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THE METHOD OF THE LAPLACE TRANSFORM MULTIQUADRICS (LTMQ) FOR THE SOLUTION OF THE GROUNDWATER FLOW EQUATION

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Abstract. This paper presents a new numerical method, the Laplace Transform MultiQuadrics (LTMQ) method, developed for the solution of the diffusion-type parabolic Partial Differential Equation (PDE) of fluid flow through porous media. LTMQ combines a MultiQuadrics (MQ) approximation scheme with a Laplace transform formulation. The use of MQ in the spatial approximations allows the accurate description of problems in complex porous media with a very limited number of nodes. The Laplace transform formulation eliminates the need for time discretization, thus allowing an unlimited time step size without any loss of accuracy. LTMQ is tested against results from three test problems of groundwater flow obtained from a standard Finite Difference (FD) model, as well as from analytical solutions. An excellent agreement between the LTMQ and the analytical and FD solutions is observed, while significant reductions in computer execution times may be achieved.

1. Introduction

MultiQuadrics (MQ) is a true scattered data, grid-free scheme for representing surfaces and bodies in an arbitrary number of dimensions by using approximations given by an expansion in terms of upper hyperboloids. It is continuously differentiable and integrable, and is capable of representing functions with steep gradients with very high accuracy. Hardy [1] first derived MQ to approximate geographical surfaces and magnetic anomalies, but it was mostly ignored until Franke [2] showed that MQ outperformed 29 other interpolation method. Micchelli [3] and Madych and Nelson [4] provided the theoretical justification for the performance of MQ. Micchelli [3] demonstrated that MQ belongs to a class of conditionally positive definite functions, and that the MQ coefficient matrix is invertible for distinct points. Madych and Nelson [4] showed that for the space of conditionally positive definite functions to which MQ belongs, a semi-norm exists and is minimized by such functions.

The extension of MQ to applications in the solution of PDE's in computational fluid dynamics is credited to Kansa [5,6], who employed MQ to solve (a) the advection-diffusion equation, (b) the von Neumann blast wave problem, and (c) Poisson's equation. He showed that MQ (a) yields excellent results with a much coarser distribution of data points, (b) is an excellent estimator of partial derivatives, (c) does not need any special stabilizing treatment for instability and numerical dispersion, (d) is far more efficient and accurate than standard Finite Difference (FD) schemes, and (e) is considerably more flexible and robust than FD in the solution of the traditionally troublesome problem of steep moving fronts.

Laplace transforms are a powerful tool in the solution of PDE's, but their application was limited to simple one-dimenional problems with homogeneous properties. By combining traditional space discretization schemes with Laplace transforms, Moridis and Reddell [7,8, 9,10,11] developed a family of new numerical methods for the solution of parabolic and hyperbolic PDE's, which includes the Laplace Transform Finite Difference (LTFD) [7,8,9], the Laplace Transform Finite Element (LTFE) [10], and the Laplace Transform Boundary Element (LTBE) methods [11]. These methods eliminate the need for time discretization of traditional numerical methods, while maintaining their flexibility in the simulation of heterogeneous systems with irregular boundaries.

The method of Laplace Transform MultiQuadrics (LTMQ) is based on the same concepts, but uses MQ as the space approximation scheme. In the present paper, the mathematical basis of LTMQ is developed for the solution of the parabolic-type PDE of groundwater flow, and the performance of the method is evaluated against results from analytical solutions and standard FD models.

2. The Laplace Transform MultiQuadrics (LTMQ) Method

The general equation of transient groundwater flow is obtained by combining appropriate forms of Darcy's Law and the equation of mass conservation [12], yielding:

$$\nabla \cdot (K\ \nabla H) = S_0\ \frac{\partial H}{\partial t} + Q, \tag{1}$$

where K is the hydraulic conductivity, H is the piezometric head, S_0 is the specific aquifer storativity, $Q = q\ \delta_c(x)\ \delta_c(y)\ \delta_c(z)$, q is the volumetric flow rate of a source or sink per unit volume, and δ_c is the Kronecker's delta. The solution of equation 1 with the LTMQ method is accomplished in the four steps described in the following sections.

2.1 Step 1: The Laplace Transform of the PDE

For a homogeneous and anisotropic two-dimensional porous medium, the Laplace transform of equation (1) expanded in cartesian coordinates yields

$$K_x \frac{\partial^2 \Psi}{\partial x^2} + K_y \frac{\partial^2 \Psi}{\partial y^2} = S_0\ \lambda\ \Psi - S_0\ H(0) + \frac{Q}{\lambda}\ , \tag{2}$$

where λ is the Laplace space variable, $\Psi = \mathcal{L}\{H\}$, and $\mathcal{L}\{\}$ denotes the Laplace transform of the quantity in brackets. It should be noted that the analysis in cylindrical coordinates is entirely analogous.

2.2. Step 2: The MQ Scheme in the Laplace Space

Following Madych and Nelson [4], we expand the continuous function Ψ in terms of MQ basis functions and an appended constant, i.e.

$$\Psi(\mathbf{x}) = a_1 + \sum_{j=2}^{N} \hat{g}(\mathbf{x} - \mathbf{x}_j) a_j, \tag{3}$$

where

$$\hat{g}(\mathbf{x} - \mathbf{x}_j) = g(\mathbf{x} - \mathbf{x}_j) - g(\mathbf{x} - \mathbf{x}_1), \qquad j = 2, \ldots, N, \tag{4}$$

$$g(\mathbf{x} - \mathbf{x}_j) = \left[(x - x_j)^2 + (y - y_j)^2 + r_j^2\right]^{1/2}, \quad r_j^2 = r_{min}^2 \left(\frac{r_{max}^2}{r_{min}^2}\right)^{(j-1)/(N-1)}, \quad j = 1, \ldots, N, \tag{5}$$

N is the number of basis functions (i.e. data points in space), and r_{max}, r_{min} are input parameters [6]. The set of linear equations relating the expansion coefficients a_j to the set of discretized values Ψ_i, $1 \leq i \leq N$ is

$$\Psi_i = \sum_{j=1}^{N} G_{ij}\ a_j, \quad G_{i1} = 1 \quad \text{and} \quad G_{ij} = \hat{g}(\mathbf{x}_i - \mathbf{x}_j) \quad \text{for} \quad 2 \leq j \leq N. \tag{6}$$

where the G_{ij} is i-th row of the coefficient matrix G. The first and second partial derivatives of Ψ_i with respect to x are

$$\left(\frac{\partial \Psi}{\partial x}\right)_i = \sum_{j=2}^{N} \left(\frac{\partial \hat{g}_{ij}}{\partial x}\right) a_j = \sum_{j=2}^{N} \left(\frac{\partial g_{ij}}{\partial x} - \frac{\partial g_{i1}}{\partial x}\right)\ a_j, \tag{7}$$

$$\left(\frac{\partial^2 \Psi}{\partial x^2}\right)_i = \sum_{j=2}^{N} \left(\frac{\partial^2 \hat{g}_{ij}}{\partial x^2}\right) a_j = \sum_{j=2}^{N} \left(\frac{\partial^2 g_{ij}}{\partial x^2} - \frac{\partial^2 g_{i1}}{\partial x^2}\right)\ a_j, \tag{8}$$

where

$$\frac{\partial g_{ij}}{\partial x} = (x_i - x_j)\ \ \left[(x_i - x_j)^2 + (y_i - y_j)^2 + r_j^2\right]^{-1/2}, \tag{9}$$

and

$$\frac{\partial^2 g_{ij}}{\partial x^2} = \left\{1 - \frac{(x_i - x_j)^2}{[(x_i - x_j)^2 + (y_i - y_j)^2 + r_j^2]}\right\} \left[(x_i - x_j)^2 + (y_i - y_j)^2 + r_j^2\right]^{-1/2}. \qquad (10)$$

The partial derivatives with respect to y are obtained in exactly the same manner. Substitution in equation (2) leads to the matrix equation

$$\mathbf{W}\,\vec{a} = \vec{b}, \qquad (11)$$

where the elements of the fully populated coefficient matrix $\mathbf{W}$ and the vector $\vec{b}$ are

$$\begin{aligned} W_{i1} &= -S_0\,\lambda \\ W_{ij} &= K_x\,\frac{\partial^2 \hat{g}_{ij}}{\partial x^2} + K_y\,\frac{\partial^2 \hat{g}_{ij}}{\partial y^2} - S_0\,\lambda\,\hat{g}_{ij}, \quad \text{for } 2 \le j \le N \\ b_j &= Q/\lambda - S_0\,H(0)_{ij}, \quad \text{for } 1 \le j \le N. \end{aligned} \qquad (12)$$

2.3 Step 3: The Solution in the Laplace Space

The MQ approximation of the PDE in the Laplace space results in N simultaneous equations. Since the matrix $\mathbf{W}$ is non-singular for distinct points, the vector of the MQ expansion coefficients $\vec{a}$ is given by

$$\vec{a} = \mathbf{W}^{-1}\,\vec{b}. \qquad (13)$$

The computation of $\mathbf{W}$, $\mathbf{W}^{-1}$ and $\vec{b}$ necessitates values for the Laplace paremeter λ. For a desired observation time t, λ is provided by the first part of the Stehfest [13] algorithm as

$$\lambda_\nu = \frac{\ln 2}{t}\nu\,, \quad \nu = 1, \ldots, N_S\,, \qquad (14)$$

where N_S is the number of summation terms in the algorithm and N_S is an even number between 6 and 20. Solution of (14) returns a set of N_S vectors of the transformed pressures $\vec{a}_\nu$

$$\vec{a}_\nu = \vec{a}_\nu(\lambda_\nu) = [\mathbf{W}(\lambda_\nu)]^{-1}\,\vec{b}_\nu(\lambda_\nu)\,, \quad \nu = 1, \ldots, N_S\,. \qquad (15)$$

To obtain a solution at a time t, all vectors $\vec{a}_\nu$, $\nu = 1, \ldots, N_S$ are needed, i.e. the system of simultaneous equations has to be solved N_S times.

2.4 Step 4: The Laplace Space Predictions at Desired Points

Once the $\vec{a}_\nu$ vectors are known, the Laplace space solutions $\vec{\Psi}_\nu$ at the original $\mathbf{x}_j$, $j = 1, \ldots, N$ points are obtained from equation (6). Then the transformed dependent variable at any point $\mathbf{x}_\kappa$ in the domain of interest is computed by direct substitution in the MQ equation (6).

2.5 Step 5: The Numerical Inversion of the Laplace Solution

The vector of the unknown heads $\vec{H}$ at any time t is obtained by using the Stehfest [13] algorithm to numerically invert the Laplace solutions $\vec{\Psi}_\nu$, yielding

$$\vec{H}(t) = \frac{\ln 2}{t}\sum_{\nu=1}^{N_S} V_\nu\,\vec{\Psi}_\nu, \quad \text{where } V_\nu = (-1)^{\frac{N_S}{2}+\nu} \sum_{\kappa=\frac{1}{2}(\nu+1)}^{\min\{\nu,\frac{N_S}{2}\}} \frac{\kappa^{\frac{N_S}{2}}(2\kappa)!}{(\frac{N_S}{2}-\kappa)!\kappa!(\kappa-1)!(\nu-\kappa)!(2\kappa-\nu)!}\,. \qquad (16)$$

The vector $\vec{\Psi}_\nu$ may include solutions at the original $\mathbf{x}_j$, $j = 1, \ldots, N$ points, predictions at another set of points $\mathbf{x}_\kappa$, $k = 1, \ldots, K$, or both.

Inverting known functions, Stehfest [13] determined the optimum $N_S = 18$ for double precision variables. However, Moridis and Reddell [7,8,9] determined that the performance of Laplace transform based numerical methods is precetically insensitive to N_S for $6 \leq N_S \leq 20$.

The solution in the Laplace space removes the need for time discretization, and eliminates the stability and accuracy problems caused by the treatment of the time derivative. An unlimited time step size is thus possible without any loss of accuracy. Due to the absence of a time truncation error, LTMQ offers a stable, non-increasing roundoff error irrespective of the time of observation t_{obs} because a single solution (involving N_S matrix inversions) is required, with a $\Delta t = t_{obs}$. On the other hand, in a standard MQ method or any other traditional numerical method solutions must be obtained at all the intermediate times of the discretized time domain, requiring longer execution times and continuously accumulating roundoff error in the process.

3. Verification and Evaluation

The LTMQ method was tested in three problems of groundwater flow for which analytical solutions exist. The LTMQ solution was verified through comparison to the analytical solutions, as well as the solutions obtained from a standard implicit FD simulator. Direct solvers were used to solve simultaneous equations in the LTMQ and FD methods. Double precision variables with 20 significant figures were used in all simulations.

3.1 Verification & Test Case 1

Test case 1 investigated the one-dimensional radial flow problem towards a well of radius $r_w \to 0$ in a homogeneous circular aquifer with infinite boundaries, the analytical solution to which was given by Theis [14]. The geometry, properties, and a FD solution of this problem can be found in Moridis and Reddell [8]. A single observation was made at $t_{obs} = 10\ days$. We used a $N = 7$ points and a $N_S = 8$ for the LTMQ solution.

The drawdown $s = H - H(0)$ results for both the analytical and the numerical solutions (LTMQ and FD) appear in Figure 1. For a more representative comparison, the LTMQ curve (in this and the remaining test cases) is computed from the MQ interpolation at the locations of the FD grid centers. The Theis solution and the LTMQ solution practically coincided, while the FD solution tended towards the LTMQ and the Theis solutions with an increasing number of time-steps corresponding to smaller Δt's.

Figure 2 shows the effect of N_S on the accuracy of the LTMQ scheme. The difference between the Theis and the LTMQ solutions is negligible for $6 \leq N_S \leq 20$. This implies that (a) the accuracy of LTMQ for this one-dimensional problem is practically insensitive to the value of N_S, and (b) a $N_S = 6$ suffices for an accurate solution. This drastically reduces the execution time and makes the LTMQ method even more efficient than theoretically predicted [13].

3.2 Verification & Test Case 2

The second test case involved one-dimensional groundwater flow from a point of high head (at the left boundary) towards a low head at the right hand boundary. The initial head is $H_1 = H(x, 0)$; at $t = 0$ the head at the right boundary is lowered to H_2. The piezometric head $H(x,t)$ is then given by

$$H(x,t) = H_1 + (H_2 - H_1)\ \text{erfc}\left\{(L - x)\ (S_0\ Z)^{1/2}\ (4\ K_x\ Z\ t)^{-1/2}\right\}, \tag{17}$$

where L is the length of the system, and Z is its thickness. The size and properties of this system appear in Figure 3, which compares the LTMQ solution to the (a) analytical solution and (b) the FD solution (obtained with a domain discretization in 52 equally-spaced gridblocks). For the LTMQ solution, $N = 10$ and $N_S = 8$. The accuracy of the LTMQ solution is demonstrated by its virtual coincidence with (a) the analytical solution, and (b) the FD solution obtained with a large number of small Δt's. For larger Δt's, the FD solution shows insufficient accuracy caused by larger truncation errors in the approximation of the time derivative.

3.3 Verification & Test Case 3

Test case 3 represented transient flow into a homogeneous and anisotropic aquifer with a fully penetrating well and constant discharge conditions. The origin of this two-dimensional, infinite-acting system is placed at the well. Assuming that the axes of the cartesian system coincide with the principal axes of the permeability tensor, the piezometric head distribution at $t = 20\ days$ is predicted along the $x = y$ axis, i.e. at an angle of 45° from the

x-axis. Only one quarter of the infinite domain (i.e. x in $[0, \infty)$, y in $[0, \infty)$) needs to be simulated in LTMQ and FD. For the LTMQ solution, $N = 35$ and $N_S = 8$. A total of 625 gridblocks were used in the FD simulation.

Figure 4 presents (a) the analytical solution [15], (b) the LTMQ solution, (c) the FD solutions, as well as (d) relevant information on the parameters used in this simulation. The same pattern observed in the two previous test cases is obvious: LTMQ produces an accurate solution, a fact indicated by its (a) virtual coincidence with the analytical solution and (b) the FD solution for a large number of small Δt's.

4. Summary and Discussion

A new numerical method, the Laplace Transform MultiQuadrics (LTMQ) method, has been developed for the solution of the diffusion-type parabolic Partial Differential Equation (PDE) of transient, near-incompressible fluid flow through porous media. LTMQ combines a MultiQuadrics (MQ) approximation scheme for the solution of the PDE with a Laplace transform formulation for the elimination of the need for time discretization. The use of MQ in the spatial approximations allows the accurate description of problems in complex porous media with a very limited number of gridded or scattered nodes. The Laplace transform formulation eliminates the time dependency of the problem, and consequently the need for time discretization. An unlimited time step size is thus possible without any loss of accuracy.

LTMQ proceeds in five steps: (1) a Laplace transform is performed on the PDE, (2) the transformed PDE is approximated using MQ, (3) the resulting system of simultaneous equations of the expansion coefficients is solved and the transformed vector of unknowns is determined in the Laplace space, (4) the transformed dependent variable at any point in the domain of interest is obtained by substitution in the MQ equation, and (5) the solution/prediction vector obtained in steps 3 and 4 is inverted numerically using the Stehfest algorithm [13]. The solution in the Laplace space renders the effects of the time step size on stability and accuracy irrelevant because time is no longer a consideration. LTMQ was tested against results from three one- and two-dimensional test problems obtained from a standard Finite Difference (FD) model, as well as from analytical solutions. An excellent agreement between the LTMQ, the FD and analytical solutions was observed. Due to its formulation, LTMQ requires solution of the simultaneous equations N_S times and a linear combination of the resulting N_S solutions. Although N_S theoretically ranges between 8 and 18, it was determined that a $N_S = 8$ is sufficient to provide an extremely accurate solution, and that only a marginal improvement is observed for a $N_S > 8$.

Compared to a standard MQ model, LTMQ does not increase the computer storage requirement because (1) the values of the unknowns at the previous time steps are not needed since no time discretization occurs, and (2) the N_S sets of unknowns are summed and stored in a single array. Compared to a standard FD method, LTMQ requires drastically fewer (at least one order of magnitude) gridded or scattered nodes for the same level of accuracy but produces fully populated matrices (as opposed to sparse banded matrices in FD). Execution times may be reduced by orders of magnitude because solutions in the LTMQ scheme are necessary only at the desired observation times, while in standard numerical and MQ schemes solutions are needed at all the intermediate times of the discretized time domain. The disadvantages of having to obtain N_S solutions for a single time step are outweighed by greater accuracy and an unlimited time step size.

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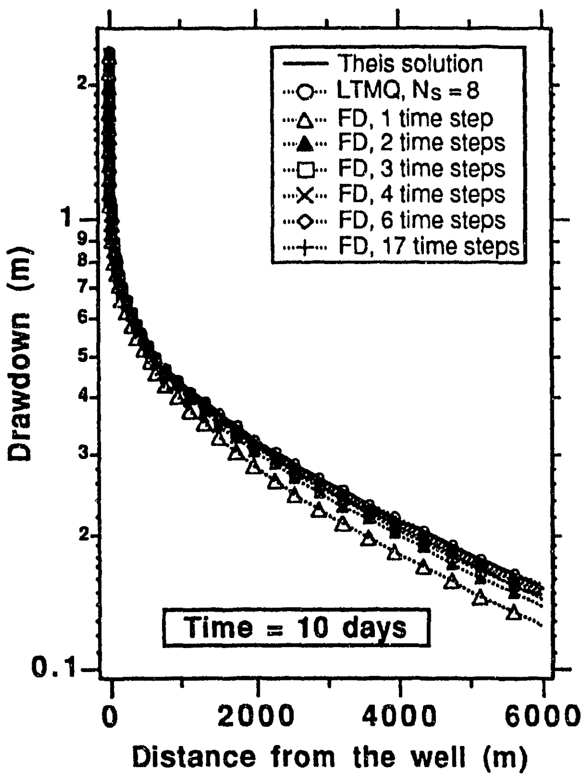

Fig. 1. Comparison of the LTMQ solution to the Theis and FD solutions in Teast Case 1.

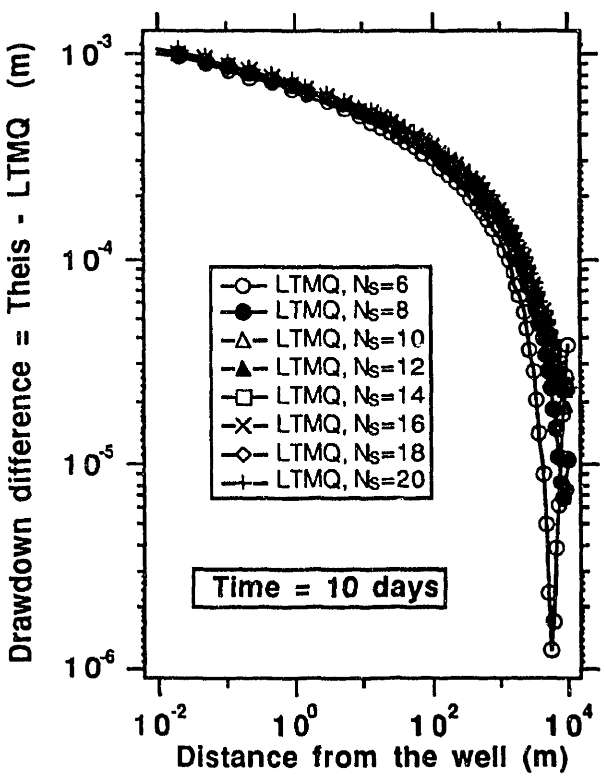

Fig. 2. Effect of N_S on the accuracy of the LTMQ method in Test Case 1.

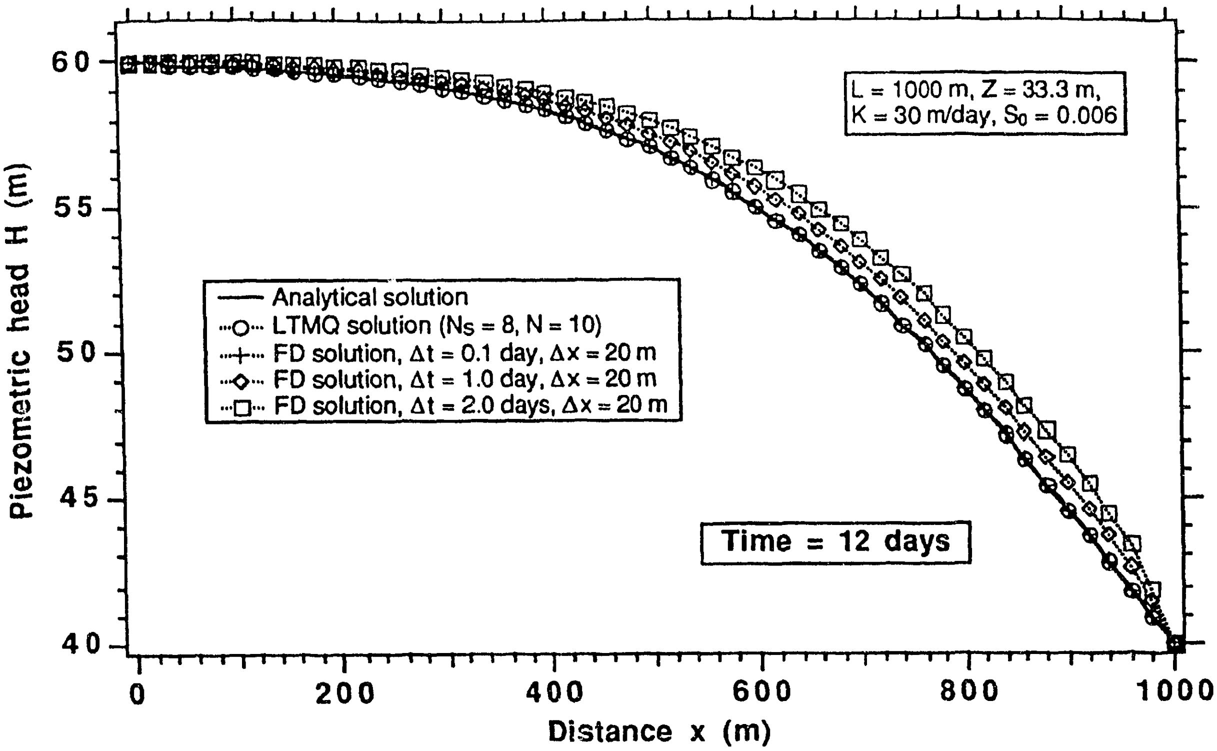

Fig. 3. Comparison of the LTMQ solution to the analytical and the FD solutions in Test Case 2.

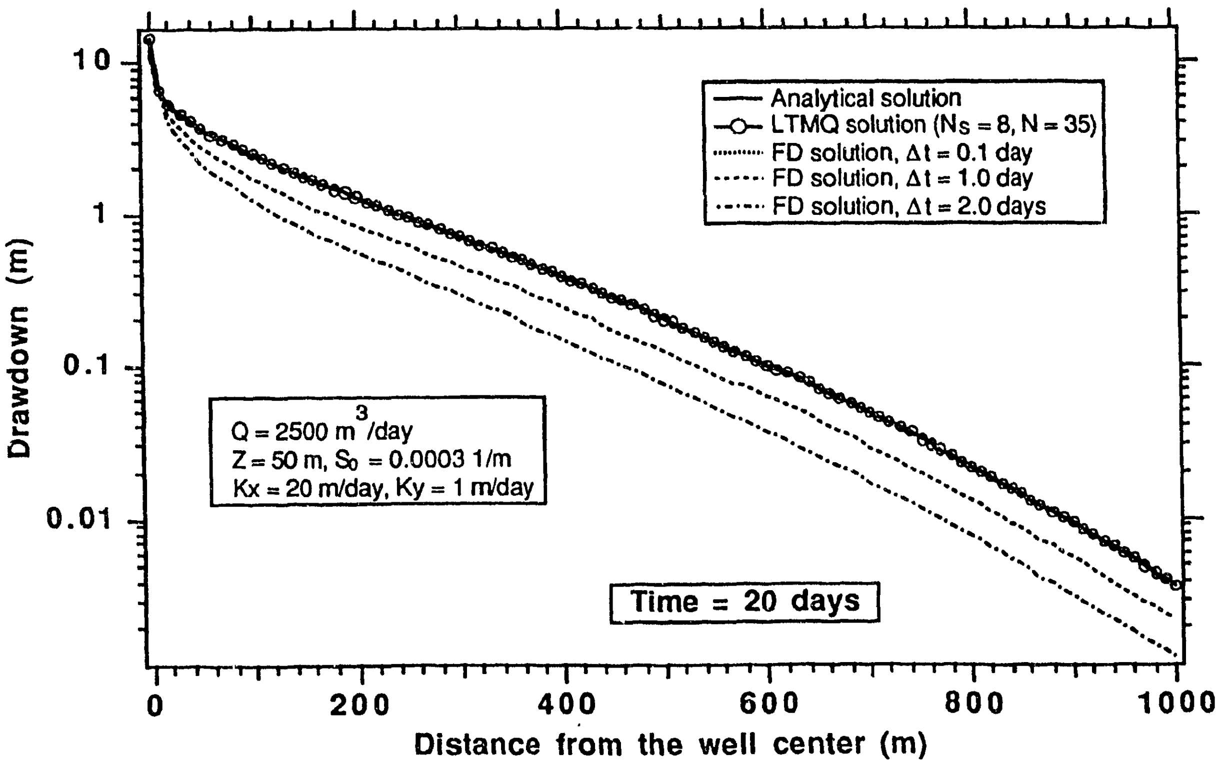

Fig. 4. Comparison of the LTMQ solution to the analytical and the FD solutions along the $x = y$ axis in Test Case 3.

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