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New developments in mathematical modeling of groundwater systems

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EXTENDED ABSTRACT

The numerical modeling of groundwater flow in unconfined aquifers is much more involved than in confined aquifers. This is because the governing equation (i.e., Richard's equation) is highly nonlinear and is subject to nonlinear boundary conditions as well. This nonlinearity is related to the dependence of the relative permeability and the water retention in the unsaturated zone on the pressure head. Moreover, fully saturated models are typically associated with boundary conditions such as constant head, pumping/injection flow rates, and leakage flux through a semi-confining bed. These are essentially linear and do not pose additional challenges to standard numerical solution techniques. This is not the case for unconfined flow models where some boundary conditions are nonlinear and therefore are unknowns a priori; thus, they are an integral part of the numerical solution. A typical example is the free and moving water table boundary. Another complication in modeling unconfined groundwater flow is to locate the position of seepage faces when the water table reaches the land surface. The seepage boundary faces are not known prior to the numerical solution and are, therefore, not fixed as typically done with other boundary conditions. Additionally, wells pumping groundwater from unconfined aquifers might become dry as the water table drops below the well screens, and natural or artificial drains may stop draining groundwater as the levels drop below predefined elevations. These are typical examples that necessitate additional bookkeeping procedures during the nonlinear iterative solution process when solving for an unconfined groundwater flow model. Furthermore, natural groundwater flow occurs mostly in highly heterogeneous and anisotropic materials, thus increasing the nonlinearity of the resulting discrete algebraic systems of the equations. Hence, robust and advanced numerical methods are needed in this context.

Modeling unconfined groundwater flow subject to free and moving boundaries is performed using two broad classes of methods. The first category assumes a fixed mesh. Within this class, an algorithm should determine the spatial and temporal distribution of three types of cells: wet, dry, and partially wet cells (i.e., crossed by the water table). The second category considers a moving mesh that adapts to the dynamics of the water table boundary. Hence, unlike for a fixed mesh method, the dry zone (i.e., approximate unsaturated zone) is not part of the computational domain. The main advantage of an adaptive mesh technique is to solve a saturated groundwater flow equation, hence a linear system of algebraic equations, during each iteration of the mesh adaption process. Meanwhile, more elaborate algorithms are needed for mesh adaption and the interpolation of hydraulic properties between moving cells.

The fixed mesh approach is probably the most widespread owing to the availability of many computer

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implementations such as MODFLOW developed by the USGS at the United States of America. Legacy versions of MODFLOW were criticized for an unphysical representation of unconfined groundwater flow dynamics, leading to a numerical instability for highly nonlinear problems. This was due, in part, to the heuristics upon which the decision to rewet a previously dry cell are based. Second, Picard iteration for some highly nonlinear problems may converge at a very slow rate or not at all. The latest releases include, however, a new Newton–Raphson-based formulation that substantially improves the computational stability. Another known difficulty within the fixed mesh approach derives from the way to artificially hide the flow patterns in the dry cells. Because this is not possible as the mesh is fixed, different approaches have been developed to tackle this problem. Desai (1988) developed a two-dimensional finite element model that linearizes the relative permeability function and recast it as a function of hydraulic head. The same approach was used by scientists in the framework of three-dimensional finite element models. Other authors used a sharp representation of this function; that is, the hydraulic conductivity in all dry cells is multiplied by a small residual factor (i.e., ~10−2–10−3). New developments presented the numerical solution of 3D unconfined seepage problems with the smoothed finite element method borrowed from solid mechanics (Kazemzadeh-Parsi, 2013). A limitation of the fixed mesh approach is that the exact position and shape of the water table could only be determined by post-processing computed groundwater heads. Hence, it is expected that a moving mesh technique will always lead to a more accurate position and a smooth shape of the phreatic surface when compared with a fixed mesh approach using the same resolution.

The second class of methods solve a series of linear equations on a deforming mesh. The mesh is adapted iteratively to fit the water table position. Here, again, many sub-approaches have been developed that could be categorized as rigorous or simplified. As described in standard textbooks of Bear (1972), the phreatic surface does not only fulfill the zero-pressure condition, but it is a kinematic boundary condition too. In other words, it is an interface through which the effects of unconfined storage, net recharge, and nonlinear effects related to the changing shape of the surface geometry are balanced. To the best of our knowledge, the only published numerical model taking into account both conditions was presented by Knupp (1996); such kinematic boundary condition, even under steady-state conditions, cannot be neglected.

Solving unconfined groundwater flow with a moving mesh technique using a finite difference method has some limitations. These problems do not exist when using a conforming (i.e., nodal-based) finite element technique such as the Galerkin weighted residual approach. However, while the groundwater head and the water table shape obtained by the conforming FEM using a moving mesh method might be accurate, it is well known that this is not the case for the specific discharge field. Moreover, the conforming FEM is not exactly mass conservative, which is problematic for nodes sharing elements with a high contrast of hydraulic conductivities. Post-processing techniques were introduced to derive continuous nodal-specific discharge fields, but it was reported that this procedure has a high computational cost. Mixed finite element methods were introduced to simultaneously approximate a scalar variable and its first-order derivative fields. Promising results highlighting a higher accuracy of this approximation technique when compared with alternative techniques were obtained for flow problems. The mixed finite element method leads, however, to an indefinite system of algebraic equations which is difficult to solve with direct or iterative methods. A hybridization technique avoids this problem by reformulating the mixed problem with primary unknowns on the faces of the mesh and using local algebraic relationships to recover the cell-centered heads and the normal specific discharge components. This gives rise to a method formally known as the mixed hybrid finite element method (MHFEM). Previous works established the outstanding behavior of this method to tackle groundwater flow problems in highly heterogeneous and anisotropic formations. While the MHFEM approximation was used for many classes of groundwater flow problems such as unsaturated flow and two-phase flow, to the best of the authors' knowledge, this is the first time that it has been used in combination with a deforming mesh approach to solve an unconfined flow in phreatic aquifers.

The objective of this paper is to introduce a new state-of-the-art three-dimensional MHFEM numerical model for confined–unconfined groundwater flow in complex aquifer systems characterized by irregular geometries, heterogeneous and anisotropic materials, and nonlinear boundary conditions of a practical relevance. These include, in particular, the nonlinear kinematic and seepage face boundary conditions generally ignored or weakly dealt with in previous studies. The work also deals with the model formulation and numerical discretization on layered unstructured grids.

In summary, determining the water table shape and position in unconfined aquifers is fundamental to many groundwater flow assessment studies. The commonly used industry standard fixed mesh models, contrary to popular belief, do not provide an accurate description of the phreatic surface. When using such models, the water table position is post-processed from the simulated groundwater heads, leading to an approximation error. This error becomes larger for coarse vertical grids.

This paper introduces a novel moving mesh technique to simulate the groundwater table in three-dimensional unconfined aquifers under steady-state or transient conditions. We adopt the face-based mixed-hybrid finite element discretization approach in space, leading to a more accurate approximation of the specific discharge field. The model uses an adaptive unstructured but layered mesh which is iteratively adjusted until its top fits the phreatic surface. The developed algorithm accounts for a linearized form of the kinematic boundary condition prescribed on the moving boundary and also supports usual boundary conditions as well. The model was compared to the existing analytical, fixed mesh, and previously published solutions. The obtained results show that the developed model is superior in terms of its numerical stability, convergence behavior, and accuracy. Furthermore, the simulated phreatic surface is free from a cellwise interpolation error and independent of the vertical grid size as used in fixed mesh methods. We also found that the ro-bustness of the moving mesh method cannot be surpassed by a fixed mesh alternative. The model's efficiency is supported by an almost quadratic rate of convergence of the outer iteration loop. Several theoretical and realistic examples are provided to demonstrate the model's accuracy, efficiency, and capability to successfully simulate unconfined groundwater flow with this novel moving mesh technique.

Keywords: Numerical modelling; Unconfined flow; Kinematic boundary condition; Water table position; Moving mesh; 3D mixed hybrid finite elements