Abstract

In this work, the possibility of using techniques to reduce linear systems to achieve more efficient groundwater flow modeling in systems of conjunctive use of water is studied. Thus, the main focus of this investigation is to relate the parameterization of the surface-ground water relationships with the characteristics of the reduced models and to find the consequences of such parameterization on the efficiency of the model's reduction.

The first proposed methodology, called Eigenvalue Method with Selective Compression and Modal Masking (EVM-SCMM), dramatically reduces the size of a groundwater flow model, increasing its execution's efficiency and decreases its required virtual memory. For practical purposes, EVM-SCMM uses the following new concepts: (*i*) effective modes, (*ii*) residual modes, (*iii*) modal participation limit, (*iv*) effective modes mask and (*v*) percentage of mass conservation. Those concepts not just allow to identify the modes that contribute to the most of the aquifer response to the external excitations; they also help to achieve a faster aquifer flow simulation than it is obtained with classical EVM. The main advantage of EVM-SCMM is that, augmenting the number of cells, allows to consider a more detailed description on the spatial variability of the aquifer's hydraulics parameters in groundwater flow modeling, having a little effect on the computational efficiency of the simulations, especially when a system of conjunctive use of surface and ground water is modeled. The EVM-SCMM has been tested on simple homogenous rectangular aquifers. The results have an accuracy similar to those obtained using EVM or Finite Differences (FD), but the simulation is more efficient. A sensitivity analysis of the impact of changing the parameterization of the river's boundary conditions, in function of the riverbed's conductance, over some control parameters as heads, stored volumes and internal fluxes is presented. It has been found that decreasing the riverbed's conductance improves the performance of EVM-SCMM because fewer modes are needed to obtain accurate results.

The conceptual framework of the EVM-SCMM allows to develop physically based criteria to generate effective modes more efficiently, to remove residual modes and to build the modal mask that accelerates the execution of the simulations. Based on the above ideas, algorithms to generate effective modes and to configure modal masks are proposed. These algorithms are based on iterative methods to solve a sparse symmetric generalized eigenvalue problem (SSGEVP), combined with physical indexes that allow to evaluate the effectiveness of any generated mode and to stop a sequence of the eigenpair's generation. The detection of the effective modes is carried out evaluating their participation factors and comparing them with the modal participation limit. The stop of the effective modes generation process is evaluated calculating the aggregate percentage of mass conservation on the aquifer and comparing it with a lower limit previously imposed to the reduced model. The advantage of include those criteria on solving a SSGEVP are that, first, they avoid to perform unnecessary iterations and, second, they approximate accurately the mass conservation equation for the water volume entering to the aquifer from the External Actions (EA). Another advantage of using iterative based on the sparse matrix-vector product methods for solving SSGEVP is that the disperse matrix structure of the model can be use to save arithmetic operations and storage in the generation of modes.

In this work, two iterative sparse generators of effective modes have been implemented. The first generator of effective modes is based on a modification of the deflated conjugate gradient iteration; it uses ILU preconditioning to accelerate the vector iterations and to minimize the Rayleigh quotient. This vector generation has proven to work very fast when a small amount of the lesser magnitude effective modes are needed. The algorithm generates sequentially each mode, calculates the modal allocation coefficients to check if such mode is effective, computes the accumulated allocation coefficients and checks the stop criteria to finish the generation. On the other hand, the second generator of effective modes is based on the rational Lanczos iteration with explicit restart to calculate sequentially sets of modes. The explicit restart deflates a new initial Lanczos vector to prevent the convergence towards one of the already available eigenvectors. Once each restart has built another set of modes, the generator calculates the allocation coefficients for each new mode and checks which of them are effective. This process is repeated for all new modes. Then, the accumulated allocation coefficients are calculated and the generator checks if the stop criteria has been achieved for all EA to stop the generation. If the stopping criteria has not been achieved, another restart is performed using a new spectral shift to improve the modal convergence. The results of many numerical experiments have shown that rational Lanczos generator is very efficient, even for large scale models where the spatial domain of the aquifer has been discretized using tens of thousands of nodes belonging to a FD network. The two proposed generators of effective modes have been applied to reduce models for: (*i*) a rectangular homogeneous aquifer connected with an straight river, (*ii*) a rectangular heterogeneous aquifer connected with a straight river and (*iii*) a highly heterogeneous aquifer with irregular boundaries connected with a sinuous sloped river. The results of the simulations show that the iterative generation of effective modes is more efficient than calculating the complete spectra of the respective SSGEVP.

An extension of the Rational Lanczos Reduction Method (RLANRM) to simulate efficiently surface-ground water relationships in models of conjunctive use systems is proposed. The classical RLANRM is used to form an orthogonal base of a Krylov reduction subspace. Also, the accumulated volumetric allocation factors of the Lanczos vectors are used as criteria for stopping the generation of the Krylov subspace, evaluating if the mass conservation equation for the income volume from the external excitations is satisfied properly. The reduction scheme is applied on the groundwater flow model to obtain a sequence of reduced systems of linear equations, whose solutions represent the states of the aquifer along the simulation horizon. To allow the calculation of the aggregated exchange volumes of water between aquifer and river during each simulation step, a discrete time pendent integration procedure of the aquifer's Lanczos states has been proposed. The concept of control parameters is included on the RLANRM to accelerate the calculations of surface-ground water relations and other required state variables. Finally, the RLANRM has been tested on simple homogenous rectangular aquifers. The results are compared to those obtained using: (*i*) embedded multi-reservoir models, (*ii*) models solved using classical EVM and (*iii*) models solved using FD. It was found that RLANRM behaves better than FD, achieving a comparable performance to the exhibited by the truncated EVM, but it is less efficient than the embedded multi-reservoir models. An analysis of the impact of changing the parameter of the river's boundary conditions, in function of the riverbed's conductance, over some control parameter as heads, stored volumes and internal fluxes is presented. It has been found that decreasing the conductance improves the performance of RLANRM because fewer Lanczos vectors are needed to obtain accurate results.

The EVM-SCMM and the RLANRM have proven to be powerful tools to reduce groundwater models. Here, EVM-SCMM and RLANRM have been applied to reduce groundwater models of two complex highly discretized linear heterogeneous aquifers. The former is a rectangular aquifer, connected with a straight river with three bands of homogenous values for the hydraulic properties; the second one is a highly heterogeneous aquifer with irregular boundaries connected with a sinuous sloped river. In both aquifers, the application of each reduction technique consisted in an sensitivity analysis of the influence of the river boundary condition's parameterization, in function of the riverbed's conductance and the reduction's parameters (modal participation limit for the EVM-SCMM and the size of Krylov reduction subspace for the RLANRM) in a more accurate representation of some selected control parameters as heads, stored volumes and surface-ground water relationships. The results have shown the power of both techniques to reduce efficiently groundwater flow models, but the main differences between them are: (*i*) EVM-SCMM is more computationally demanding than RLANRM to calculate the reduction subspace, but the execution of the flow model is faster, (*ii*) RLANRM calculates more accurately distributed aquifer's state variables as heads, stored volumes and internal fluxes if the parameterization of the rational Lanczosíteration is set appropriately, (*iii*) EVM-SCMM obtains global surface-ground water relations more efficiently and accurately than RLANRM. The main conclusion of these applications is that the choice of any of both methodologies depends on the type of the problem to be solved and/or the desired control parameters to be better represented in the reduced simulations.