's dispersion model for symmetric curves and low dispersion degrees. The results constitute a rough calculation to the study of dispersion processes in porous media columns.

The optimization carried out in the worksheet to estimate the dispersion module by minimizing difference between experimental and calculated accumulative dimensionless conductivity using Equation (1) showed a good agreement with the values obtained in ACUAINTRUSION TRANSPORT.

REFERENCES

[1] Boluda-Botella, N.; León, V.M.; Cases, V.; Gomis, V.; Prats, D. 2010. Fate of Linear Alkylbenzene Sulfonate in agricultural soil columns during inflow of surfactant pulses. J. Hydrol, 395, 141-152.
[2] Boluda Botella, N., Gomis Yagües, V. and Ruiz Beviá, F. 2008. Influence of the transport parameters and chemical properties of the sediment in experiments to measure reactive transport in seawater intrusion. J. Hydrol, 357, 29-41.
[3] Departamento de Ingeniería Química. Universidad de Alicante. 2007. ACUAINTRUSION TRANSPORT. Available in http://hdl.handle.net/10045/2691.
[4] Levenspiel, O. 2009. Ingeniería de las reacciones químicas. 3ª ed. Limusa Wiley, 670 pp.
[5] Lapidus, L. and Amundson, N.R. 1952. Mathematics of adsorption in beds. VI. The effect of longitudinal diffusion in ion-exchange and chromatographic columns. J. Phys. Chem. 56 (8), 984-988.