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Abstract In this paper some analytical solutions of the advection-dispersion equation are proposed and adopted to solve a non-linear parameter estimation problem. To test the robustness of the analytical solutions if adopted in inverse problems, the anisotropic dispersion coefficients are estimated using sets of experimental data simulated by Monte Carlo techniques. Cylindrical geometry is considered since large columns are the most common devices adopted to study both dispersion and kinetics mechanisms and, even if the solutions are expressed in terms of Bessel function expansion and equations solved only for particular initial and boundary conditions, they give very good results in terms of reliability and precision of our estimates. Discussion of results is based on the analysis of residuals, variance-covariance matrix and bias of parameters. The influence of location and time of sampling, number of samples and data uncertainty on the dispersion coefficients estimates is also analyzed by means of ANOVA tests.

***Keywords**:* Parameter estimation; Column outflow experiments; Solute transport.

1. INTRODUCTION

Contaminant transport in aquifers has become of arising interest in the last few years for scientist working in environmental engineering, hydrology and chemical engineering. Some analytical solutions of the advection-dispersion equation have been proposed in literature with the aim of studying the mechanism of contaminant transport, the movements of pollutants in groundwater and to estimate chemical-physical parameters. In particular, the estimation problem, i.e. the situation in which unknown parameters are to be estimated from experimental data, is a very difficult task if the theoretical physical-mathematical model of the described process is expressed by a PDE: since the minimum problem descending from the optimisation procedure has to be solved under constraints being represented by the PDE itself, only numerical computations can be adopted and, moreover, convergence to optimum is not always reached. For these reasons the investigation about the possibility of using analytical solutions not only for prediction but specially for solving inverse problems is a challenging task.

The analytical solutions of the mathematical models describing pollutant transport are rarely possible if some important hydraulic/chemical effects are considered together, so two or three dimensional solutions of the convection-dispersion equations are given often for non-reacting contaminants or for simple degradation or decay and isotropic dispersion (Broadbridge et al. [2002]); otherwise solutions taking into account of nonlinear chemical adsorption/desorption are found only for a

monodimensional advection-dispersion scheme (Van der Zee [1990], Bosma and Van der Zee [1993]).
The authors recently studied and proposed (Massabò et al. [2004]) some analytical solutions for the transport equation in cylindrical geometry for a reacting solute under chemical decay or linear adsorption-like reaction by taking into account of dispersion in both radial and axial directions. Bessel function expansion is used to solve the second order PDE model with different initial conditions corresponding to usual experimental practices. This mathematical model represents one of the most adopted experimental device to investigate about pollutant transport phenomena and so it can be used to fit experimental data from large columns in which contaminant flows through a saturated porous media.
The use of analytical solutions of the advection-dispersion equation in estimation problems is very limited. Parameter estimation is difficult when flow and transport parameters are to be optimised simultaneously because of slow convergence rates and unstable estimates. So, usually the flow parameters are assumed to be known. Murphy and Scott [1977] introduced an inverse approach in order to estimate the dispersivities from observed concentration values. Strecker and Chu [1986] were the first to estimate both flow and transport parameters dividing the optimisation procedure in two separate stages, while Wagner and Gorelick [1987] estimated flow and transport parameters simultaneously by inverse modelling, making use of nonlinear regression based on the least squares method.
In this work the analytical solutions of the transport equation proposed by the authors are used for parameter estimation. In order to investigate solutions suitability if adopted in inverse problems, only the dispersion coefficients are considered at this time: the analytical solutions contain the full Bessel expansion also in this case; so, disregarding of the kinetic term does not influence the reliability of the entire procedure.
Discussion of results is based on the analysis of residuals, variance-covariance matrix of parameters and variance-covariance matrix of the experimental data. The influence of sampling methodology on the parameter estimates is analyzed in terms of number of samples, their location in the model space *(x, r, t)* and the experimental error.

2. THEORETICAL FRAMEWORK

2.1 The estimation problem

Let us consider the situation in which unknown parameters $\boldsymbol{\theta}$ are to be estimated from experimental data **w*** and the theoretical model describing the experimental campaign is defined by an implicit model.
If the theoretical implicit model is expressed by a PDE, we have the following situation.
Let the experimental data **w*** be connected by a linear mapping (or be the same of) to the solution **u** of a PDE, expressed as follows:

$$L_{\vec{\theta}}(\mathbf{u}) = 0 \tag{1}$$

$$A\mathbf{u} + \mathrm{B}\frac{\partial \mathbf{u}}{\partial \mathbf{n}} = \mathrm{f}\ (\xi) \quad \text{on the boundary S'} \tag{2}$$

defined by coordinates $\boldsymbol{\xi}$ and where the subscript $\boldsymbol{\theta}$ indicates the vector of the unknown parameters (the dispersion coefficients here discussed) in the differential equation, S' is the domain in which the generical mixed boundary condition is defined; **n** indicates the direction normal to S'.
Let F be the linear mapping:

$$\mathrm{F} : \mathbf{u}_{\vec{\theta}} \rightarrow \mathbf{w}_{\vec{\theta}} \tag{3}$$

where $\mathbf{w}_{\boldsymbol{\theta}}$ is to be compared with the experimental data **w*** to carry out some kind of regression analysis by minimizing some convenient objective function Φ ; e.g.:

$$\Phi = \left\| \mathbf{w}_{\vec{\theta}} - \mathbf{w}^* \right\| \tag{4}$$

The formal solution of problem (1) + (2) is given by

$$\mathbf{u}_{\vec{\theta}}(\mathbf{x}) = \int_{\mathbf{P}} \mathrm{G}''_{\vec{\theta}}(\mathbf{x}, \xi) f(\xi) d\xi \tag{5}$$

where G" indicates the $\boldsymbol{\theta}$-dependent Green's function of the second kind and **x** the independent variables of the domain on which **u** is defined. As there are no general solution methods for complex PDE's, if exact or approximate analytical solutions are not available, only numerical solutions for problem (1) + (2) can be used to solve the inverse estimation problem (4). Solving problem (4) where $\mathbf{w}_{\boldsymbol{\theta}}$ depends on $\mathbf{u}_{\boldsymbol{\theta}}$ by the linear mapping (3) and where $\mathbf{u}_{\boldsymbol{\theta}}$ is the solution of problem (1) + (2) means an optimization procedure which cannot be easily solved by numerical algorithms: we have the typical convergence difficulties of a constrained optimization algorithm plus the

typical numerical errors of the PDEs solver, both affecting the search for the global minimum.
In fact, if the model remains in implicit form, a maximum likelihood estimation procedure leads to a nonlinear, constrained minimization problem where constraints are given by the equation model itself, i.e. equations (1) + (2) + (3); and **w*** are the measured values of all the model variables regardless their kind, i.e. time, spatial coordinates and state variables (t, **x**, **ξ**, **u**) and **θ** is the vector of the unknown parameters.
Only if:

i) the model can be solved in reduced form (explicit analytical solution);
ii) the errors on the independent variables and on space and time measures are neglected;
iii) the errors on the remaining variables are independent (Bard[1974]);

the estimation problem reduces to an unconstrained minimization problem of the kind weighted or not-weighted least squares. Hence the importance of finding analytical solutions for problem (1) + (2) so to satisfy condition (i). Conditions (ii) and (iii) can be easily satisfied if ad hoc experimental conditions are observed.
It is also important to notice that linear differential models and their analytical solutions are particularly important in data analysis because the experimental conditions can be often forced to keep in the linear domain (relaxation experiments)

2.2 Model equations and analytical solutions

Under the hypothesis that large columns are adopted to investigate anisotropic dispersion (showed in photograph 1), we assume that the initial conditions do not depend on the angular variable; as a consequence, the process preserves symmetry around the longitudinal axis. The advection-dispersion PDE expressing the mass balance of a generic solute in terms of dimensional concentration *C(r,x,t)*, can be written as follows:

$$\frac{\partial C^*}{\partial t^*} + u^* \frac{\partial C^*}{\partial x^*} = D_R \left(\frac{\partial^2 C^*}{\partial r^{*2}} + \frac{1}{r^*} \frac{\partial C^*}{\partial r^*} \right) + D_L \frac{\partial^2 C^*}{\partial x^{*2}} \quad (6)$$

Here the constant advective term is represented by the average pore water velocity *u** and anisotropic dispersion is described by means of the two mechanical dispersion coefficients D_R and D_L. They represent different dispersion mechanisms such as molecular diffusion, hydrodynamic dispersion, eddy diffusion or mixing. Using typical dimensionless variables, the equation becomes:

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} = \frac{\eta}{Pe_R} \left(\frac{\partial^2 C}{\partial r^2} + \frac{1}{r} \frac{\partial C}{\partial r} \right) + \frac{1}{Pe_L} \frac{\partial^2 C}{\partial x^2} \quad (7)$$

where:

$$Pe_R = \frac{U_0 R}{D_R}; \quad Pe_L = \frac{U_0 L}{D_L}; \quad \eta = \frac{L}{R}; \quad (8)$$

where *R* and *L* are respectively the radius and the length of the column and U_0 and C_0 the scales of velocity and concentration.

Photograph 1: Large column adopted to investigate anisotropic dispersion.

Boundaries and initial conditions are necessary to have a unique solution. We assume:

$$\left. \frac{\partial C(r,x,t)}{\partial r} \right|_{r=1} = 0; \quad (9)$$

$$\lim_{x \to +\infty} C(r,x,t) = 0; \quad (10)$$

$$\lim_{x \to +\infty} \frac{\partial C}{\partial x} = 0; \quad (11)$$

The first condition represents the mathematical formulation of the impermeability of the column wall while the other two are the simplest boundary conditions representing a semi-infinite system. By considering the following further initial and boundary conditions describing the pollutant release:

$$C(r,0,t) = C_0 H(t); \qquad (12)$$

$$C(r,x,0) = 0; \qquad (13)$$

where C_0 is the concentration of contaminant in the inlet section and *H(t)* is the Heavyside function. For this case a particular Bessel series expansion of the concentration function is used giving the following analytical solution:

$$\begin{aligned} C(r,x,t) = & \sum_{k=0}^{+\infty} A_k J_0(Z_k^1 r)\frac{1}{2}\exp\left[\frac{xuPe_L}{2}\right]\cdot \\ & \cdot\left\{\exp\left[x\sqrt{\frac{u^2Pe_L^2}{4}+\eta\left[Z_k^1\right]^2\frac{Pe_L}{Pe_R}}\right]\cdot\right. \\ & \cdot erfc\left[\frac{1}{2}x\sqrt{\frac{Pe_L}{t}}+\sqrt{\frac{U^2Pe_Lt}{4}+\eta\frac{\left[Z_k^1\right]^2}{Pe_R}t}\right]+ \\ & +\exp\left[-x\sqrt{\frac{u^2Pe_L^2}{4}+\eta\left[Z_k^1\right]^2\frac{Pe_L}{Pe_R}}\right] \\ & \left.\cdot erfc\left[\frac{1}{2}x\sqrt{\frac{Pe_L}{t}}-\sqrt{\frac{U^2Pe_Lt}{4}+\eta\frac{\left[Z_k^1\right]^2}{Pe_R}t}\right]\right\} \qquad (14) \end{aligned}$$

where J_0 is the zero-order Bessel function, Z_k^1 is the k-th zeros of the first order Bessel function and the Bessel's coefficients are:

$$A_k = \frac{2\int_0^1 \rho f(\rho) J_0(Z_1^k \rho)\, d\rho}{\left[J_0\left(Z_1^k\right)\right]^2}, \quad k = 1,2,...$$

$$A_0 = \int_0^1 \rho f(\rho)\, d\rho \qquad (15)$$

3. THE ESTIMATION PROCEDURE

Since we have the analytical solution of the PDE describing the column behaviour (i.e. condition I of paragraph 2.1), we can estimate the unknown parameters Pe_L and Pe_R by solving an unconstrained minimization problem (least squares) only if also conditions ii) and iii) of paragraph 2.1 hold true. We can easily suppose that errors on measures of time and space are negligible with respect to measures on concentration in the body of the large column. Concentration measures in the liquid phase could be carried out with HPLC or Atomic Absorption if we use, for example, hydrocarbons of heavy metals as contaminants, in case of reactive flow (not developed in this paper), or bromide if we refer to conservative tracers. The overall estimation procedure has been carried out using simulated experimental data with errors belonging to a Gaussian distribution with zero mean and 0.01 or 0.05 variance. We considered different sampling points in the column length and radius (preserving symmetry around the longitudinal axis) and repetitions at different time as shown in figure 1.

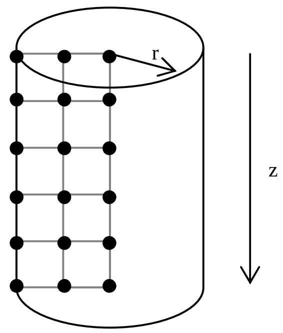

Figure 1: Grid of possible space points in the soil column.

30 Monte Carlo runs for each experimental situation hypothesized have been carried out. The scheme of the adopted data simulation with two levels on the number of measurement points in the spatial domain (S) and two levels on the experimental error variance (V) is resumed in Table 1.

Situation	**nx**	**nr**	**nt**	σ^2
S1V1	5	3	4	0.01
S2V1	5	5	4	0.01
S3V1	10	3	4	0.01
S4V1	10	5	4	0.01
S1V2	5	3	4	0.05
S2V2	5	5	4	0.05
S3V2	10	3	4	0.05
S4V2	10	5	4	0.05

Table 1: The experimental situations analyzed for parameter estimation.

The true values for parameters Pe_L and Pe_R, i.e. values adopted to generate the experimental solute concentration by adding experimental errors to the output of equation (9), are both set to 100. A Marquardt's modified algorithm (Marquardt [1963], Bard [1974]) with analytical first order derivatives supplied by the user has been adopted to solve the nonlinear optimization problem.

In Table 2 the results of the parameter estimation procedure are briefly summarized, where Pe^*_L and Pe^*_R are the mean values (over the 30 Monte Carlo runs) of the estimated parameters and σ^2_{PeL} and σ^2_{PeR} are the related calculated variances.

Situation	Pe^*_L	Pe^*_R	σ^2_{PeL}	σ^2_{PeR}
S1V1	99,94	99,91	1,75	0,26
S2V1	99,96	99,92	1,23	0,20
S3V1	99,81	99,89	0,55	0,11
S4V1	99,87	99,91	0,33	0,08
S1V2	101,44	99,20	31,84	7,18
S2V2	101,35	99,50	21,11	4,90
S3V2	100,45	99,78	20,36	3,60
S4V2	100,09	99,91	13,00	2,69

Table 2: Results of the estimation procedure.

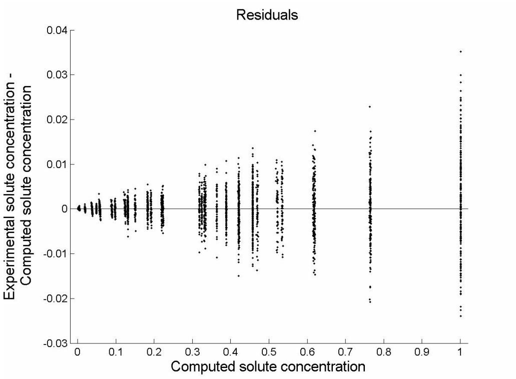

Figure 1: Example of residuals plot, when nx=5, nr=3, nt=4 and σ^2=0,01.

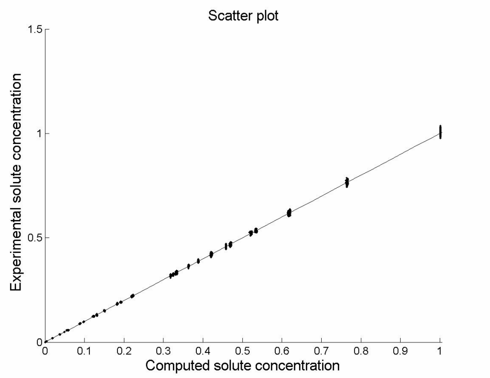

Figure 2: Example of scatter plot, when nx=5, nr=3, nt=4 and σ^2=0,01.

For all the situations and for each run a complete analysis of the residuals has been carried out. Also the computed variance-covariance matrix of the parameters, obtained from the Hessian matrix at minimum (Bard 1974), has been compared with the calculated values of variance of Table 2. In Figures 1 and 2 one example of residuals and one scatter plot are shown.

4. VALIDATION AND DISCUSSION OF RESULTS

From the analysis of the objective function at minimum and its derivatives, residuals, variance-covariance matrix of the parameters, mean value and bias of the parameters, we can say that the proposed procedure for the estimation of the dispersion parameters seems to work very well. The use of the analytical solution of the advection-dispersion equation for parameters estimation gives values of dispersion coefficients very close to the true ones and with low standard deviation. No over- or under-estimation has been found.

In order to analyse the relation between number of samples and data uncertainty on the residuals of parameter values in comparison to their mean, these residuals have been also analyzed by means of ANOVA tests. ANOVA has been done for all the situations described in Table 1 in order to establish which is the factor, among those enumerated above, to which most of the variance of the residuals is to be ascribed.

Fischer tests on ANOVA results show that we have a minimum confidence level of 95% only when we compare the bigger influence of data uncertainty due to Monte Carlo runs with the number of points on x-axis.

One example of ANOVA and Fischer test results for Pe_L, in the case of nx=5, nr=3, nt=4 and σ^2=0,01, is shown in Table 3 and Table 4.

	Variance of mean deviation PeR	**Degree of freedom**	**Mean Square**
Factor 1: Data uncertainty	11.8314	29	0.4079
Factor 2: N° of points on r-axis	1.0059	1	1.0059
Factor 3: N° of points on x-axis	6.6849	1	6.6849

Table 3: ANOVA results for Pe_L when nx=5, nr=3, nt=4 and σ^2=0,01.

Factor comparison	**Fischer distribution value**	**Confidence level**
1-2	16.3854	99.96%
1-3	2.4656	87.28%
2-3	6.6453	76.44%

Table 4: Fischer tests results for Pe_L when nx=5, nr=3, nt=4 and σ^2=0,01.

5. CONCLUSIONS

The procedure here proposed to estimate the longitudinal and transversal dispersion coefficients in pollutant transport problems and based on analytical solutions of the advection-dispersion equation, gave very good results in terms of: parameters values very closed to the true ones, low standard deviation, robustness and reliability of the estimation procedure in all the simulated experimental situations. Even if the analytical solutions are possible only with simple boundary conditions, with some expedients the real experimental conditions can be forced to keep in that domain.

The influence of sampling methodology on the parameter estimates has been also analyzed in terms of number of samples, their location and experimental error to give information about the choice of the sample domain that, especially when field campaigns are to be performed and the position of the piezometric wells are to be fixed, strongly influence the whole cost of experimentation.

Further analyses will regard some consideration on the precision of the analytical model in terms of model output sensitivity, also using the available analytical solution (Massabò et al. [2004]) with kinetic terms. Besides, in future works, the extension of the estimated parameter set, by considering, for example, the pore water velocity, will be analysed. The analytical solution could be used also to test parameter estimation procedures carried out using numerical algorithms for the solution of the 2D advection dispersion equation.

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