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Guidelines for validation and verification of groundwater mathematical studies (GULLIVER): a case study

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Abstract

The goal of this work is to define a set of guidelines for "validating" mathematical models that are to be used in real-world problems of subsurface flow and contaminant transport. Groundwater models today are being used to study increasingly complex problems involving large temporal and spatial scales and with many uncertainties inherent in the data and in the models themselves. It becomes important therefore to establish procedures and benchmark tests with which to assess a given model's adequacy for simulating a specific groundwater problem. In the GULLIVER project we propose to create a public library of phenomenological schemes (PS), each one satisfactorily solved by an established model. A user with a specific application and model at hand can select the PS that most closely corresponds to his application, and corroborate his model against the established solution. The user's model is considered validated when the two numerical solutions match according to specified criteria. In this paper we describe this methodology and present its application to a 2D saturated flow and transport test case based on data from a field study site in Calabria, Italy.

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1 Introduction

In addressing groundwater protection and remediation problems, a deep dichotomy exists between the research world, where groundwater problems are approached from a phenomenological point of view, and real-world practitioners or model end-users, who have to confront the problems in all their data, parameter, and boundary condition complexities [8]. This imbalance has hindered the full application of advanced numerical techniques to real cases. There is a wide literature that demonstrates a close link between mathematical model and data; if the aim of a mathematical model is to efficiently and reliably describe the behaviour of a physical system under different stresses and forcings, the aim of field study is to obtain accurate measurements (directly, or, more commonly in the case of groundwater, indirectly) of the characteristic parameters of a system.

Reliability of a model solution depends mainly on the model being "valid", in the sense of adequately representing the underlying physical processes of interest and being based on accurate and consistent numerical algorithms, but it also depends on data precision, in the same way that data reliability depends to some extent on model requirements. The phenomenological model through which the characteristic parameters are determined must be the same as the phenomenological model used in simulation, and the model is sensitive to those parameters directly involved in the equations governing the phenomenon [9]. The issue of the degree of reliability required of a mathematical model that is used to solve a groundwater problem raises long-standing questions concerning whether groundwater models can actually be validated [3, 5]. It is broadly accepted that a mathematical model can be a useful too in addressing groundwater flow and pollution problems. A similar consensus is lacking however in attempts to establish procedures and rules for the validation of such models. Indeed there seems to be little agreement both on what validation is and how a theory, and thus a model, can be validated.

A way out of this dilemma is to focus not on verification of a model's validity (valid model), but to assess instead the usefulness of a model in its specific context (validated model): "...a model is developed for real problems and applied to specific situations, it is entirely instrumental. We have not to question if it is valid, only if it is useful - we validate, not verify" [7]. In other words validation should "guarantee" the ability of a model to make reliable predictions. It should thus be viewed as a verification process, whereby we assess whether the model has an adequate predictive accuracy within its domain of applicability and over characteristic time and space scales.

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2 The GULLIVER project

Within this context of "validation", the goal of this work is to define guidelines for assessing and evaluating mathematical models used in hydrogeology for simulation of groundwater flow and transport processes. The GULLIVER project proposes to create a public library of "phenomenological schemes" (PS) which have been solved satisfactorily by established models used in academic and research centers. A user can validate a groundwater model solving the PS that most closely corresponds to the specific problem at hand (e.g., unsaturated flow, 2D groundwater flow with injection/extraction points, density-dependent flow and transport, etc). The user's model is considered validated when the two numerical solutions match according to specified criteria.

Each PS includes a PS proposal set and a PS solution set. The PS proposal set contains:

- A metadata description of the problem;
- An accurate graphical and physical description of the problem (flow and transport domain, boundary conditions, parameters, load conditions, pollutant types, etc).

The PS solution set includes:

- One or more analytical, experimental, or numerical solutions;
- Data validation and prediction intervals with given probabilities;
- Detailed description of the simulation results;
- A bibliography for the mathematical models used;
- A listing of the commercial codes that have been validated on the specific PS.

The proposed validation procedure will benefit the large community of users needing to adopt simulation models to address groundwater management, protection, and remediation problems, providing them with better indications of the reliability of various models. We limit ourselves in this paper to presenting a case study of 2D saturated flow and transport based on data from a field site in Calabria, Italy. A numerical model based on the method of cells [4] is validated against a finite element reference model [2].

3 Numerical simulation models

3.1 Governing equations

Using indicial notation where the indices i and j denote summation over the three coordinate dimensions ($i, j = 1, 2, 3$), the equation for groundwater

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flow can be written as

$$\frac{\partial}{\partial x_i}\left(k_{ij}\frac{\partial h}{\partial x_j}\right) = S_s\frac{\partial h}{\partial t} - q \tag{1}$$

where k_{ij} is the hydraulic conductivity tensor, x_i is the ith Cartesian coordinate, S_s is the specific elastic storage of the medium, t is time, and q represents distributed source or sink terms. Initial and boundary conditions of Dirichlet or Neumann type complete the mathematical formulation.

Using the Darcy velocities v_i, defined as

$$v_i = -k_{ij}\frac{\partial h}{\partial x_j} \tag{2}$$

we can write the conservation equation for the contaminant. With the dispersion part of the contaminant velocity expressed as $-D_{ij}(\partial c/\partial x_j)$, we obtain the equation describing transport of a non-reactive solute

$$\frac{\partial}{\partial x_i}(D_{ij}\frac{\partial c}{\partial x_j}) - \frac{\partial}{\partial x_i}(v_i c) = n\frac{\partial c}{\partial t} - qc_1 - f \tag{3}$$

where $D_{ij} = n\tilde{D}_{ij}$, n is the porosity of the medium, $\tilde{D}_{ij}$ is the dispersion tensor, c is the concentration of the solute, c_1 is the concentration of solute injected (withdrawn) with the fluid source (sink), and f is the distributed flow rate of the solute per unit volume. The dispersion tensor for a two-dimensional porous medium is given by [1]

$$D_{ij} = \alpha_T\,|v|\,\delta_{ij} \; + \; (\alpha_L - \alpha_T)\frac{v_i v_j}{|v|} \; + \; D_o\, n\, \tau\, \delta_{ij} \tag{4}$$

where α_L is the longitudinal dispersivity, α_T is the transverse dispersivity, δ_{ij} is the Kronecker delta, τ is the tortuosity ($\tau = 1$ usually assumed), D_o is the molecular diffusion coefficient, and $|v| = \sqrt{v_1^2 + v_2^2}$. Initial and boundary conditions of Dirichlet, Neumann or Cauchy type can be specified.

3.2 Finite element model

In the two-dimensional finite element discretization of the flow equation an approximate solution $\hat{h}$ for h is defined as

$$h \approx \hat{h} = \sum_{i=1}^{l} \hat{h}_i(t) N_i(x_1, x_2) \tag{5}$$

where $N_i(x_1, x_2)$ are linear shape or basis functions for triangular finite elements, $\hat{h}_i$ are the unknown nodal potential heads, and l is the number of nodes. Substituting $\hat{h}$ in equation (1) and prescribing an orthogonality condition between the residual

$$L(\hat{h}) = \frac{\partial}{\partial x_i}\left[k_{ij}\left(\frac{\partial \hat{h}}{\partial x_j}\right)\right] - S_s\frac{\partial \hat{h}}{\partial t} + q \tag{6}$$

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and each basis function yields the Galerkin integral:

$$\int_V L(\hat{h})N_i \, dV = 0, \qquad i = 1, \ldots, l \tag{7}$$

where V is the flow region or integration domain. Assuming the coordinate directions x_j to be parallel to the principal directions of hydraulic anisotropy and applying Green's lemma we arrive at a system of linear equations that can be written as

$$H\hat{h} + P\frac{\partial \hat{h}}{\partial t} + q^* = 0 \tag{8}$$

where H is the stiffness matrix, P is the capacity matrix, and vector q^* accounts for the prescribed boundary flux, the withdrawal or injection rate, and the coupling with the transport equation. Integration in time of (8) by a weighted finite difference scheme yields

$$\left(\nu H_{t+\Delta t} + \frac{\nu P_{t+\Delta t} + (1-\nu)P_t}{\Delta t}\right)\hat{h}_{t+\Delta t} =$$
$$\left(\frac{\nu P_{t+\Delta t} + (1-\nu)P_t}{\Delta t} - (1-\nu)H_t\right)\hat{h}_t - \nu q^*_{t+\Delta t} - (1-\nu)q^*_t \tag{9}$$

where for stability reasons the weighting parameter ν must satisfy the condition $0.5 \leq \nu \leq 1$. Selecting $\nu = 0.5$ leads to the Crank-Nicolson scheme while $\nu = 1$ gives the fully implicit backward difference scheme.

Finite element integration of the transport equation (3) follows the same procedure as the flow equation, and yields the discretized system of equations

$$(A + B + D)\hat{c} + C\frac{\partial \hat{c}}{\partial t} + r^* = 0 \tag{10}$$

where matrices A, B, and D account for the dispersion, convection, and Cauchy boundary condition terms, respectively. The vector r^* accounts for point and distributed contaminant sources and sinks. Integration in time of equation (10) is again performed using a weighted finite difference scheme:

$$\left[\nu(A+B+D)_{t+\Delta t} + \frac{\nu C_{t+\Delta t} + (1-\nu)C_t}{\Delta t}\right]\hat{c}_{t+\Delta t} =$$
$$\left[\frac{\nu C_{t+\Delta t} + (1-\nu)C_t}{\Delta t} - (1-\nu)(A+B+D)_t\right]\hat{c}_t - \nu r^*_{t+\Delta t} - (1-\nu)r^*_t \tag{11}$$

where as before $1/2 \leq \nu \leq 1$. Unlike the flow equation, the transport equation is quite sensitive to the value of the weighting parameter ν. A value close to $1/2$ leads to accurate but unstable solutions while values close to 1 yield good stability but with larger numerical dispersion [6].

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3.3 The method of cells

If we consider a cell complex in which the most nonuniform cells are the smallest, we may use as an approximation the same constitutive law used in the differential context. Since a numerical process produces approximate expressions of physical laws, consideration of small reasonably uniform regions enables us to obtain a natural discretized form. The forming of densities and rates and the passage to the limit to form field functions, typical of field and continuum theories, deprives physical variables of their geometrical content. From these considerations it follows that to obtain a discrete formulation of the fundamental equation of a physical theory, it is not necessary to go down to the differential form and then to go up again to the discrete form. It is enough to apply the elementary physical laws to small regions in which the uniformity of the field is attained to a sufficient degree, linked to the accuracy of the input data and to the degree of approximation requested of the solution.

Let T be a triangulation of the domain into N cells. For example, a 2D domain may be discretized via a Delaunay triangulation. In this case the cells are the Voronoi polygons, whose union is the dual of the Delaunay triangulation. Note that by definition the boundary of a Voronoi cell is orthogonal to the edge of a Delaunay triangle. For each cell $\bar{v}_h$ the discrete equation enforcing conservation of the fluid mass m_h in the time interval $\bar{\Delta}t = \bar{t}_{n+1} - \bar{t}_n$ is

$$\bar{\Delta}_t m_h + \sum_\alpha \bar{d}_{h\alpha}\Phi_\alpha = 0 \tag{12}$$

where $\bar{\Delta}_t m_h = (m_h(\bar{t}_{n+1}) - m_h(\bar{t}_n)/\bar{\Delta}t$ and Φ_α represent the mass flux across boundary α of $\bar{v}_h$. The discrete form of Darcy's law (2) over boundary α can be written as

$$q_\alpha = K\frac{H_\alpha}{\ell_\alpha} \tag{13}$$

where H_α, called the head coboundary, is the head difference discretizing the opposite of the gradient normal to boundary α and ℓ_α is the size of the boundary of the Delaunay simplex (the triangle edge). The mass flux Φ_α is then given by

$$\Phi_\alpha = \rho q_\alpha s_\alpha \tag{14}$$

where s_α is the size of the boundary α of the Voronoi cell. If this direction does not coincide with the principal axis of anisotropy, a rotation of the local reference frame is performed to maintain the diagonal form of the conductivity tensor.

For a confined aquifer, we can write:

$$\rho S_s \bar{v}_h \bar{\Delta}_t h_h + \sum_\alpha \Phi_\alpha = 0 \tag{15}$$

where for simplicity we have written $\bar{v}_h$ to indicate the volume of cell $\bar{v}_h$. This equation can be written for every cell of the domain discretization,

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thus yielding a system of equations with h_h as unknowns

$$\bar{H}h_h + \bar{P}\bar{\Delta}_t h_h = \bar{q} \tag{16}$$

where $\bar{H}$ and $\bar{P}$ are the stiffness and capacity matrices of the method of cells. This system can be solved using an approach entirely similar to the Crank-Nicolson scheme used for the finite element equation (9) with $\nu = 0.5$.

The discrete form of the solute mass conservation equation may be written as

$$\bar{\Delta}_t m_{c_h} + \sum_\alpha \bar{d}_{h\alpha}\Phi_{c_\alpha} = \Phi^*_{ch} \tag{17}$$

The solute mass variation in time is

$$\bar{\Delta}_t m_{c_h} = n\,\rho_s\,\bar{v}_h \frac{C(t_{n+1}) - C(t_n)}{t_{n+1} - t_n} \tag{18}$$

where ρ_s is the density of the solute and C_h is the concentration within cell $\bar{v}_h$. The total flux Φ_{c_α} is the sum of the dispersive flux $\Phi^{disp}_{c_\alpha}$ and the convective flux $\Phi^{conv}_{c_\alpha}$. The latter is given by

$$\Phi^{conv}_{c_\alpha} = \frac{\Phi_\alpha}{\rho} C_h \tag{19}$$

while the dispersive flux is

$$\Phi^{disp}_{c_\alpha} = D_\alpha \bar{s}_\alpha \frac{C_\alpha}{l_\alpha} \rho_s \tag{20}$$

where C_h is the concentration coboundary and D_α is the projection of the dispersion tensor (4) along the α-direction. If this direction does not coincide with the principal axis of anisotropy, a rotation of the local reference frame is performed to maintain the diagonal form of the dispersion tensor.

Again, assembling the equations for all the cells in the discretized domain yields a system of equations with C_h as unknowns

$$(\bar{A} + \bar{B} + \bar{D})C_h + \bar{C}\bar{\Delta}_t C_h = \bar{f} \tag{21}$$

for which all the considerations reported in the finite element case still apply.

4 Validation exercise

In this section we report an example of a validation process using a two dimensional saturated flow test and a corresponding contaminant transport problem. The two PS sets have been defined starting from field data based on a real site for which experimental measurements are available.

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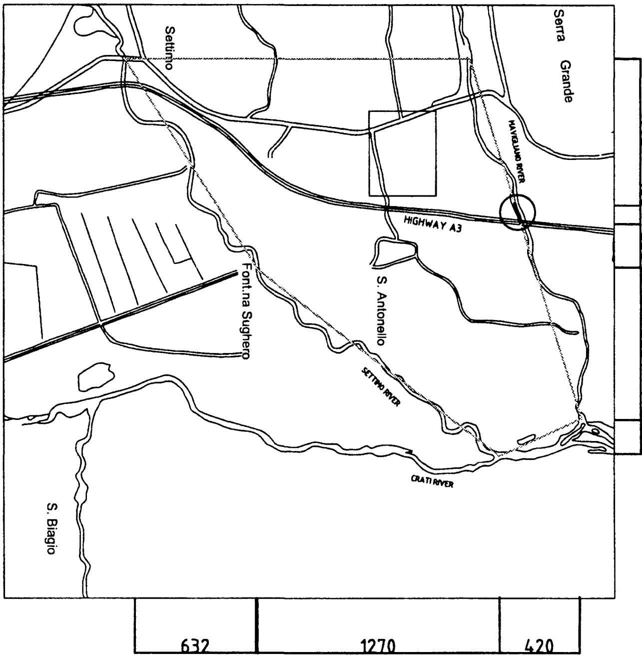

Figure 1: Location of the study area used for the validation exercise. The boundary of the numerical model is shown as a dotted line.

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The study area (Figure 1) is located near the town of Montalto Uffugo in Calabria, Italy. It is a valley at the confluence of the Settimo River on the south, the Mavigliano River on the north and the Crati River on the east. The geology is formed by three layers: sand (0–7 m), clay (7–11 m), and silt (11 to about 40 m) [10]. A basal clay underlies the silty sand. A local perched water table is in the alluvium above the clay layer, and the silty sand layer constitutes a confined aquifer above the basal clay. Measurements of the hydraulic conductivity and its distribution have been made over the past few years using a kriging approach with external drift methodology applied to electrical-resistivity data [11]. The domain for the flow and transport model application is defined as the area enclosed by the surface water system as shown in Figure 1. In the flow model a heterogeneous isotropic porous medium is assumed. Dirichlet boundary conditions are according to the water levels in the surface water system. Two permeability zones are assumed in the flow fields, and are indicated in Figure 1. Zone 1 is characterized by $K_{11} = K_{22} = 10^{-5}$ m/s, $S_s = 10^{-2}$ m/s, while in zone 2 $K_{11} = K_{22} = 10^{-6}$ m/s, $S_s = 10^{-3}$ m/s. One extracting well, located at coordinates $x = 1640$ m and $y = 2525$ m and pumping at a rate of $q_{out} = 0.003$ m^3/s, is coupled with another well, located at $x = 1140$ m and $y = 2250$ m, where the head is kept constant at 138 m. In the transport test case we simulate a contaminant injection from the Mavigliano River, just east of Highway A3 (see Figure 1), where a contaminant source of 300m of length is kept at constant concentration. A second contaminant point source is located at $x = 1467$ m, $y = 2413$ m. The parameters used in the simulations are: $n = 0.2$, $\alpha_L = 50$ m, and $\alpha_T = 10$ m.

The benchmark code for this test case has been run on a number of successively refined computational grids so that a reliable solution is obtained. The results for the flow test case at time $t = 230$ days are shown in Figures 2, 3 whereas Figures 4, 5 deal with the transport problem. The solutions obtained with the two methods are not significantly different so that the method of cells can be considered verified for this PS set. However, more meaningful and objective comparison procedures need to be devised, as the contour plots give only a qualitative picture. Appropriate simulation quantities useful for these purposes could be, for example, mass balance measures (both local and global), stability measures (e.g., negative concentrations in transport problems, existence of negative transmissibilities in stiffness matrices), accuracy measures (e.g. outgoing fluxes from zero Neumann boundaries), and so on. Only by means of these quantities, unique and clear guidelines for an unbiased comparisons of numerical code results can be defined. In the flow test case, one such measure could be the drawdown at one of the wells: for the extracting well, the benchmark drawdown is $\Delta h_b = 6.46$ m, while in the method of cell solution it is $\Delta h_c = 6.06$ m, and thus the relative difference is $\epsilon = 6\%$. A range of differences could be specified, within which the proposed code is to be considered verified.

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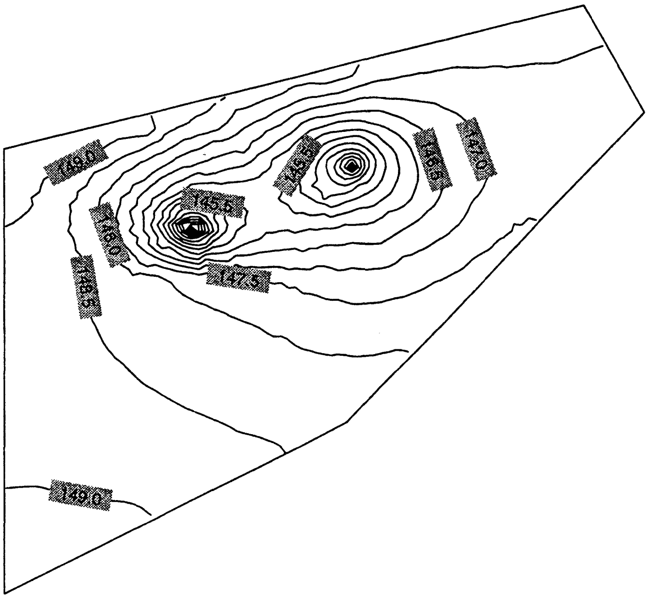

Figure 2: Results of the flow problem at $t = 230$ days: benchmark solution.

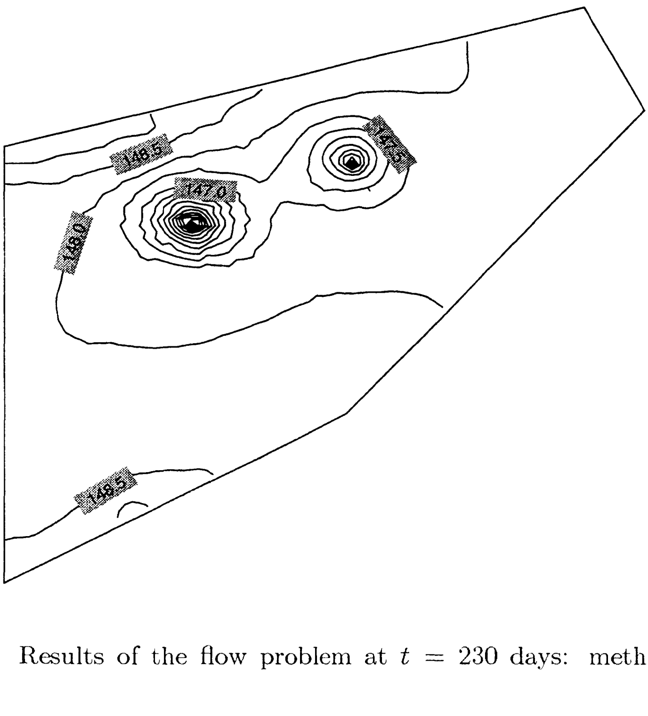

Figure 3: Results of the flow problem at $t = 230$ days: method of cell solution.

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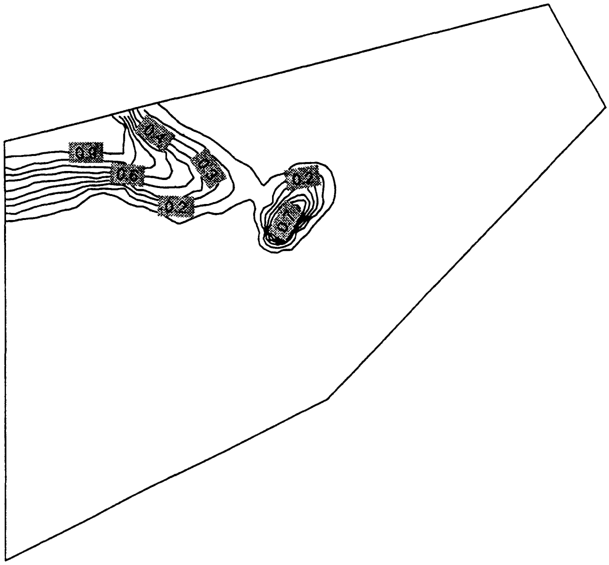

Figure 4: Results of the transport problem at $t = 2.3 \times 10^5$ days: benchmark solution

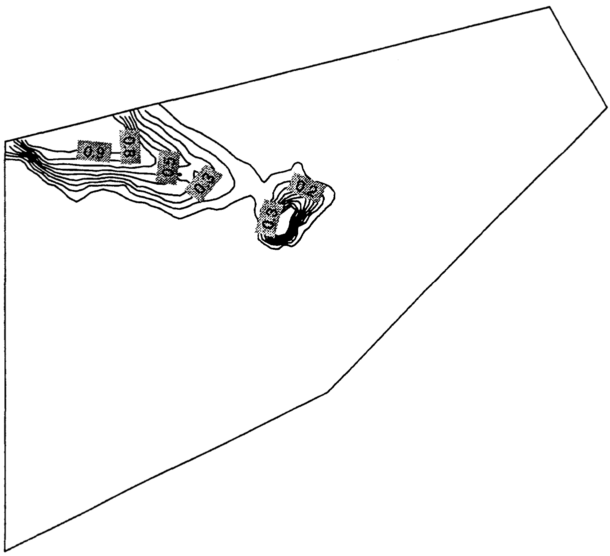

Figure 5: Results of the transport problem at $t = 2.3 \times 10^5$ days: method of cell solution

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This value should in any case be coupled with a reliability assessment of the results in the PS solution set.

5 Conclusions and Future work

The GULLIVER project proposes the creation of a public library of phenomenological schemes to be used as benchmark tests for the verification of mathematical and numerical models for groundwater engineering applications. We have discussed the possibility of creating a "rigorous" procedure for model verification based on the definitions of these PS. Applicability of this approach is shown by means of a preliminary flow and contaminant transport sample test using well-established Finite Element codes for finding the benchmark solution and a recently proposed scheme (the method of cells) as code to be verified. The PS library is intended to be a dynamic library to be filled in the future with increasingly complex PSs.

The sample application raises, however, several interesting questions that need to be addressed in the future. The most important one concerns the definition of appropriate simulation quantities that can be used to objectively control the validity of the numerical solutions. This will be subject for future studies.

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