Well bore boundary conditions for variably saturated flow modeling

R. Therrien a,*, E.A. Sudicky b

a Département de Géologie et Génie Géologique, Université Laval, Que., Canada G1K 7P4
b Department of Earth Sciences, University of Waterloo, Waterloo, Ont., Canada N2L 3G1

Abstract

Well bore boundary conditions are incorporated in a three-dimensional finite element model that solves the variably saturated groundwater flow equation. One-dimensional line elements, which are used to discretize the flow equation along the well screen, are superimposed onto three-dimensional porous media elements. The use of line elements allows the inclusion of well bore storage effects, and also avoids the need of a second iteration step during the solution of the nonlinear flow equation to achieve the correct head and flux distribution along the well screen. Verification of the formulation is done by comparing results from the numerical model to an analytical solution for pumping in an unconfined aquifer. Simulation of convergent–divergent flow into a heterogeneous unconfined aquifer illustrates that the model accounts for the aquifer heterogeneity by producing a variable fluid flux distribution along the well screen. This result has implications for the correct modeling of contaminant transport to the well. © 2000 Elsevier Science Ltd. All rights reserved.

Keywords: Groundwater flow; Variably saturated; Modeling; Well; Boundary conditions

1. Introduction

For an unconfined aquifer, where variably saturated conditions exist, a complete mathematical representation of groundwater flow to a well requires consideration of time-dependent drainage from above the water table, vertical components of flow in the saturated zone, and possible effects of well bore storage [10]. Since the relationship between discharge and drawdown is linear for a fully penetrating well in a confined aquifer, mathematical superposition can be used to solve the governing flow equation. However, the discharge–drawdown relationship is nonlinear for partially penetrating wells in confined aquifers, and also for variably saturated flow conditions. One must therefore resort to other mathematical techniques to correctly handle well bore boundary conditions in these nonlinear cases.

Cooley [1] presented a method to solve for flow to a well in a variably saturated flow model. In his two-dimensional finite difference model, the well bore constitutes a boundary of the domain. A uniform hydraulic head, corresponding to the water level in the well, is assumed to exist along the well screen. In the numerical solution, the model iterates to obtain this unknown hydraulic head and fluxes at the well screen, which need to be consistent with the prescribed pumping rate and the hydraulic properties of the aquifer. The model also allows a seepage face to develop at the well screen, which is the result of well bore storage effects. The height of the seepage face is determined iteratively during the solution. Neuman and Witherspoon [13] also presented an iterative method based on the same principle, including well bore storage, for a finite element saturated flow model. Another approach to represent well bore conditions consists in using elements, or finite difference cells, that have the same spatial dimension as the aquifer elements (see, for example, [10,11]). The size of these elements is equal to that of the well screen and they are assigned a very high permeability.

A fully coupled technique, termed the discrete well bore approach, has been presented in [4] to solve multiphase flow problems. With this approach, the well bore is represented by a second set of nodes, different from the porous medium nodes. Using these nodes, laminar Navier–Stokes flow is simulated along the well bore, as well as fluid exchange between well bore nodes and porous medium nodes. The approach allows the calculation of well bore saturation and pressure values different from the surrounding porous material.

In this study, the technique of Sudicky et al. [15] presented for saturated flow is extended to handle well
bore boundary conditions for three-dimensional variably saturated flow. With this method, one-dimensional elements representing the well are superposed onto the three-dimensional porous medium elements. This approach differs from those mentioned above, except the work from [4], because it fully couples the well and porous medium flow equations and eliminates the extra iteration step to determine the correct well bore flux distribution for heterogeneous media. The approach also allows the inclusion of well bore storage effects. Furthermore, the model can simulate time-dependent drainage from above the water table and vertical components of flow in the saturated zone, which are considered nonnegligible [10].

We will first present the governing equations describing variably saturated flow for the porous medium and the well screen, and summarize the numerical scheme proposed for their solution. A comparison of the method to an analytical solution for pumping in an unconfined aquifer will then be presented. Finally, we will illustrate the capability of the proposed method by simulating variably saturated flow in a heterogeneous aquifer undergoing pumping and injection.

2. Governing equations

The three-dimensional variably saturated groundwater flow equation, derived from mass conservation, is [1,12]

\[
\frac{\partial}{\partial x_i} \left( K_{ij} \frac{\partial (\psi + z)}{\partial x_j} \right) + Q \pm q_n \big|_{r_s} = S_w r_s \frac{\partial \psi}{\partial t} + \theta_s \frac{\partial S_w}{\partial t},
\]

\[i, j = x, y, z,\]

where \(x_i\) and \(x_j\) are the spatial coordinates, \(K_{ij}\) the porous medium hydraulic conductivity tensor \([L/T]\), \(K_{rw}\) the medium relative permeability, and \(\psi\) and \(z\) are the pressure and elevation head \([L]\), respectively. The specific storage coefficient of the medium is \(S_w [L^{-1}]\), the water saturation is given by \(S_w\), and \(\theta_s\) is the saturated water content, which is equal to the porosity. Fluid sources or sinks in the domain are represented by \(Q\) and fluid exchange between the aquifer material and the well screen is represented by the term \(q_n\) in Eq. (1). This equation is nonlinear since the water saturation and the relative permeability are functions of the unknown pressure head. It is assumed here, for generality, that these relationships can be described by any arbitrary function, such as those presented in [18].

Also based on mass continuity principles and making the assumption that flow is laminar along the well screen for the sake of convenience, the equation describing flow along the axis of a well having a finite storage capacity is [8]

\[
\pi \left( \frac{r_s^2}{L_s} + r_s^2 S_w \right) \frac{\partial (\psi_w + z)}{\partial t} - \pi r_s^2 K_w \frac{\partial^2 (\psi_w + z)}{\partial l^2} \pm q_n|_{r_s} \\
\pm Q \delta(l - l') = 0,
\]

where \(r_s\) and \(r_c\) are the radii of the well screen and well casing, respectively, and \(L_s\) is the total length of the screen. The pressure head in the well screen is given by \(\psi_w\) and the discharge or injection rate \(Q\) is applied at elevation \(l\) in the well screen. Eq. (2) was used by Lacombe et al. [8] to represent wells located in a fully saturated porous medium. To account for cases where the water level drops below the top of the well screen, a concept similar to a relative permeability is used to restrict flow along the well. This concept is described in more detail in Section 3.

The hydraulic conductivity of the well is obtained from the Hagen–Poiseuille formula [15]

\[
K_w = \frac{r_s^2 \rho g}{8 \mu},
\]

where \(\rho\) and \(\mu\) are the fluid density and viscosity, respectively, and \(g\) is the gravitational constant.

The first term on the left-hand side of (2) represents the storage coefficient of the well bore and comprises two parts: the storage resulting from the compressibility of the fluid and storage caused by the variation of the water level in the casing. Although it can be assumed that the former contribution is negligible, it is retained in the formulation. Similar to [15], the storage contribution arising from the change in water level is redistributed along the well screen.

3. Numerical formulation

To solve the coupled equations (1) and (2), the three-dimensional variably saturated flow model presented in [16] has been modified to incorporate the well bore equation (2). The model is based on the control volume finite element method [2] to discretize the flow equation. For variably saturated flow, it can be shown that the control volume finite element method, described in [2] and used in the model of Therrien and Sudicky [16], leads to the same discretized equations as produced by the Galerkin finite element method with lumping of the mass matrix. Therefore, the model presented here is similar to a standard finite element model. The control volume finite element formulation is chosen here because the Newton iteration technique can be efficiently programmed since the fluid flux terms between nodes are explicitly computed [3]. The Newton method is more robust than other techniques, for example, the Picard method, for the solution of nonlinear equations. Only the main steps of the numerical solution of the variably saturated flow equation are presented here; details can be found in [16].
An approximating function, \( \hat{\psi} \), is first defined for the unknown pressure head in the porous medium and in the well, according to

\[
\psi(x_i, t) \simeq \hat{\psi}(x_i, t) = \sum_j N_j(x_i) \psi_j(t),
\]

\[
\psi_w(x_i, t) \simeq \hat{\psi}_w(x_i, t) = \sum_{K \in \Omega} \Omega_K(t) \psi_{wK}(t),
\]

where \( N \) and \( \Omega \) are linear interpolation functions defined for the porous medium and the well screen, respectively. Nodal values of pressure head for the porous medium are \( \psi_j \), with nodal index \( J \) ranging from unity to the total number of nodes, \( n \). The pressure head in the well is \( \psi_{wK} \), with \( K \) being the set of nodes located on the well screen. The standard Galerkin technique (see, for example, [5]) is used to discretize Eqs. (1) and (2) over the domain of interest. The divergence theorem allows the reduction the order of the derivatives in Eqs. (1) and (2) and a lumped approach is taken to represent the storage terms. The time derivative is approximated by an implicit finite difference representation.

The porous medium is discretized in three dimensions with either rectangular prisms, triangular prisms or tetrahedra, and one-dimensional line elements are used to represent the well screen. Similar to [15], nodes attached to the well elements are coincident with those on the adjacent porous medium elements, and duplicate nodes are not employed. After carrying out the discretization procedure for all elements, the matrix contributions arising from the discretization of the well screen are superimposed onto those stemming from the discrete form of Richards' equation (1). Continuity in pressure head is therefore ensured at the well screen/porous media interface and thus avoids the need for a direct evaluation of the exchange fluxes between the well and the porous medium elements.

Upon assembly of all elemental contributions, the following discrete system of equations for the superimposed well and porous medium elements is obtained:

\[
\sum_{I=1}^{n} \left( \frac{(\psi_{I}^{L+1} - \psi_{I}^{L})}{\Delta t} \right) S_{wI}^{L+1} \left( \sum_{E_i} S_i \int_{E_i} N_I \, dE \right) + \sum_{I=1}^{n} \left( \frac{(S_{wI}^{L+1} - S_{wI}^{L})}{\Delta t} \right) \theta_I \int_{E_i} N_I \, dE \\
+ (\psi_{I}^{L+1} + z_I) \sum_{\eta_I \in \Omega_I} K_{I\eta} \int_{E_i} \frac{\partial N_I}{\partial x_i} \frac{\partial N_j}{\partial x_j} \, dE \\
+ \sum_{K=1}^{N_w} \left[ \frac{(\psi_{wK}^{L+1} - \psi_{wK}^{L})}{\Delta t} \pi \left( r_w^2 + r_w^2 S_w \right) \int_{E_k} \Omega_K \, dE \right] \\
+ (\psi_{wK}^{L+1} + z_K) \sum_{\eta_K \in \Omega_K} \pi r_w^2 K_w \int_{E_k} \frac{\partial N_I}{\partial x_i} \frac{\partial N_K}{\partial x_K} \, dE = 0,
\]

where the set of porous medium elements containing node \( I \) in their incidence list is given by \( E_I \), and \( \eta_I \) represents the set of nodes connected to node \( I \) through those elements. Similarly, \( n_w \) represents the total number of nodes associated with the well elements, \( E_K \) is the set of one-dimensional well elements containing node \( K \) in their incidence list and \( \eta_K \) represents the set of nodes connected to node \( K \) through those well elements. Note that because the control volume finite element formulation is used here, Eq. (6) is for a node, while the standard finite element formulation results in an elemental equation. As mentioned above, both formulations are identical when the mass matrix is lumped for the finite element method. The time level in Eq. (6) is given by superscript \( L \), with \( L + 1 \) representing the unknown time for which the solution is sought. For an implicit time discretization, all integrals in (6) are evaluated at time \( L + 1 \).

To simulate the portion of the well above the water table, where there is no flow in the well bore, a correction term analogous to a relative permeability is used to reduce the hydraulic conductivity of the well in Eq. (6). Numerical experiments have shown that if a zero relative permeability is used for those well nodes that are above the water table and have negative pressure heads, convergence difficulties arise in the Newton iteration. To avoid these difficulties, but still restrict flow in the well above the water table, the correction term is chosen such that the equivalent hydraulic conductivity of the well becomes lower than that of the surrounding porous matrix, typically by two orders of magnitude. The well nodes that are above the water level therefore have a negligible contribution to the total flow.

The discretized nonlinear equations are solved using the Newton iteration method and the final system of linearized matrix equations is solved by a preconditioned GMRES solver [17]. A self-adjusting adaptive time-step algorithm, based on the maximum permissible change in pressure or saturation during a given time step, permits an efficient time-step selection procedure for transient simulations [16].

### 4. Verification problem

The numerical formulation for representing wells in unconfined formations was verified by comparing to results from the analytical solution of Kroszynski and Dagan [6]. This solution directly accounts for both the unsaturated and saturated portions of a pumped aquifer. The verification is made for the problem described in [6], which consists of pumping an unconfined aquifer with a single partially penetrating well.

The aquifer has a constant thickness of 13.0 m and its lateral extent is assumed infinite in the analytical
solution. A single well having a radius of 0.3 m is located in the aquifer, with its screen extending between the intervals of 5.0–7.0 m above the base of the aquifer. The aquifer is homogeneous, with a horizontal hydraulic conductivity equal to 40.0 m/day and a vertical hydraulic conductivity equal to 10.0 m/day. The solution of Kroszynski and Dagan [6] is limited to unsaturated properties described by the following equations:

\[
k_{rw} = e^{a(\psi - \psi_c)},
\]

\[
S_w = e^{a(\psi - \psi_c)},
\]

(7)

where \(a\) is a parameter describing the unsaturated characteristics of the aquifer and \(\psi_c\) is the air-entry pressure. The values of \(a\) and \(\psi_c\) for the verification problem are 2.0 m\(^{-1}\) and \(-0.35\) m, respectively. The water content of the aquifer ranges from a saturated value of 0.3 to a residual value equal to 0.1. For this problem, in accordance with [6], the elastic contribution to storage in the aquifer is neglected.

Because of the symmetry of the problem, only one quadrant of the aquifer is discretized, with the pumping well located at the origin. The three-dimensional domain has dimensions of 160.0 m in both the \(x\) and \(y\) directions, and a thickness of 13.0 m in the \(z\) direction. The nodal spacing varies, with a finer horizontal discretization near the pumping well, and additional resolution vertically at the extremities of the well screen and near the water table. A total of 12 nodes in each of the \(x\) and \(y\) directions are used, and 30 nodes are used in the \(z\) direction. The three-dimensional grid thus contains a total of 4320 nodal points and 3509 rectangular prism elements, while four line elements are used to discretize the well screen.

Prior to pumping, static conditions are assumed in the aquifer according to equilibrium drainage, and the water table is initially located 3.0 m below the ground surface and overlain by a 0.35 m thick capillary fringe. It is assumed that no infiltration occurs at the surface, and all other boundaries of the model are impermeable. Care was taken to locate the lateral boundaries far enough to eliminate boundary effects during the pumping period. Pumping of the aquifer occurs at a constant rate of 800 m\(^3\)/day for a period of two days, with an initial time step equal to \(4 \times 10^{-5}\) days. During the simulation, a variable time-stepping option with a maximum permissible change in saturation equal to 0.05 is used. With the variable time-stepping, a total of 27 time steps were needed for the two-day simulation.

The drawdown at six observation points was recorded over the duration of the simulation and was compared to drawdowns computed with the solution presented in [6]. The location of these observation points is given in Table 1. The drawdown curves, presented in Fig. 1, are for the case where well storage is neglected because the analytical solution does not incorporate this effect. It can be seen that, at these locations, there is a very good agreement between the numerical model presented here and the analytical solution.

In a second simulation, we included the effect of well bore storage. Fig. 2 shows the comparison of drawdown calculated at the pumping well with and without well bore storage. It can be seen that, for this scenario, well bore storage reduces the drawdown in the well until a time equal to approximately 0.01 day (or 15 min). Also, the drawdown curve when storage is considered results in a straight line of slope close to 1.0 when plotted on logarithmic scales. This shape is typical of cases for which the effect of well bore storage cannot be neglected (see, for example, [7]).

![Fig. 1. Comparison to the analytical solution of Kroszynski and Dagan [6] for pumping in an unconfined aquifer. Lines represent the analytical solution, symbols represent the numerical results, and the numbers of each curve designate the different observation well locations provided in Table 1.](image-url)
The hydraulic conductivity of the aquifer varies spatially with a geometric mean equal to $1.0 \times 10^{-4}$ m/s and a variance equal to 1.0 for the log-transformed $K$ value. The elemental hydraulic conductivities were randomly generated with the algorithm described in [14], using an exponentially decaying autocorrelation function with correlation lengths $\lambda_x = \lambda_y = 1.0$ m and $\lambda_z = 0.2$ m. For simplicity, it is assumed that the unsaturated properties of the aquifer are uniform and are described with the following van Genuchten [18] relationships:

$$\theta = \left[ \frac{1}{1 + (\alpha \beta \psi)^n} \right]^m,$$  \hspace{1cm} (8)

$$k_{rw} = \theta^{1/2} \left[ 1 - (1 - \theta^{1/m})^{2n} \right]^2.$$  \hspace{1cm} (9)

The following parameter values were used for the aquifer material: $\alpha = 3.11$ m$^{-1}$, $m = 0.72$ and $n = 3.664$. The aquifer porosity is equal to 0.25 and a value of 0.07 is used for the residual water content.

The top and bottom boundaries of the system consist of an impermeable base at $z = 0.0$ m and the ground surface at $z = 2.0$ m, which is also impermeable because it is assumed that no infiltration occurs at the surface during the simulation. A natural gradient is assumed to exist in the system prior to the pumping and withdrawal, with horizontal flow oriented in the direction of increasing $x$ values. Fixed hydraulic head boundary conditions, with a value equal to 1.5 m at $x = 0.0$ m, and a hydraulic head equal to 1.29 m at $x = 9.0$ m, produce a gradient equal to 0.023. The two remaining lateral boundaries at $y = 0.0$ and 9.0 m are aligned in the direction of mean flow and are assumed to be no-flow boundaries.

Steady-state flow is simulated, with a constant injection rate of $1.0 \times 10^{-4}$ m$^3$/s, and a pumping rate equal to $1.5 \times 10^{-4}$ m$^3$/s. To check convergence of the Newton iteration, the maximum change of pressure head between successive iterations is calculated over the whole domain. Also, the residual value of Eq. (6) is computed at each iteration. Convergence is attained when both the maximum change in pressure head and the maximum residual value, in absolute values, are smaller than $1.0 \times 10^{-7}$. A total of four Newton iterations were required to reach convergence.

Results are shown in Fig. 3(a) in the form of a contour plot highlighting steady-state hydraulic head distribution for two planes; one vertical plane at $y = 4.5$ m, in the direction of regional flow and intersecting the two wells, and one horizontal plane located at $z = 0.5$ m. It can be seen that in spite of the heterogeneous hydraulic conductivity distribution, the hydraulic head contours appear quite regular. Fig. 3(b) shows more closely the vertical cross-section located in the direction of flow, at

5. Illustrative example

To illustrate the usefulness of the proposed algorithm to represent well bore conditions along a partially penetrating screen, a simulation of convergent–divergent flow in a heterogeneous unconfined aquifer is now presented. This scenario is chosen because it is representative of conditions prevailing during two-well tracer tests, a commonly used technique to determine flow and solute transport properties of heterogeneous aquifers (see, for example, [9,19]). The analysis and interpretation of these tests usually rely on measured breakthrough concentrations at the extraction well, or at intermediate observation wells. The observed concentrations are influenced by the flux distribution along the well screen arising from local aquifer heterogeneities. Since numerical models are often used as interpretative tools to reproduce the breakthrough data through the adjustment of the advective–dispersive properties of the system, it becomes important that the correct flux distribution around and along the well screen be represented by the model.

For this hypothetical example, the domain considered has dimensions of $9.0$ m $\times$ $9.0$ m in the $x$ and $y$ horizontal directions, and $2.0$ m in the $z$ direction. Two partially penetrating wells, having each a radius equal to 0.1 m, are located in the aquifer. The injection well is located at $x = 2.0$ m and $y = 4.5$ m, and is screened from elevations $z = 0.0$–$0.9$ m. The pumping well is located at $x = 7.0$ m and $y = 4.5$ m, with a screen extending from $z = 0.0$ to 1.1 m. The domain is discretized with rectangular prism elements having constant dimensions of 0.25 m in the $x$ and $y$ directions, and 0.05 m in the $z$ direction. This generates a total of 56129 nodes and 51840 elements.

Fig. 2. Comparison of drawdown in the pumping well with and without well bore storage.
y = 4.5 m, and illustrates the hydraulic head contours and the position of the water table. The water table is gently dipping towards the pumping well, with a break in slope occurring very near the pumping well (at x = 7.0 m). At the pumping well, the water table is located below the top of the screen, indicating the formation of a seepage face, and a zone of desaturation close to the top of the well screen.

Fig. 4 illustrates the flux distribution along the axis of the two wells. This distribution is back-calculated after solution by using the computed heads in Eq. (1) for the porous medium, reassembling the matrix, and then computing the resulting well fluxes $q_w$. It can be noted that there is an order of magnitude change in the flux along the screen in the two wells. The implications of this flux variation along the well screens are significant if one were to perform solute transport simulations to reproduce results from a two-well tracer test, using the present scenario. For example, nodal concentrations at the pumping well would need to be averaged by the corresponding fluid fluxes to get an estimate of the total well concentration. Since the fluxes can vary by an order of magnitude (Fig. 4), a simplification in determining the fluid fluxes could lead to large errors when calculating the concentration in the well.

6. Conclusions

An extension of the numerical approach proposed in [15] is presented to handle well bore boundary conditions in an unconfined aquifer for variably saturated conditions. The method consists of superposing one-dimensional line elements representing the well screen, onto three-dimensional porous medium elements. This ensures continuity of heads and fluxes at the nodes common to the well screen and the porous medium, and allows the simultaneous solution of the equation describing flow along the axis of the well screen and that representing three-dimensional variably saturated flow in the aquifer. The algorithm has been verified by reproducing results from an analytical solution for pumping in a variably saturated aquifer. An illustrative example focusing on divergent–convergent flow in a heterogeneous unconfined aquifer demonstrates that a realistic variable flux distribution along the well screen can be obtained with the proposed method. These results can in turn be used in the analysis of solute migration between wells in unconfined heterogeneous aquifers.

The method has not been thoroughly tested against the dual node method presented by Forsyth and Sudicky [4] for the solution of the variably saturated flow problem. Although the dual node method is required to solve multiphase flow problems, the very small volumes associated with the well bore nodes can lead to convergence problems during the Newton iterations, which is not the case with the present method where well contributions are added to the porous matrix contributions. Our experience with the Forsyth and Sudicky [4]...
model suggests that the present method is a viable alternative to simulate well bore conditions in variably saturated media.

Acknowledgements

This work was supported by the Natural Science and Engineering Research Council of Canada (NSERC) research grants to R. Therrien and E.A. Sudicky. The insightful comments of two anonymous reviewers have helped improve the paper.

References