

A COMPARISON OF ITERATION SCHEMES FOR THREE-DIMENSIONAL FINITE-DIFFERENCE SATURATED-UNSATURATED FLOWS WITH NON-ORTHOGONAL GRIDS

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ABSTRACT

The finite-difference method offers advantage in terms of simplicity of discretization and has been widely used for simulating saturated-unsaturated flow. However, geometrically complex flow domains have not been expressed well by conventional finite-difference models which are basically defined on orthogonal coordinate system. To overcome this shortcoming, a finite-difference saturated-unsaturated flow model that can treat non-orthogonal grids using a coordinate transformation method was presented. Picard iteration scheme is a widely used for Richards' equation. This method is simple to implement but converges slowly. The Newton method is comparatively complex but converges faster than the Picard method. One of our purposes in this study is evaluating the performances of two methods for FDM using the coordinate transformation technique. Another object is about treating cross-derivative terms. The cross-derivative terms derived in the coordinate transformation procedure are quite difficult to treat in implicit manner in practical aspect because 19-stencil is given in three-dimensional problems, which make the programming extremely complex. Therefore, the cross-derivative terms are usually evaluated in explicit manner and the other terms are evaluated in implicit manner. However, the Newton-Krylov method does not require forming 19-stencil directly. Instead of it, it is required to calculate the matrix-vector product which can be approximated by taking differences of the original nonlinear function in the procedure of Newton-Krylov method. It is a major advantage of the Newton-Krylov method that all the terms can be evaluated in implicit manner without forming 19-stencil matrix, which may give higher convergence speed and allow larger time step than the scheme evaluating the terms in partially implicit manner. But there is additional cost of the Newton-Krylov method for calculating the original nonlinear function at every Krylov iteration step. In this study, the performances of the Newton method, the Picard method, which are evaluating the equation in partially implicit manner and the Newton-Krylov method were assessed through steady-state test problems with curvilinear flow domain.

1 INTRODUCTION

Modeling of saturated-unsaturated flow through porous media is an important research topic and involved in various branches of water resources engineering, agricultural engineering, chemical contaminant tracing, and rainfall-runoff modeling. Although several analytical solutions of the governing equation of saturated-unsaturated flow through porous media have been reported (Broadbridge & White, 1988; Hogarth & Parlange, 2000; Menziani et al. 2007; Parlange, 1972; Philip, 1957), it is found that these solutions are generally obtained under simple initial and boundary conditions. Hence, numerical models are usually used to investigate saturated-unsaturated flow in porous media, where analytical solutions are not appropriate. Particularly in hydrological engineering, the saturated-unsaturated subsurface flow model are used as a tool to investigate the processes related with new findings obtained by observation studies. For example, to more deeply understand the hydrological processes of a hillslope including the nonequilibrium and preferential flow, the saturated-unsaturated subsurface flow model has been widely used in many recent researches (Gerke & Van Genuchten, 1993; Gwo et al., 1995; Jarvis, 1998; Keim et al, 2006; Kosugi et al., 2004; Liang et al., 2009; Simunek et al., 2003). Over the past three decades, many numerical models including finite-difference models (FDMs) and finite-element models (FEMs) have been developed for simulating saturated-unsaturated flow (Celia et al., 1990; Clement et al. 1994; Forsyth et al., 1995; Jones & Woodward, 2001; Tocci et al., 1997). Other approaches such as a finite-volume approach, a mixed finite-element approach, and an Eulerian-Lagrangian approach have also been developed for simulating saturated-unsaturated flow (Bause et al., 2004; Farthing et al., 2003; Huang et al., 1994; Manzini & Ferraris, 2004). In particular, this thesis will focus on modeling of FDMs. FDMs have certain advantages with respect to the ease of coding and understanding owing to its simplicity of discretization as compared to the other models. However, a disadvantage of FDMs has been also

pointed out; FDMs do not accurately represent all geometrically complex flow domains with low resolution, especially in multidimensional simulations.

Because saturated–unsaturated flow equation systems are highly nonlinear, implicit temporal discretization and iterative procedures are generally needed for numerical stability. The Picard and Newton iteration methods are common approaches for modeling of the saturated–unsaturated flow. These two methods have their own advantages and disadvantages. The Picard method is simple to implement and cost-efficient (per iteration basis). However, it converges slowly than the Newton method. On the other hand, the Newton method is comparatively complex to implement and consumes more CPU resources than the Picard method. But it converges fastly. Paniconi et al. (1991) and Paniconi & Putti (1994) compared FEMs using two iteration methods in one, two and three-dimensional problems and assessed their performances. They showed that if initial guess at the first iteration is good, the Newton method is more robust and converges fastly than the Picard method. However, the Newton method is more sensitive to initial guess than the Picard method and often fails to converge in particular problems, especially in steady-state problems. They also insisted that the hybrid of the Picard and Newton method can overcome the disadvantages of both methods while keeping advantages of both methods. To overcome this disadvantage, An et al. (2010) applied the coordinate transformation method to FDM of simulating saturated–unsaturated flow. Their model showed good performance for curvilinear flow domain and proved that FDM with the coordinate transformation method is an attractive numerical model.

Coordinate transformation represents diffusion with cross-derivative terms. Therefore, the transformed equation requires a 19-point stencil instead of a 7-point stencil, which is required by the conventional FDM with an orthogonal grid. All the terms including the cross-derivative terms are quite difficult to treat in implicit manner in practical aspect because it makes the programming extremely complex. Therefore, the cross-derivative terms are usually evaluated in explicit manner and the other normal-derivative terms are evaluated in implicit manner. In this approach, the 7-point stencil is calculated implicitly by the iterative calculation, as in the case of the conventional FDM. However, there is another way to avoid complexity of programming besides the 7-point stencil strategy. The Newton-Krylov method does not require forming 19-stencil matrix directly. Instead of it, it is required to calculate the matrix-vector product which can be approximated by taking differences of the original nonlinear function in the procedure of Newton-Krylov method. Newton-Krylov method is combination of Newton method for linearization and Krylov subspace method for solving linearized simultaneous equation. It is a major advantage of the Newton-Krylov method that all the terms can be evaluated in implicit manner without forming 19-stencil matrix, which may give higher convergence speed and allow larger time step than the scheme evaluating the terms in partially implicit manner. But there is additional cost of the Newton-Krylov method for calculating the matrix-vector product at every Krylov iteration step. Hence, it is expected that there is a trade-off between the Newton-Krylov method and the 7-point stencil Newton iteration method.

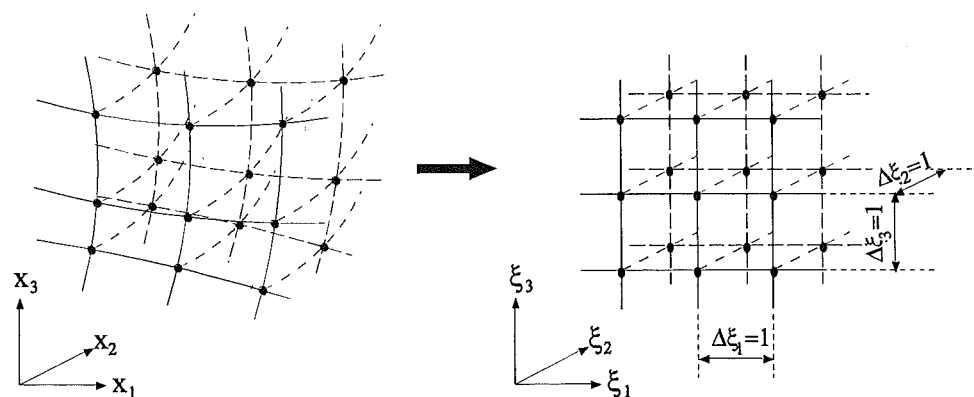


Figure 1. Concept of coordinate transformation: an arbitrarily shaped mesh in physical space is transformed into an orthogonal mesh in computational space.

2 ITERATION METHOD

Referring to An et al. (2010), coordinate-transformed Richards' equation from physical space, $(x_1, x_2, x_3) = (x, y, z)$, to computational space, $(\xi_1, \xi_2, \xi_3) = (\xi, \eta, \zeta)$ as Fig 1. is written as

$$\frac{1}{J} \frac{\partial \theta}{\partial t} - \sum_{p=1}^3 \sum_{q=1}^3 \frac{\partial}{\partial \xi_p} \left\{ G^{p,q} K \frac{\partial \psi}{\partial \xi_q} \right\} - \sum_{p=1}^3 \frac{\partial}{\partial \xi_p} H^p K = 0, \quad (1)$$

where ψ is the pressure head, θ is the volumetric moisture content, K is the hydraulic conductivity function of ψ , t denotes the time, G and H are defined as

$$\frac{1}{J} = \frac{\partial(\xi_1, \xi_2, \xi_3)}{\partial(x_1, x_2, x_3)}, \quad G^{p,q} = \sum_{r=1}^3 \sum_{s=1}^3 \frac{K_{r,s}^e}{J} \frac{\partial \xi_p}{\partial x_r} \frac{\partial \xi_q}{\partial x_s}, \quad H^p = \sum_{r=1}^3 \frac{K_{r,3}^e}{J} \frac{\partial \xi_p}{\partial x_r}, \quad (2)$$

where $K_{r,s}^e$ is anisotropy tensor element of the hydraulic conductivity. If the diagonal entries of $K_{r,s}^e$ equal one and off-diagonal entries zero, it express an isotropic medium. J is the Jacobian determinant, meaning the ratio of the control volume in the physical space to that in the computational space, and $G^{p,q}$ and H^p represent the mesh skewness and the anisotropy tensor. The terms with $p = q$ of Eq. (3.6) represent normal-derivative contributions and the other terms ($p \neq q$) represent cross-derivative contributions. The backward Euler approximation of coordinate-transformed Richards' equation is written as

$$\frac{1}{J} \frac{\theta^{n+1} - \theta^n}{\Delta t} - \sum_{p=1}^3 \sum_{q=1}^3 \frac{\partial}{\partial \xi_p} \left\{ G^{p,q} K^{n+1} \frac{\partial \psi}{\partial \xi_q} \right\}^{n+1} - \sum_{p=1}^3 \frac{\partial}{\partial \xi_p} H^p K^{n+1} = 0, \quad (3)$$

where superscripts n denotes the time level.

2.1 Newton Method

In the Newton method, all nonlinearities of equation are taken into consideration as follows:

$$f(\psi^{n+1,m}) - \frac{df(\psi)}{d\psi} \Big|^{n+1,m} \delta\psi^m = 0, \quad (4)$$

where $f(\psi)$ is Richards' equation, superscripts m denotes the iteration level and $\delta\psi^m (\psi^{n+1,m+1} - \psi^{n+1,m})$ is updating value. Nonlinearities of Richards equation is involved with the term of $\theta(\psi)$ and $K(\psi)$. Applying Eq. (4) to Eq.(3) gives

$$\begin{aligned} & \frac{1}{J} \frac{\theta^{n+1} - \theta^n}{\Delta t} - \sum_{p=1}^3 \sum_{q=1}^3 \frac{\partial}{\partial \xi_p} \left\{ G^{p,q} K^{n+1,m} \frac{\partial \psi}{\partial \xi_q} \right\}^{n+1,m} - \sum_{p=1}^3 \frac{\partial}{\partial \xi_p} H^p K^{n+1,m} \\ & + \frac{C^{n+1,m}}{J \Delta t} \delta\psi^m - \sum_{p=1}^3 \sum_{q=1}^3 \frac{\partial}{\partial \xi_p} \left\{ G^{p,q} K^{n+1,m} \frac{\partial(\delta\psi^m)}{\partial \xi_q} \right\} \\ & - \sum_{p=1}^3 \sum_{q=1}^3 \frac{\partial}{\partial \xi_p} \left\{ G^{p,q} \delta\psi^m \frac{\partial K}{\partial \psi} \right\}^{n+1,m} \frac{\partial \psi}{\partial \xi_q} \Big|^{n+1,m} - \sum_{p=1}^3 \frac{\partial}{\partial \xi_p} \left\{ H^p \delta\psi^m \frac{\partial K}{\partial \psi} \right\}^{n+1,m} = 0. \end{aligned} \quad (5)$$

2.2 Picard Method

The nonlinearities came from $K(\psi)$ are not considered in the Picard iteration method as follows:

$$\begin{aligned} & \frac{1}{J} \frac{\theta^{n+1} - \theta^n}{\Delta t} - \sum_{p=1}^3 \sum_{q=1}^3 \frac{\partial}{\partial \xi_p} \left\{ G^{p,q} K^{n+1,m} \frac{\partial \psi}{\partial \xi_q} \right\}^{n+1,m} - \sum_{p=1}^3 \frac{\partial}{\partial \xi_p} H^p K^{n+1,m} \\ & + \frac{C^{n+1,m}}{J \Delta t} \delta \psi^m - \sum_{p=1}^3 \sum_{q=1}^3 \frac{\partial}{\partial \xi_p} \left\{ G^{p,q} K^{n+1,m} \frac{\partial (\delta \psi^m)}{\partial \xi_q} \right\} = 0. \end{aligned} \quad (6)$$

The values of $K(\psi)$ are estimated at previous iteration step and their nonlinearities are not considered in implicit manner. Comparing Eqs. (5) and (6), it is found that the Picard method can be viewed as an approximate the Newton method neglecting the terms involving nonlinearities of $K(\psi)$, which are 6th and 7th terms of the left side of Eq.(5). It is well known that the Newton scheme converges quadratically whereas the Picard scheme converges linearly. A comparison of these two schemes used in FEM is well described in Lehmann, & Ackerer (1998), Paniconi et al. (1991), and Paniconi & Putti(1994).

2.1 Newton-Krylov Method

The Newton-Krylov method is combination of Newton iteration method for linearization of nonlinear system and Krylov subspace method for solving linear simultaneous equation. The link between the two methods is the Jacobian-vector product, which can be approximated from original nonlinear equation without estimating real Jacobian matrix. The history and details of Newton-Krylov method are well reviewed in Knoll & Keyes (2004).

In Newton-Krylov approach, a Krylov subspace method is used to solve the linear simultaneous equation. To solve the Eq. (4), an initial residual vector is defined as

$$f(\psi^{n+1,m}) - A \delta \psi^0 = r_0, \quad (7)$$

where A is matrix of $df(\psi)/d\psi$, $\delta \psi^0$ is an initial guess of $\delta \psi$, r_0 is an initial residual vector, and the time index n and iteration index m are dropped because the Krylov iteration is performed at fixed n and m . Then, based on Krylov subspace method, the solution of Eq. (4) can be expressed as

$$\delta \psi^l = \sum_{k=0}^{l-1} \beta^k (A)^k r_0, \quad (8)$$

where superscript l denotes Krylov iteration step, and β^k is scalar values determined to minimize the residual in Generalized Minimal RESidual (GMRES) algorithm. It is found that Eq. (8) requires the matrix A only in the form of matrix-vector product, which can be approximated by taking differences of the original nonlinear function as Brown and Saad (1990) and Chan and Jackson (1984):

$$Av \approx \frac{f(\psi + \varepsilon \psi) - f(\psi)}{\varepsilon}, \quad (9)$$

where v is an vector of $(A)^{k-1} r_0$, and ε is scalar value much smaller than the scalar elements of v . Eq. (9) is simply rewritten form of taking a first-order Taylor series expansion approximation of $f(\psi + \varepsilon \psi)$. The error in this approximation is proportional to perturbation ε and there are various options for choosing the perturbation parameter (Knoll & Keyes, 2004). The following formulation was used in this study as referring to Brown & Saad (1990):

$$\varepsilon = \frac{b}{\|\psi\|_2} \max \left[|\psi \cdot v|, \|v\|_1 \right] \text{sign}(\psi \cdot v), \quad (10)$$

where b is a constant whose magnitude is within a few orders of magnitude of the square root of machine roundoff, typically 10^{-6} for 64-bit double precision.

The matrix of $df(\psi)/d\psi$ does not required to be formed to solve nonlinear system in Newton-Krylov approach, which is the most attractive feature of Newton-Krylov method especially

for complex systems such as the transformed equation in this study. However, it should be also pointed out that there might be additional cost for calculating Eq. (9) at each Krylov iteration compared with the exact Newton iteration method, in which A is formed and the calculation cost for Av is neglectable.

3 NUMERICAL SIMULATION

Three linearization schemes, the Picard method with 7-point stencil, the Newton method with 7-point stencil and the Newton-Krylov method, are evaluated throughout test simulation. Van Genuchten (1980)'s equation for the soil water retention curve and Mualem (1976)'s equation for the unsaturated hydraulic conductivity function were used in this study. The sandyloam soil property referring to Carsel & Parrish (1988) was used in test simulation.

The performances of three iteration methods for steady state problem are investigated. Curvilinear domain with $21 \times 21 \times 21$ mesh is considered as shown in Fig. 2. The initial condition is $\psi_0(z) = 45 - z$ (m). All side boundaries are Dirichlet boundaries as $\psi_{\text{bound}}(z) = 45 - z$ (m) and no flux boundaries for top and bottom. Pumping well is placed at $(x = 626; y = 626)$ and water levels at the well are varied as $L = 10, 20$, and 30 (m). Well nodes are set as $\psi_{\text{well}}(z) = L - z$ (m) in $z \leq L$ and seepage face boundary in $z > L$.

Fig. 3 describes pressure head results performed by the Newton method. The results performed by the other two methods were very similar to Fig. 3. Table 1 lists total iteration number and CPU time taken by three iteration methods with line search method. Fig. 4 shows the convergence behavior of three iteration methods. The Newton-Krylov method more fastly converged than the other two methods as expected. The Newton method converged faster than the Picard method. At first few iterations the Newton and Picard method showed similar convergence behavior. But after few iterations the Newton converged more drastically than the Picard method. Even though the Newton-Krylov methods converged most fastly, the Newton method consumed least CPU resources in this test simulation. Average CPU cost per iteration of Newton-Krylov and Newton method were 1.38 and 0.19 sec in this simulation. Comparing the Newton method, the Newton-Krylov method requires additional cost for solving the matrix-vector product, Eq. (9), at Krylov iteration when linear equation is calculated. In this test simulation, 70-90 Krylov iterations were required to be solved for one outer iteration which is equivalent to the Picard or Newton iteration. This additional calculation consumed more than 80 % of CPU resources in Newton-Krylov iteration method. In conclusion, the Newton method was the most efficient iteration method in this test simulation. It is also found that the Picard method is not attractive iteration method for steady-state problems compared with the Newton method.

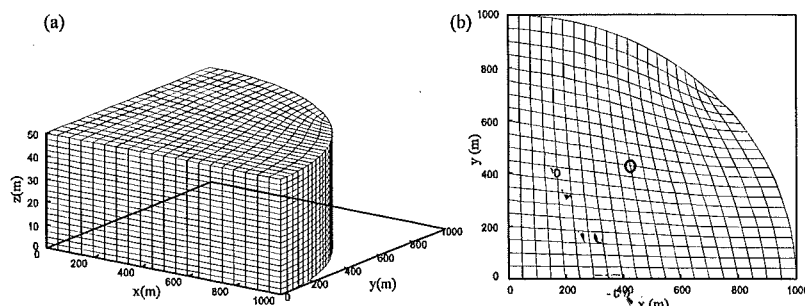


Figure 2. Curvilinear flow domain and grid used in test. (a) perspective view; (b) plane view and circle represents the place of pumping well

Table 1. Total iteration numbers and CPU times performed by three iteration methods.

Scheme	Total iteration number			CPU time (s)		
	L = 10	L = 20	L = 30	L = 10	L = 20	L = 30
Picard	342	151	83	76	30	15
Newton	36	25	21	8	5	3
Newton-Krylov	22	13	11	34	17	14

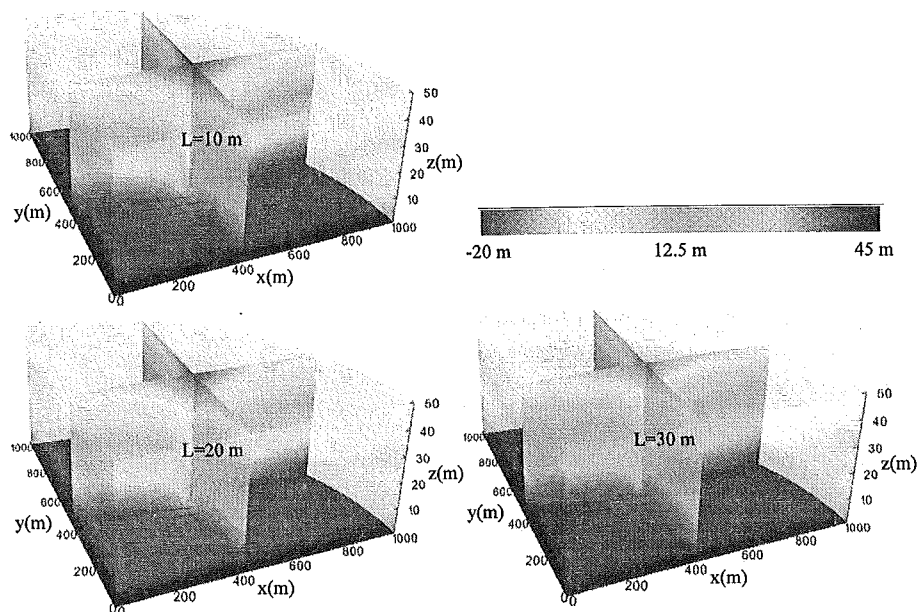


Figure 3. Pressure head results performed by the Newton method. A cross sectional distribution for $x = 626$, $y = 626$ and $z = 0$ m.

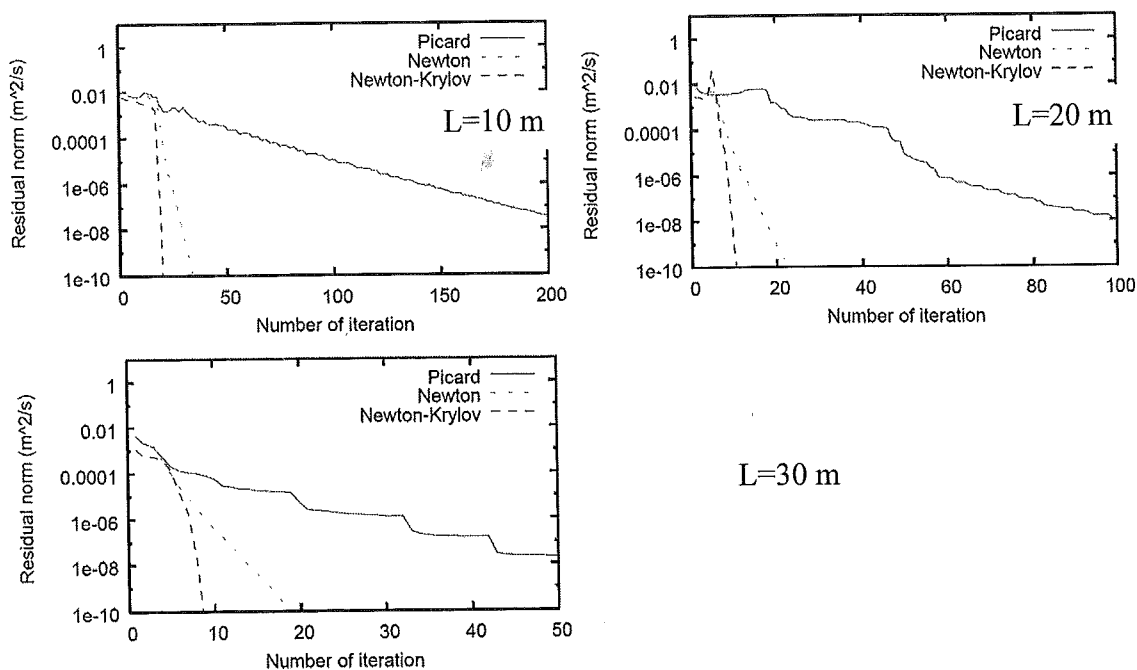


Figure 4. Convergence behavior of three iteration methods; L_1 residual norm are plotted

4 CONCLUSION

The performances of three iteration methods, the Picard, Newton and Newton-Krylov methods, for three-dimensional non-orthogonal finite difference model were compared. The Picard and Newton methods implemented 7-stencil strategy in which the cross-derivative terms are evaluated in explicit manner to avoid extremely complex programming and cost for forming 19-stencil matrix. On the other hand, Newton-Krylov method considered all terms in implicit manner while saving the cost for forming 19-stencil and avoiding complexity of coding because it requires calculating matrix-vector product instead of directly calculating 19-stencil exact Newton method. Theoretically, the results of the Newton-Krylov method are the same resulted by 19-stencil exact Newton method. However there is additional cost for calculating matrix-vector product per Krylov iteration compared with the exact Newton

method. Steady-state pumping well problem was considered as test simulation varying problems difficulties to compare convergence behavior of three iteration methods. The models using all three methods solved the problems stably. The Newton-Krylov method converged more fastly than the other two methods. However the Newton-Krylov required much more CPU resources per iteration than the other two methods. The Picard method converged much more slowly than the other two methods. As a result, the Newton method was most cost-efficient in our test case. This paper presented the performances of three iteration methods for steady-state problem. Further research on the performances of three iteration methods for unsteady-state case is ongoing.

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