Pré-Publicações do Departamento de Matemática
Universidade de Coimbra
Preprint Number 04–15

APPLICATION OF THE ADVECTION-DISPERSION EQUATION TO CHARACTERIZE THE HYDRODYNAMIC REGIME IN A SUBMERGED PACKED BED REACTOR

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ABSTRACT: The hydraulic characteristics of a laboratory submerged packed bed, filled with a volcanic stone, pozzuolana, have been experimentally investigated through tracer tests. Sets of essays at flow rates from 1 to 2.5 l/h in clean conditions were performed. The results showed a considerable amount of dispersion through the filter as the hydraulic loading was changed, indicating a multiplicity of hydrodynamic states, approaching its behavior to plug flow.

An analytical solution for the advection-dispersion equation model have been developed for a semi-infinite system and we have considered an appropriate physical boundary condition. A numerical simulation using finite difference schemes is done taking into account this particular boundary condition that changes according to the flow rates. Proper formulation of boundary conditions for analysis of column displacements experiments in the laboratory is critically important to the interpretation of observed data, as well as for subsequent extrapolation of the experimental results to transport problems in the field.

KEYWORDS: advection-dispersion equation, finite differences, hydraulic loading.

1. Introduction

The experiments were carried out on a pilot scale packed bed (Fig. 1) made of tubular acrylic glass with 7 cm internal diameter, 41 cm total packing length, submerged with 3 cm of water level. The filter was filled with a homogeneous pozzuolana material with 4 mm of effective diameter and porosity of 0.52. Five ports have been used to collect samples. The flow rates were measured by a peristaltic pump.

Experiments have been performed at flow rates of 1.0, 2.0 and 2.5 l/h, at different carbon concentrations for a 33 cm packing length. These experiments will allow the studying of the hydrodynamic characteristics along the filter.

We injected 10 ml of a tracer (Blue Dextran) impulse immediately above the liquid level being the response evaluated by measuring the absorbance at 610 nm of collected samples at equal time periods.

Received May 4, 2004.

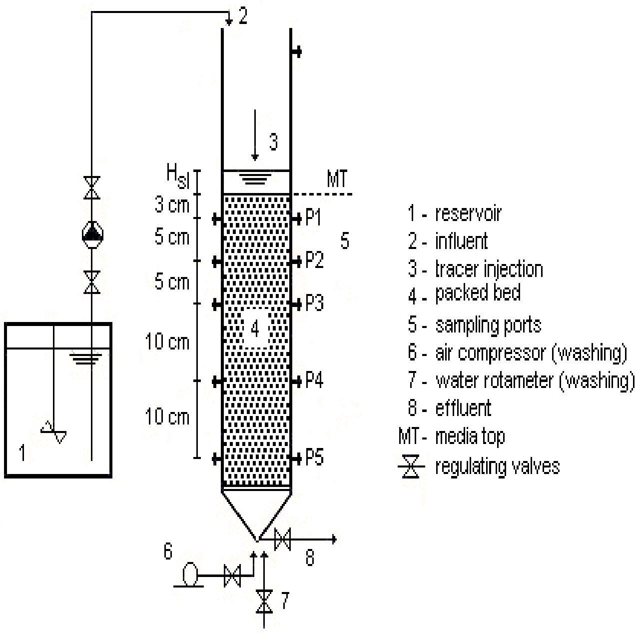


FIGURE 1. Schematic representation of the experimental apparatus

In vertical columns, especially if the ratio length/diameter is too large (Bedient et al [1]), the effects of liquid flow in the horizontal direction x is considered not important compared with the flux in the vertical direction z. In these conditions, the mechanism of advection, dispersion and exchange reaction in an isotropic and homogeneous packed bed under steady-state conditions, are generally described by the well-known advection-dispersion equation, see for instance, Ogata and Banks [5], van Genuchten and Alves [6], van Genuchten and Parker [7], Levespiel [3], Bedient et al [1],

$$R\frac{\partial C}{\partial t} + V\frac{\partial C}{\partial z} = D\frac{\partial^2 C}{\partial z^2}, \tag{1}$$

where C is the solute concentration, D is the dispersion coefficient, V is the average pore-water velocity, t is the time and z is the distance. The parameter R accounts from possible interactions between the chemical and the solid phase of the soil. Here, we consider there is no interactions between the chemical and the solid phase and therefore $R = 1$.

We consider a dimensionless parameter, called Péclet number,

$$Pe = \frac{VL}{D}, \tag{2}$$

where L is the packing length.

The Péclet number describes the relative influence of the effects caracterised by advection-dispersion problems which involve a non-dissipative component and a dissipative component. The Péclet number also determines the nature of the problem, that is, the Péclet number is low for dispersion-dominated problems and is large for advective dominated problems.

2. The model problem

Our interest is in the solution of

$$\frac{\partial C}{\partial t} + V\frac{\partial C}{\partial z} = D\frac{\partial^2 C}{\partial z^2} \tag{3}$$

for $t > 0, z \geq 0$ with an initial condition

$$C(z,0) = f(z) \tag{4}$$

and subject to the boundary conditions

$$\lim_{z\to\infty} C(z,t) = 0 \quad \text{and} \quad C(0,t) = g(t),\ t \geq 0. \tag{5}$$

The exact solution of the problem (3)-(5) can be found using Laplace Transforms in t and we will get the solution

$$\begin{aligned} C(z,t) \;=\; & \frac{1}{\sqrt{\pi}}\int_0^t g(t-\hat{\tau})G^*(z,\hat{\tau})d\hat{\tau} + \frac{1}{\sqrt{\pi}}\int_{\frac{Vt-z}{2\sqrt{Dt}}}^{+\infty} f(z - Vt + 2\sqrt{Dt}\xi)e^{-\xi^2}d\xi \\ & -\frac{1}{\sqrt{\pi}}\int_{\frac{Vt+z}{2\sqrt{Dt}}}^{+\infty} f(-z - Vt + 2\sqrt{Dt}\xi)e^{Vz/D}e^{-\xi^2}d\xi, \end{aligned} \tag{6}$$

where the function $G^*(z,\hat{\tau})$ is given by

$$G^*(z,\hat{\tau}) = \frac{z}{2\sqrt{D}\hat{\tau}^{3/2}}e^{-(z-V\hat{\tau})^2/4D\hat{\tau}}.$$

For our particular problem the initial condition is given by $f(z) = 0$ and we need to determine the boundary condition, $g(t)$, which represents the solute concentration on the inflow boundary.

We have the following physical parameters: V_{inj} denotes the volume of injected tracer; V_{sl} is the volume of the liquid on the top of the packed bed; M_0 is the mass injected; C_{sl} is the concentration of the liquid level where the tracer is absorbed before going into the packed bed through the media top and Q denotes the flow rate.

We have that

$$C_{sl} = \frac{M_s}{V_{inj} + V_{sl}} \tag{7}$$

and the physical boundary condition is given by the following exponential decay

$$g(t) = C_{sl} \mathrm{e}^{-Qt/V_{sl}}. \tag{8}$$

This condition is obtained considering that the inflow concentration is governed by the differential equation,

$$\frac{dg}{dt} = -\frac{Q}{V_{sl}} g \quad \text{with} \quad g(0) = C_{sl} \tag{9}$$

which describes the inflow decay by a rate of Q/V_{sl}.

Note that for our specific case where the initial condition is given by $C(z,0) = 0$ and the inflow is governed by (8) we have the analytical solution

$$C(z,t) = \frac{1}{\sqrt{\pi}} \int_0^t g(t-\hat{\tau}) G^*(z,\hat{\tau}) d\hat{\tau}. \tag{10}$$

3. Numerical solution using a finite difference scheme

To derive a finite difference scheme we suppose there are approximations $\mathbf{U}^n := \{U_j^n\}$ to the values $C(x_j, t_n)$ at the mesh points

$$x_j = j\Delta x, \ \ j = 0, 1, 2, \ldots .$$

If we choose a uniform space step Δx and time step Δt, there are two dimensionless quantities very important in the properties of a numerical scheme

$$\mu = \frac{D\Delta t}{(\Delta x)^2}, \qquad \nu = \frac{V\Delta t}{\Delta x}.$$

The quantity ν is usually called the Courant (or CFL) number.

We use the usual central, backward and second difference operators,

$$\Delta_0 U_j := \frac{1}{2}(U_{j+1} - U_{j-1}), \ \ \Delta_- U_j := U_j - U_{j-1}, \ \text{and} \ \delta^2 U_j := U_{j+1} - 2U_j + U_{j-1}$$

to describe the finite difference scheme.

Consider the approximation formula

$$U_j^{n+1} = [1 - \nu\Delta_0 + (\frac{1}{2}\nu^2 + \mu)\delta^2 + \nu(\frac{1}{6} - \frac{\nu^2}{6} - \mu)\delta^2\Delta_-]U_j^n. \tag{11}$$

This scheme was first proposed by Leonard [2] using control volume arguments. However, it can also be obtained using a cubic expansion by interpolating U^n_{j-2} as well as U^n_{j-1}, U^n_j and U^n_{j+1}, as we can see in Morton and Sobey [4].

The model problem we are interested in is defined on the half-line with an inflow boundary condition

$$C(0,t) = g(t), \tag{12}$$

where $g(t)$ is defined by (8). Consequently we consider

$$U^n_0 = g(n\Delta t). \tag{13}$$

The scheme (11) is a higher order scheme and it uses two points upstream. Therefore it can not be applied on the first interior point of the mesh. At this particular point we need to apply a numerical boundary condition. To determine the numerical boundary condition we use for interpolation the points U^n_0, U^n_1, U^n_2 and U^n_3 and we bring in a forward third difference instead of a backward third order difference to yield

$$U^{n+1}_1 = [1 - \nu\Delta_0 + (\frac{1}{2}\nu^2 + \mu)\delta^2 + \nu(\frac{1}{6} - \frac{\nu^2}{6} - \mu)\delta^2\Delta_+]U^n_1, \tag{14}$$

where Δ_+ is the forward operator defined by $\Delta_+ U_j := U_{j+1} - U_j$. For more information on this and other numerical boundary conditions see for instance Sousa and Sobey [8].

The use of this downwind third difference does not affect accuracy since still based on a cubic local approximation. However, it does have some penalties in terms of stability. Some more interesting discussions could be done on the right choice of the numerical boundary condition which is independent of the physical boundary condition (13).

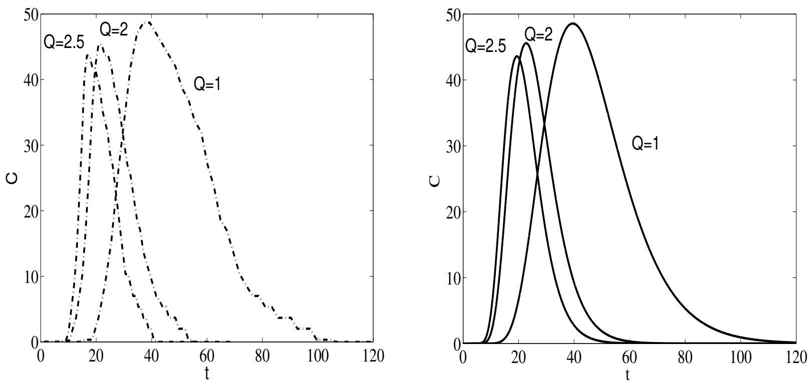
4. Numerical results versus experimental results

In this section we present the numerical results that adjust the essays for three different flow rates.

Table 1 shows the values of different parameters necessary to the evaluation of the inflow boundary condition defined by (8). We can observe that we have a different boundary condition for each flow rate Q.

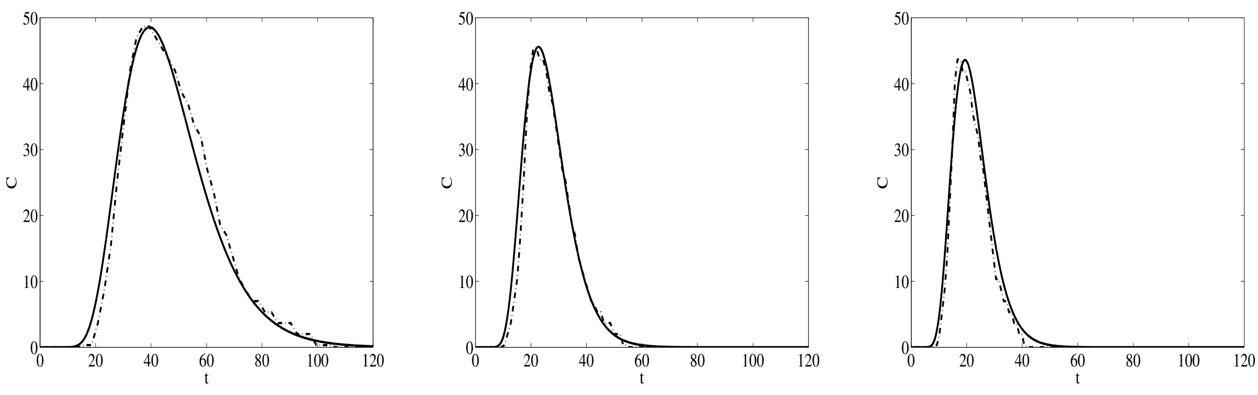
Q (l/h)	V_{inj} (ml)	V_{sl} (ml)	M_s (mg)	C_{sl}(mg/l)
1	10	112	32.5	267.26
2	10	112	32.5	267.26
2.5	10	112	32.5	267.26

Table 1. Parameters related to the determination of the physical inflow boundary condition.



(a) (b)

FIGURE 2. (a) Experimental results for flow rates $Q = 1, 2, 2.5$;
(b) Numerical simulation for flow rates $Q = 1, 2, 2.5$.



(a) (b) (c)

FIGURE 3. The same as Fig. 2 but with the numerical results and experimental results in the same figure:
(a) $Q = 1$: $V = 0.00828$, $D/VL = 0.065$, $Pe = 15.3$
(b) $Q = 2$: $V = 0.01440$, $D/VL = 0.056$, $Pe = 17.8$
(c) $Q = 2.5$: $V = 0.01680$, $D/VL = 0.054$, $Pe = 18.5$

We show, in Fig. 2 and Fig. 3, the experimental results and the numerical simulations for different flow rates. The numerical results allow us to determine the Péclet number, that is helpful in the characterization of the hydraulic conditions.

5. Conclusion

The results lead us to conclude that, according to the range of hydraulic loading applied, a large amount of diffusion occurs in the filter bed. This occurrence is associated to the likely combination of factors such as dead zones, immobile zones, short-circuiting and diffusion (both mechanical dispersion and molecular diffusion).

The analytical solution represented by (6) for the semi-infinitive system can accurately predict the experimental curves and may be applied to results from finite experiments as the one here mentioned. To the numerical simulation we use a numerical scheme quite appropriated since when we have significant values of diffusion we need a larger stability region, that is, we need the method to converge to the analytic solution in a region where we can have great accuracy and at the same time we are allowed to have significant diffusion.

More experiments are in progress considering different organic loadings at different hydraulic loadings.

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