Spatial moment analysis: an application to quantitative imaging of contaminant distributions in porous media

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With the aim of characterizing complex solute transport problems in porous media, a two-dimensional physical model has been designed and constructed and will be described in this paper along with some results relative to the estimation of the dispersive parameters and the pore water velocity. The experimental setup, simulating a fixed bed, uses a transmitted light imaging technique in conjunction with a fluorescent dye tracer (sodium fluorescein) to monitor solute movements. Besides, to establish the relationship between the image intensity, detected by the CCD camera, and tracer concentration in the physical model, a calibration was conducted over the whole imaged area for two different sets of glass beads (simulating the porous media). In this procedure, background levelling is needed to enhance the contrast in intensity values between the background porous media and the tracer itself. The results successfully model a reagent or a contaminant plume (generated by a pulse input) within a homogeneous porous bed. For each experimental run, concentration distributions are determined from the calibration curve. Estimates of the solute mass, pore water velocity and longitudinal and transverse dispersion coefficients are calculated by using spatial moment analysis. The results confirm the reliability of the proposed procedure and testify that the method can efficiently characterize the porous medium.

1. Introduction

Laboratory scale flow tank experiments, used extensively in literature at different spatial scales (Corapcioglu et al. (1999), Jia et al. (1999), Huang et al. (2002), Theodoropoulou et al. (2003), Gaganis et al. (2004), Jones and Smith (2005)) have shown that techniques based on coloured dye tracers could be successfully used to study solute transport in a porous media confined in a transparent container satisfying the requirements of high spatial resolution and accuracy. These advances in the study of mass transport processes are based on image analysis at a laboratory scale that relies on extremely detailed sampling to map temporal and spatial variations in concentration distributions achieving up to two/three orders of magnitude more sampling points than conventional analysis methods.
A two-dimensional experimental apparatus, able to quantitatively explain solute transport in a porous matrix through a transmitted light imaging technique, has been designed and constructed and will be described in this paper along with some results relative to the estimation of the dispersive parameters and to the pore water velocity. The relationship between luminous intensity and solute concentration, taking into account luminous dispersion and non uniform lighting, was assessed by a pixel-by-pixel calibration. The injection of a pulse-like plume in conjunction with an analysis of the spatial moments permits to confirm the reliability of the method, through a comparison between what estimated and what directly measured; moreover, the analysis of second order central spatial moment allows to evaluate soil parameters as the longitudinal and transverse dispersion coefficients.

The findings of this work are useful for characterizing the porous medium and can have implications on the management and remediation of groundwater quality, as the estimated values of physical parameters can drastically influence the choice of the remediation criteria.

2. Materials and Methods

2.1 Experimental Setup

The experimental apparatus, placed in a dark room to capture only the luminous intensity emitted by the fluorescent dye and represented in Figure 1, is composed by:

Tracer: the fluorescent tracer chosen was sodium fluorescein (formula \( C_20H_{10}Na_2O_8 \)), as it has a moderately high resistance to sorption (so it is possible to consider it as a conservative tracer) and doesn’t undergo any detectable photobleaching phenomenon in the performed experimental conditions.

Porous matrix: a Perspex box of internal dimension 200 x 280 x 10 mm\(^3\) was packed with glass beads of constant diameter (1 mm or 2 mm), simulating a two-dimensional homogeneous porous media (the 10mm thickness is sufficiently thin to approximate a two-dimensional system). Before inserting glass beads in the box, their mass was measured in order to determine the porosity \( n \) of the porous matrix (\( n = 0.36 \) for 1 mm beads and \( n = 0.43 \) for 2 mm beads).

Source injection pipe: a 6 mm diameter stainless steel pipe was inserted through the entire thickness of the model. The pipe has three equidistant holes, 1 mm diameter, thus obtaining a uniform distribution of the tracer all along the model thickness.

Luminous source: two 18 W Arcadia FMB18 light tubes were utilized as light source to excite the conservative tracer. Their wavelength peak is tuned to the absorption band of the tracer itself (480 nm).

Pump: the effluent from the model was removed by a Gilson standard low-pulse peristaltic pump placed downstream which permits a steady flow rate to be applied to the model in a variable range (from 0.3 \( \mu \)l/min to 30 ml/min).

Camera: the images were recorded by a Hamamatsu C5405 CCD (Charge Coupled Device) camera, with a resolution of 752(H) x 582(V) and a minimum object illumination of 0.3 lux. The light emitted by the dye was filtered by an Edmund Optics bandpass filter to select the emission peak of the tracer in the green part of the spectrum at a central wavelength of 520 nm with a bandwidth of 10 nm. The distance between CCD camera and the model was set at 80 cm.
Figure 1 - Schematic of experimental apparatus. Fluorescent dye, injected in the injection point on the right (source) of the model, is excited by linear light sources, images are captured by a CCD camera, placed perpendicularly above the centre of the porous matrix, and then translated and processed by a personal computer.

2.2 Calibration

The intensity of the fluorescence $F$, after background levelling, is equal to the intensity of absorbed light $(I_0 - I)$, multiplied by the fluorescence quantum yield, $\gamma$ (ratio between the number of emitted quanta and the number of absorbed quanta), where $I_0$ and $I$ are the intensities of the light entering and leaving the sample. These intensities are linked to the solute concentration $C$ through the Lambert-Beer’s law, $I / I_0 = 10^{-\varepsilon CF}$, where $\varepsilon$ is the molar extinction coefficient of the dye, $l$ is the path length of the light and $f$ is an optical or geometric factor related to the light path in the glass bead porous media. The relationship between the imaged luminous intensity and the tracer concentration is thus established:

$$F - F_b = gI_0 (1 - 10^{-\varepsilon CF}) \gamma$$

(1)

where $g$ is the detection efficiency of the CCD camera, comprehensive of filter effects and $F_b$ is the background intensity.

Non-uniform illumination, vignetting and luminous dispersion make unfeasible the use of a unique calibration curve all along the physical model, as they invalidate the hypothesis of spatial uniformity for the distribution of the luminous intensity imaged by the CCD camera. A background levelling procedure, coupled with a pixel-by-pixel calibration, tend to eliminate these effects.

2.3 Spatial Moments Analysis

The image analysis procedure was applied to determine concentration maps for a laboratory-scale flow experiment, consisting in an injected pulse-like tracer. Two flow velocity of $4.35 \times 10^{-4}$ m/s and $2.22 \times 10^{-4}$ m/s were established for the 1mm diameter porous medium, while, for 2mm diameter porous medium, the flow velocity was imposed to be $4.58 \times 10^{-4}$ m/s or $2.36 \times 10^{-4}$ m/s. The system configuration was also varied for different initial concentrations ($C_{init1} = 100$ mg/l, $C_{init2} = 50$ mg/l) for both
different diameters of the glass beads. After switching the peristaltic pump on and reaching a steady flow condition, a selected volume of sodium fluorescein solution at known concentration was introduced by means of a syringe pump through the source pipe and image acquisition started recording the pollutant plume at regular time steps of 5 seconds. These images have been analysed by inverting equation (1) to estimate the concentration. The total mass of the solute inserted in the model was compared to the mass calculated by zero-order spatial moment analysis of the measured concentration profile, defined as:

\[ M_0 = \int \int C(x, y)H \, dx \, dy \]  

(2)

where \( C \) is the solute concentration (indirectly measured from inversion of (1)) and \( H \) is the thickness of the porous medium. \( M_0 \) multiplied by the porosity \( \eta \), gives an estimate of the total mass of the plume.

By evaluating the derivatives of the first-order spatial moments with respect to time, it was possible to calculate the pore water velocity of the centroid of the system and compare it with the discharge \( Q \) (and therefore with the Darcy's velocity \( q = Q/A \), where \( A \) is the cross section), measured at the outflow chamber. Finally, the evaluation of the second central spatial moments along \( x \)- and \( y \)-direction \( (S_{xx} \) and \( S_{yy} \)) permit to assess the spread of the solute body around its centroid. As the plume's dimensions increase with time, by differentiating the dependence of these moments with respect to the time, it is possible to estimate both longitudinal \( (D_L) \) and transverse \( (D_T) \) dispersion coefficients:

\[ D_L = \frac{1}{2} \frac{dS_{xx}}{dt} ; \quad D_T = \frac{1}{2} \frac{dS_{yy}}{dt} \]  

(3)

3. Results and Discussion

3.1 Zero-order moment (solute mass)

An analysis of the total mass of the solute inserted in the model has been performed through the computation of the zero-order spatial moment, calculated with equation (2). The comparison between estimated mass with injected mass for different average flow rates and source concentration is shown in Figure 2. It may be observed that the pixel-by-pixel calibration permits to accurately estimate the total mass, even if mass is not well estimated at high initial concentrations that correspond to high \( F \) values. In fact, due to non-linearity of the calibration curve and its tendency to level off at high \( C \) values, a small error on \( F \) can lead to large error bars on the concentration value.

3.2 First-order moment (solute pore water velocity)

Figure 3 shows a comparison between the specific discharge estimated for the first spatial moment along \( x \)-direction and the real one for different average flow rates and source concentration. Substantially, the error in estimating Darcy's velocity along \( x \)-axis by the use of first order spatial moments is acceptable, even if some differences between estimated and measured values are detected. Potential reasons for these discrepancies
resides in luminous dispersion, causing a non perfect identifiability of the fringe of the plume, and preferential paths in porous media determining local variation of velocity.

**Figure 2** – Comparison between estimated and injected mass for 1mm (upper panel) and 2mm (lower panel) glass beads, with error bars on estimated mass.

**Figure 3** – Comparison between estimated and measured pore scale velocity for 1mm (upper panel) and 2mm (lower panel) glass beads, with error bars on estimated pore scale velocity.

### 3.3 Second-order moment (longitudinal and transverse dispersion parameters)

From equation (3), longitudinal and transverse dispersion coefficients are obtained using the first derivative of the solute variance with respect to time. Both $D_l/D_m$ and $D_t/D_m$ (where $D_m$ is the molecular diffusion coefficient of fluorescein in water, equal to $5 \times 10^{-10}$ m²/s) increase approximately in a linear way with Peclet number $Pe = (qd)/(nD_m)$ (Figure 4), where $q$ is the specific discharge, $d$ is the diameter of the glass beads and $n$ is the porosity. This behaviour is in accordance with what reported by Bear (1972), confirming the validity of the proposed approach.
Figure 4 – Longitudinal and dispersion coefficients as a function of the Peclet number.

4. Conclusion

We reported a detailed description of an experimental setup based on an optical detection technique which is accurate, not invasive and of relative low cost to investigate tracer transport in porous media. It is characterised by high spatial resolution (two/three orders of magnitude more sampling points than conventional analysis methods) and consents to understand mechanisms of solute transport in porous media. The spatial moments for transport of a non reactive solute (sodium fluorescein) in this experimental apparatus are presented. The behaviour of effective properties of solute velocity, longitudinal and transverse dispersion coefficient is analyzed. The temporal behaviour of these properties is found to follow a linear regime, testifying the achievement of the Fickian condition.

5. References