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Research Note

Finite Volume Discretization of Flow in Porous Media by the MATLAB System

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In this paper, a finite volume scheme is used to discretize flow in porous media. A numerical method for treating advection-dominated contaminant transport for flow of groundwater is described. This system combines the advantages of numerical discretization and the finite volume method (like local mass conservation). The equations are discretized using a finite volume approach. The resulting nonlinear differential system is integrated in time using a solver. The conservation of energy (convection-diffusion) equation is solved using a special method for reducing the oscillations induced by the standard finite volume method. Consequently, a mathematical model for multi-component flow transport in an anisotropic media is presented, which couples the equations for multi-component diffusion and Darcy's law for flow in a porous medium. Furthermore, application of an integrated matlab system in several studies has been provided. The integrated matlab system is based on open data formats and standards and may be used for many other application areas, especially where modeling in 2D and 3D is involved. Numerical simulations are performed to validate the model and investigate the effect. The final purpose of this paper is to discuss and compare the difference between the finite volume scheme for uniform and for unstructured grids, which is shown to be less than 0.2 percent.

INTRODUCTION

Porous media flow models are applied to important areas of interest, including environmental studies and industrial applications. However, large-scale experiments are usually expensive or even impossible; therefore, computer simulations should be considered. Protection of groundwater is a major source of concern to regulatory bodies such as the Environmental Agency. There are many possible causes for groundwater contamination, including chemical spills, leakage of petrol and diesel fuel from underground storage tanks and contamination from disused mines. The process of seepage of a contaminant into the soil is called solute transport. Then, the contaminant spreads through the groundwater in the prevailing flow direction forming a plume [1]. Numerical models have become a standard tool for predicting the response of wells to changes in pumping rate, their number or densit, effects of prolonged drought or changes in land use practices. Here, the focus is on the numerical model of flow in unsaturated, heterogeneous soil. Some results concerning the modeling aspects are summarized briefly and a numerical approach is described for solving these kinds of problem. Simulation results are presented at the end of the paper. In recent years, there has been a growing interest in the finite volume method (also called control-volume or box scheme), which is mostly due to the requirement of many applications for having locally conservative discretization. In the case of different methods used in various parts of the domain, this means finding a stable way of gluing together the solutions in the subdomains [2]. Then, an approximation for the mathematical formulation that would be stable, convergent and accurate is sought. Finally, constructing and studying efficient solution methods for the resulting algebraic problem are considered. Many authors have studied convection-diffusion equations and proposed different numerical solution techniques, such as a non-conforming finite element [3], combined finite volume and finite element methods [4] or finite volume schemes [5]. Powerful advanced computing application software, such as MATHWORK, MATLAB [6] and JAVA [7] have made it possible to write numerical models and utilize

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tested built-in functions and algorithms for standard tasks. It is now no longer necessary for programmers to write their own algorithms to solve integrals or compute statistical parameters. This reduces errors in programming and makes it easier to configure the model with input data and verify the results. The authors of this paper have carried out numerical work for several years and have applied different underground water methods like TRUST [8], TRUMP [9], PORFLOW [10], UNSAT [11], SUTRA [12], MODFLOW [13] and etc. on several fields in Iran. The authors have designed an FVMP model to solve problems of available underground water models. Every groundwater flow model must be calibrated to ensure that it is a reasonable representation of actual flow conditions in the aquifer. One of the most common methods of calibrating wells in the field, is to calculate the water level for those points in the model. In this way, the validity of the modeling results can be assessed and the model credibility as a predictive tool can be established [14]. The above mentioned model (FVMP) has been calibrated by different methods and its correctness has been certified.

FINITE VOLUME VERSUS FINITE DIFFERENCE AND FINITE ELEMENT APPROACH

Numerical solutions of problems in fluid dynamics are usually formulated using one of three methods: finite-volume method, finite-difference method and finite-element method [15]. In the finite-difference approach, a finite-difference approximation of the differential equation is solved. When this numerical method is applied, the equation is first transformed from the physical domain to a uniform computational domain and the differential form of the equation is usually solved at the node points. By contrast, the finite volume approach solves the integral form of the equation, which can capture discontinuities in the solution. The main advantage of the finite-volume approach over the finite-difference approach is its better suitability for complex geometries, as the solution can be obtained in "physical space" [4]. The finite volume method produces the numerical equations at a given point, based on the values at neighboring points, whereas the finite element method produces equations for each element independently of all the other elements. It is only when the finite element equations are collected together and assembled into the global matrices that the interaction between elements is taken into account. The finite element method takes care of derivative boundary conditions when the element equations are formed and then the fixed values of variables are applied to the global matrices. The finite volume approach is written to combine the setting of the equations and their solutions. The decoupling of these two phases, in finite element programs, allows the programmer to keep the organization of the program very clear and the addition of new element types is not a major problem. Adding new cell types to a finite volume program can be a major task involving a rewrite of the program; therefore, some finite volume programs can exhibit problems if they have multiple cell types [17].

MATHEMATICAL MODEL

The groundwater models have been designed, based on mathematical models. As the mathematical models improve, these models also improve. Meanwhile, the progress in numerical methods for solving algorithms has also contributed towards completing these models. Presenting new methods of numerical solutions, including finite volume methods, has created greater capabilities for studying the current in porous media. Using these capabilities in making a model results in an increase in accuracy and a decrease in computer memory requirement. Thus, studying the interactive effects among different elements and new researches, which was not possible using the old models, is made easily accessible using these methods.

Mathematically, the processes can be modeled by numerically solving both Laplace and the solute transport equations as a coupled set. Here, first, the Laplace equation is solved to find the steady-state values of the hydraulic head. Then, using Darcy's law, seepage velocities are obtained for inclusion in the time-dependent solute transport equation, which is solved using finite volume techniques [15]. This enables one to track the movement of the plume front through the aquifer. For the purpose of reference, the mathematical model of two fluids is presented here (pure water and concentrated brine) with the following flow equation:

$$\phi\partial_t p + \nabla.(\rho q) = Q. \tag{1}$$

Here, the velocity (q) of the aqueous mixture is explicitly given by Darcy's law:

$$q = -\frac{k}{\mu}(\vec{\nabla} p - \rho\vec{g}). \tag{2}$$

This is coupled with the transport equation in porous media:

$$\phi\partial_t(\rho c) + \nabla(\rho c q - \rho D \nabla c) = Q, \tag{3}$$

with the density of (incompressible) the mixture given by a functional dependance,

$$\rho = \rho(c). \tag{4}$$

The transport problem that includes sources/sinks of contaminant, due to some chemical reaction (or exchange processes between different phases) and the injection/extraction well, can be described by the following equation.

$$\partial_t(\theta C) + \nabla(qC - D\nabla C) + \lambda C = r + Q\widetilde{c}. \tag{5}$$

These equations arise from the modeling of the transport of dissolved salt in flowing groundwater. The unknown functions are the mass fraction $c = c(x,t)$, which represents the contaminant concentration and the pressure $p = p(x,t)$. A detailed discussion of the model can be found in [18]. Equation 1 is called the transport equation and Equation 2 is called the flow equation. In particular, the permeability tenser, K, and gravity, $g \in R^d$, are obtained. In general, the viscosity and the density, μ, ρ, are nonlinear functions of C, i.e., $\mu = \mu(c), \rho = \rho(c)$ with $\mu, \rho \succ 0$. To the authors' knowledge, up to now, no theory of existence, uniqueness, long-time behavior etc. of solutions of Equations 1 to 3 exists. The parameter $\theta(\theta :\rightarrow (0,1))$ determines properties like porosity (or retardation factor); the velocity (q) describes the movement of the flow in porous media. The dispersion-diffusion tensor, D, can include a molecular diffusion (together with a tortuosity matrix) and a velocity dependent dispersion matrix [18]. Next, λ represents an effective reaction rate of sinks, due to chemical reactions and r describes, analogously, the source terms of the contaminant. Finally, Q describes the injection or extraction wells of the fluid, where the injection concentration, $\widetilde{c}$, must be given explicitly for $Q > 0$ and replaced by $\widetilde{c} = c$ for the extraction well ($Q < 0$). The system is completed by the initial condition $c(0) = c_0$ and boundary conditions for the unknowns (c, ρ), where the latter are of different types at various parts of the boundary of volume (A).

FINITE VOLUME DISCRETIZATION

To derive the discretization, Equation 3 is integrated over the finite volumes $A_i (i = 1, 2, 3, ..., n)$ and, then, Green's formula is applied. The equation then becomes:

$$\int_{A_i} \phi \frac{\partial \rho c}{\partial t} dx + \int_{\partial A_i} \rho c n.q ds - \int_{\partial A_i} \rho n.D\nabla c ds = \int_{A_i} Q dx. \tag{6}$$

The arising integrals over A_i and along the boundary ∂A_i are approximated. In particular, for the first one, the quadrature rule is used:

$$\int_{A_i} u dx \approx u(x_i)|A_i|, \tag{7}$$

where $|A_i|$ is the area of subdomain A_i. The boundary integrals are approximated by:

$$\int_{\partial A_i} \rho c n.q ds - \int_{\partial A_i} \rho n.D.\nabla c ds \approx \sum_{j,e} \left|\Gamma_{ij}^e\right| n_{ij}^e \times \left(\frac{1}{2}\rho_{ij}^e q_{ij}^e (c_i + c_j) - L_{ij}^e \rho_{ij}^e D_{ij}^e \nabla_{C_{ij}}^e\right), \tag{8}$$

where $\left|\Gamma_{ij}^e\right|$ is the length of the boundary segment Γ_{ij}^e. The outer normal (w.r.t) A_i on Γ_{ij}^e is called n_{ij}^e. For the indices, $j \in A_i$ is obtained where j is the index of all neighbor nodes X_i and $e \in A_{ij}$. With variable L, a scalar function is denoted, dependent on the local Peclet number ($L(0) = 1$ & $L(0) \geq 1$). Variable L describes different types of upwind. For $L = 1$, upwind approximates have not been used, which means the integral is approximated by a standard quadrature rule [19].

For the sake of a short notation, $C_i := C_h(x_i)$, $p_i := p_h(x_i), C_{ij}^e := C_h(x_{ij}^e), p_{ij}^e := p_h(x_{ij}^e), \ldots$. Also, Composite functions are abbreviated by $\rho_h := \rho(C_h)$, $\rho_h(x) := \rho(C_h(x)), \rho_i := \rho(C_i), \rho_{ij}^e := \rho(C_{ij}^e), \ldots$. Therefore, the following discrete equation is arrived at:

$$|A_i|\,\phi_i \partial_t(\rho_i c_i) + \sum_{j,e} \left|\Gamma_{ij}^e\right| n_{ij}^e.(\frac{1}{2}\rho_{ij}^e q_{ij}^e (c_i + c_j) - L_{ij}^e \rho_{ij}^e D_{ij}^e \nabla_{C_{ij}}^e) = |A_i|\,Q_i, \tag{9}$$

where q is defined as in Equation 2.

The flow equation can be treated in the same way as the transport equation in the previous section. Therefore, for the semi-discrete problem, $(C_h(t), p_h(t)) \in V_h := V_h \times V_h$ must be found, such that for all $t \in (0,T)$ holds:

$$|A_i|\,\phi_i \partial_t(\rho_i) + \sum_{j,e} \left|\Gamma_{ij}^e\right| n_{ij}^e.(\rho_{ij}^e q_{ij}^e) = |A_i|\,\widetilde{Q}, \tag{10}$$

$$|A_i|\,\phi_i \partial_t(\rho_i c_i) + \sum_{j,e} \left|\Gamma_{ij}^e\right| n_{ij}^e.\left(\frac{1}{2}\rho_{ij}^e q_{ij}^e (c_i + c_j) - L_{ij}^e \rho_{ij}^e D_{ij}^e \nabla_{C_{ij}}^e\right) = |A_i|\,Q_i, \tag{11}$$

with suitable initial and boundary conditions as for the continuous problem. The Darcy velocity is defined in a discrete form of Equation 2.

The following assumption is considered regarding the existence and uniqueness of a solution. There exist numbers $T > 0$ and $q > 1$, such that Problems 10 and 11 possess a unique solution:

$$\begin{pmatrix} c_h(t) \\ p_h(t) \end{pmatrix} \in V_h, \quad t \in (0,T).$$

The arising system of ordinary differential equations is solved by an implicit Euler discretization. For reason of simplicity, further restriction is considered as the case Q, $\widetilde{Q} \equiv 0$, Dirichlet boundary conditions and triangular volumes [16].

FVMP MODEL (FINITE VOLUME METHOD DISCRETIZATION OF FLOW IN POROUS MEDIA)

After introducing the mathematical model and relations governing the current in porous media, the FVMP program has been designed by the authors of this paper. This model has been designed, based on a mathematical model and current discretization using the finite volume method. The objective of designing this program is to solve several problems in relation to the simulation of a current in porous media. Available programs have been prepared based on finite elements or finite difference. Regarding the need for networks to model particular media, these programs occupy a huge volume of the memory. Each of them has some problems and deficiencies. The authors of this paper have applied different models in the study of various fields for about eight years. Considering the obtained experience, the FVMP model has been designed to solve these problems. FVMP is a computer program for simulation of a multi-component multi-dimensional reactive transport in porous media. The code is written entirely in the MATLAB system using the finite volume method. The use of matlab language allows for runtime allocation of memory for arrays, thus, minimizing memory requirements while maximizing the number of options which can be selected at runtime. Using an automatic reading of a thermodynamic and kinetic database, the code can be used for reactive transport problems with arbitrary complexity and size.

The Main Features

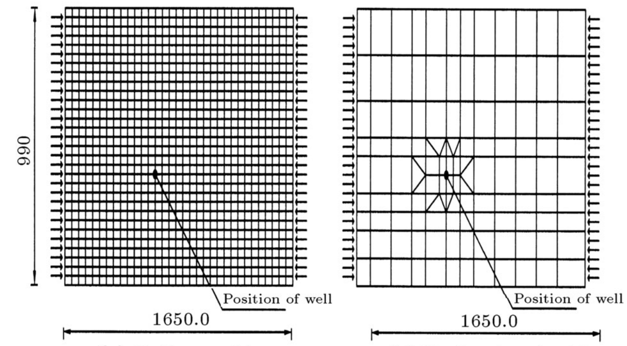
Main features of the code include:

- Simulation of advective, dispersive, diffusive transport in up to two dimensions using the global implicit option or three dimensions using time-splitting of transport and reaction,
- Non-isothermal transport and reaction,
- Multi-component aqueous complexation,
- Kinetically-controlled mineral precipitation and dissolution,
- Multi-component exchange on multiple sites,
- Multi-component diffusion with an electrochemical migration term to correct for electro neutrality where diffusion coefficients of charged species differ,
- Unstructured spatial grids (triangles/quadrilaterals),
- Variable time step sizes,
- Schemes of different order in space/time.

UTILIZATION PROGRAM FOR A CASE STUDY

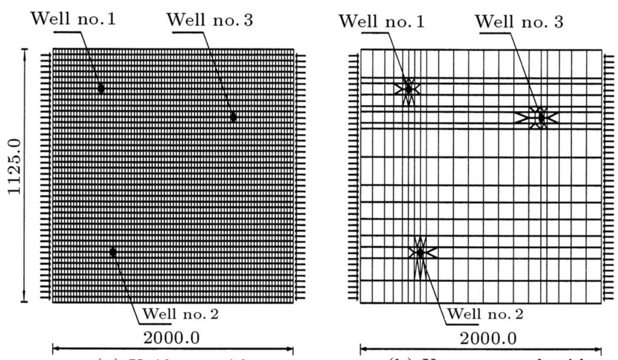
A numerical test is used for the case study and research on the correctness of the designed model. Two types of finite volume are used in these numerical tests. When the difference between the results of the two volumes is low, it could be said that the model can be implemented. Another possibility is using less volume and, as a result, smaller computer memory would be required. Despite this fact, the accuracy of the model using finite volume does not change.

Two kinds of numerical experiment were conducted. First, a uniform algorithm was considered for the finite volume discretization of flow and transport equations. In the second part of the experiment, an unstructured algorithm was considered for the finite volume discretization of flow and transport equations. Finally, the finite volume discretization of the uniform and unstructured algorithm were compared. In the first numerical experiment, a region with a 1650*990 meter dimension was taken into consideration. This region has a single well with a flow rate of -200 (l/s). This well is located at (660,396), where 660 is the x coordinate and 396 is the y coordinate. The hydraulic conductivity can be highly nonlinear and can vary with space according to the soil type. Moreover, in this experiment, hydraulic conductivity in all dimensions is 10^{-3} (m/s). FVMP actually provides the ability to control and adjust the numerical solution process by manipulating the solver parameters and convergence criteria while the solution is in progress. In addition, it provides a real-time graphical display of the solution convergence data. The convergence criteria in this numerical experiment is adjusted as 10^{-6}. The coefficient of correction that is considered for the present stage (and the stage before) of solution, is selected as 1.8. First, the mesh is constructed using uniform finite volumes. The reticulation foregoing is shown in Figure 1a. To continue reticulation of the foregoing system, unstructured finite volumes are used, which are illustrated in Figure 1b. In the second experiment, a region with a 2000*1125 meter dimension is considered. This region has three wells. The first well has a flow rate of -100 (l/s), located at (400, 950), where 400 is the x coordinate and 950 is the y coordinate. The second well has a flow rate of -200 (l/s), located at (500, 225). The third well has a flow rate of -150(l/s), located at (1500, 835), where 1500 is the x coordinate and 835 is the y coordinate. Now, the mesh is constructed by



(a) Uniform grid (b) Unstructured grid

Figure 1. Uniform and unstructured grids for systems having one well.



(a) Uniform grid (b) Unstructured grid

Figure 2. Uniform and unstructured grids for system having three wells.

uniform finite volumes. The reticulation foregoing is shown in Figure 2a. To continue the reticulation of the foregoing system, unstructured finite volumes are used, shown in Figure 2b. The convergence criteria and coefficient of correction correspond to those values in the first experiment. Now, the region in the xy-plane is considered where the water moves towards the well in such a way that the velocity vector is in the xy-plane. At the top and bottom of the xy region, it is assumed that there is no flow through these boundaries. However, assume that there is an ample supply from the left and right boundaries, so that the pressure is fixed.

IMPLEMENTATION OF DESCRIPTIVE MODELS BY FVMP

The graphical output features of the FVMP program have been carefully designed to allow one to visually analyze modeling results. The right combination of output features can be selected to create project specific maps and graphs. The FVMP program will produce report-quality maps and graphs that can be saved in DXF, BMP or WRL file formats. Saving output in a different graphic file format gives the flexibility of importing it into other graphic programs for additional post-processing. Before printing the graphic, it can be annotated with shapes and texts, which can help in describing the graphic to the target audience and draw attention to key areas of the model or graph.

The first output graphs for the first experiment are plots of hydraulic head pressure as a function of x and y. In Figure 3, the head contour lines output for a uniform grid is shown. The grid consists of 1500 nodes. The solution is compared with the result of an unstructured grid, consisting of 139 nodes, in Figure 4.

The output graphs for the second experiment are plots of hydraulic head pressure as a function of x and y. In Figure 5, the head contour lines output for a uniform grid is shown. The grid consists of 3600 nodes. The solution is compared with the result of an unstructured grid, consisting of 336 nodes, in Figure 6.

The qualitative behavior of the solution is the same, with significantly less computational cost, as the unstructured procedure. Consequently, using the unstructured grid, the number of nodes is reduced. This process does not decrease the precision of the solution. Considering that the number of solution cycles is reduced in this way, the probability of numerical errors is weak. Discretization error is also known as numerical error. A consistent numerical

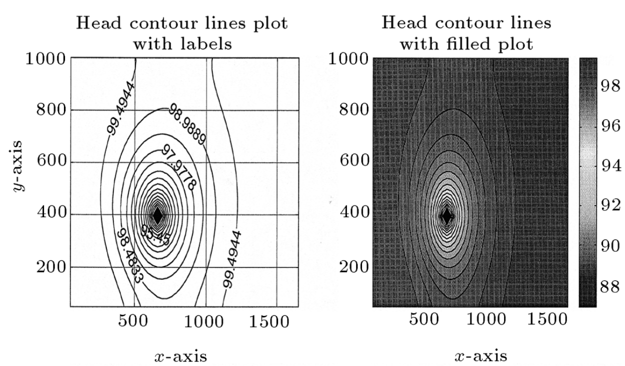


Figure 3. Different types of head contour lines for a uniform grid in systems with one well.

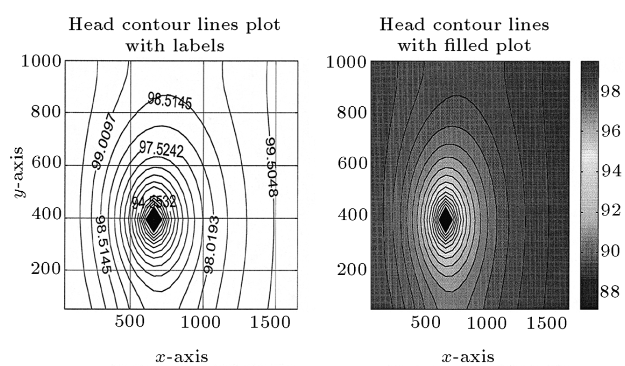


Figure 4. Different types of head contour lines for an unstructured grid in systems with one well.

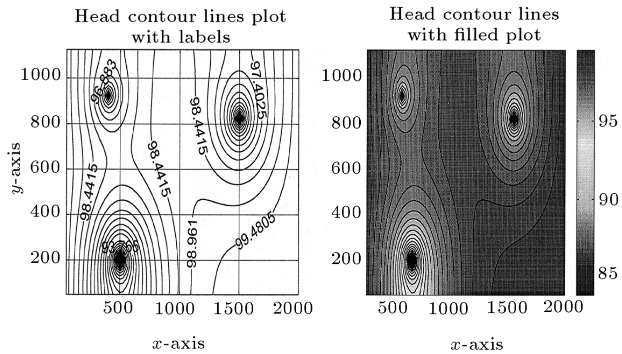


Figure 5. Different types of head contour lines for a uniform grid in systems with three wells.

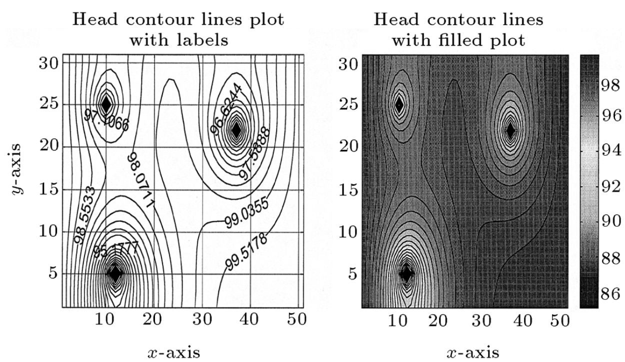


Figure 6. Different types of head contour lines for an unstructured grid in systems with three wells.

method will approach the continuum representation of the equations and zero discretization error, as the number of grid points increase and the size of grid spacing approaches zero. As the unstructured grid is refined, the solution should become less sensitive to grid spacing and approach the continuum solution. This is unstructured grid convergence [20].

NUMERICAL RESULTS FOR THE UNIFORM AND UNSTRUCTURED GRIDS

The purpose of this section is to discuss and compare the differences between the finite volume method for uniform grid and for unstructured grid. The main advantage of an unstructured mesh over a uniform mesh is in the handling of complex geometrical domains. Each grid point can be identified by its coordinate and indices and all neighboring points are easily located. In contrast to the uniform grid system, the mesh points in an unstructured grid system are not organized in an orderly manner. The main difference between the uniform and the unstructured grid system is in the identification of the points forming the computational volume and its neighbors.

First, the results for the uniform grid case are discussed. Figure 7a shows that the pressure near the well for experiment no.1 has dropped from 100 meters

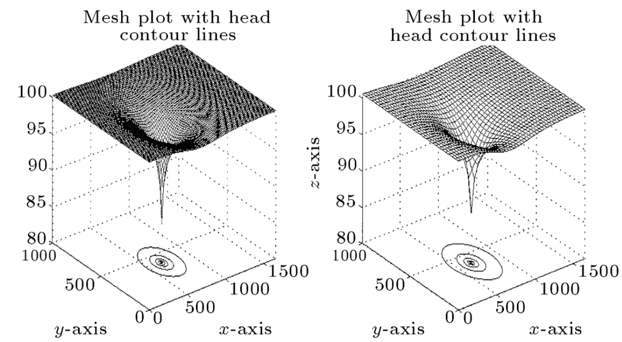


Figure 7. 3D view of the head for systems with one well.

to 88.5 meters. Figure 7b demonstrates this case for the unstructured grid. The difference between the two grids, in this case, is less than 0.15 percent. In the second stage, the results for the uniform grid case for experiment no. 2 are discussed. Figure 8a shows that the pressure near well number 2 has dropped from 100 meters to 86.3 meters. Figure 8b illustrates this case for the unstructured grid. The difference between the two grids, in this case, is less than 0.2 percent.

CONCLUSIONS

In this paper, a numerical solution has been presented for the flow in unsaturated, anisotropic porous media using the finite volume method. The main difficulties appear in treating the degeneracy of the model and the heterogeneity of the medium. The FVMP program focuses on unstructured finite volume computation of 2D and 3D flows with moving boundaries that are fundamentally encountered for flows in porous media. An interface capturing procedure is formulated with a stabilized finite volume scheme to solve the 2D and 3D flow equation in porous media. The idea of using the FVMP is to avoid updating the constructed mesh over the flow domain as the front of the interface advances with time through the discretized flow domain. The FVMP is embedded into the finite volume scheme by adding an extra advection equation and an additional unbounded degree of freedom to the number of the unknowns.

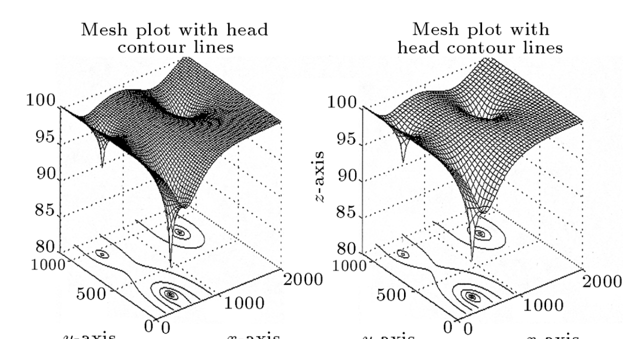


Figure 8. 3D view of the head for systems with three wells.

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