

Experimental Determination of Hydrodynamic Dispersion Coefficients for Modelling of Fixed-bed Biosorption

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The aim of this work was to determine the hydrodynamic dispersion coefficient at different interstitial velocities for its application in a mass transport model to predict heavy metal biosorption onto *Posidonia oceanica* and peat. Tracing experiments with lithium chloride (LiCl) were performed in biosorbent packed beds of 10 and 27 cm length and flow rates between 10 and 100 cm³ h⁻¹. Hydrodynamic dispersion coefficients were obtained by solving the mass balance equation for one-dimensional transport in the axial direction. Potential equations relating dispersion coefficient and interstitial velocity were obtained for both biosorbents, which were successfully coupled to a mass transport model to simulate the breakthrough curves for the sorption of copper onto *Posidonia oceanica* and peat at several flow rates.

1. Introduction

Fixed-bed column is the most effective configuration for operations such as adsorption and ion exchange, so it is widely used in the chemical industry. The performance of this kind of systems depends on the combined effects of thermodynamic and rate factors. Rate factors, that include mass-transfer limitations, reaction kinetic limitations, and hydrodynamic dispersion, determine the efficiency of the real process. In fixed beds, axial mixing is often described in terms of the axial dispersion coefficient that accounts for molecular diffusion, convective mixing and nonuniformities in the fluid velocity across the fixed bed (LeVan et al., 1997).

The main objective of this work was to obtain a relationship between the interstitial velocity and the axial dispersion coefficient in fixed-bed columns of two biosorbents, *Posidonia oceanica* and peat, by a tracing method. In order to check the feasibility of this relationship, it was coupled with a mass transport model that assumes rate control by the intraparticle mass transfer to simulate the breakthrough curves for the sorption of copper onto both biosorbents at several flow rates.

2. Experimental

Tracing experiments were carried out in Pyrex glass columns of 1.0 cm inner diameter. Two biosorbent fixed-bed lengths were used (10 and 27 cm). The system was operated in the up flow mode, using lithium chloride (LiCl) as the tracer, which has been shown as a reliable tracer (Inglezakis et al., 2001). Effluent conductivity measurements were used for monitoring the operation and to obtain tracer breakthrough curves. These experiments were carried out with different flow rates ranging between 10 to 100 cm³ h⁻¹.

Continuous biosorption experiments were performed in the same columns. Several experiments were carried out with an inlet copper concentration of 20 mg dm⁻³ and flow rates of 20, 40 and 80 cm³ h⁻¹, using *Posidonia oceanica* and peat as biosorbents with bed lengths around 10 cm.

Effluent samples were periodically collected. Copper concentration was measured by Atomic Absorption Spectrometry.

3. Results and discussion

3.1 Tracing experiments

In order to estimate the hydrodynamic dispersion coefficient, the mass transport equation assuming no chemical reaction was solved for the tracing experiments. Thus, the convection-dispersion equation for one-dimensional transport in the axial direction with a steady-state flow was applied.

For each experiment, the hydrodynamic dispersion coefficient was estimated by minimizing the relative error between predicted and experimental data.

As an example, Figure 1 shows the predicted curves together with the experimental data, as normalized effluent conductivity (K/K_0) versus operation time for the 27 cm bed length. The simulated breakthrough curves fit the experimental data properly with a relative error between 3.0% and 6.0%.

The hydrodynamic dispersion coefficients for *Posidonia oceanica* fixed bed resulted in values from 0.13×10^{-6} to 4.50×10^{-6} m² s⁻¹ for interstitial velocities between 0.40×10^{-4} and 3.79×10^{-4} m s⁻¹. For the peat bed, the values were from 5.00×10^{-8} to 2.95×10^{-6} m² s⁻¹ for interstitial velocities between 0.56×10^{-4} and 5.03×10^{-4} m s⁻¹. Potential equations were obtained to describe the relationship between liquid velocity and dispersion coefficient for both biosorbent as it has been previously reported by other authors (Yoshida and Takemori, 1997; Inglezakis and Pouloupoulos, 2005):

$$D = \alpha u_i^\beta \quad (1)$$

Table 1 summarizes the values of the parameters of equation (1) together with the correlation coefficients for both biosorbents.

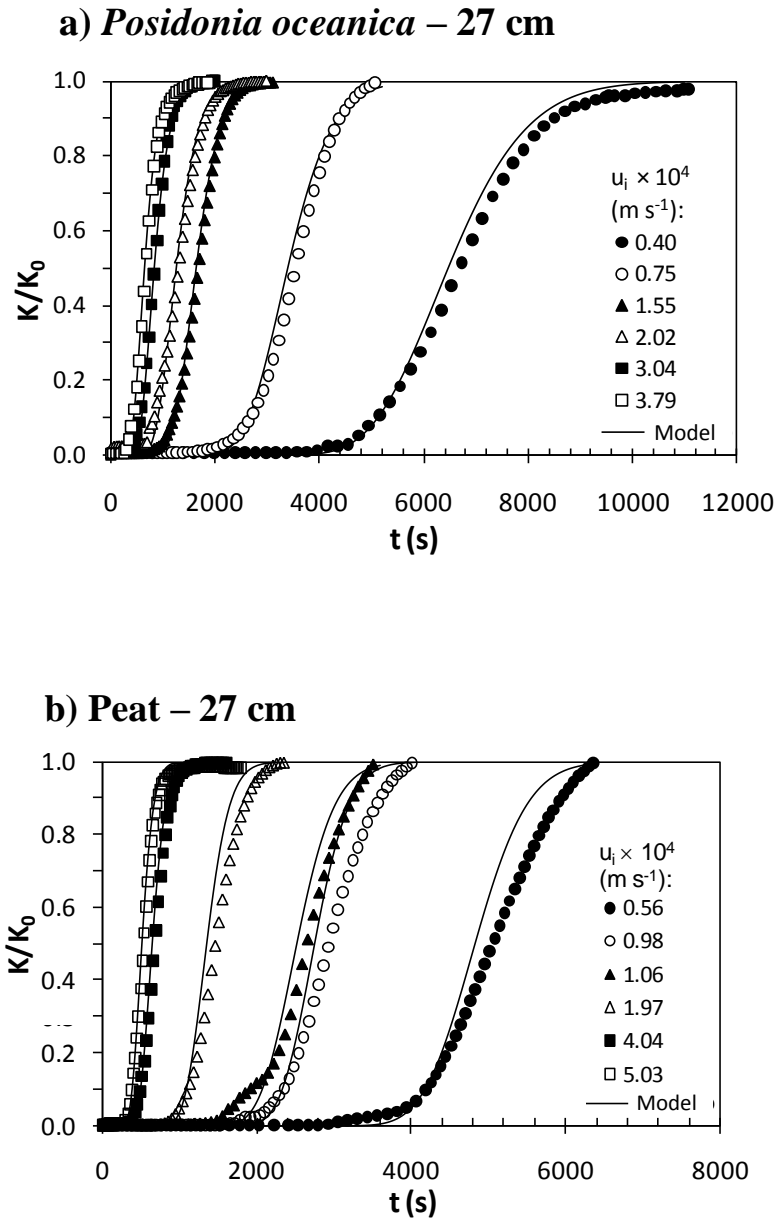


Figure 1: Breakthrough curves of tracing experiments at different interstitial velocities (u_i) with a bed length of 27 cm for a) *Posidonia oceanica* and b) peat

Table 1 Parameters of the potential equation that relates the hydrodynamic dispersion coefficient (D) with the interstitial velocity (u_i) for *Posidonia oceanica* and peat.

Biosorbent	α	β	R^2
<i>Posidonia oceanica</i>	0.404 ± 0.223	1.476 ± 0.062	0.984
Turba	3.311 ± 3.011	1.827 ± 0.105	0.971

3.2 Copper sorption experiments and modelling

As a result of copper sorption experiments, breakthrough curves were obtained and were depicted as normalized effluent copper concentration (C/C_0) versus time. Biosorption breakthrough curves presented the typical S-shape, with early breakthrough and tailing, revealing non-ideal transport.

Both biosorbents presented high retention capacity without detecting copper in the effluent for a long period.

The performance for copper removal was remarkable with an average copper sorption capacity of 55 mg g^{-1} for *Posidonia oceanica* and 45 mg g^{-1} for peat.

A mass transport model has been developed to predict column performance for copper biosorption. The model assumes one-dimensional convective-dispersive transport and rate controlled biosorption.

Intraparticle mass transfer is assumed to be the rate limiting step and it is described by a linear driving force approximation, considering that the most important transport resistance lies in the solid phase rather than in the liquid phase. Biosorption equilibrium is represented by Langmuir isotherms which were previously determined for *Posidonia oceanica* (Izquierdo et al., 2010a) and peat (Izquierdo et al., 2010b) in fixed bed experiments.

The dispersion coefficient was evaluated from the experimental relationship obtained in the tracing experiments (Table 1).

The model was solved for the experiments performed at flow rate of $40 \text{ cm}^3 \text{ h}^{-1}$ and the mass transport coefficient was estimated by minimizing the relative error at the breakthrough point ($C/C_0 = 0.05$), which is in practice the final point for industrial applications.

Mass transfer coefficient resulted in $1.0 \times 10^{-4} \text{ s}^{-1}$ for *Posidonia oceanica* and in $1.1 \times 10^{-5} \text{ s}^{-1}$ for the peat, and it was assumed to be independent on the flow rate. As an example, model predictions for the three flow rates are shown in Figure 2 together with the experimental data for *Posidonia oceanica* experiments.

The mathematical model successfully predicts the breakthrough point and reproduces the shape of the experimental breakthrough curve.

Relative error in the prediction of the breakthrough point resulted in values between 0.9 % and 3.3 %; the total mass balance was predicted with deviations between 5.5 % and 9.5 %.

Similar results were obtained using peat as biosorbent.

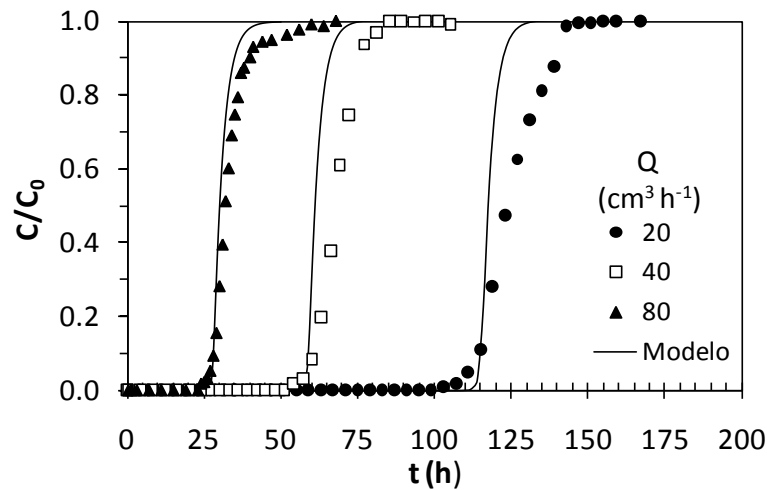


Figure 2: Experimental and simulated breakthrough curves of copper sorption experiments at different flow rates (Q) with copper concentration of 20 mg dm^{-3} and *Posidonia oceanica* as biosorbent

4. Conclusions

A tracing method was applied for the determination of the experimental dispersion coefficient of *Posidonia oceanica* and peat fixed beds. A potential equation which relates the dispersion coefficient and the liquid interstitial velocity was obtained for each sorbent.

These potential equations were coupled successfully with a mass transport model in order to predict the experimental breakthrough curves in sorption experiments performed at different flow rates; the simulated curves accurately predict the breakthrough point and the shape of the curve.

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