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**IMPLEMENTATION AND TESTING OF TECHNIQUES FOR
IMPROVING THE PERFORMANCE OF RICHARDS'
EQUATION SOLVERS AND THE HANDLING OF
HETEROGENEOUS SOILS**

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TECHNIQUES FOR IMPROVING RICHARDS' EQUATION SOLVERS

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Abstract. Efficient, robust simulation of groundwater flow in the unsaturated zone remains computationally expensive, especially for problems characterized by sharp fronts in both space and time. Standard approaches that employ uniform spatial and temporal discretizations for the numerical solution of these problems lead to inefficient and expensive simulations. Accurate solution of the pressure-head form of Richards' equation is very difficult using standard time integration methods, because the mass balance errors grow unless very small time steps are used in the time integration process. Richards' equation may be solved for many problems more economically and robustly with variable time step size instead of constant time step size. But variable step-size methods applied to date have relied upon empirical approaches to control step size which do not explicitly control truncation error of the solution. In the first part of this thesis, we solve Richards' equation using the method of lines with a finite difference approach. We show how a differential algebraic equation implementation of the method of lines can give solutions to Richards' equation that are accurate, have good mass balance properties, and are more economical for a wide range of solution accuracy. We have implemented the method of lines using the higher order time integration ode solver **ode15s** to (i) assure robustness for difficult nonlinear problems and computational efficiency; (ii) develop high order adaptive methods for the time discretization taking into account the different time scales that may appear in the process; (iii) investigate the advantage of using higher-order methods in time. The numerical results demonstrate that the proposed method provides a robust and efficient alternative to standard approaches for simulating variably saturated flow in one spatial dimension.

In the 2nd part of the thesis, we to investigate the convergence and mass balance behavior in Richards' equation-based solvers. As hydrological models become increasingly sophisticated (e.g., coupling with various meteorological, ecological, or biogeochemical components) and are applied in ever more computationally demanding contexts (e.g., the many realizations that are typically generated in parameter estimation, uncertainty analysis, data assimilation, or scenario studies), the need for robust, accurate, and efficient codes is greater than ever. The Richards equation for subsurface flow is highly nonlinear and requires iterative schemes for its solution.

These schemes have been the subject of much research over the past two decades, but an effective all-purpose algorithm has thus far proven elusive. Ideally, rapid (quadratic as opposed to linear) and global (insensitive to initial guess) convergence is sought, in addition to applicability over a range of conditions (dry soils, storm-interstorm simulations, geological heterogeneity, 3D domains with complex boundary conditions, etc). Richards equation can be mathematically formulated and numerically discretized in a variety of manners, and the specific form and scheme chosen will affect the mass balance behavior of the model. We implement and test a promising nested Newton-type algorithm for solving Richards' equation. In the current state of the art, the Picard iteration method is widely used for solving the nonlinear equation governing flow in variably saturated porous media because this method is simple to code and computationally cheap. But the convergence is slow and sometimes fails. On the other hand, the Newton method is more complex and expensive than Picard. As a result the Picard method is more attractive than Newton. However, especially for strongly nonlinear flow problems, the robustness and higher rate of convergence makes Newton an attractive alternative in some cases. In this work the Picard and Newton schemes are compared with results of a nested Newton-type algorithm. Three test cases are presented and each problem is solved over a wide range of vertical discretization. The results highlight the different aspects of the performance of the iterative methods and the different factors that can affect their convergence and efficiency, including problem size, spatial and temporal discretization, convergence error norm, mass lumping, time weighting, conductivity, moisture content characteristics, and boundary conditions. It is suggested that nested Newton-type methods can be effectively implemented and used alongside Picard and Newton and numerical models of Richards' equation.

In the final part of the thesis, we studied the performance of a lookup table option, as an alternative to analytical calculation, for evaluating the nonlinear soil characteristics needed in the Picard and Newton schemes. This assessment is conducted for the CATHY (CATchment Hydrology) 3D Richards-based subsurface flow solver. The lookup table method can be a cost-effective alternative to analytical evaluation in the case of heterogeneous soils, but it has not been examined in detail in the hydrological modeling literature. Two layered soil test problems

are considered, and the robustness and accuracy of the lookup table method are assessed for uniform and nonuniform distributions of lookup points in the soil retention curves.

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1. INTRODUCTION

Modeling of variably saturated flow is an important problem of practical interest for which significant issues remain unresolved. Among them are the appropriate formulation of governing equations and constitutive relations [148]. While important formulation issues remain, the standard approach to model variably saturated flow is through the use of numerical solution to Richards' equation. Richards' equation represents the movement of water in unsaturated soils, and was formulated by Lorenzo A. Richards in 1931. Richards' equation is derived by combining Darcy's law with a mass conservation equation in porous media. It is a highly nonlinear parabolic partial differential equation (PDE) which is often difficult to approximate since it does not have a closed-form analytical solution.

The highly nonlinear nature of Richards' equation due to the dependence of the hydraulic conductivity and diffusivity on the moisture content, in combination with the non-trivial forcing conditions that are often encountered in engineering practice, makes Richards' equation practically impossible to solve using analytical approaches except for a few special cases [2, 92, 77]. The practical utility of analytic and semi-analytic solutions is limited by their respective assumptions, which most notably, are homogeneity of the soil medium and a simple mathematical form for the constitutive and forcing equations. Most of the analytic solutions are obtained using by the exponential hydraulic model. The governing flow equation becomes linearized by this exponential model, which allows us to determine the analytical solution.

Although analytical solutions may have limited practical applications, they do serve as a means for verifying many numerical models for unsaturated flow. These are especially useful for infiltration in very dry, layered soils where numerical models often suffer from lack of convergence and mass balance problems. In addition, the analytical solutions may enhance our understanding of the infiltration process under a transient state in layered soils.

The analytical solutions mentioned above are restrictive in nature and also limited to one-dimensional problems. Consequently, numerical treatments are needed to solve more complicated problems. Numerical methods for solving Richards' equation have been developed in the last few decades. It is desirable to develop appropriate numerical schemes for moisture flow in unsaturated porous media. As a result, a multitude of numerical algorithms has been proposed to approximate Richards' equation [2, 22].

The numerical solution of Richards' equation requires decisions about the form of the equation to be solved, the constitutive relations used to close the equation, the spatial approximation, the temporal approximation, the nonlinear equation solution, and the linear equation solution methods. Standard approaches have evolved for each of these decisions, together with potentially attractive alternatives to the standard choices in some cases [148].

For the numerical solution of Richards' equation, it is convenient to decouple the issues of temporal and spatial accuracy. The most common approaches for approximating Richards' equation use low-order finite difference or finite element spatial approximations and low-order time integration [53, 112]. In addition, most variably saturated flow simulators currently in use are based upon fixed spatial grids and either fixed time-step or an empirically based adaptive time stepping method [1, 22]. The numerical stability of the finite element models is improved by mass lumping since previous findings indicate that consistent mass formulation could cause numerical oscillations [22, 68, 91]. Previous studies highlight the importance of proper treatment of the time derivative for reliable numerical simulations [22, 74]. Typically used time stepping schemes are the backward Euler and Crank-Nicolson schemes. Other time stepping schemes used for Richards' equation include the three-level Lees scheme, the Douglas-Jones predictor corrector method, implicit Runge-Kutta schemes and backward difference formulae [72, 92].

The solution of the non-linear algebraic systems that arise in implicit numerical discretizations of Richards' equation has been the subject of significant research studies. Iterative schemes (e.g., Picard, Newton iteration methods, fast secant and relaxation methods) as well as non-iterative

methods (e.g., the implicit factored scheme) have been proposed to resolve the nonlinearities [9, 38, 74]. In practice, the fixed-point iteration scheme, or Picard method, prevalent due to its simplicity and satisfactory performance [81].

A differential algebraic equation-based method of lines (DAE/MOL) solution of Richards' equation can result in a more robust and efficient solution to Richards' equation than traditional approaches in some cases [135]. In this approach, estimates of temporal truncation error were used explicitly to control the solution order, which ranged from first to fifth order in time, and the time-step size.

Despite the above remarks, significant issues of robustness and efficiency remain for certain classes of difficult test problems, especially those that give rise to sharp fronts that propagate through the domain [148]. These sharp fronts in both space and time can require significant changes in spatial adaption as a function of temporal evolution of the problem. Numerical methods for Richards' equation were mainly limited to simple time stepping schemes coupled with finite difference or finite element spatial approximations. The two commonly used simple time stepping strategies, namely fixed time step and heuristic, within numerical hydrological simulations are crude and wasteful of computational resources [92]. This has paved the way to the introduction of adaptive algorithms, which adjust to the behavior of the solution and are generally more reliable and efficient than uncontrolled approaches. Adaptive spatial approximations for Richards' equation include mesh refinement, moving mesh, and subspace enrichment schemes. The most effective approaches often use a mixture of two or three of the basic methods. Theoretically, combined ψ and θ -based methods offer the fastest possible convergence rates. However, the complexity of data structures for some combined adaptive methods can be substantial [83].

Adaptive time integration methods include variable-step variable-order (up to fifth) differential-algebraic equation solver (DASPK) integrators [72, 74, 135, 148]. In all cases, formal truncation error control leads to considerable gains in accuracy and efficiency over fixed step and heuristic

time stepping algorithms, and also improves the mass balance of schemes based on the ψ formulation of Richards' equation. It suffices to say that unconditional stability is an important property of an effective time stepping scheme for Richards' equation, due to the stiffness of spatially discrete parabolic partial differential equations [74]. Hence, most production and research codes employ the implicit Euler algorithm, which is first order accurate but very stable.

1.1. Richards' equation for flow in variably saturated porous media.

Richards' equation can be cast in several forms, depending on whether pressure (ψ -based form), moisture (θ -based form), or both (mixed form) are used as state variables. Assuming the porous media and water are incompressible, the temporal variation of the water saturation is significantly larger than the temporal variation of the water pressure. We also assume that the air phase is infinitely mobile, so the air pressure remains constant, and we neglect source or sink terms.

With this assumptions the mixed form of Richards' equation can be written as :

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} \left[K(\psi) \left(\frac{\partial \psi}{\partial z} + 1 \right) \right] \quad (1.1)$$

where ψ is the pressure head $[L]$, $\theta(\psi)$ is the volumetric soil moisture content $[L^3 L^{-3}]$, $K(\psi)$ is the nonnegative hydraulic conductivity $[LT^{-1}]$, t is the time $[T]$, and z is the vertical coordinate assumed positive upward $[L]$.

Taking the advantage of the differentiability of the soil retention function, one may write as follows:

$$c(\psi) \frac{\partial \psi}{\partial t} = \frac{\partial}{\partial z} \left[K(\psi) \left(\frac{\partial \psi}{\partial z} + 1 \right) \right] \quad (1.2)$$

where $c(\psi) = \frac{d\theta}{d\psi}$ is the moisture capacity $[L^{-1}]$.

This version is referred to as the head-form (ψ -form) of Richards' equation. Another formulation of the Richards equation is based on the water content θ ,

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} \left[D(\theta) \frac{\partial \theta}{\partial z} \right] + \frac{\partial K}{\partial z} \quad (1.3)$$

where $D = \frac{K}{c(\psi)} = K \frac{d\psi}{d\theta}$ is the soil water unsaturated diffusivity [$L^2 T^{-1}$].

Generally, to solve the ψ -based form is the most commonly used because it has the advantage of being applicable to both saturated and unsaturated conditions and of accommodating heterogeneous soils. However, these approximations generally exhibit very poor preservation of mass balance problems, unacceptable time-step limitations [91], and relatively slow convergence [8] which seriously undermines its physical basis [73].

In contrast, the θ -based form is a conservation form by construction, i.e., it follows the mass conservation law. In this form, mass balance is improved significantly and rapidly convergent solutions can be obtained. But unfortunately they are strictly limited to unsaturated conditions, since in a saturated condition the water content becomes constant and D approaches infinity. Furthermore, for multi-layered soils, θ cannot be guaranteed to be continuous across interfaces separating the layers. Thus, this form may be useful only for homogeneous media [50].

The mixed form of Richards' equation is also mass conserved. It is applicable to both saturated and unsaturated porous media. This form of Richards equation is generally considered superior to the other two forms because of robustness with respect to mass balance [22, 83, 91]. However, conservation of mass alone does not ensure acceptable numerical solutions, as shown by some studies [22, 83].

1.1.1. *Constitutive relationship.*

To complete the model formulation of Richards' equation, we must specify the constitutive relationship to describe the interdependence among fluid pressures, saturations, and relative permeabilities. Many experimental data sets have been described using the van Genuchten [138] relation and many sets of parameters are available in the literature [139]. The standard range of the pore size distribution parameter n in the van Genuchten relationship varies from near to 1.0 [139] to near or even greater than 10.0 [76, 87]. If the values of n are increasing then the distribution of pore size is uniformly increasing. Most of the natural unconsolidated media tested showed $n < 2.0$ [139]. Convergence of the common numerical approaches to Richards equation faces difficulties because the van Genuchten and similar relations are not smooth [140, 141].

The computational cost is very high for the complex power functions in the van Genuchten and other constitutive relations [113]. If function values are tabulated and intermediate values are evaluated either by linear or higher order interpolation then the computational cost can be reduced during the simulation. The higher order effective interpolation is the cubic spline interpolation which constructs the C^2 continuous interpolation polynomials. Hence the polynomial value and function value are the same at each spline knot [113]. When $n < 2$ for the van Genuchten relation, cubic spline interpolation is very difficult to maintain the accuracy but this approach works very well for most porous media conditions. With this condition, at $\psi = 0$, the permeability and specific moisture capacity functions are not continuously differentiable and are thus less smooth than for $n \geq 2$. If we use cubic spline interpolation, then the solutions of the system of linear equations gives the 2nd derivatives of the interpolation polynomials at each of the spline knots whose dimension is equal to the number of spline knots. Near the non smooth region of the relation we can see significant oscillation for this type of problem which in this case occurs near the saturated-unsaturated transition area. To interpolate the intermediate function values we loss accuracy for these oscillations. If high accuracy is required then the convergence difficulties occurs for the nonlinear solver.

Generally, the pressure head becomes negative (capillary pressure increases) as the soil water content decreases. The water retention curve is defined as the relationship between the negative pressure head and the volumetric water content for a sample. This curve represents the behavior of a sample as water is added or removed from it. In practice, volumetric water content is plotted on an arithmetic scale and negative pressure head is plotted on either an arithmetic or logarithmic scale. These curves are determined experimentally and they are typically nonlinear regardless of how they are plotted. The shape changing of water retention curves depends on the nature of the soil such as drying (air replacing draining water) or wetting (entry of water to displace the air).

As mentioned, there are several mathematical relationships for the constitutive or water retention curves that are used in modeling. The most commonly used relationships are the Brooks-Corey [14] and the van Genuchten [138] equations. These two models illustrated in detail as follows:

1.1.2. *The Brooks-Corey model.*

The constitutive relationships proposed by Brooks and Corey [14] are given by:

$$\theta(\psi) = \theta_r + (\theta_s - \theta_r) \left(\frac{\psi_d}{\psi} \right) \quad \text{if} \quad \psi \leq \psi_d \quad (1.4a)$$

$$\theta(\psi) = \theta_s \quad \text{if} \quad \psi > \psi_d \quad (1.4b)$$

$$K(\psi) = K_s \left[\frac{\theta(\psi) - \theta_r}{\theta_s - \theta_r} \right]^{3+2/n} \quad \text{if} \quad \psi \leq \psi_d \quad (1.5a)$$

$$K(\psi) = K_s \quad \text{if} \quad \psi > \psi_d \quad (1.5b)$$

$$c(\psi) = n \frac{\theta_s - \theta_r}{|\psi_d|} \left(\frac{\psi_d}{\psi} \right)^{n+1} \quad \textbf{if} \quad \psi \leq \psi_d \quad (1.6a)$$

$$c(\psi) = 0 \quad \textbf{if} \quad \psi > \psi_d \quad (1.6b)$$

where θ is the actual volumetric water content, θ_r is the residual volumetric water content, θ_s is the porosity, $\psi_d = -\frac{1}{\alpha}$ is the bubbling or air entry pressure head (L) and is equal to the pressure head to desaturate the largest pores in the medium, and $n = 1 - \frac{1}{m}$ is a pore-size distribution index, whose value for many natural porous media ranges from 1.0 to 2.0 when determined using standard laboratory approaches and fitted using standard inverse techniques [139].

All of the above material parameters affect the shape of the soil hydraulic functions and satisfy $0 \leq \theta_r < \theta_s$ and K_s , α , $n > 0$.

1.1.3. *The van Genuchten model.*

Perhaps the most widely used empirical constitutive relations for moisture content and hydraulic conductivity are those of van Genuchten [138]. He proposed a method of determining the functional relationship of relative hydraulic conductivity to the pressure head by using the field observation knowledge of moisture retention. In turn, the procedure would require curve-fitting to the proposed moisture retention function with the experimental/observational data to establish certain parameters inherent to the resulting hydraulic conductivity model.

The model is given by:

$$\theta(\psi) = \theta_r + \frac{\theta_s - \theta_r}{[1 + |\alpha\psi|^n]^m} \quad \textbf{if} \quad \psi \leq 0 \quad (1.7a)$$

$$\theta(\psi) = \theta_s \quad \textbf{if} \quad \psi > 0 \quad (1.7b)$$

$$K(\psi) = K_s \left[\frac{\theta - \theta_r}{\theta_s - \theta_r} \right]^{\frac{1}{2}} \left\{ 1 - \left[1 - \left(\frac{\theta - \theta_r}{\theta_s - \theta_r} \right)^{\frac{1}{m}} \right]^m \right\}^2 \quad \text{if} \quad \psi \leq 0 \quad (1.8a)$$

$$K(\psi) = K_s \quad \text{if} \quad \psi > 0 \quad (1.8b)$$

$$c(\psi) = \alpha m n \frac{\theta_s - \theta_r}{[1 + |\alpha \psi|^n]^{m+1}} |\alpha \psi|^{n-1} \quad \text{if} \quad \psi \leq 0 \quad (1.9a)$$

$$c(\psi) = 0 \quad \text{if} \quad \psi > 0 \quad (1.9b)$$

where θ is the actual volumetric water content, θ_r is the residual volumetric water content, θ_s is the porosity, α is the mean pore size, $n = 1 - \frac{1}{m}$ is the uniformity of the pore-size distribution, whose value for many natural porous media ranges from 1.0 to 2.0 when determined using standard laboratory approaches and fitted using standard inverse techniques [139]. All the material parameters affect the shape of the soil hydraulic functions and satisfy $0 \leq \theta_r < \theta_s$ and $K_s, n, \alpha > 0$.

1.1.4. Permeability approximation.

For the case of $n < 2$, in the numerical simulation of saturated/unsaturated flow to evaluate the interblock permeabilities in the vicinity of saturation is another problem. In this region, for a small change of capillary pressure, the relative permeabilities can vary greatly. The method of estimating interblock permeabilities is very important to achieve nonlinear solver convergence.

In much of the existing numerical literature, the arithmetic average of the two neighboring cell permeability is used as the interblock relative permeability [56, 146, 152]. This procedure, however, results in an overestimation of interblock permeability and a smearing of the steep wetting front [152].

There are alternative approaches to estimate the interblock permeabilities such as geometric mean [56, 152], harmonic mean [56, 152], one and two-point upstream weighting [56], a Kirchhoff integral method [152], and a weighted averaging scheme based upon matching Darcy fluxes [146]. Some comparisons among the above methods have been completed but the general guidance is not yet available [152].

Since permeabilities vary in space as a function of ψ , so the estimation of the permeabilities is an important issues of the numerical approach within the spatial discretization scheme. Several procedures are available to evaluate the values of $K_{i\pm\frac{1}{2}}$ in the literature [56, 146, 152]. Three possible methods are as follows:

The arithmetic mean technique is [56, 146, 152] : $K_{i\pm\frac{1}{2}} = \frac{K_i + K_{i\pm 1}}{2}$ which is simple and inexpensive to compute.

Because K varies in space as a function of ψ , an integral representation of mean interblock values(KINT) can be computed as

$$K_{i\pm\frac{1}{2}} = \frac{1}{|\psi_i - \psi_{i\pm 1}|} \int_{\min(\psi_i, \psi_{i\pm 1})}^{\max(\psi_i, \psi_{i\pm 1})} K d\psi \text{ if } \psi_i \neq \psi_{i\pm 1}$$

$$K_{i\pm\frac{1}{2}} = K_z(\psi_i) \text{ if } \psi_i = \psi_{i\pm 1}$$

This approach is computationally expensive and thus not commonly used [119, 146, 152].

A third method considered for estimating $K_{i\pm\frac{1}{2}}$ is termed the arithmetic mean saturation (KAMS) and is computed by $K_{i\pm\frac{1}{2}} = K_z\{\frac{Se_i + Se_{i\pm 1}}{2}\}$. This approach is easy to compute and has appeared in the literature [152].

In this study, we used the arithmetic mean technique for all of the different numerical schemes.

For unsaturated media, hydraulic conductivity is not constant; it is strongly dependent on the degree of saturation. When the pressure head is close to zero, that is, the media is near to saturation then the hydraulic conductivity takes its maximum value. The hydraulic conductivity decreases when the media is dry; i.e., the water content reduces including the more negative pressure head and the pores of media filled by air. The approach of the volumetric water content to residual results in a water phase that may not even be continuous through the sample, giving a hydraulic conductivity that is close to zero. Therefore the concept of relative permeability or relative hydraulic conductivity has proven useful in capturing the relationship existing between hydraulic conductivity (K) and negative pressure head ($-\psi$) in the unsaturated zone. Hence relative hydraulic conductivity for unsaturated media can be defined using by the relation as follows:

$$K_r(\psi) = \frac{K(\psi)}{K_s} \quad \text{if} \quad \psi \leq 0 \quad (1.10a)$$

$$K_r(\psi) = 1 \quad \text{if} \quad \psi > 0 \quad (1.10b)$$

Where $K_r(\psi)$ is the relative hydraulic conductivity, which varies between 0 and 1, K_s is the saturated hydraulic conductivity, and $K(\psi)$ is the unsaturated hydraulic conductivity.

The moisture capacity is the analytical differentiation of water content with respect to the pressure head . When using this analytical expression for some simulations, severe difficulties arise near the saturation due to the shape of the water capacity function and the relative hydraulic conductivity function [142]. The slopes changes from $-\infty$ for $\frac{\partial \theta}{\partial \psi}$ and ∞ for $K_r(\psi)$ when $n < 2$ to zero when $n > 2$. In order to overcome this difficulty, two variants of a chord slope technique combined with a centred difference formula can be used [63, 110]. One variant uses the pressure head at the previous time step, the other at the previous nonlinear iteration.

1.1.5. *Approximation of specific moisture capacity $C(\psi)$.*

There are two different ways to evaluate the specific moisture capacity function. The first method is the tangent approximation which can be obtained with the analytical differentiation

of $\theta(\psi)$ (i.e, $C(\psi) = \frac{d\theta}{d\psi}$). The second method is the standard chord slope approximation [110]. The standard chord slope method is expressed by $C_i^{n+1,m} = \frac{\theta_i^{n+1,m} - \theta_i^n}{\psi_i^{n+1,m} - \psi_i^n}$, n is the time index and m is the Picard iteration index. Compared to the tangent method, the standard chord slope method can improve the mass balance of numerical schemes for ψ -based forms of Richards' equation [110]. Analytical differentiation is used to evaluate $C(\psi)$ in this study for all the cases.

In a numerical method, the flow domain is often divided into many cells. The differential equation as well as the boundary and initial conditions are approximated by discrete equations. Solving these discrete equations (on a computer) yields the head in discrete locations (nodes) and time. Popular numerical methods include the finite difference and finite element methods.

1.2. Numerical solution of Richards' equation.

Finite difference, finite element, and finite volume methods are the modern tools for solving partial differential equations. These methods often suffer to some degree from mass balance errors as well as from numerical oscillations and dispersion. Additional numerical problems may appear when the gravitational term becomes important. Finite elements are advantageous for several domains in two and three dimensions. In one dimension finite difference is advantageous because it needs no mass lumping to prevent oscillations. A mass conservative model for solving the mixed form of Richards' equation using a finite difference method has been presented in [22].

Numerical simulation of groundwater flow and transport requires solutions of large, sparse systems of equations. Thus, the complexity and size of problems that can be solved numerically are often constrained by the efficiency of the algorithm used to solve the resulting systems of equations. A number of studies have compared the efficiency of iterative algorithms used to solve a variety of two and three-dimensional, linear and nonlinear groundwater flow problems [55, 78, 88]. These investigations typically compared two or more iterative solvers such as the strongly implicit procedure, successive over-relaxation, conjugate gradient methods, and preconditioned conjugate gradient methods. Results of these comparisons varied depending on the specific problems, but there is general agreement that preconditioned conjugate gradient methods provide competitive convergence rates.

1.2.1. *Spatial discretization.*

The method of finite differences is the most popular numerical approach for the simulation of large reservoir systems. Conceptually finite difference methods are straightforward and there are several practical reasons for this popularity. The fundamental concepts are readily understood and do not require advanced training in applied mathematics. Because of their extensive history, they boast a firm theoretical foundation. In addition the form and algebraic simplicity of the equations arising from difference approximations has led to several clever algorithms being developed for their solution.

The use of the finite differences in subsurface simulation began in earnest with the development of the alternating direction algorithms [106]. The importance of numerical simulation in the forecast of reservoir performance was recognized early by the oil industry. In the period following the classic paper [106], there was astounding growth in the numerical methodologies proposed and the physical systems considered. Early work focused on single-phase reservoir simulation [18]. This was followed by black oil reservoir simulation, which involved two components, a volatile gas soluble in the oil phase and a nonvolatile component (black oil). Important details are found in [24, 32, 127, 129].

Moreover, models have been developed for forecasting reservoir behavior under tertiary recovery operations. Many of these simulators are chemically, thermodynamically, and hydrodynamically, e.g., thermal oil recovery simulation [47, 128], polymer flood behavior forecasting [12]. For problems of this complexity and degree of nonlinearity the simplicity and computational efficiency of finite difference methods has a justifiable attraction. Three excellent monographs on the application of finite difference theory to reservoir engineering have been published and the interested reader is referred to these publications for technical details [6, 26, 105].

The first application of finite difference theory to groundwater flow was published in the paper [111]. This work and those that followed shortly thereafter [11, 41, 108] focused on a description of the thermodynamics of single-phase fluid flow. Hence at that time numerical simulators

represented a natural extension of the electric analog network models that were widely used for groundwater flow forecasting.

During the same time as these groundwater flow models were being developed, there was a parallel effort under way in soil physics. In the late fifties a number of researchers appear to have been interested in the unsaturated flow equations, which are similar to those encountered in multiphase oil reservoir simulation. Early papers that represent some of this work include [3, 53, 107, 114, 150]. The numerical approach was made attractive with the ability to accommodate spatially variable material properties, and the finite difference approach, being the only well-established numerical methodology available at that time, was the obvious choice. A review article [54] comparing six of the most frequently used numerical schemes reported significant differences in computational efficiency.

The majority of saturated-unsaturated groundwater flow simulators [27, 44] assumed an immobile air phase. This obviously reduces the number of dependent variables and the associated solution time compared to approaches where the air and water phase equations are solved simultaneously using the same basic methodology employed in the oil industry for two-phase flow [19, 48].

There is extensive literature on the use finite difference methods for the solution of the mass transport equation. The governing equation is applicable to oil, groundwater, and unsaturated flow simulation. A scheme is presented that circumvented some of the well-known numerical difficulties [129].

Multidimensional groundwater transport models [101, 126] including density-dependent formulations [45, 65] have also been published. Also a transport model based on a polygonal finite difference net was employed [100] and appears to represent the first large-scale application of transport modeling in regional groundwater simulation.

The simulation of mass transport in saturated-unsaturated media is of more recent vintage [130]. A number of important papers followed, such as [147]. The majority of papers now appearing in the literature in this topical area seem to have abandoned finite difference methods in search of more accurate simulation tools.

We have yet to consider the use of finite difference methods in non isothermal flow. The simulation of geothermal reservoir behavior is probably the most exotic problem to be considered along these lines. The majority of geothermal reservoir models are formulated using finite differences. It is difficult to establish with certainty the geothermal reservoir model development chronology. Among the earliest papers were those of [16, 39, 80, 133, 134]. A closely related yet distinctly different simulator was presented in [25] to forecast oil reservoir behavior subject to steam flooding. Because of the highly nonlinear nature of the geothermal equations and their considerable mathematical complexity, it is not surprising that finite difference methods remain today the generally accepted numerical approach for this class of problems.

In all numerical solutions the continuous partial differential equation (PDE) is replaced with a discrete approximation. In this context the word "discrete" means that the numerical solution is known only at a finite number of points in the physical domain. The number of those points can be selected by the user of the numerical method. In general, increasing the number of points not only increases the resolution (i.e., detail), but also the accuracy of the numerical solution.

To simulate the movement of water in variably saturated porous media, several numerical models have been developed. In the majority of the applications, the pressure-based form of the variably saturated flow equation is used [63, 64, 95] which, as already mentioned, is known to have poor mass-balance properties in unsaturated media [22, 75]. One-dimensional (vertical), variably saturated flow problems [29, 30, 42, 54, 57, 150] have been widely solved in many studies by using finite-difference approximations.

Six finite difference numerical schemes are analyzed to solve Richards' equation [54]. They have compared the calculated and measured infiltration profiles for a sandy soil. They found that the observed water content profiles and computed different numerical schemes are very closely agreed. The six schemes are numerically reliable tools for prediction of infiltration of water into the soil. In fact, the agreement between implicit approximation and quasi-analytical solution implies that the numerical schemes can yield accurate results.

The ψ -based form of Richards' equation is solved using a fully implicit (backward Euler) with Picard iteration method [22]. The solution of the ψ -based form of Richards' equation can give an efficient mass conservative solution if the moisture capacity is evaluated by appropriate methods [110]. The ψ -based form employing standard chord slope (SCS) approximation of moisture capacity showed excellent mass balance results [110].

Seldom have researchers used finite differences to solve variably saturated flow problems in higher dimensions [27, 43, 44, 75, 115]. Most of the existing two-dimensional finite difference solutions to variably saturated flow problems have limitations. The finite difference models of Freeze [43, 44] and Cooley [27] incur numerical instabilities and convergence difficulties, therefore they are not robust. Primarily these problems arise from inefficiencies of the line successive over-relaxation and alternating direction implicit schemes used in solving the two-dimensional nonlinear equations. The most successful and efficient example of a finite difference solution to two-dimensional, variably saturated flow problems was presented, in the author's opinion, by Kirkland et al. [75]. Nevertheless the objective of Kirkland et al. [75] was to develop competitive numerical procedures to solve infiltration problems in dry soils. The effect of specific storage is not accounted for by the fundamental flow equation, i.e., Richards' equation solved by Kirkland et al. [75], hence it cannot be used to model accurately a wide variety of variably saturated flow problems, including many transient drainage and seepage face phenomena in large domains.

Several researchers have successfully used finite elements to solve the general variably saturated flow equation [27, 63, 64, 95]. Be that as it may, all of these finite element models

are pressure-based, with finite difference Euler time marching algorithms to approximate the transient term, which can produce high mass-balance errors. Recent advances in finite element modeling techniques for variably saturated problems was discussed in [102].

The application of the finite element method to subsurface problems followed two distinctly different paths. In the petroleum industry, Galerkin's method, the theoretical foundation upon which most modern finite element models are built, was used almost exclusively with rectangular elements. Enhanced accuracy was achieved using higher degree polynomial basis functions, occasionally augmented with analytical solutions. In subsurface hydrology and subsidence, on the other hand, the tendency was to use triangular or isoparametric irregular quadrilateral elements. The resulting dichotomy of approaches has led to two quite different bodies of literature.

The Galerkin finite element concepts appear to have been introduced into the oil reservoir engineering [109]. This approach had much greater potential appeal even though the author's objective was to overcome problems generally associated with finite difference solutions to the convection-dominated transport equation. Subsequently the method was applied to a two-phase flow water flooding problem [33]. This concept was then extended to two-dimensional two-phase flow [84]. Whereas solutions of high accuracy were generally achieved, it was also concluded that the Galerkin finite element schemes were, for the most part, noncompetitive with finite difference algorithms in terms of their computational efficiency. Subsequent work changed this prognosis, for instance alternating direction procedures [33] and Lobatto quadrature for evaluation of the coefficient matrices [151].

In groundwater hydrology, finite element theory has been employed using triangular and isoparametric elements. In contrast to work in the petroleum industry, most, but not all, groundwater simulations use first-degree Lagrange polynomials as basis functions. The classic and the earliest publication describing the use of triangular finite element theory in porous media flow is [66]. Shortly thereafter the application is demonstrated of this methodology to the analysis of free surface Darcy groundwater flow [96, 131]. It is extended to deal with non-Darcy

free surface flow [60, 143]. The finite element method is particularly suited to this application because of the simplicity of deforming the mesh and updating the element matrix coefficients to accommodate the changing geometry of the solution domain and the changing element properties due to nonlinear material behavior. This advantage is even more evident when the method is applied to the simulation of land subsidence. In such instances, the finite element grid deforms as the land subsides [117, 118]. Furthermore it is straightforward to extend the finite element stress analysis to deal with the elastoplastic material properties and anisotropic behavior which are frequently encountered in practice.

It appears that the unsaturated flow problem that exhibits a dynamic air phase was not solved using finite elements. But the problem solved by McMichael and Thomas [84], however, is conceptually very similar. The single-equation static air phase was considered by Neuman [95]. He found that in solving these nonlinear equations an enhanced solution was obtained when the time matrix was modified to resemble a finite difference formulation on an irregular subspace.

The unsatisfactory finite difference solutions obtained for the convective-diffusive transport equation motivated the original work on Galerkin's method [109]. This approach was also investigated for solving the heat transport equation at about the same time [5]. The work involved a considerably more challenging natural convection problem in higher dimensions. Both of the preceding investigations employed the Galerkin approach in the sense adopted by the petroleum industry. The finite element approach has also been applied to the simulation of mass and energy transport in two and three dimensions [52, 121, 132]. The Galerkin finite element approach is, finally, widely used in both the petroleum industry and the hydrologic community for the solution of multidimensional transport in both single and multiphase systems [34, 51, 151].

The finite element method has also been used for the simulation of nonisothermal flow in geothermal reservoirs [61, 89, 90, 144]. Other nonisothermal applications include the simulation of coupled moisture and thermal transport in unsaturated soils [52] and the simulation of

seasonal thermal energy storage [62, 145].

In recent years the simulation of pressure propagation and mass and energy transport in fractured reservoirs has received increased attention. There are two avenues of approach to the problem; one requires identification and mathematical definition of the geometry of each fracture in the porous medium and the second assumes the fractures and porous blocks represent two overlapping continua.

Finite element methods have been used to solve the equations arising from both models. The flexibility inherent in the finite element approach is particularly useful in the discrete fracture case [98, 149]. Several researchers have extended the earlier work to investigate the transient coupling effect of fluid flow and solid deformation and to understand the nonlinear mechanical behavior of fractures or joints [4, 46, 58]. These include a finite element formulation to simulate the double continuum-based fractured porous media equations [10, 34, 99]. In this case, the finite element scheme was not an essential aspect of the mathematical simulators as it was in the discrete model formulation.

The simulation of mass transport with chemical reactions is an exceedingly challenging problem. Although early work in this area employed finite difference approximations [79], subsequent work has used approaches based on, for instance, Galerkin theory [116] or orthogonal collocation [97]. In these problems the enhanced accuracy of the finite element Galerkin methodology appears to offset the somewhat increased numerical complexity.

1.2.2. *Linearization techniques.*

Solving the highly nonlinear Richards equation requires the use of the iterative schemes and the efficient simulation can be obtained only if time step adaptation is incorporated into the numerical code.

In linearization schemes such as Picard and Newton, the number of iterations needed to converge is a determining factor for the simulation efficiency. To this purpose, convergence is often enhanced by providing the solver with an initial estimate that is closer to the final solution for the current time step. For problems involving flow to a pumping well an extrapolation method for doing so is presented in [27, 63]. The extrapolation method with varying order was investigated together with the effects of these improved initial guesses for the Picard scheme [31]. A suitable initial guess can also be obtained by taking the solution from the previous time step and choosing a sufficiently small time step size [9]. Thus, numerical algorithms often include an empirical time step adaptation criterion [31, 40, 74, 104].

The two-dimensional Richards equation has been solved by the mixed hybrid finite element method with a combination of Picard and Newton linearization techniques [9]. The governing equation generally tends to elliptic shape in near steady state or in unsaturated regions and typically ill conditioning may arise. Hybridization is used to overcome this ill-conditioning. It has been shown that for the many situations when a good initial guess is obtained either from the Picard scheme or relaxation techniques then convergence is achieved faster by the mixed hybrid finite element Newton approach.

The Picard and Newton schemes are the most common nonlinear iterative solvers. Aside from these standard schemes, the initial-slope Newton scheme, Newton-Kreylov methods, and combined Picard-Newton schemes have also been used successfully as iterative solvers for the nonlinear Richards equation [9, 38, 67]. In practice, Picard iteration is prevalent due to its simplicity and generally acceptable performance [81]. However, Picard and Newton solvers in uncontrolled time stepping schemes show poor convergence or complete failure for non smooth

constitutive functions describing some soils, for example certain unconsolidated loams and clay loams. To overcome convergence problems for such difficult simulations, more sophisticated variable-order variable-step schemes with chord iteration solvers can be used [92, 135]. Iterative solvers become computationally expensive if frequent Jacobian evaluation is not avoided because at each time step, multiple iterations are necessary including the recalculation and inversion of the Jacobian.

Several non iterative schemes have been compared with the traditional Newton and Picard iteration methods to solve the Richards equation [103]. Non iterative methods offer potential efficiency advantages over iterative scheme since they require a single formulation and inversion per time step. Two first order accurate linearization methods, a second order accurate two-level implicit-factored scheme, and a second order accurate three-level Lees method have been examined and it was found that the second order accurate scheme is quite competitive with the conventional Picard and Newton iteration methods [103]. However, to solve the Richards equation, it is not easy to apply the implicit factored scheme and this method has difficulties at the saturated-unsaturated interface. The solution of Richards' equation shows stability problems when using the Lees scheme, a three-level non iterative second-order method [103]. Despite these difficulties, the non iterative implicit factored scheme is an attractive and most promising alternative to traditional iterative methods for solving Richards' equation [74, 103]. A second order accurate non iterative adaptive algorithm is proposed [74] and for solving Richards' equation such adaptive algorithms allow accurate and cost-effective solution of problems that standard algorithms cannot easily handle. A more recent second-order non iterative linearization was found to be more efficient than first order approximation and competitive with the variable order variable step DASPK-KAM [93] algorithm. Ease of incorporation into widely used backward Euler codes and adaptive time step variation are particularly important in variably saturated solvers and are found to be some of the key merits of non iterative implicit time stepping schemes with adaptive temporal control [72].

1.2.3. *Performance measures.*

Different criteria are considered for evaluation of the performance of numerical methods. These criteria are root mean square error (RMSE), mass balance conservation, number of linear and nonlinear iterations, and execution time.

To investigate the robustness and efficiency of the method of lines approach, we studied the behavior of the ODE solver along different factors: the number of successful steps, failed attempts, function evaluations, partial derivatives, LU decompositions, solutions of linear systems, and CPU for all simulations.

A low mass balance error is a necessary but not sufficient condition to ensure accuracy of the solution. In other words, accurate solutions ensure small mass balance error. In this work, we consider the following formula for measures of RMSE :

$$\| E \|_2 = \left(\frac{1}{N} \sum_{i=1}^N (\psi_{exact} - \psi_i)^2 \right)^{\frac{1}{2}}$$

We considered ψ_{exact} is the base solution, which is made by dense-grid resolution of the vertical soil column and N is the total number of nodes.

Another evaluation method is the ability to conserve global mass over the domain of interest (mass balance conservation). Mass balance (MB) measurement for determination of the ability of a scheme for mass conservation can be defined as follows:

$$MB = (\text{Total additional mass in the domain}) / (\text{Total net flux into the domain})$$

Here the additional mass is evaluated with respect to the initial mass in the system. For the finite difference approximations, this is calculated by the following formula:

$$MB(t^n) = \frac{\sum_{i=2}^N (\theta_i^n - \theta_i^0) \Delta z}{\sum_{j=0}^n \left\{ -K_{N-1/2}^j \left(\frac{\psi_{N-1}^j - \psi_N^j}{\Delta z} + 1 \right) + K_{3/2}^j \left(\frac{\psi_1^j - \psi_2^j}{\Delta z} + 1 \right) \right\}}$$

where $K_{N-1}^j = \frac{K_N^j + K_{N-1}^j}{2}$ and $K_{3/2}^j = \frac{K_1^j + K_2^j}{2}$, N is the number of nodes, n is the number of time steps, ψ_N^j is the pressure head in the j^{th} time and N^{th} node, and θ_i^0 and θ_i^n are the initial and final values of moisture content at node i respectively.

1.3. Thesis layout.

The thesis is organized in four chapters. The first chapter (**Introduction**) addressed some background and the work on the numerical solution of Richards' equation that has been published. We introduced Richards' equation, which is the basic equation describing underground water movement. We present general formulations of the equation including advantages and disadvantages of the three forms and give some popular models that hydrologists use. In order to complete the numerical model we must specify the equations for soil hydraulic properties and these properties are described by the more well known van Genuchten and Brooks-Corey models. The constitutive models are illustrated in detail. Numerical solution techniques for the equation are introduced. Several approaches for solving Richards' equation have been introduced in the past few decades, e.g., finite difference methods or finite element methods. In our research, we discretized the equation and derived the Picard, Newton, and nested Newton-type algorithms as nonlinear iterative techniques. RMSE and mass balance error criteria are formulated for the numerical evaluation of accuracy and efficiency of the techniques.

The second chapter (**Solution of Richards' equation by the method of lines**) gives a general overview of the method of lines. The discretized system of ODE is derived using the method of lines. The system of algebraic equations is solved by the Matlab temporal ode solver ode15s. The general information on various Matlab ode solvers is discussed. For implementing the approach, two test problems are considered. Computational statistics are illustrated by the tables. The accuracy and efficiency are presented and summarized by the tables and figures.

In the third chapter (**Assessment of nested Newton-type scheme**), we evaluate the accuracy and computational efficiency of three strategies: the iterative Picard and Newton methods and the nested Newton scheme. The working procedures of the CATHY code are presented. The evaluations are based on the three test problems of one-dimensional unsaturated flow. The proposed nested Newton-type linearization procedure involves outer and inner iterations. Outer iterations are designed to handle nonlinearities and inner iterations are employed to solve a linear problem for every outer iteration. In addition to accuracy and efficiency, we also discuss

briefly other features of the three strategies, including symmetry and stability properties and mass balance.

In the last chapter (**Using lookup tables for heterogeneous soils**), we show the applications of lookup table options in CATHY for solving layered soil problems. Different strategies are discussed for implementing the lookup table option, including nonlinear tolerance and allowable maximum number of iterations per time step with time reduction and increase factors. In this part, we focus on the numerical behavior as well as on better choice of nodal distribution in the domain of soil moisture curves. Two problems are considered for evaluating the accuracy and efficiency of the strategy. The computational statistics for both uniform and nonuniform cases are presented in tables, and time stepping, nonlinear convergence, mass balance errors, and RMSE are illustrated by tables and figures.

2. SOLUTION OF RICHARDS' EQUATION BY THE METHOD OF LINES

2.1. Introduction.

To solve Richards' equation, the time step size is required to satisfy the limitations of truncation error otherwise to achieve convergence of the nonlinear or linear solver can change by several orders of magnitude over the course of simulation [135]. Therefore fixed time-step methods are wasteful of computational resources and have been superseded by methods that adapt some combination of the time-step size and order of the discrete temporal approximation [71, 73, 93, 110]. Combination of a formal error estimation and convergence characteristics of the iterative nonlinear and linear algebraic solvers is a usual strategy. Temporal adaptation can be implemented with a number of combinations, in some sense defying a clear, concise, and unambiguous classification of approaches, e.g., fixed low order based on empirical methods; fixed-order methods based upon an error estimator; variable order, variable step size methods based upon an error estimator.

A very common useful method is fixed low order which is based on empirical methods. It is more popular than fixed time step methods because of the simplicity of its implementation and its clear advantages [9, 75, 110]. The adjustments of time stepping for all the methods have differences on the basis of algorithm used. A common approach is to increase the time step by a constant multiple if an allowable number of nonlinear solver iterations is not met, and to decrease the time step size by a constant multiple if an upper limit on the number of nonlinear solver iterations is exceeded [1, 9, 23, 75, 110]. Another adjustment approach is to use a constant multiple over a time step but have it depend upon the changes in a dependent or related variable, such as pressure head or volumetric moisture content [75]. Estimating and controlling the temporal step size based upon non-dimensional numbers that characterize the nature of the solution and adjusting the step size to stay within allowable bounds is another empirical approach [35]. This class of approach is an improvement over fixed time-step methods, however no explicit control of truncation error is provided and advantage is not taken of cases in which higher-order methods are more efficient than low-order methods.

A promising alternative to purely empirical approaches are the methods that estimate truncation error and control the step size to achieve user defined tolerances. Predictor corrector methods based upon the joint use of explicit and implicit methods is one of the error estimators that can be derived by comparing solutions with different step sizes, different orders, or other differences in approximation methods [7]. These approaches are well known and commonly used in the ordinary differential equations community [74, 123]. Moreover, Richards' equation can be approximated using by low-order time-integration methods based upon error estimators [72, 73].

Controlling the time step size and the order of the approximation to satisfy a user-specified error criterion and achieve efficiency is a more sophisticated approach for temporal integration [13, 124]. Such approaches usually contain heuristic algorithms to follow order selection and recover from failures to meet error criteria or tolerances in nonlinear or linear solvers. These types of heuristic algorithms are intended to achieve efficiency and robustness and are necessarily lacking a rigorous theory of an optimal algorithm, which is an elusive problem-dependent proposition [13, 135]. Significant effort is needed for implementing such a variable order, variable time-step solver with formal error estimation [70]. With these considerations, for the solution of a wide range of problems in science and engineering, such techniques are common and more effective [17, 69].

2.2. Implementation.

Generalizing equation (1.1) to saturated and unsaturated porous media and using pressure head as the dependent variable we obtain:

$$\frac{\partial \psi}{\partial t} = \frac{1}{c(\psi) + S_s(\frac{\theta}{\theta_s})} \frac{\partial}{\partial z} \left[K(\psi) \left(\frac{\partial \psi}{\partial z} + 1 \right) \right] \quad (2.1)$$

or,

$$\frac{\partial \psi}{\partial t} = \frac{1}{c(\psi) + S_s S_a(\psi)} \frac{\partial}{\partial z} \left[K(\psi) \left(\frac{\partial \psi}{\partial z} + 1 \right) \right] \quad (2.2)$$

where $S_a(\psi) = \frac{\theta(\psi)}{\theta_s}$ and S_s is the specific storage coefficient, which accounts for fluid and matrix compressibility. In accounting for the effects of specific storage, the governing differential is an

extension of the classical Richards equation.

To solve this equation, we need to consider auxiliary conditions of the form:

$$\psi(z, t = 0) = \psi_0(z) \quad (2.3)$$

$$\psi(z = 0, t > 0) = \psi_1 \quad (2.4)$$

$$\psi(z = Z, t > 0) = \psi_2 \quad (2.5)$$

where Z is the length of the domain, and ψ_0 (defined as initial condition) may be a function of space, but ψ_1 (bottom boundary condition) and ψ_2 (top boundary condition) are constants. These simple conditions are adequate to develop a meaningful set of test problems.

2.2.1. *Method of lines.*

A general procedure for the solution of time dependent partial differential equations is the method of lines. This technique is more effective with respect to accuracy and computational time than the regular finite difference method and is regarded as a special finite difference method. It is a well established numerical technique or rather a semi analytical method to solve practical complex field problems. Mathematicians originally developed the method, and it has been used for boundary value problems in physics, fluid flow, electromagnetics and other research areas. It basically involves discretising a given differential equation in one or two dimensions whilst using an analytical solution in the remaining direction. The method of lines has the merits of both analytical and finite difference methods. It does not yield spurious modes nor have the problem of relative convergence.

The semi analytical character of the formulation by the method of lines leads to a simple and compact algorithm, which yields accurate results with less computational effort than other techniques. It is easy to establish stability and convergence for a wide range of problems, by separating discretisation of space and time. By using well documented and reliable ordinary differential equations solvers, such as Matlab ode solvers (**ode15s**, **ode113**, **ode23t**, **ode23tb**, **ode23s**, etc), the programming effort can be substantially reduced. There is no need to solve a

large system of equations since only a small amount of discretisation lines are necessary in the computation, hence computing time is small.

The method of lines can be used to solve parabolic and elliptic equations, although it is commonly used in the electromagnetic community for solving hyperbolic equations. In this work, we consider the simple case of applying the method of lines to solve a parabolic partial differential equation, namely Richards' equation using the Matlab ode solver **ode15s**.

For the solution of problems involving flow and transport in porous media, including Richards' equation, lately the method of lines has become an attractive alternative approach [70, 93, 135, 137, 148]. For solving Richards' equation, the method of lines has been proven to be significantly more efficient than standard fixed time-step or fixed order empirically adaptive approaches [135]. For finite difference and mixed finite element spatial discretization approaches [36, 137], the issues involving the solution of the resulting system of algebraic equations [36, 37] are aspects of multidimensional and heterogeneous systems which have been investigated. With such developments, temporal integration of Richards' equation is considered relatively mature.

The basic idea of the method of lines (MOL) is to replace the spatial (boundary value) derivatives in the partial differential equations (PDE) with algebraic approximations. Once this is done, the spatial derivatives are no longer stated explicitly in terms of the spatial independent variables. Thus, in effect only the initial value variable, typically time in a physical problem, remains. In other words, with only one remaining independent variable, we have a system of ordinary differential equations (ODEs) that approximate the original PDE using standard approaches (e.g., finite difference, finite element, or finite volume methods). The challenge, then, is to formulate the approximating system of ODEs. Once this is done, we can apply any integration algorithm for initial value ODEs to compute an approximate numerical solution to the PDE. In this approach one can specify the temporal accuracy; therefore the error checking, robustness, order selection, and time-step adaptivity features available in sophisticated ODE codes can be applied to the time integration of the PDE. However, MOL approaches have received

only limited application in the subsurface science literature, and significant implementation issues require resolution before such approaches realize their full potential in routine applications for difficult nonlinear problems, such as Richards' equation. MOL approaches for Richards' equation require a formulation such as (1.2), which is a single equation in one unknown and is independent of the particular method of discretization in space. Mixed forms of Richards' equation, such as (1.1), simultaneously advance ψ and θ in time with a standard, low-order time integration method (e.g., fully implicit or Crank-Nicolson methods) so as to preserve mass balance. Equation (1.1) is formally one equation in two unknowns and as such cannot be given to an ODE solver. Therefore, mixed methods typically use first-order schemes to advance θ and obtain mass balance [22, 110]. The method of lines will permit higher-order integration when based upon a high-order ODE solver.

A method of lines approach based on reduction of the original equation to a set of explicit ODEs would typically require rewriting equation (1.1) to the form given by equation (2.2), which yields an explicit set of ODEs after the spatial derivatives are approximated. This approach is the obvious one; however, the preliminary work found it to be an ineffective and relatively costly approach for computing solutions to Richards' equation. The problem with the approach is that $S_a(\psi) = \frac{\theta(\psi)}{\theta_s}$ can become very small for cases when saturated conditions develop and fluid compressibility is small.

The effects of small $S_a(\psi) = \frac{\theta(\psi)}{\theta_s}$ can be loss of accuracy in time integration and/or ill conditioning of the Jacobian matrix of the nonlinear system that must be solved at each time step. The size of the time step depends in part on how the nonlinear solver performs during a corrector step; the latter in turn depends on the norm of the inverse Jacobian and the Lipschitz constants of the Jacobian [74]. Division by the small function $S_a(\psi) = \frac{\theta(\psi)}{\theta_s}$, can affect both of these parameters, and ill-conditioned Jacobians can lead to loss of accuracy in the solution itself. Moreover, analytic Jacobians are easier to compute if we do not have to divide by $S_a(\psi) = \frac{\theta(\psi)}{\theta_s}$ before computing the Jacobian.

A differential algebraic equation (DAE) approach, which we advocate here, discretizes (1.1) in space, but does not divide by $S_a(\psi) = \frac{\theta(\psi)}{\theta_s}$. Popular methods based on (1.1) are however restricted to low-order methods in time [77, 92].

We consider a uniform spatial discretization comprised of $N - 1$ intervals of length Δz , with $\Delta z = Z/(N - 1)$, and $z_i = (i - 1)\Delta z$ for $1 \leq i \leq N$.

The spatial operator :

$$O_s(\psi) = \frac{\partial}{\partial z} \left[K(\psi) \left(\frac{\partial \psi}{\partial z} + 1 \right) \right] \quad (2.6)$$

is approximated at $z = z_i$ for $1 < i < N$ by

$$\begin{aligned} O_{si}(\psi) &= \frac{(K \frac{\partial \psi}{\partial z})_{i+1/2} - (K \frac{\partial \psi}{\partial z})_{i-1/2}}{\Delta z} + \frac{K_{i+1/2} - K_{i-1/2}}{\Delta z} \\ &= \frac{K_{i+1/2} \frac{(\psi_{i+1} - \psi_i)}{\Delta z}}{\Delta z} - \frac{K_{i-1/2} \frac{(\psi_i - \psi_{i-1})}{\Delta z}}{\Delta z} + \frac{K_{i+1/2} - K_{i-1/2}}{\Delta z} \\ &= \frac{1}{\Delta z^2} [K_{i-1/2} \psi_{i-1} - (K_{i-1/2} + K_{i+1/2}) \psi_i + K_{i+1/2} \psi_{i+1}] \\ &\quad + \frac{1}{\Delta z} [K_{i+1/2} - K_{i-1/2}] \\ &= r [(K_i + K_{i-1}) \psi_{i-1} - (K_{i-1} + 2K_i + K_{i+1}) \psi_i + (K_i + K_{i+1}) \psi_{i+1}] \\ &\quad + \frac{1}{2\Delta z} [K_{i+1} - K_{i-1}] \end{aligned} \quad (2.7)$$

where $r = 1/2\Delta z^2$ and N is the total number of spatial nodes in the solution, ψ_i is the approximation to $\psi(z_i)$, $K_i = K(\psi_i)$ and

$$K_{i+1/2} = \frac{1}{2} [K(\psi_{i+1}) + K(\psi_i)] \quad (2.8)$$

$$K_{i-1/2} = \frac{1}{2} [K(\psi_i) + K(\psi_{i-1})] \quad (2.9)$$

The differential algebraic equations system that we solve is a system of $N - 2$ differential equations for the $N - 2$ unknown functions of $\psi_i(t)$, subject to the boundary conditions ψ_1 and ψ_N . The i^{th} equation is

$$A(\psi_i) \frac{d\psi_i}{dt} = O_{si}(\psi_i) \quad (2.10)$$

where O_{si} is a spatial operator given by (2.7) and

$$A(\psi_i) = C(\psi_i) + S_s S_a(\psi_i) \quad (2.11)$$

2.2.2. ODE solver.

The above set of equations (2.10) may be solved by an implicit ODE or DAE integrator, with a stiff solver being the most reasonable choice. To solve this set of equations one can use the packages LSODE, VODE, DASSL, DASPK (is the latest version of DASSL), which are all public domain time integrators available through netlib (<http://www.netlib.org/>). All are based upon forms of the backward differentiation formulas (BDFs). LSODE and VODE are ODE solvers, while DASSL is a DAE solver. All of these solvers are well suited to stiff systems of differential equations of the type encountered in the method of lines solution of Richards' equation.

The method of lines involves discretising the spatial domain and thus replacing the PDE with a vector system of ordinary differential equations, for which efficient and effective integrating packages have been developed [120, 122]. The MATLAB package has strong vector and matrix handling capabilities, a good set of ODE solvers, and an extensive functionality which can be used to implement the method of lines [122].

We used a standard finite difference discretization in space and the **ode15s** for temporal integration. The ODE solver **ode15s** is a variable order solver based on the numerical differentiation formulas (NDFs). Solver **ode15s** uses the backward differentiation formulas (BDFs, also known as Gears method) that are usually less efficient. In other words, it is a quasi-constant step size implementation of the NDFs in terms of backward differences. Like **ode113**, **ode15s**

is a multi step solver. When **ode45** fails, or the solution is very inefficient, and/or one suspects that the problem is stiff, or when solving a differential-algebraic problem, then **ode15s** is an appropriate ODE solver [122, 123, 124, 125], but the accuracy of **ode15s** is low to medium.

In this work, we used a general syntax $[T,Y]=\mathbf{ode15s}(\text{odefun}, \text{tspan}, y_0, \text{options})$, with time interval $\text{tspan} = [t_0, t_f]$, that integrates the system of differential equations $y' = f(t, y)$ with initial conditions y_0 . The integration proceeds by steps, taken to the values specified in tspan . Note that the step size (the distance between consecutive elements of tspan) does not have to be uniform. Here odefun is a function handle, where the function $f = \text{odefun}(t, y)$, for a scalar t and a column vector y , and the solution returns as a column vector f corresponding to the given function $f(t, y)$. Each row in the solution array Y corresponds to a time return in column vector T . That is solutions will be stored at the specific times $t_0, t_1, t_2, \dots, t_f$ (all increasing or all decreasing), corresponding to $\text{tspan} = [t_0, t_1, t_2, \dots, t_f]$. The vector options is built by means of the function odeset that accepts name-value pairs. An option can have more than one data type as a value. odeset allows options to be set in any order and default values are used for any quantity not explicitly set by the user. It allows integration with the BDFs and integration with a maximum order less than the default of 5.

The most commonly used options are RelTol (Relative error tolerance) and AbsTol (Absolute error tolerance), tolerances associated with the error control. Specification of the error control is a default matter discussed in [123]. In MATLAB, the local error e'_i in y_i is calculated in each step and made to satisfy $|e_i| \leq r |y_i| + a_i$, where $r = \text{RelTol}$ and $a_i = \text{AbsTol}(i)$. The scalar relative error tolerance RelTol has a default value of 10^{-3} . The vector of absolute error tolerances AbsTol has by default all its values equal to 10^{-6} . If a scalar absolute error tolerance is input, the code understands that the value is to be assigned to all entries of the RelTol vector. In this study, we used $\text{RelTol} = 1.0 \times 10^{-5}$ and $\text{AbsTol} = 1.0 \times 10^{-7}$.

2.3. Description of test problems.

Aspects of the method of lines solution to Richards' equation were evaluated for two sets of test problems reported by [135]. We denoted the numerical test problems are Problem A and

Problem B. The simulation conditions are described in Table 1, including constitutive relation properties, spatial and temporal domains, and auxiliary conditions. Problem A was previously examined by [92, 110, 135] and material properties were used by [22] as well. The material properties for Problem B correspond to a dune sand as reported by [76], while the auxiliary conditions vary to yield a range of solution behavior.

TABLE 1. Soil hydraulic properties for Problem A and Problem B.

	Problem A	Problem B
θ_r (-)	0.102	0.093
θ_s (-)	0.368	0.301
α (m ⁻¹)	3.35	5.47
n (-)	2.00	4.26
K_s (m/days)	7.97	5.40
S_s (m ⁻¹)	0.00	1.0×10^{-6}
z (m)	[0 0.3]	[0 10]
t (days)	[0 0.25]	[0 0.20]
ψ_0 (m)	-10.0	-z
ψ_1 (m)	-10.0	0.00
ψ_2 (m)	-0.75	0.10

The unsaturated hydraulic conductivity for both problems was described by the van Genuchten model. Both sets of simulation conditions yield a difficult sharp-front problem. Problem A is considered because it is a standard test problem [135]. It is a common test problem and very helpful in clearly illustrating some important aspects of the method of lines.

Problem B is a vertical infiltration problem and has been analysed by [71, 92, 93, 135]. It has constant head boundary conditions at both top and bottom boundaries and a hydrostatic equilibrium initial condition. The combination of the initial and boundary conditions along with the constitutive relationships makes it a very difficult problem to solve accurately, since the solution includes an extremely sharp front in space that moves through the domain as a function of time.

However, Problem A is substantially easier than Problem B because the domain is much shorter, the media is not as uniform (i.e., n is smaller for Problem A), and saturated conditions are not achieved for Problem A. These factors, combined, suggest that while both problems are

relatively difficult sharp-front problems, Problem B is considerably more difficult than Problem A and will provide a stringent and meaningful test for the methods proposed in this work.

2.4. Results.

The analytic evaluation of constitutive relations represents a significant portion of the computational effort required to solve Richards' equation numerically, due to the complicated power functions involved. To increase the efficiency of the overall simulation, these relations are often evaluated by tabulating a set of analytic values and then interpolating intermediate values as they are required during the simulation. Linear interpolation is often used, yet higher-order methods such as cubic or Hermite spline interpolation may be required for higher-accuracy solutions. This tabulation and interpolation procedure results in significant savings in computational effort without lost accuracy, compared to direct function evaluations. In this work, we used analytic evaluation to ensure robust and accurate solutions.

In order to assess the robustness and efficiency of the method of lines approach, we used four sets of spatial nodes for each of the test cases. We studied different factors of behavior of the ODE solver including the number of successful steps, failed attempts, function evaluations, partial derivatives, LU decompositions, and solutions of linear systems. We also studied characteristics of the method relative to changes in the refinement level and the number of cells in the coarse grid. Thus CPU time was considered as a suitable choice of work measure. The number of nodes in the grid is also an important parameter for comparison in this work, since our main objective is to obtain accurate results. The accuracy for each of the simulations is evaluated by means of the root mean square error (RMSE) and mass balance (MB) calculated with respect to the surrogate exact solution. The deviation between the fine and several sets of coarse solutions are quantified using a root mean square error formula, defined earlier in the performance measure section, where ψ_i is a test solution generated using a coarser grid and ψ_{exact} is the true solution, and N is the total number of grid points. The RMSE are measured at the four different times for both test problems. In addition, a traditional mass balance approach was also used to track the numerical error. A good closure of mass in the domain can be maintained even though the internal structure of the solution is different from the fine solution. Therefore,

in this work, we used the RMSE to quantify the deviations between coarse and fine solutions. In this study, all of the numerical codes have been written in MATLAB 7.6.0 (2008a) software and executed on a Dell INSPIRON, 2.56 GHz system.

2.4.1. Test Problem A.

The van Genuchten soil moisture curves for the test Problem A are shown in Figure 1.

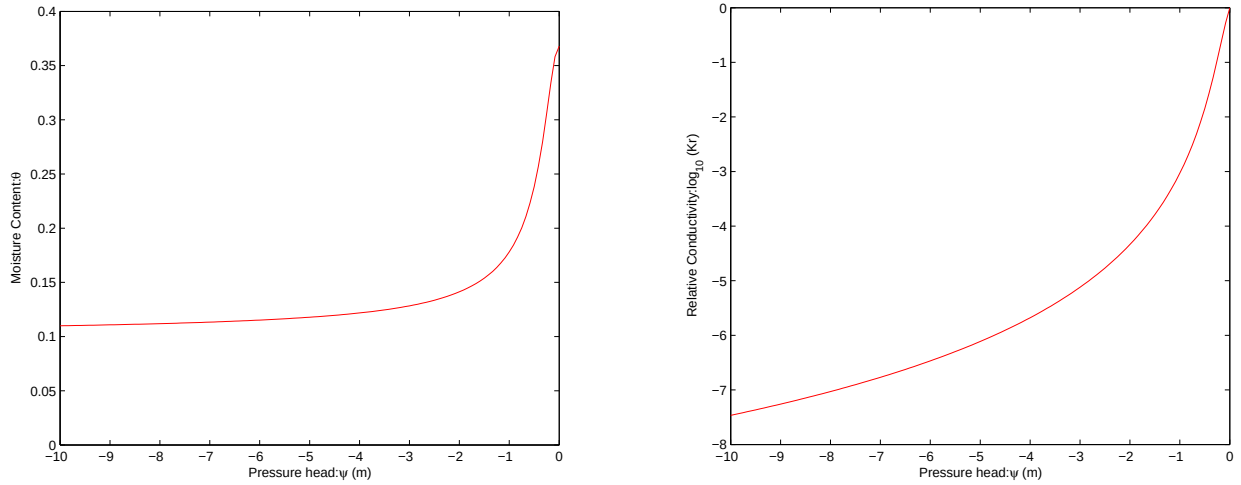


FIGURE 1. Soil moisture retention curves for test Problem A: Moisture content (left) and log hydraulic conductivity (right).

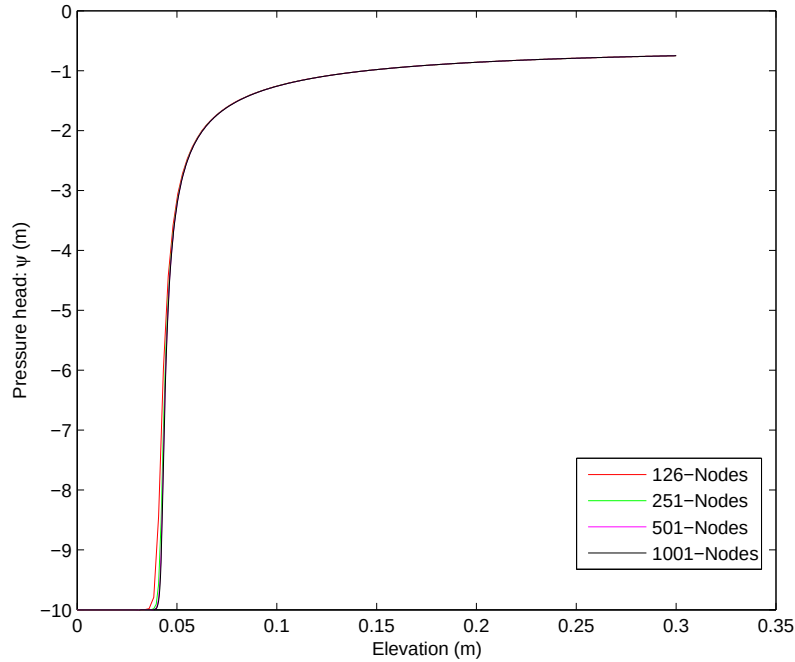
The four sets of vertical discretization are $N = 126, 251, 501$, and 1001 where the exact solution is made by 2001 nodes, i.e., $\psi_{exact} = 2001$. The RMSE is evaluated at $t = 0.10, 0.20$ and 0.25 days with respect to the reference solution.

The computational performance of the ODE solver **ode15s** for the several vertical discretizations of Problem A are reported in Table 2. Table 2 shows that when doubling the number of layers, the successful steps of ODE solver increase by approximately 1.5 times. The average number of function evaluations and average number of solution of linear systems per step (including failed steps) is 2.40, 8.18, 21.54, 57.18 and 1.95, 2.00, 2.05, 2.07 for 125, 250, 500, and 1000 layers respectively. The CPU increases rapidly with the increasing number of layers.

TABLE 2. Computational statistics for Problem A.

No. of layers	125	250	500	1000
No. of successful steps	1485	2255	3150	4111
No. of failed attempts	93	202	255	366
No. of function evaluations	6425	20104	73350	256014
No. of partial derivatives	27	61	133	247
No. of LU decompositions	281	484	616	818
No. of solutions of linear systems	3076	4914	6982	9260
CPU (s)	2.60	18.08	755.72	7102.34

The computed solution profile for 4 different numbers of layers is presented in Figure 2. The solution profiles agree well with the published report [22, 135]. As the solution figure indicates, there is no significant difference between the 500 and 1000 layer profiles at the near bottom of the soil column. Also note that the solution profiles gradually get smoother with the increasing number of nodes.

FIGURE 2. Pressure head profile at $t=0.25$ days.

The evaluated RMSE graph (Figure 3) is drawn for 125, 250, 500, and 1000 layers where we considered 3 different times $t=0.10$, 0.20 , and 0.25 days for each distinct set of layers. Clearly from Figure 3, the highest to lowest errors are shown by 125 and then 250 and then 500 and

then 1000 layers. At time $t=0.10$ days, the maximum error= 2.933 m is found at $z=0.1416$ m for 125 layers, on the other hand for 1000 layers, at $z=0.1428$ m the maximum error= 0.1021 m, as expected. At the end of the simulation, that is, at $t=0.25$ days, except in the neighborhood of $z=0.0432$ m, the error continuously decreases for all the different layers. For example, for the 125 layers case, we found error= 4.15×10^{-2} m at $z=0.055$ m and then it is 7.40×10^{-5} m at $z=2.52$ m and finally it is 0 at the end point of the given domain. We obtained excellent behavior for the 1000 layers case at $t=0.25$ days. In this case, the maximum error is 0.047 m at $z=0.0432$ m and then the errors are 2.93×10^{-3} m, 8.05×10^{-5} m, 8.64×10^{-6} m and 2.83×10^{-6} m at $z=0.05$ m, 0.10 m, 0.20 m, and 0.25 m respectively, and at $z=0.3$ m the error is 0.

The RMSE for Problem A of the four sets of layers at 3 different time levels are presented in the Table 3. Clearly from the error table, the error is reduced with increasing number of nodes. From these statistics in Table 3 it can be concluded that all runs have adequate and comparable accuracy. Also, the RMSE error graph at the 3 different times for 4 different numbers of layers are shown in Figure 3 (top graph) including a zoom part (bottom graph) of the error for clear observation of error behavior for all layers.

TABLE 3. Computed error table for Problem A.

Time (days)	0.10	0.20	0.25
No. of Layers	–	Error	–
125	0.4971	0.4285	0.4023
250	0.2364	0.1942	0.1821
500	0.0980	0.0779	0.0725
1000	0.0316	0.0248	0.0230

The mass balance error values for Problem A at different number of layers at different times are shown in Table 4. Table 4 clearly shows, for all four discretizations, that the MB are acceptably small.

TABLE 4. Computed mass balance for Problem A.

No. of Layers	125	250	500	1000
MB	7.3×10^{-3}	3.7×10^{-3}	1.8×10^{-3}	9.3×10^{-4}

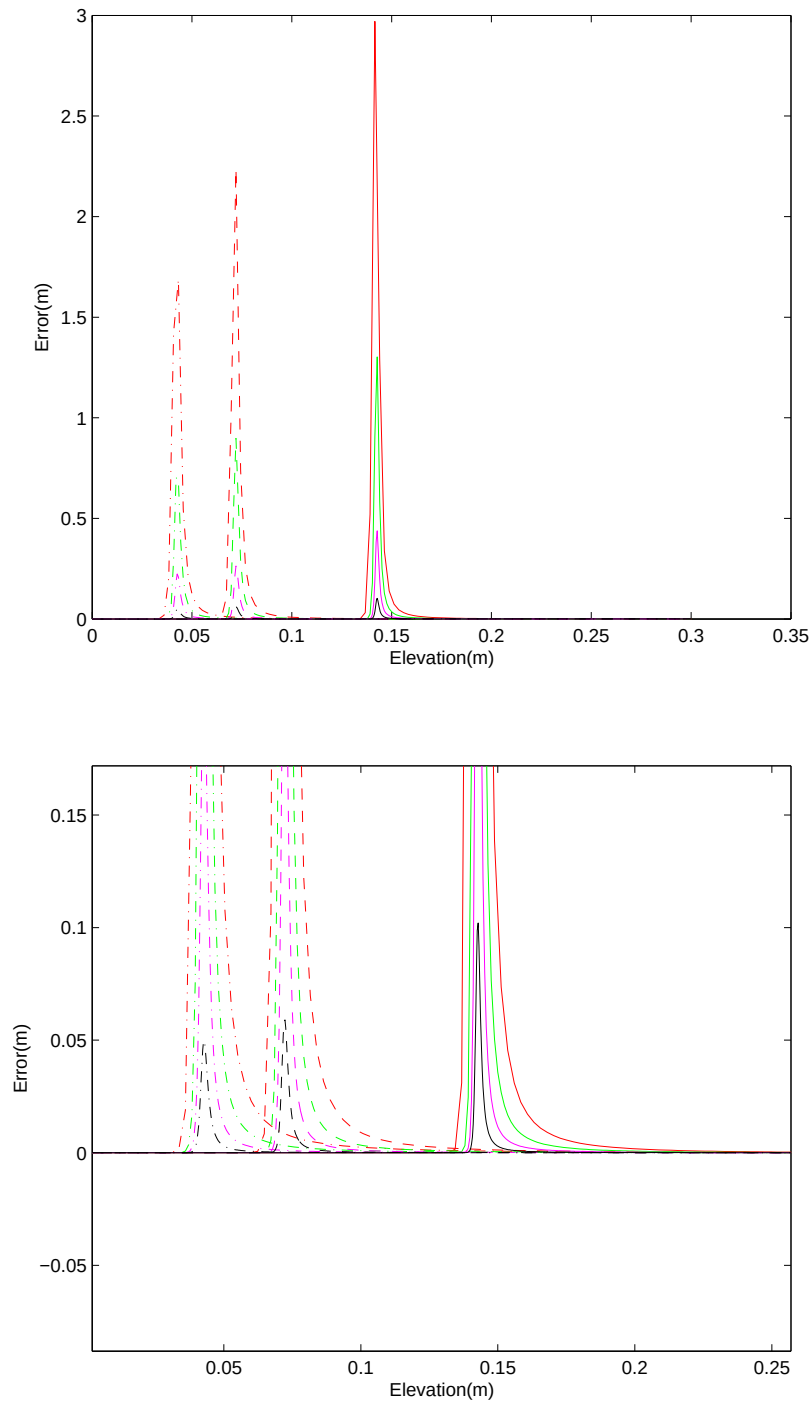


FIGURE 3. Computed RMSE for Problem A (top graph) and its zoom graph (bottom graph). Here solid lines, dashed lines, and dash-dotted lines represent the error at $t=0.10$, 0.20 , and 0.25 days respectively for each distinct set of layers with red, green, magenta, and black colors representing 125, 250, 500, and 1000 layers respectively.

2.4.2. Test Problem B.

Figure 4 shows the van Genuchten soil moisture curves for test Problem B. The first subplot shows the moisture content profile and the second subplot shows the hydraulic conductivity profile as a function of pressure head ψ .

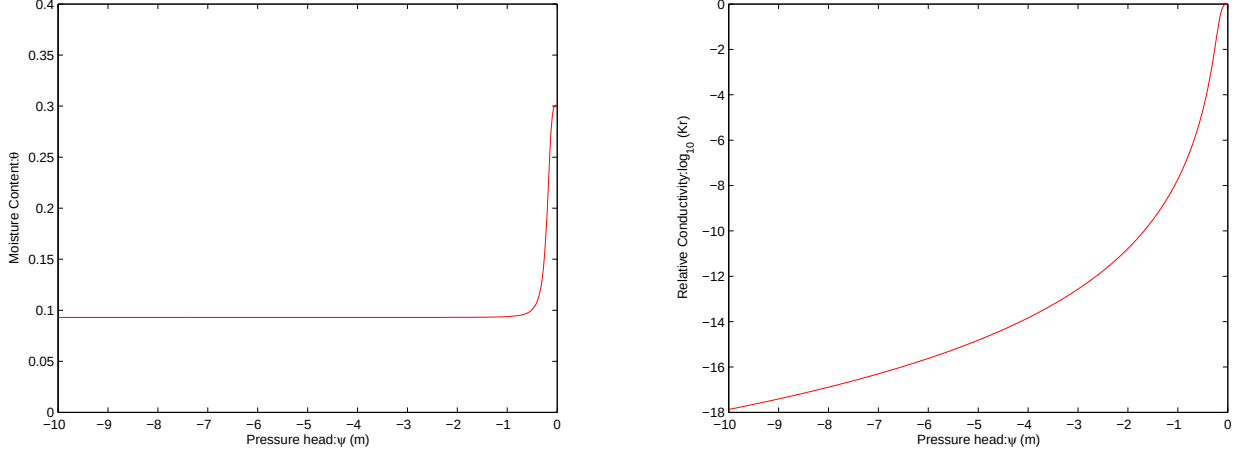


FIGURE 4. Soil moisture retention curves for test Problem B: Moisture content (left) and log hydraulic conductivity (right).

To solve this difficult sharp front infiltration problem and get more accuracy, we have taken four sets of vertical discretization, $N = 101, 201, 401$, and 801 nodes and the exact solution is made by 1601 nodes for determination of solution accuracy.

A comparison of computational statistics of the ode solver 'ode15s' for Problem B, such as the number of nodes, the number of successful steps taken, failed steps, the number of function evaluations, the number of Jacobians, the number of LU decomposition, the number of solutions of linear systems, and the total CPU for the various runs for the method of lines approach are tabulated in Table 5. The number of steps and failed steps approximately double along the four sets of discretizations. The failed steps indicate that the solver often needs to reduce the time step. The average function evaluations and average linear systems solved per step (successful and failed steps) are 13.76, 19.51, 25.65, 32.37 and 2.08, 2.04, 2.03, 2.02 for 101, 201, 401, and 801 nodes respectively. The CPU time column shows that the computational cost

dramatically increases with increasing number of nodes.

TABLE 5. Computational statistics for Problem B.

No. of layers	100	200	400	800
No. of successful steps	2223	3911	7350	14132
No. of failed attempts	654	1034	1710	2979
No. of function evaluations	39583	96472	232389	553833
No. of partial derivatives	336	432	535	649
No. of LU decompositions	988	1613	2775	4975
No. of solutions of linear systems	5873	10064	18382	34617
CPU (s)	64.00	250.13	3040.58	15468.60

Figure 5 (left graph) is a comparison of solution profiles for pressure head for all runs of Problem B that agrees well with the published papers [22, 135]. The right graph of Figure 5 clearly shows that the smoothness is developed by 801 nodes resolution of the soil column.

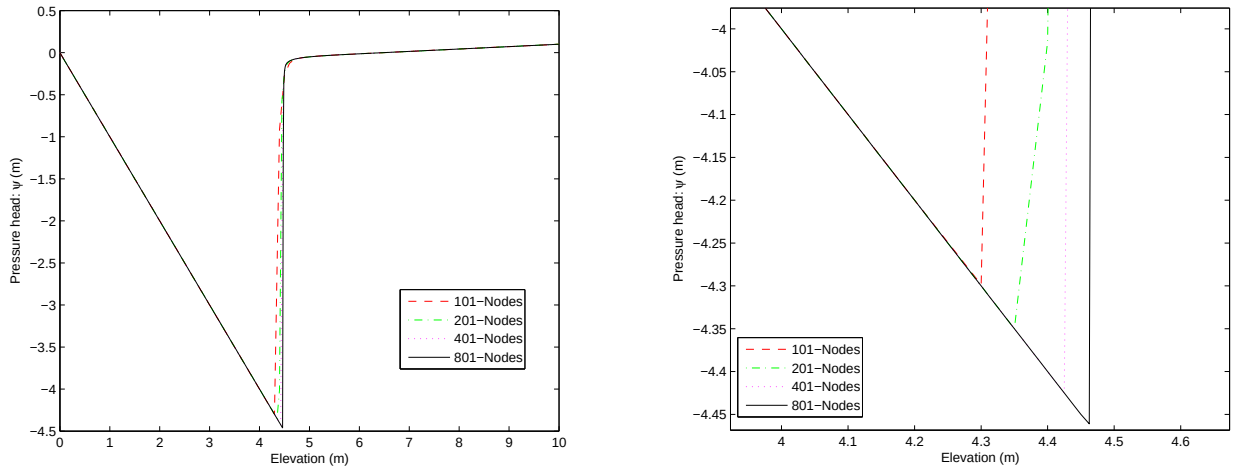


FIGURE 5. Computed pressure head for all sets of layers for Problem B (red dashed, green dash-dotted, magenta dotted, and black solid lines represent 101, 201, 401, and 801 nodes respectively).

The accuracy factor RMSE is evaluated at 3 different times, $t = 0.10, 0.15$, and 0.20 days for all the different numbers of nodes, and the errors are summarized in Table 6. This table shows that the efficiency of solutions can be improved by increasing the number of nodes. The error graph (Figure 6) of 800 layers shows the acceptable error. For example, we found at $t=0.10$

days, the error is 5.02×10^{-3} m at $z=0.10$ m, 0 m error at $z=5$ m, 1.5×10^{-4} m, 1.16×10^{-5} m and 0 m at $z=6$ m, 8 m and 10 m respectively. The maximum errors were concentrated at the front and these dominated the overall error as they were orders of magnitude greater than the rest of the domain. The computed RMSE profile is plotted in Figure 6. The first subplot of Figure 6 is the complete representation of error behavior of all the runs at the three times and the second subplot is a zoom portion.

TABLE 6. Computed error table for Problem B.

Time (days)	0.10	0.15	0.20
No. of Layers	—	Error	—
100	1.2082	0.7747	0.3546
200	0.8779	0.4068	0.3026
400	0.6013	0.4142	0.3175
800	0.2783	0.1694	0.1288

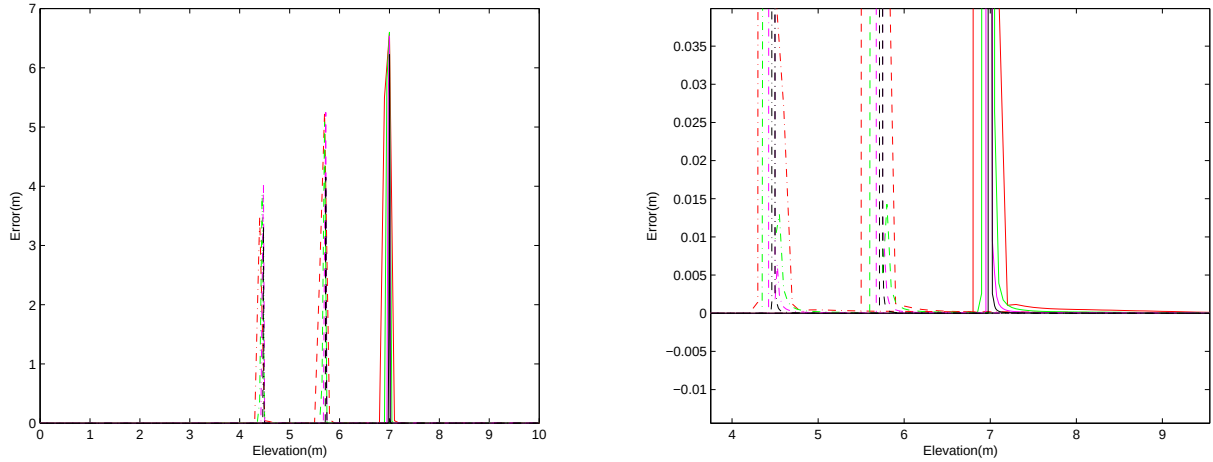


FIGURE 6. Computed error for Problem B. The errors at 0.10, 0.15, and 0.20 days are denoted by the solid, dashed, and dash-dotted lines respectively while the red, green, magenta, and black colors are for 101, 201, 401, and 801 nodes.

One of the main motivations for solving Problem B is to test the mass conservation properties of the method of lines algorithm. The mass balance for different runs measured against the fine mesh solution is presented in Table 7. The mass balance for the method of lines is good, indicating that the approach did not result in a significant deterioration of mass conservation

properties compared to a fine mesh solution.

TABLE 7. Computed mass balance for Problem B

No. of Layers	100	200	400	800
MB	6.63×10^{-5}	3.24×10^{-5}	1.59×10^{-5}	7.88×10^{-6}

2.5. Conclusions.

Problem B is more difficult to solve than Problem A, as noted by the computational performance measures. These measures reflect the smaller time step needed to solve the system but do not reflect the additional effort needed because Problem B used a larger number of nodes than Problem A. Including differences related to spatial discretization in the performance measures would further increase the difference between the performance required to solve Problem B and that required to solve Problem A.

In this work we formulated a spatial discretization approach for a one-dimensional finite difference solution of Richards' equation and the method implemented. We solved two difficult test problems using the method of lines for a wide variety of error tolerances and spatial discretizations without any difficulty. Thus, to solve difficult sharp-front problems that arise in the Richards equation, the method of lines approach is an attractive alternative. Hence a method of lines approach similar to that used in this work may provide efficient solutions for other difficult nonlinear subsurface flow and transport problems.

3. ASSESSMENT OF NESTED NEWTON-TYPE SCHEME

3.1. Introduction.

Catchment modeling typically refers to surface flow modeling, but such modeling approaches fail when surface and subsurface interactions are a key component of the hydrological cycle. These cases require the modeling of both surface and subsurface flow. Recently several models that couple surface and subsurface flow have been developed using different coupling approaches. Generally speaking, we can consider coupling schemes to be of three different types: sequential and noniterative; sequential and iterative; and first-order coupled, with the presumption that the sequential iterative and the first-order coupled approaches are to be more accurate, whereas the sequential noniterative approach is easier to implement and should be more efficient on a per time step basis. However, the simpler approaches can be more sensitive to mass balance errors; whilst the first-order coupling raises parameterization concerns (new exchange terms are introduced).

Therefore a need arises to assess in detail the advantages and disadvantages of different coupling approaches. To address some of these important issues, we can use the CATHY (CATchment HYdrology) model that features elements of both the sequential noniterative and sequential iterative coupling schemes. CATHY is a physically-based hydrological model where the surface module resolves the one-dimensional (1D) diffusion wave equation and the subsurface module solves the 3D Richards equation. Coupling between these two equations is based on an extension of the boundary condition switching procedure used in some subsurface models for the handling of atmospheric inputs on the land surface boundary of the catchment. The chief aim of this work is to assess, via sensitivity analysis, the accuracy and mass balance limitations for the CATHY model over a range of temporal and spatial discretizations and for a variety of hydrological configurations, with particular attention to the case of high exchange fluxes under Dirichlet boundary conditions. Such a boundary condition is not flux-limited and may lead to a poor estimation of exchange fluxes and consequently to poor overall mass balance.

There are two types of numerical discretization used, finite element and finite difference for the given test problems. To obtain the numerical solution of Richards' equation we used CATHY. For solving the highly nonlinear partial differential equation, Richards' equation, we used Picard and Newton as iterative schemes. We investigated various aspects of solution behavior, that is, how many steps to complete the simulations, what are the appropriate time step sizes for the solver to get convergence, how many nonlinear iteration to take each time step, what is the number of linear iterations in each nonlinear iteration for every time step, what is the mass balance error behavior, etc.

A finite difference discretization of the mixed form of Richards equation leads to a nonlinear numerical model which yields exact local and global mass conservation. The resulting nonlinear system requires sophisticated numerical strategies, especially in a variable saturated flow regime. In [21] a nested, Newton-type algorithm for the discretized Richards equation is derived. With a judicious choice of the initial guess convergence is obtained for any time step size and for all flow regimes. The nested Newton algorithm converge quadratically for each time step and for all flow. In this case we discretized the Richards equation using a standard finite difference method. By this algorithm, a base solution is made for every test problem using the same number of nodes, time step size, and tolerance as we did for CATHY, in order to evaluate the root mean squared error and compare with the results of the Picard and Newton cases.

We have solved 3 difficult test problems for wide a range of cases. In every test case, we have taken different number of nodes, and for each set of nodes, different number of time step sizes are used. We also made the base solution for a sufficient number of points maintain strict tolerance.

We cannot compare all the behavior of solution between CATHY and nested Newton because according to the nested Newton algorithm we evaluated the solution profile, total number of outer iterations (i.e., number of mildly nonlinear iterations), total number of inner iterations (number of linear iterations), and average outer and inner iterations.

3.2. Implementation.

3.2.1. Numerical model for flow in variably saturated porous media.

Introducing a general storage term $S(\psi) = \frac{d\theta}{d\psi} + (\frac{\theta}{\phi})S_s$ and write pressure head as a dependent variable in equation (1.1) to handle flow in both saturated and partially saturated media, we obtain

$$S(\psi)\frac{\partial\psi}{\partial t} = \frac{\partial}{\partial z} \left[K_s K_r \left(\frac{\partial\psi}{\partial z} + 1 \right) \right] \quad (3.1)$$

where $\frac{d\theta}{d\psi}$ =specific soil moisture capacity, S_s =Specific storage= $\rho g(c_w + c_f)$, ρ =density of water, c_w =compressibility of water, and c_f =effective formation compressibility.

In equation (3.1) we have expressed the hydraulic conductivity as $K(\psi) = K_s K_r(\psi)$, a product of the conductivity at saturation and the relative conductivity.

The specific storage component of the general storage term accounts for the slight compressibility of water. Richards' equation is highly nonlinear due to pressure head dependencies in the specific soil moisture capacity and relative hydraulic conductivity terms, the latter term contributing a nonlinearity to both the diffusion-type component $\frac{\partial}{\partial z} (K(\psi) \frac{\partial\psi}{\partial z})$ and the gravitational gradient term $\frac{\partial K(\psi)}{\partial z}$.

For the numerical solution of Richards' equation (3.1), we discretize the spatial domain using finite element Galerkin discretization and a finite difference discretization of the time derivative term. To develop the finite element model there are $M - 1$ discretized elements for M global nodes in the problem domain.

The approximating function is:

$$\psi(z, t) = \psi(\hat{z}, t) = \sum_{j=1}^M N_j(z) \psi_j(t) \quad (3.2)$$

where $\psi_j(t)$ are undetermined global nodal values of ψ and $N_j(z)$ are the corresponding Lagrange basis functions. To get the unknown coefficients we used the weighted residual method. The approximating function for each element (e) is:

$$\begin{aligned}\hat{\psi}^{(e)} &= \sum_{i=1}^2 N_i^{(e)}(\xi) \psi_i^{(e)}(t) \\ &= \frac{1}{2}(1 - \xi) \psi_1^{(e)}(t) + \frac{1}{2}(1 + \xi) \psi_2^{(e)}(t)\end{aligned}\tag{3.3}$$

where $-1 \leq \xi \leq 1$

The vector form of the equation (3.3) is:

$$\hat{\psi}^{(e)} = (\mathbf{N}^{(e)}(\xi))^T \psi^{(e)}\tag{3.4}$$

The global function of (3.2) is

$$\hat{\psi} = \sum_{e=1}^{M-1} (\mathbf{N}^{(e)})^T \psi^{(e)} = \sum_{e=1}^{M-1} \hat{\psi}^{(e)}\tag{3.5}$$

If we apply the symmetric weak formulation of the Galerkin method in (1.1) then the system of ordinary differential equations is

$$\mathbf{A}(\psi)\psi + \mathbf{F}(\psi)\frac{d\psi}{dt} = \mathbf{q}(\mathbf{t}) - \mathbf{b}(\psi)\tag{3.6}$$

where ψ is the vector of undetermined coefficients corresponding to the values of pressure head at each node, $\mathbf{A}$ is the stiffness matrix, $\mathbf{F}$ is the storage or mass matrix, $\mathbf{q}$ contains the specified Darcy flux boundary conditions, and $\mathbf{b}$ contains the gravitational gradient component. Over local sub domain element $\Omega^{(e)}$ we have

$$\mathbf{A}^{(e)} = \int_{\Omega^{(e)}} \mathbf{K}_s^{(e)} \mathbf{K}_r(\hat{\psi}^{(e)}) \frac{dN^{(e)}}{dz} \left(\frac{dN^{(e)}}{dz} \right)^T dz\tag{3.7}$$

$$\mathbf{b}^{(e)} = \int_{\Omega^{(e)}} \mathbf{K}_s^{(e)} \mathbf{K}_r(\hat{\psi}^{(e)}) \frac{dN^{(e)}}{dz} dz\tag{3.8}$$

$$\mathbf{F}^{(e)} = \int_{\Omega^{(e)}} \mathbf{S}(\hat{\psi}^{(e)}) \mathbf{N}^{(e)} (\mathbf{N}^{(e)})^T dz \quad (3.9)$$

The system matrices $\mathbf{A}$ and $\mathbf{F}$ are symmetric. This symmetry of the overall system is lost for some of the iterative and linearization strategies. Since linear Lagrange basis functions are used the matrices $\mathbf{A}$ and $\mathbf{F}$ have a banded structure with a bandwidth of three. The fraction of nonzero entries for each of these matrices will be $3/M$.

Either lumped or distributed matrices can be used in the numerical models. The models can handle a variety of boundary conditions, including atmospheric inputs, seepage faces, and source/sink terms.

3.2.2. Time differencing.

Equation (3.6) can be integrated in time by the weighted finite difference scheme. We obtain

$$\mathbf{A}(\psi^{\mathbf{k}+\lambda}) \psi^{\mathbf{k}+\lambda} + \mathbf{F}(\psi^{\mathbf{k}+\lambda}) \frac{\psi^{\mathbf{k}+\lambda} - \psi^{\mathbf{k}}}{\Delta t} = \mathbf{q}(\mathbf{t}^{\mathbf{k}+\lambda}) - \mathbf{b}(\psi^{\mathbf{k}+\lambda}) \quad (3.10)$$

where

$$\psi^{\mathbf{k}+\lambda} = \lambda \psi^{\mathbf{k}+1} + (1 - \lambda) \psi^{\mathbf{k}} \quad (3.11)$$

with $0 \leq \lambda \leq 1$ (λ is a weighting parameter) and k and $k+1$ denote the previous and current time levels.

The time step size to ensure a stable solution will be dependent on the spatial discretization, and for nonlinear equations there will in general also be a dependency on the form of the solution itself at any given time. Equation (3.10) is $O(\Delta t)$ accurate except for $\lambda = \frac{1}{2}$. When $\lambda = \frac{1}{2}$, the discretized scheme (3.10) corresponds to Crank-Nicolson scheme.

The system of equations (3.10) is nonlinear in $\psi^{\mathbf{k}+1}$ except when $\lambda = 0$, which corresponds to an explicit Euler scheme. When $\lambda > 0$, the schemes become implicit. Some iteration or

linearization strategy is needed to solve a system of nonlinear equations for the implicit case. For $\lambda = 1$, the scheme corresponds to backward Euler.

Let us consider $f(\psi^{\mathbf{k}+\lambda}) = 0$, then the equation (3.10) becomes

$$f(\psi^{\mathbf{k}+\lambda}) \equiv \mathbf{A}(\psi^{\mathbf{k}+\lambda})\psi^{\mathbf{k}+\lambda} + \mathbf{F}(\psi^{\mathbf{k}+\lambda})\frac{\psi^{\mathbf{k}+1} - \psi^{\mathbf{k}}}{\Delta t} + \mathbf{b}(\psi^{\mathbf{k}+\lambda}) - \mathbf{q}(\mathbf{t}^{\mathbf{k}+\lambda}) = 0 \quad (3.12)$$

To solve the nonlinear system (3.12), we need to use some iterative or other linearization techniques. The most common iterative scheme to use is either Picard or Newton.

The Picard iterative scheme is more popular than Newton because the formulation of Picard is simple and it preserves symmetry of the finite element matrices. On the other hand, the Newton method requires the evaluation of Jacobian matrices and yields a nonsymmetric system. That is why on a per iteration basis, the Picard method is less costly than the Newton method. The Picard method converges linearly whereas Newton converges quadratically. So for some problems or under certain accuracy constraints Newton gives better convergence behavior than Picard.

3.2.3. Newton scheme.

Applied to (3.12), the Newton scheme [103] can be written as

$$\mathbf{f}'(\psi^{\mathbf{k}+1,(\mathbf{m})})(\psi^{\mathbf{k}+1,(\mathbf{m}+1)} - \psi^{\mathbf{k}+1,(\mathbf{m})}) = \mathbf{f}(\psi^{\mathbf{k}+1,(\mathbf{m})}) \quad (3.13)$$

where superscripts m and $m + 1$ denote the previous and current iteration level. The Jacobian for the system is

$$f'_{ij} = \frac{1}{\Delta t}F_{ij} + \sum_s \frac{\partial A_{is}}{\partial \psi_j^{k+1}}\psi_s^{k+\lambda} + \frac{1}{\Delta t} \sum_s \frac{\partial F_{is}}{\partial \psi_j^{k+1}}(\psi_s^{k+1} - \psi_s^k) + \frac{\partial b_i}{\partial \psi_j^{k+1}} \quad (3.14)$$

expressed here in terms of the ij^{th} component of the Jacobian matrix $\mathbf{f}'(\psi^{\mathbf{k}+1})$.

The Newton iteration scheme is a updating parallel chord method, that is, the tangent f' is the iteration matrix which is updated at each iteration. The simplified Newton method is

defined as the Newton scheme without updating. On the other hand for modified Newton we do not need to update the iteration matrix at each iteration, and selective iteration is used. If the Jacobian or iteration matrix is approximated by the finite difference formula we get another variant of Newton which is known as the secant method. Generally, when the Jacobian term cannot easily be derived analytically then these variant methods can be used and some more costly numerical technique is required to compute it.

For Richards' equation the nonlinearities are contained in the characteristics equations, and these expressions can be analytically differentiated. We therefore use the original, unmodified Newton method in our work.

The Newton scheme can be derived by imposing a quadratic convergence criterion on a general fixed point iteration method. Alternatively, the Newton scheme can be derived from a Taylor series expansion of (3.12) as its fixed point. Good initial solution estimates are important in the successful convergence of the Newton and other iterative schemes. Unlike iterative techniques for linear systems, where theorems exist which specify conditions that guarantee global convergence, such results are not available for nonlinear iterative methods. That is, convergence is guaranteed provided the initial estimate is close enough to the solution.

3.2.4. *Picard scheme.*

The Picard scheme has a simple formulation which can be obtained directly from (3.10) by iterating with all linear occurrences of $\psi^{\mathbf{k}+1}$ taken at the current iteration level $(m+1)$ and all nonlinear occurrences at the previous level (m) . We get

$$\begin{aligned} \left(\lambda \mathbf{A}^{\mathbf{k}+\lambda,(\mathbf{m})} + \frac{1}{\Delta t} \mathbf{F}^{\mathbf{k}+\lambda,(\mathbf{m})} \right) \psi^{\mathbf{k}+\lambda,(\mathbf{m}+1)} \\ = \mathbf{q}^{\mathbf{k}+\lambda} - \mathbf{b}^{\mathbf{k}+\lambda,(\mathbf{m})} - \lambda \mathbf{A}^{\mathbf{k}+1,(\mathbf{m})} \psi^{\mathbf{k}} + \frac{1}{\Delta t} \mathbf{F}^{\mathbf{k}+1,(\mathbf{m})} \psi^{\mathbf{k}} \end{aligned} \quad (3.15)$$

If we compare the equations (3.13) and (3.15), it seems that the Picard scheme looks like the approximation of Newton method. It is found that under appropriate conditions the Newton

scheme is quadratically convergent and Picard scheme converges only linearly. The linearization of Newton produces a nonsymmetric system matrix, whereas picard yields a symmetric system. Since different storage and linear solver algorithms can be used to exploit these structural differences, this factor is very important to assess the relative efficiency of the two schemes. For the Newton scheme we need to evaluate three derivative terms in the Jacobian, implying that the Newton scheme is more costly and algebraically complex than Picard.

The dynamic time step sizes need to be adjusted according to the convergence behavior of the nonlinear iteration scheme. During any time step, a nonlinear convergence tolerance Tol is specified, along with a maximum number of iterations, $maxit$. The starting simulation time step size is Δt_0 and continues until we reach the simulation time T_{max} . If the convergence is achieved in a fewer number of iterations than another pre-assigned number of iterations $maxit_1$, then the current time step size is increased by a specified magnification factor, denoted by Δt_{mag} and this is repeated until we reach the maximum time step size Δt_{max} . It remains unchanged if the convergence required falls between $maxit_1$ and $maxit_2$ iterations. The time step size is decreased by a reduction factor of Δt_{red} to a minimum of Δt_{min} if the convergence required more than $maxit_2$ iterations. If convergence is not achieved within the maximum number of iterations, then back-stepping occurs that is, the solution is recomputed at the current time level using the reduced time size factor Δt_{red} to a minimum of Δt_{min} . For the iterative procedure, the initial conditions are used as the first solution estimate for the first time step of a transient simulation or for the steady state problems. For the subsequent time steps of a transient simulation, the first estimate is the previous time step pressure head solution. Therefore, the convergence behavior is dependent on the quality of the initial estimate and is directly affected by the time step size.

The infinity norm (l_∞) is used as the convergence termination criterion for both of the nonlinear iterative methods Newton and Picard, that is, when

$\| \psi^{k+1, (m+1)} - \psi^{k+1, (m)} \|_\infty \leq Tol$ is satisfied then convergence is achieved. This represents an absolute convergence criterion.

3.2.5. *Nested Newton scheme.*

The number of iterations needed to converge is a determining factor for the simulation efficiency in linearization schemes such as the Picard and the Newton. Therefore convergence rate is often enhanced by providing the solver with an initial estimate that is closer to the final solution for the current time step. This can be achieved by taking the initial estimate from the previous time step and by selecting a sufficient small time step [9]. Hence numerical algorithms often include an empirical time step adaptation criterion [28, 50, 63, 64]. In this section we illustrate the nested Newton-type algorithm proposed by [21] in detail.

[21] used a finite volume approach, but in this work we have used a finite difference spatial approximation. According to [21] the moisture capacity $c(\psi)$ is defined as $c(\psi) = p(\psi) - q(\psi)$, a difference of two nonnegative, nondecreasing, and bounded functions. Accordingly, the moisture content is defined as a difference of volumes $\theta(\psi) = \theta_1(\psi) - \theta_2(\psi)$, where $\theta_1(\psi)$ and $\theta_2(\psi)$ are integrals of $p(\psi)$ and $q(\psi)$, respectively. Then a nested Newton-type algorithm of Richards' equation is derived by linearizing, in order, $\theta_1(\psi)$ and $\theta_2(\psi)$ in the inner and in the outer cycle, respectively. For a wide class of constitutive relationships and all flow regimes, convergence of the iterations is ensured for any time step size.

The approximation of the time derivative of water content in the mixed form of Richards' equation is :

$$\frac{\partial \theta}{\partial t} = \frac{\theta(\psi_i^n) - \theta(\psi_i^{n-1})}{\Delta t} \quad (3.16)$$

where Δt is the time step size and n is the time index.

Using the discretized relation (2.7) and (3.16), a fully implicit formulation, at every time step n , for all $i = 1, 2, \dots, M$, the finite difference form of the mixed form of Richards' equation is taken to be

$$\theta(\psi_i^n) - r [\{K_{i-1}^n + K_i^n\}\psi_{i-1}^n - \{K_{i-1}^n + 2K_i^n + K_{i+1}^n\}\psi_i^n + \{K_i^n + K_{i+1}^n\}\psi_{i+1}^n] = b_i^n \quad (3.17)$$

where

$$b_i^n = \theta(\psi_i^{n-1}) + \frac{\Delta t}{2\Delta z} [K(\psi_{i+1}^n) - K(\psi_{i-1}^n) + S_i^n] \quad (3.18)$$

and $K_i^n = K(\psi_i^n)$ and so on.

For the given initial conditions ψ_i^0 equation (3.17) constitutes a fully nonlinear system of equations at every time step $n = 1, 2, 3, \dots$, to be solved for ψ_i^n . To solve (3.18), one can set $\psi_i^{n,0} = \psi_i^{n-1}$. Then the Picard iterations are taken to be

$$\begin{aligned} \theta(\psi_i^{n,m}) - r(\{K_{i-1}^{n,m-1} + K_i^{n,m-1}\}\psi_{i-1}^{n,m} - \\ \{K_{i-1}^{n,m-1} + 2K_i^{n,m-1} + K_{i+1}^{n,m-1}\}\psi_i^{n,m} + \{K_i^{n,m-1} + K_{i+1}^{n,m-1}\}\psi_{i+1}^{n,m}) = b_i^{n,m-1} \end{aligned} \quad (3.19)$$

where

$$b_i^{n,m-1} = \theta(\psi_i^{n-1}) + \frac{\Delta t}{2\Delta z} [K(\psi_{i+1}^{n,m-1}) - K(\psi_{i-1}^{n,m-1}) + S_i^{n,m-1}] \quad (3.20)$$

At each iteration $m = 1, 2, 3, \dots$, system (3.20) constitutes a mildly nonlinear system [49] for $\psi_i^{n,m}$, with the diagonal nonlinearity being presented by the volumes $\theta(\psi_i^{n,m})$. This system of equations represents a consistent and conservative discretization of (1.1). Therefore in spite of the chosen spatial and temporal accuracy, each Picard iterate $\psi_i^{n,m}$ is a conservative approximation for the new pressure. Generally an inexact solution of (3.19) will not be conservative.

In the current study, to ensure the resulting mass balance error will be negligible, local and global mass conservation will be enforced at each Picard iteration by solving (3.19) to the best possible accuracy. As a result convergence of the Picard iterations is not essential, however a

few steps can be allowed with the only purpose to update the hydraulic conductivity to the n^{th} time level [21].

Excluding the Picard iteration index m and the time index n , system (3.19), at every time step and for each Picard iteration, can be written in matrix form as :

$$\theta(\psi) + T\psi = \mathbf{b} \quad (3.21)$$

where $\psi = (\psi_i)$ is the unknown vector, $\theta(\psi) = \theta(\psi_i)$ is a nonnegative vectorial function representing the discrete fluid volumes, T is the diffusive flux matrix, and $\mathbf{b}$ is a known vector whose elements are the right-hand side of (3.19), properly augmented by the known Dirichlet boundary conditions.

Moisture capacity :

By denoting with θ_r the residual moisture content and by $c(\psi) = \frac{\partial \theta}{\partial \psi}$ the (nonnegative) specific moisture capacity, the moisture content can be expressed in terms of $c(\psi)$ as :

$$\theta(\psi) = \theta_r + \int_{-\infty}^{\psi} c(\xi) d(\xi). \quad (3.22)$$

So that $\theta_s = \theta_r + \int_{-\infty}^{\psi} c(\xi) d(\xi)$ is the soil porosity and $\theta(\psi) \leq \theta_s$ for all $\psi \in \mathfrak{R}$.

Assumption C1 : $c(\psi)$ is defined for all $\psi \in \mathfrak{R}$ and is a nonnegative function with bounded variations.

Assumption C2 : There exists $\psi^* \in \mathfrak{R}$ such that $c(\psi)$ is strictly positive and non decreasing in $(-\infty, \psi^*)$ and nonincreasing in $(\psi^*, +\infty)$.

Thus, $c(\psi) = \frac{\partial \theta}{\partial \psi} \geq 0$ and $\theta_r < \theta(\psi) \leq \theta_s$ for all $\psi \in \mathfrak{R}$.

The most commonly used constitutive equations, relating the moisture content to the pressure head, satisfy Assumptions $C1 - C2$. Since $c(\psi)$ are nonnegative functions with bounded variations, they are almost everywhere differentiable, admit only discontinuities of the first kind, and can be expressed as the difference of two nonnegative, nondecreasing, and bounded functions, say $p(\psi)$ and $q(\psi)$, so that $c(\psi) = p(\psi) - q(\psi) \geq 0$ and $0 \leq q(\psi) \leq p(\psi)$ for all $\psi \in \Re$. When $c(\psi)$ satisfies Assumptions $C1 - C2$, the corresponding Jordan decomposition is given by

$$p(\psi) = c(\psi), \quad q(\psi) = 0 \quad \text{if} \quad \psi \leq \psi^* \quad (3.23a)$$

$$p(\psi) = c(\psi^*), \quad q(\psi) = p(\psi) - c(\psi) \quad \text{if} \quad \psi > \psi^* \quad (3.23b)$$

In addition, fluid volumes $\theta(\psi) = \theta_1(\psi) - \theta_2(\psi)$ where each component of $\theta_1(\psi)$ and $\theta_2(\psi)$ respectively, is given by

$$\theta_1(\psi) = \theta_r + \int_{-\infty}^{\psi} c(\xi) d(\xi) \quad \text{and} \quad \theta_2(\psi) = \int_{-\infty}^{\psi} q(\xi) d(\xi) \quad (3.24)$$

or, equivalently

$$\theta_1(\psi) = \theta(\psi), \quad \theta_2(\psi) = 0 \quad \text{if} \quad \psi \leq \psi^* \quad (3.25a)$$

$$\theta_1(\psi) = \theta(\psi^*) + c(\psi^*)(\psi - \psi^*), \quad \theta_2(\psi) = \theta_1(\psi) - \theta(\psi) \quad \text{if} \quad \psi > \psi^* \quad (3.25b)$$

So that $\theta(\psi) = \theta_1(\psi) - \theta_2(\psi)$, $p(\psi) = \frac{d\theta_1(\psi)}{d\psi}$, and $q(\psi) = \frac{d\theta_2(\psi)}{d\psi}$.

Let $C(\psi)$, $P(\psi)$, and $Q(\psi)$ denote the diagonal matrices whose diagonal entries are $c(\psi)$, $p(\psi)$, and $q(\psi)$ respectively. Thus $C(\psi) = P(\psi) - Q(\psi)$ represents the Jacobian of $\theta(\psi)$ almost everywhere; $P(\psi)$ is almost everywhere the Jacobian of $\theta_1(\psi)$; and $Q(\psi)$ is almost everywhere

the Jacobian of $\theta_2(\psi)$.

Finally let $\mathbf{0}$ and $\mathbf{O}$ denote the zero vector and zero matrix of appropriate size respectively. The following easy property is stated here for later reference.

LEMMA 1.

Let $c(\psi)$ satisfy the Assumptions $C1$ and $C2$, and let $p(\psi)$ and $q(\psi)$ be the Jordan decomposition of $c(\psi)$. For all $\varphi, \psi \in \Re$ one has

$$P(\psi)(\psi - \varphi) - [\theta_1(\psi) - \theta_1(\varphi)] \geq \mathbf{O}$$

$$Q(\psi)(\psi - \varphi) - [\theta_2(\psi) - \theta_2(\varphi)] \geq \mathbf{O}$$

Diffusive flux matrix :

Without loss of generality, it will be assumed that matrix T is irreducible. This may not be the case when, at any time, two or more subdomains are not connected by strictly positive diffusive flux coefficients. In such a circumstance the considerations that follow apply separately to each such subdomain where the corresponding matrix T is irreducible.

To account for Dirichlet, Neumann, and mixed Neumann boundary conditions, matrix T is assumed to be symmetric and (at least) positive semidefinite, satisfying either one of the following properties:

$T1$: T is a symmetric M -matrix (i.e., a Stieltjes Matrix), or

$T2$: T is singular, and $T + D$ is a Stieltjes matrix for all diagonal matrices $D \succcurlyeq O$ (i.e., $D \geq O$ and $D \neq O$).

When T is $T2$, the following compatibility assumption is required on $\mathbf{b}$:

$$\sum \theta_r < \sum b < \sum \theta_s \tag{3.26}$$

Inequalities (3.26) assure the physically and mathematical compatibility of the systems (3.21). This assumption states that, the resulting total fluid volume must be larger than the total residual volume and smaller than the maximum water volume when the flow boundary conditions are specified everywhere along the boundary faces [20].

Nested Iterations :

In general, to achieve faster convergence we can take as the initial guess for the iterative procedure the solution from an outer iteration loop or from the previous time step. Therefore, in order to meet the requirement $\psi^0 \leq \psi^*$ of ALGORITHM1 (see below) to get the advantage of the known solution from the previous Picard iteration, a suggested choice for the initial guess is as follows:

$$\psi^0 = \min(\psi^*, \psi^{n,m-1}) \quad (3.27)$$

where n and m represent the time and Picard iterations indices.

From the Brooks-Corey model, we see that the moisture capacity $c(\psi)$ is maximum at $\psi^* = \psi_d$ and $\psi_d = -\frac{1}{\alpha}$.

Also, from the van Genuchten model, we have $\psi^* = -\frac{1}{\alpha} \left(\frac{n-1}{n} \right)^{\frac{1}{n}}$.

According to [21] consider the matrix T is satisfied T2 with the inequalities (3.26) hold true and the moisture capacities satisfy both Assumptions C1 and C2, so the system (3.21) becomes:

$$\theta_1(\psi) - \theta_2(\psi) + T\psi = \mathbf{b} \quad (3.28)$$

Choose $\psi^0 \leq \psi^*$, to linearize $\theta_2(\psi)$, we get from (3.2.5), a sequence of outer iterates $\{\psi^k\}$ as follows:

$$\theta_1(\psi^k) - [\theta_2(\psi^{k-1}) + Q(\psi^{k-1})(\psi^k - \psi^{k-1})] + T\psi^k = \mathbf{b} \quad (3.29)$$

We can write the above equation in the form

$$\theta_1(\psi^k) + (T - Q^{k-1})\psi^k = \mathbf{d}^{k-1}, \quad k = 1, 2, \dots \quad (3.30)$$

which is a system of mildly nonlinear equations, whose solutions are $\{\psi^k\}$, and where $Q^{k-1} = Q(\psi^{k-1})$, $\mathbf{d}^{k-1} = \mathbf{b} + \theta_2(\psi^{k-1}) - Q^{k-1}\psi^{k-1}$

Now for all $k = 1, 2, \dots$ by setting $\psi^{k,0} = \psi^{k-1}$ and linearizing $\theta_1(\psi)$, we get a sequence of inner iterates $\{\psi^{k,l}\}$ derived from equation (3.30) as follows :

$$[\theta_1(\psi^{k,l-1}) + P(\psi^{k,l-1})(\psi^{k,l} - \psi^{k,l-1})] + (T - Q^{k-1})\psi^{k,l} = \mathbf{d}^{k-1} \quad (3.31)$$

Thus we can determine the inner iterates from the following linear systems :

$$(P^{k,l-1} + T - Q^{k-1})\psi^{k,l} = \mathbf{f}^{k,l-1}, \quad l = 1, 2, \dots \quad (3.32)$$

where $P^{k,l-1} = P(\psi^{k,l-1})$ and $\mathbf{f}^{k,l-1} = \mathbf{d}^{k-1} - \theta_1(\psi^{k,l-1}) + P^{k,l-1}\psi^{k,l-1}$.

The k^{th} outer residual from (3.30) is $\mathbf{r}^k = \theta_1(\psi^k) + T\psi^k - \mathbf{b}$, which satisfies (by LEMMA 1) the relation:

$$\mathbf{r}^k = -\{Q^{k-1}(\psi^{k-1} - \psi^k) - [\theta_2(\psi^{k-1}) - \theta_2(\psi^k)]\} \leq \mathbf{0} \quad (3.33)$$

The stopping criterion for the outer iterations is $\|\mathbf{r}^k\| < \varepsilon$ where ε is the user defined tolerance representing the maximum mass balance error allowed.

Similarly, the $(k, l)^{th}$ inner residual can be derived from (3.32) and it is also satisfies the LEMMA 1, so

$$\mathbf{r}^{k,l} = P^{k,l-1}(\psi^{k,l-1} - \psi^{k,l}) - [\theta_1(\psi^{k,l-1}) - \theta_1(\psi^{k,l})] \geq \mathbf{0} \quad (3.34)$$

And the stopping criteria for the inner iterations is $\|\mathbf{r}^{k,l}\| < \varepsilon$.

The above nested iterations can be summarized as ALGORITHM1:

ALGORITHM1:

```

Choose  $\psi^o \leq \psi^*$ 
Do  $k = 1, 2, \dots$ 
Set  $\psi^{k,0} = \psi^{k-1}$ 
Do  $l = 1, 2, \dots$ 
Solve  $(P^{k,l-1} + T - Q^{k-1}) \psi^{k,l} = \mathbf{f}^{k,l-1}$ 
If  $\|\mathbf{r}^{k,l}\| < \varepsilon$ , then set  $\psi^k = \psi^{k,l}$  and exit
End do
If  $\|\mathbf{r}^k\| < \varepsilon$ , then set  $\psi = \psi^k$  and exit
End do

```

3.3. Description of test problems.

To justify the proposed nested algorithm and to compare with the numerical solution of Richards' equation by the CATHY model, we consider three one-dimensional test problems. The first one-dimensional test problem deals with a sharp moisture front that infiltrates into the soil column [21, 31, 74]. The second one-dimensional test case involves flow into a layered soil with variable initial conditions [21, 82, 86]. The last one-dimensional test problem concerns flow into very dry heterogeneous soil.

3.3.1. Test Problem 1.

This problem considers a soil column of 2.0 m deep discretized with a vertical resolution $\Delta z = 0.00625$ m. The initial pressure head distribution is $\psi(z, 0) = z - 2$. At the bottom of the column, a water table boundary condition (i.e., $\psi(0, t) = 0$) is imposed, while a time-dependent Dirichlet condition is imposed at the top boundary which is presented in Figure 7.

$$\psi(2, t) = \begin{cases} -0.05 + 0.03 \sin\left(\frac{2\pi t}{100000}\right) & \text{if } 0 < t \leq 100000 \\ 0.1 & \text{if } 100000 < t \leq 180000 \\ -0.05 + 2952.45 \exp\left(-\frac{t}{18204.8}\right) & \text{if } 180000 < t \leq 300000 \end{cases}$$

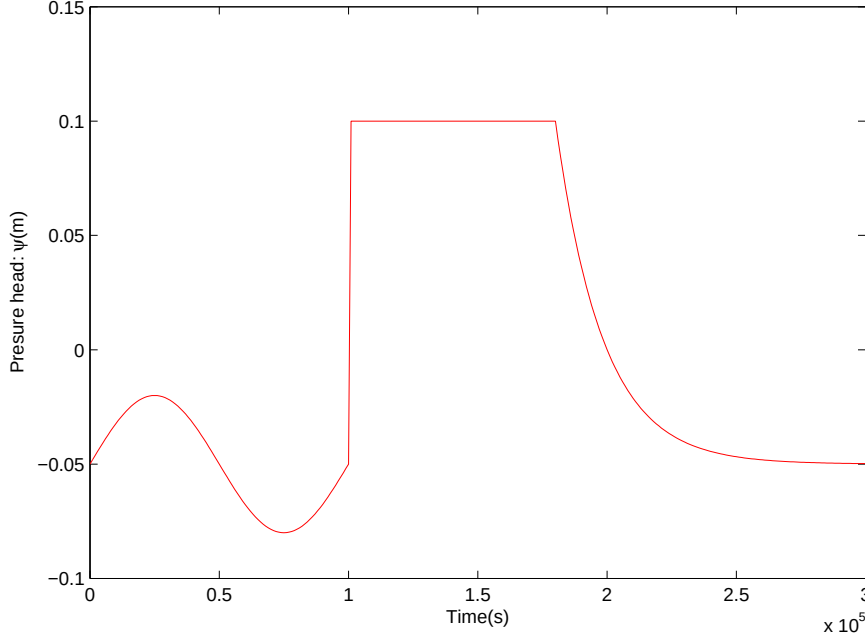


FIGURE 7. Dirichlet BC imposed at the top of the soil column for Test Problem 1.

The soil hydraulic properties are described by the van Genuchten model. The soil parameters are given in Table 8 [21, 31, 74]. The Dirichlet boundary condition leads to significant ponding between 100000 and 200000 s (27.8 and 55.6 h), and as will be seen in the results, this type of boundary condition, prominent in coupled groundwater/surface water modeling, is a source of significant difficulty in the iterative schemes.

These soil properties correspond to an unconsolidated clay loam with a nonuniform grain size distribution [136]. Previous studies [72] carried out a similar comparison using a moisture-based form of Richards equation and a different test case that does not feature time-varying boundary

TABLE 8. Soil hydraulic properties used in Test Problem 1.

Parameters	Values
θ_s	0.410
θ_r	0.095
α (m ⁻¹)	1.9
n	1.31
K_s (m/d)	0.062

conditions with surface ponding.

The second period of the simulation ($100000 < t \leq 180000$ s) is very challenging for numerical solvers. Because of sudden increase of the upper Dirichlet boundary condition to a positive value of 0.1 m (ponding), it creates a sharp moisture front that infiltrates into the soil column. At the beginning of the third period ($t > 180000$ s) ponding decreases exponentially, reaching asymptotically a final value -0.05 m, and by the end of the simulation the entire column is close to full saturation.

3.3.2. Test Problem 2.

This case involves vertical drainage through a layered soil from initially saturated conditions. At time $t = 0$, the pressure head at the base of the column is reduced from 2 to 0 m. During the subsequent drainage, a no flow boundary condition is applied to the top of the column. This problem is considered to be a challenging test for numerical methods because a sharp discontinuity in the moisture content occurs at the interface between two material layers [21, 82, 86].

During downward draining the middle coarse soil tends to restrict drainage from the upper fine soil, and high saturation levels are maintained in the upper fine soil for a considerable period of time. The Brooks-Corey model is used to prescribe the pressure-moisture relationship. The hydraulic properties of the soils are given in Table 9. The soil profile is Soil 1 for $0 < z < 0.6$ m and $1 < z < 2$ m and Soil 2 for $0.6 < z < 1.2$ m. A Dirichlet boundary condition is imposed at the base of the bottom boundary.

TABLE 9. Soil hydraulic properties used in Test Problem 2.

Parameters	Soil 1	Soil 2
θ_s	0.35	0.35
θ_r	0.07	0.035
α (cm ⁻¹)	0.0286	0.0667
n	1.5	3.0
K_s (cm/s)	9.81×10^{-5}	9.81×10^{-3}

3.3.3. Test Problem 3.

The present test problem involves a one-dimensional flow into initially dry layered soil of sand and clay. The van Genuchten model is used to prescribe the pressure-moisture relationship. The hydraulic properties of the sand and clay are given in Table 10 and initial pressure head is set to -4.80 m. The soil profile is sand for $0 < z < 1$ m and $2 < z < 3$ m, and clay for $1 < z < 2$ m. A no-flow boundary condition is applied everywhere except for a water flux rate of 0.5 m/d that is applied to the top of the vertical column. This problem was specifically devised for testing numerical algorithm's ability to survive both very dry conditions and transitions to a saturated state.

TABLE 10. Soil hydraulic properties used in Test Problem 3.

	Sand	Clay
$\theta_s(-)$	0.3658	0.4686
$\theta_r(-)$	0.0286	0.1060
α (cm ⁻¹)	0.0280	0.0104
$n(-)$	2.2390	1.3954
K_s (m/s)	6.26×10^{-3}	1.5167×10^{-4}

3.4. Results.

3.4.1. Test Problem 1.

The moisture retention curve is monotonic with a point of inflection that gives the moisture capacity function its typical shape. The soil moisture retention curves for this test problem using the van Genuchten model are represented in Figure 8.

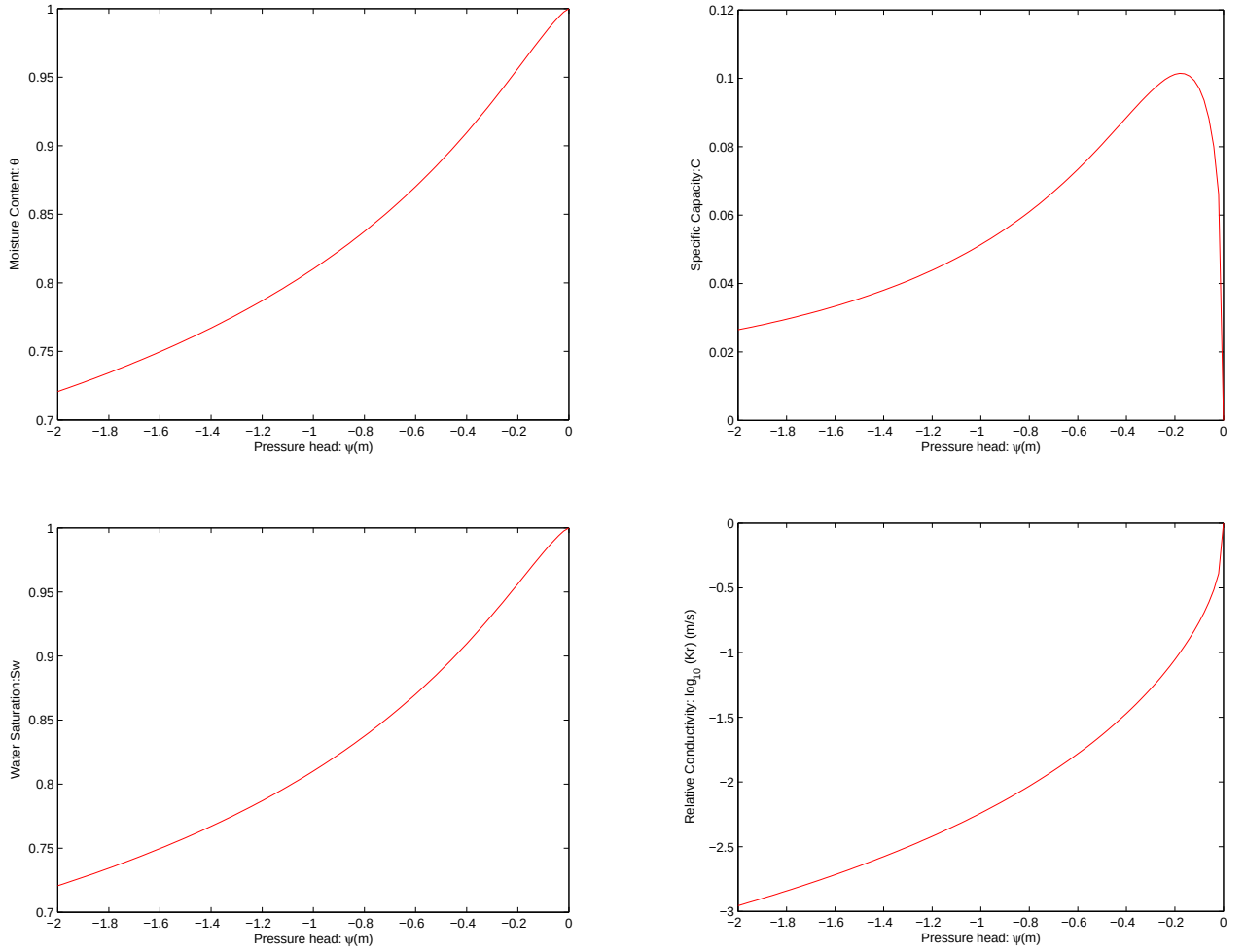


FIGURE 8. Soil moisture retention curves for Test Problem 1.

We simulated this test problem for four different vertical discretizations: 500, 250, 50, and 10 layers. For each discretization we used four different time step sizes $\Delta t_{max} = 1000$ s, 100 s, 10 s, and 1 s.

We implemented nested Newton to solve this test problem in a Matlab code and we also solved the problem with the Picard and Newton schemes in the CATHY model.

We plotted the errors at the 4 times for a wide range of solutions. The RMSE (root mean squared error) are computed against a reference solution that was generated with a 1000-layer discretization and strict time stepping and convergence criteria (for Picard and Newton, the base solution is made by CATHY and for nested Newton by the Matlab code).

We used analytical differentiation for evaluating the soil moisture characteristics for both CATHY and nested Newton. In CATHY we used $\Delta t_{mag} = 1.05$, $\Delta t_{red} = 0.50$, $\Delta t_{min} = 1.0 \times 10^{-4}$, $maxit_1 = 10$, $maxit_2 = 6$ and the maximum number of nonlinear iterations is 15 for all runs. The nonlinear convergence tolerance on the L_2 norm of the error was 1.0×10^{-4} . Backward Euler time stepping scheme and lumped mass matrix are used for all simulations. We used BiCGSTAB to solve the linear systems with 1.0×10^{-10} for the linear tolerance where the maximum number of linear iterations is 1000.

The computed pressure head and the corresponding water saturation profiles at various times obtained with a tolerance 1.0×10^{-4} are displayed in Figures 9 and 10. These solutions are very similar to those reported in the literature [21, 31, 74]. The initial conditions and pressure head solution profiles at 4 different times are shown in Figure 9. The red profile, which falls within the ponding period, shows the excess water that forms at the soil surface and the rather sharp moisture front that is generated.

In the investigation of solution behavior, we included adaptive time stepping behavior of Newton and Picard for all vertical discretizations. We found most striking here the very different behavior between the Newton and Picard schemes during the ponding period. Whereas the Newton scheme is forced to take very small step sizes only at the very beginning and end of the ponding period, the Picard scheme needs to negotiate a wide range of step sizes throughout the ponding period, and indeed for the $\Delta t_{max} = 1000$ s case it never achieves this maximum

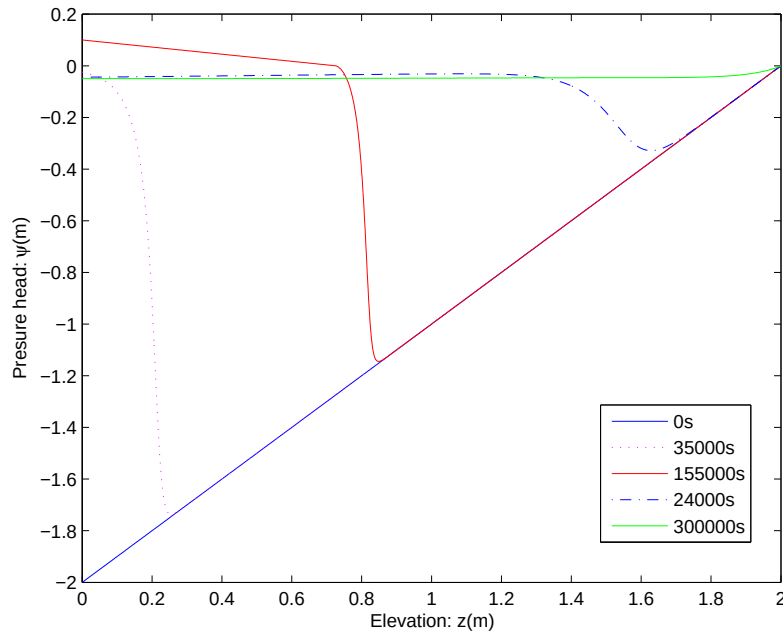


FIGURE 9. Pressure profile at various times throughout the simulation for Test Problem 1.

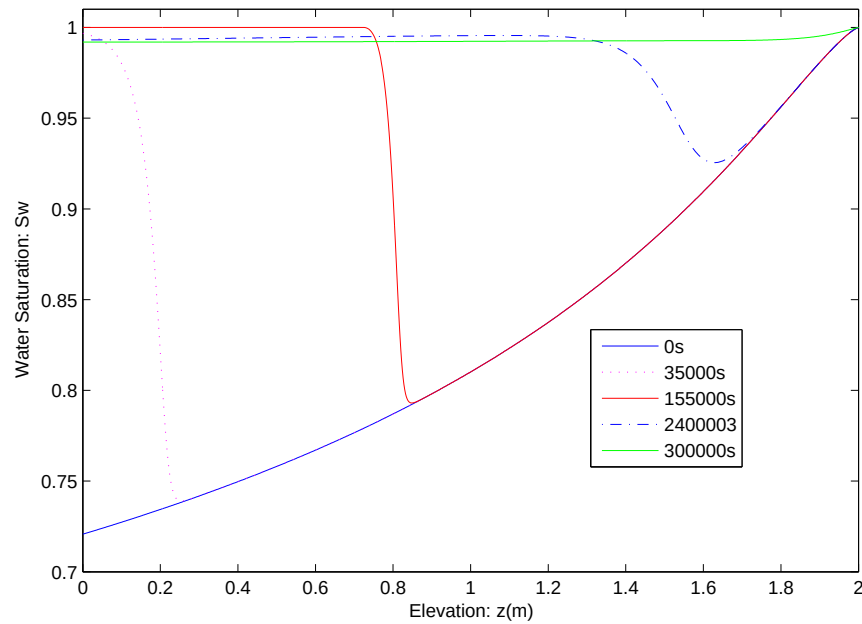


FIGURE 10. Water saturation profile at various times throughout the simulation for Test Problem 1.

value during ponding, for any of the vertical discretizations. Constraining an iteration scheme to take extremely small time steps for prolonged periods during a simulation can represent an

enormous computational burden for subsurface solvers. For simplicity, and to understand the time stepping behavior of Newton and Picard, we plotted the 250 layers case with all time step sizes in Figure 11. The time stepping behavior of Newton and Picard can be found in Figures 12 and 13 respectively.

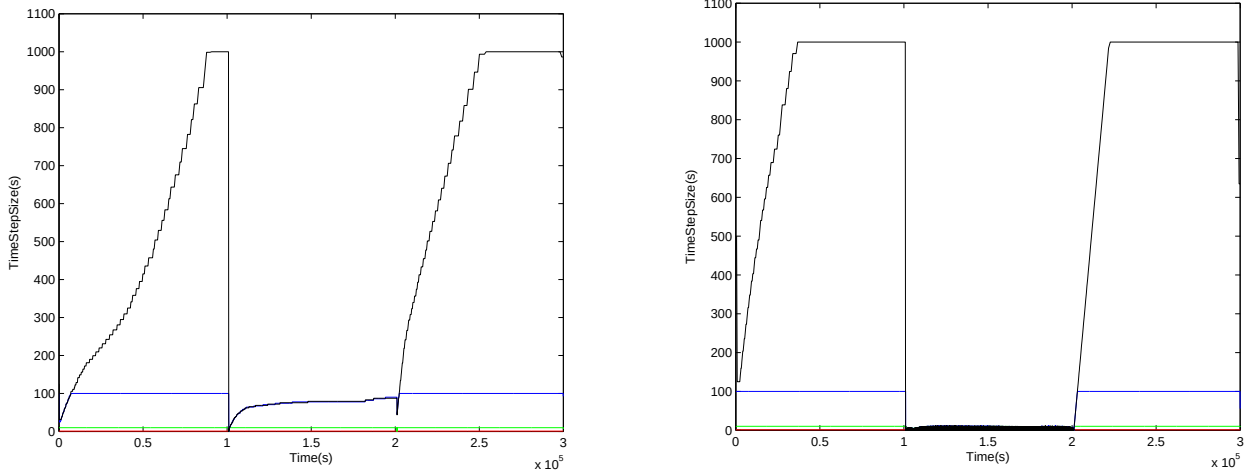


FIGURE 11. Time stepping behavior of Newton (left) and Picard (right) for 250 layer discretization of Test Problem 1. Red, green, blue, and black lines: $\Delta t_{max} = 1$ s, 10 s, 100 s, and 1000 s respectively.

We have shown graphically the convergence behavior of the Newton and Picard Figures 14 and 15 respectively schemes in terms of the number of nonlinear iterations required at each time step. In Figure 16 the inner iteration per time step is observed for the nested newton scheme. The nested Newton scheme exhibits a behavior similar to Newton, but with a smoother transition into and out of the ponding period, and without the need for time step adaptation.

It is shown that from the inner iteration behavior (Figure 16) of nested Newton the ponding period (100000 s to 200000 s) is very difficult for the numerical solver. In this period, 3 to 8 inner iterations are needed per outer iteration to get convergence for 500 layer discretizations for all time step sizes. Out of this range of simulation period, it requires few number of inner iterations per outer iteration. We have seen similar convergence behavior for the 250 and 50 layer cases. For the 10 layer case only 1 inner iteration is needed to achieve convergence per

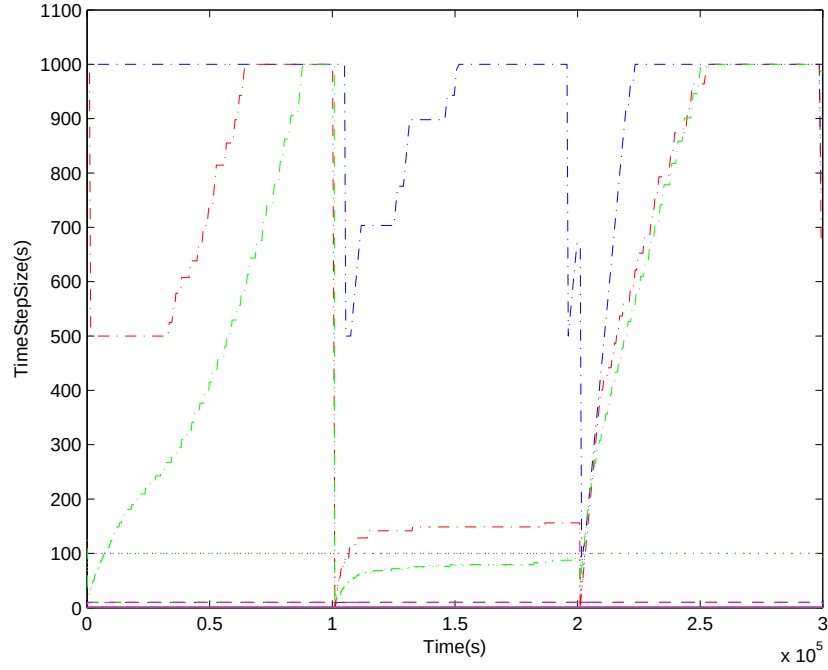


FIGURE 12. Time step size behavior of Newton scheme for Test Problem 1. Blue, red, green, and black lines: 10, 50, 250, and 500 layers respectively. Solid, dashed, dotted, and dash-dotted lines: $\Delta t_{max} = 1$ s, 10 s, 100 s, and 1000 s respectively.

outer iteration for $\Delta t_{max} = 1$ s.

The mass balance behavior is presented for the Picard and Newton schemes for the 10, 50, 250, and 500-layer discretizations and for all time step sizes. The mass balance error almost closes to zero except for a few cases around 100000 s. The cumulative mass balance error behavior for Newton and Picard is plotted in Figure 17. Note that in the 500 layer discretization, Newton is diverges for $\Delta t_{max} = 100$ s and 1000 s. Figure 18 is the combined mass balance behavior of Picard and Newton.

We have presented summary statistics for the Picard and Newton schemes run over a wide range of mesh discretizations (10, 50, 250, and 500 layers, i.e., $\Delta z = 20, 4, 0.8$, and 0.4 cm, respectively) and maximum time step sizes ($\Delta t_{max} = 1000$ s, 100 s, 10 s, and 1 s). There are 8 performance indicators (in Tables 11, 12, 13, 14) which are: total volumetric and percentage mass balance error, total number of time steps and average step size, the average number of Newton or Picard iterations taken at each time step, the average number of iterations needed

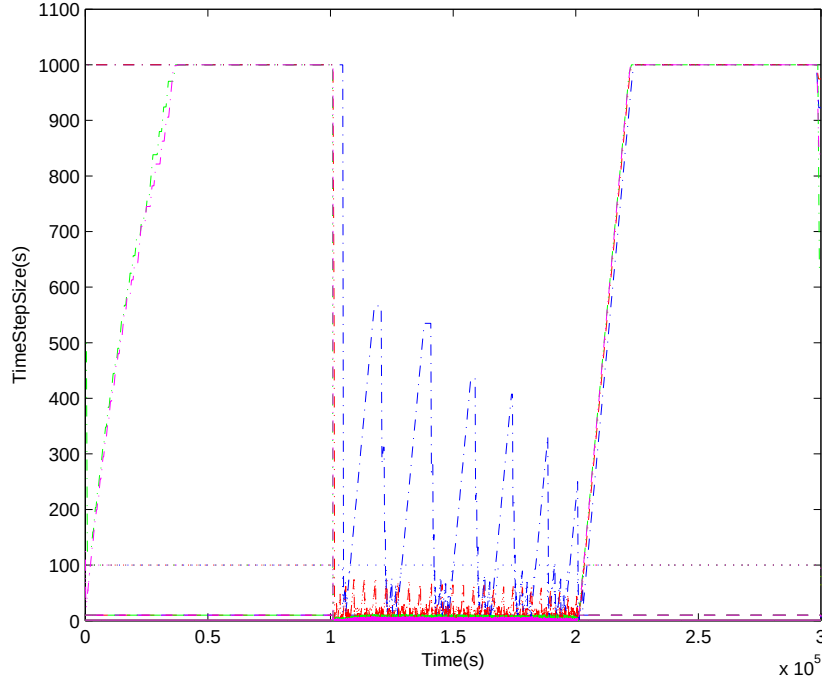


FIGURE 13. Time step size behavior of Picard scheme for Test Problem 1. Blue, red, green, and black lines: 10, 50, 250, and 500 layers respectively. Solid, dashed, dotted, and dash-dotted lines: $\Delta t_{max} = 1$ s, 10 s, 100 s, and 1000 s respectively.

to solve the linear algebraic system at each Picard or Newton iteration, the number of back-stepping occurrences (failure of Picard or Newton to converge within a preset maximum number of iterations-15 in these runs-so that the time step is repeated at a smaller step size), and the number of linear solver failures (only relevant for the Newton scheme, which generates a non-symmetric algebraic system).

TABLE 11. Computational performance of CATHY model: Picard scheme for $\Delta t_{max}=1$ s and 10 s: Test Problem 1.

Δt_{max} (s) $\rightarrow$	1	1	1	1	10	10	10	10
Δz (cm)	20	4	0.8	0.4	20	4	0.8	0.4
MBE (m^3)	-4.15e-4	-2.13e-5	9.85e-6	4.95e-6	-4.15e-4	-2.11e-5	8.12e-6	8.44e-6
MBE (perc.)	-8.38e0	-3.96e-1	1.82e-1	9.15e-2	-8.38e0	-3.91e-1	1.50e-1	1.56e-1
Time Steps	300000	303006	364601	403462	30333	42583	136622	186242
Δt (s)	1.00	0.99	0.82	0.74	9.89	7.05	2.20	1.61
NL It/Step	1.01	1.43	1.65	1.70	1.70	2.22	2.44	2.37
Lin It/NL It	2.00	3.00	3.09	3.03	3.67	4.73	4.38	4.02
Back steps	0	367	6290	9564	45	1084	7911	11419
Solver Failures	0	0	0	0	0	0	0	0

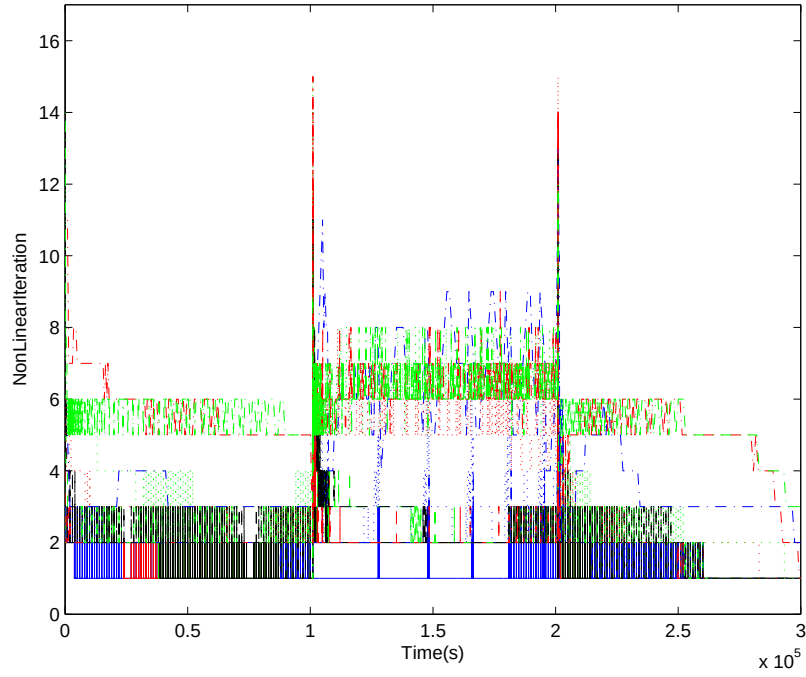


FIGURE 14. Convergence behavior of Newton scheme for Problem 1. Blue, red, green, and black lines: 10, 50, 250, and 500 layers respectively. Solid, dashed, dotted, and dash-dotted lines: $\Delta t_{max} = 1$ s, 10 s, 100 s, and 1000 s respectively.

TABLE 12. Computational performance of CATHY model: Picard scheme for $\Delta t_{max} = 100$ s and 1000 s: Test Problem 1.

Δt_{max} (s) $\rightarrow$	100	100	100	100	1000	1000	1000	1000
Δz (cm)	20	4	0.8	0.4	20	4	0.8	0.4
MBE (m^3)	-4.15e-4	-2.13e-5	9.85e-6	4.95e-6	-4.15e-4	-2.11e-5	8.12e-6	8.44e-6
MBE (perc.)	-8.38e0	-3.96e-1	1.82e-1	9.15e-2	-8.38e0	-3.91e-1	1.50e-1	1.56e-1
Time Steps	300000	303006	364601	403462	30333	42583	136622	186242
Δt (s)	1.00	0.99	0.82	0.74	9.89	7.05	2.20	1.61
NL Ite/Step	1.01	1.43	1.65	1.70	1.70	2.22	2.44	2.37
Lin Ite/NL Ite	2.00	3.00	3.09	3.03	3.67	4.73	4.38	4.02
Back steps	0	367	6290	9564	45	1084	7911	11419
Solver Failures	0	0	0	0	0	0	0	0

TABLE 13. Computational performance of CATHY model: Newton scheme for $\Delta t_{max} = 1$ s and 10 s: Test Problem 1.

Δt_{max} (s) $\rightarrow$	1	1	1	1	10	10	10	10
Δz (cm)	20	4	0.8	0.4	20	4	0.8	0.4
MBE (m^3)	-4.15e-4	-2.14e-5	9.74e-6	5.84e-6	-4.15e-4	-2.09e-5	1.40e-5	5.90e-6
MBE (perc.)	-8.37e0	-3.97e-1	1.80e-1	1.08e-1	-8.38e0	-3.87e-1	2.59e-1	1.09e-1
Time Steps	300000	300096	300083	300196	30000	30149	30247	30266
Δt (s)	1.00	0.9997	0.9997	0.9993	10.00	9.95	9.92	9.91
NL Ite/Step	1.01	1.42	1.47	1.47	1.68	1.86	2.05	2.08
Lin Ite/NL Ite	2.16	3.24	3.52	3.70	3.50	4.17	4.83	4.95
Back steps	0	2	6	13	0	6	16	14
Solver Failures	0	0	0	3	0	0	2	1

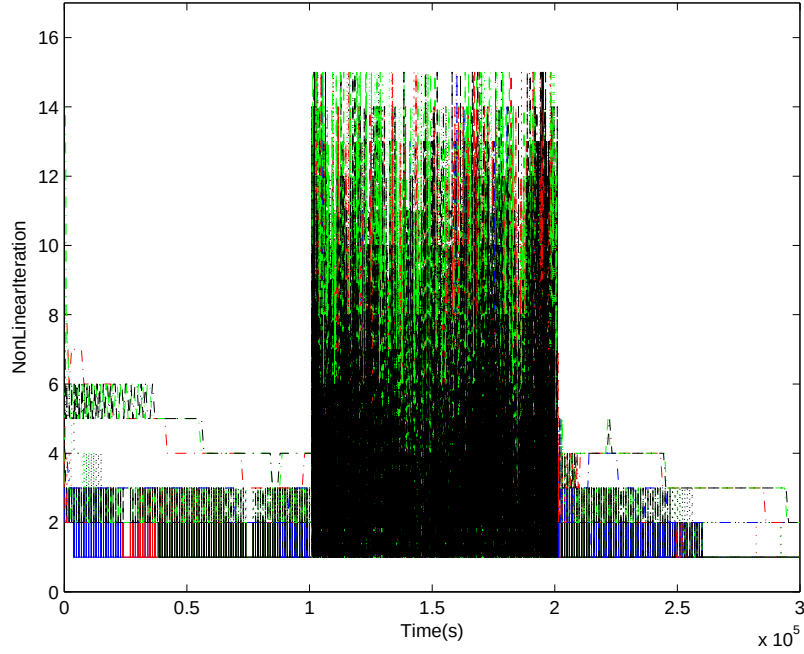


FIGURE 15. Convergence behavior of Picard scheme for Problem 1. Blue, red, green, and black lines: 10, 50, 250, and 500 layers respectively. Solid, dashed, dotted, and dash-dotted lines: $\Delta t_{max} = 1$ s, 10 s, 100 s, and 1000 s respectively.

TABLE 14. Computational performance of CATHY model: Newton scheme for $\Delta t_{max} = 100$ s and 1000 s: Test Problem 1.

Δt_{max} (s) $\rightarrow$	100	100	100	100	1000	1000	1000	1000
Δz (cm)	20.0	4.0	0.8	0.4	20.0	4.0	0.8	0.4
MBE (m^3)	-4.14e-4	-1.52e-5	2.24e-5	div	-4.05e-4	-1.65e-5	3.19e-5	div
MBE (perc.)	-8.36e0	-2.82e-1	4.13e-1	div	-8.17e0	-3.05e-1	5.87e-1	div
Time Steps	3016	3187	3737	div	357	1281	2237	div
$\Delta t(s)$	99.5	94.1	80.3	div	840.0	234.0	134.0	div
NL Ite/Step	2.12	3.38	4.26	div	4.60	5.58	5.93	div
Lin Ite/NL Ite	5.33	6.42	6.88	div	7.54	8.23	8.04	div
Back steps	0	7	12	div	1	15	22	div
Solver Failures	0	0	1	div	0	1	3	div

Nested Newton runs at a fixed time step size and there is no back-stepping. The number of time steps, the total number of outer iterations, and the total number of inner iterations required to cover the entire simulation are reported. Also the average number of outer iterations per time step and the average number of inner iterations per outer iteration are indicated (Table 15).

Particularly, the total number of inner iterations corresponds to the number of linear systems being solved within each run, so this number is directly related to the overall performance.

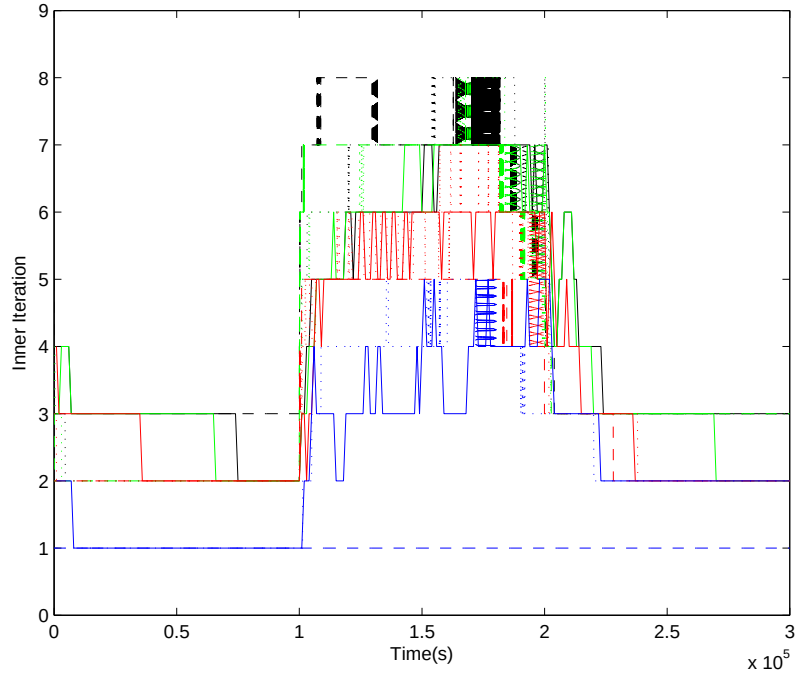


FIGURE 16. Convergence behavior of nested Newton scheme for Problem 1. Blue, red, green, and black lines: 10, 50, 250, and 500 layers respectively. Dashed, dotted, and solid lines: $\Delta t_{max} = 10$ s, 100 s, and 1000 s respectively.

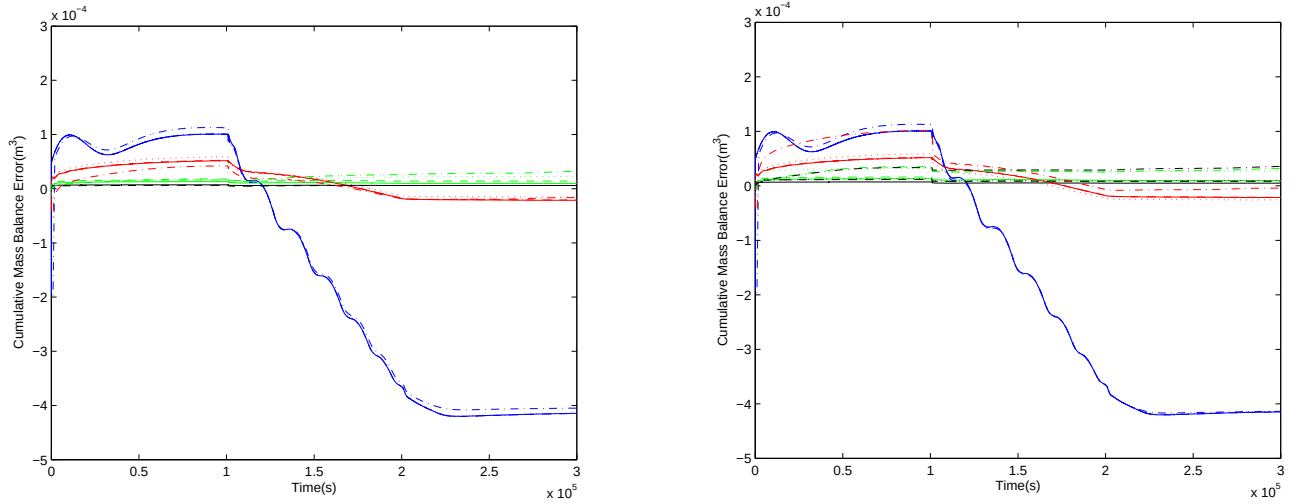


FIGURE 17. Cumulative mass balance error of Newton scheme (left) and Picard scheme (right) for Test Problem 1. Blue, red, green, and black lines: 10, 50, 250, and 500 layers respectively. Dashed, dotted, and solid lines: $\Delta t_{max} = 10$ s, 100 s, and 1000 s respectively.

The accuracy for each of the simulations is evaluated by the root mean squared error (RMSE) with respect to the exact solution. The calculated error for all the discretizations at 4 different

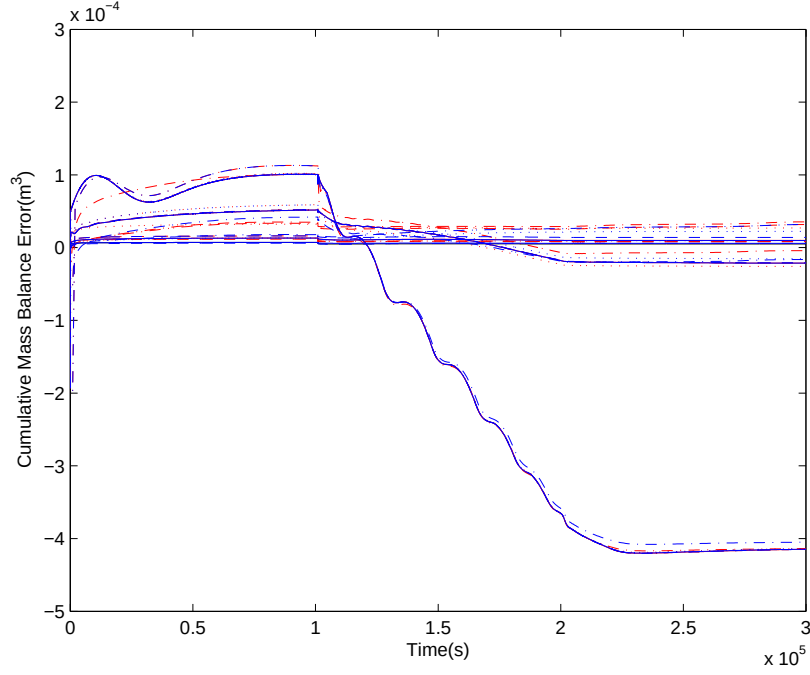


FIGURE 18. Cumulative mass balance error of Picard (red) and Newton (blue) scheme for Test Problem 1. Solid, dashed, dotted, and dash-dotted lines: $\Delta t_{max} = 1$ s, 10 s, 100 s, and 1000 s respectively.

TABLE 15. Computational performance of nested Newton scheme: Test Problem 1.

	Δt_{max} (s) $\rightarrow$	1000	100	10
Δz (cm) $\downarrow$	No. of Time Steps	300	3000	30000
20	Tot. outer iterations	670	7133	30000
	Tot. inner iterations	680	7133	30000
	Avg. outer iterations	2.23	2.38	1.00
	Avg. inner iterations	1.01	1.00	1.00
4	Tot. outer iterations	899	9920	91203
	Tot. inner iterations	1039	9929	91203
	Avg. outer iterations	3.00	3.31	3.04
	Avg. inner iterations	1.16	1.00	1.00
0.8	Tot. outer iterations	899	9920	91203
	Tot. inner iterations	1039	9929	91203
	Avg. outer iterations	3.00	3.31	3.04
	Avg. inner iterations	1.16	1.00	1.00
0.4	Tot. outer iterations	1041	12077	131712
	Tot. inner iterations	1240	12124	131731
	Avg. outer iterations	3.47	4.03	4.39
	Avg. inner iterations	1.19	1.00	1.00

times, specifically, at 35000 s, 155000 s, 240000 s, and 300000 s for Picard and Newton and for all time step sizes, is plotted. Also the error plot is made for the nested Newton scheme at the

same times with all the time step sizes. We have shown that the expected errors are highest at the coarsest spatial and temporal discretizations, and the peak errors propagate with the moisture front that is moving downwards into the soil. Picard errors are generally a little higher than Newton errors, and the sharp increase in (absolute) error during the ponding period can be noted.

To discuss about the error behavior of the Picard and Newton schemes, we attached individual error graphs of Newton and Picard for 50, 250, and 500 layers along with all different time step sizes. Figure 19 is represents 50, 250 and 500 layers respectively for the Newton and Picard methods.

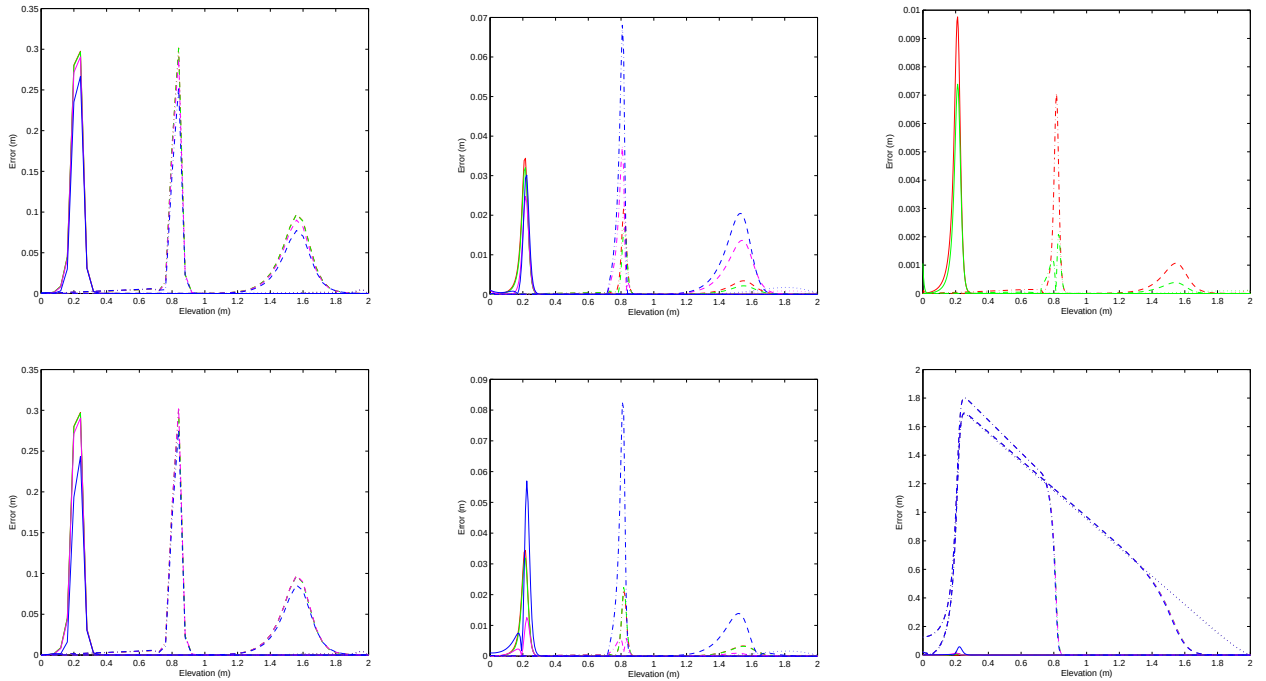


FIGURE 19. Error profile for 50, 250, and 500 layers: Newton (top three plots) and Picard (bottom three subplots) for Test Problem 1. Red, green, magenta, and blue lines: $\Delta t_{max} = 1$ s, 10 s, 100 s, and 1000 s respectively. Solid, dash-dotted, dashed, and dotted lines are at times 35000 s, 155000 s, 240000 s, and 300000 s respectively.

For the 50 layers Picard case we see that the maximum error is given in the interval $[0.08, 0.32]$ and it is 0.2973 m, 0.2967 m, 0.2903 m, and 0.2434 m at $z = 0.24$ m for $\Delta t = 1$ s, 10 s, 100 s, and 1000 s respectively at time=35000 s and then the error is always less than 10^{-5} m until the

end of the domain. At time=155000 s, the maximum error is found in the interval $[0.72, 0.92]$. Before $z = 0.72$ m, the error is less than 5.88×10^{-3} m and after $z = 0.92$ m, we found small error, which is less than 1.24×10^{-3} m. When we consider the third time=240000 s, we got 9.67×10^{-2} m as a maximum value at $z = 1.56$ m for $\Delta t = 1$ s, 10 s, 100 s and for 1000 s case, it is 8.57×10^{-2} m. Before $z = 1.2$ m, it is less than 1.11×10^{-3} m. For the time=300000 s case, the error is less than 4×10^{-6} m in the whole simulation.

In the case of 250 layers for Picard, it can be observed that, in the interval $[0, 0.296]$, maximum error is 5.7×10^{-2} m and minimum value is 1.26×10^{-2} m for $\Delta t = 1000$ s and $\Delta t = 100$ s respectively for the time=35000 s case. After this interval the error is less than 6.5×10^{-5} m. Except in the neighbourhood of $z = 0.8$ m, the calculated error for time=155000 s case is always less than 4.3×10^{-5} m. Out of the interval $[1.2, 1.64]$, we have seen the error less than 1.69×10^{-4} m for all types of time discretization for time=240000 s. For time=300000 s the maximum evaluated error value is 1.41×10^{-3} m for $\Delta t_{max} = 1000$ s but for all other time step sizes the error is less than 10^{-3} m.

Excellent error behavior is found for the 500 layers Picard case. At time=35000 s for $\Delta t_{max} = 1000$ s, the maximum error is 5.80×10^{-3} m at $z = 0.224$ m. For $\Delta t_{max} = 1$ s, 10 s, 100 s, maximum errors are 9.59×10^{-3} m, 6.30×10^{-3} m and 1.29×10^{-2} m respectively, found at $z = 0.208$ m. For $\Delta t_{max} = 1000$ s time step size, error becomes 1.96×10^{-4} m at $z = 0.3$ m and then continuously decreases, and approaches 0 m error at $z = 0.4$ m. This trend remains unchanged until the end of the simulation. The error behaves similarly for all other time step sizes in this time. For the time=300000 s case, the maximum error is recorded at $z = 0.256$ m and it is 1.81 m for $\Delta t_{max} = 1000$ s, and other time step sizes behave similarly. But for time=300000 s and $\Delta t_{max} = 1$ s, the error is always less than 10^{-5} m.

For the 10, 50 and 250 layers cases, Newton shows the same error behavior of the corresponding Picard case. Note that Newton diverges for $\Delta t_{max} = 100$ s and $\Delta t_{max} = 1000$ s for 500 layers. This scheme shows excellent error behavior, the maximum error is 9.76×10^{-3} m at $z = 0.212$

m is recorded for all the cases in the whole domain.

The nested Newton scheme error graphs are plotted for 4 different sets of layers with 3 different time step sizes $\Delta t_{max} = 10$ s, 100 s, 1000 s at the same 4 times as for the Picard and Newton cases. For 500 layers, nested Newton error behavior is the same as the Picard method. Layer-wise error graphs are presented in Figure 20.

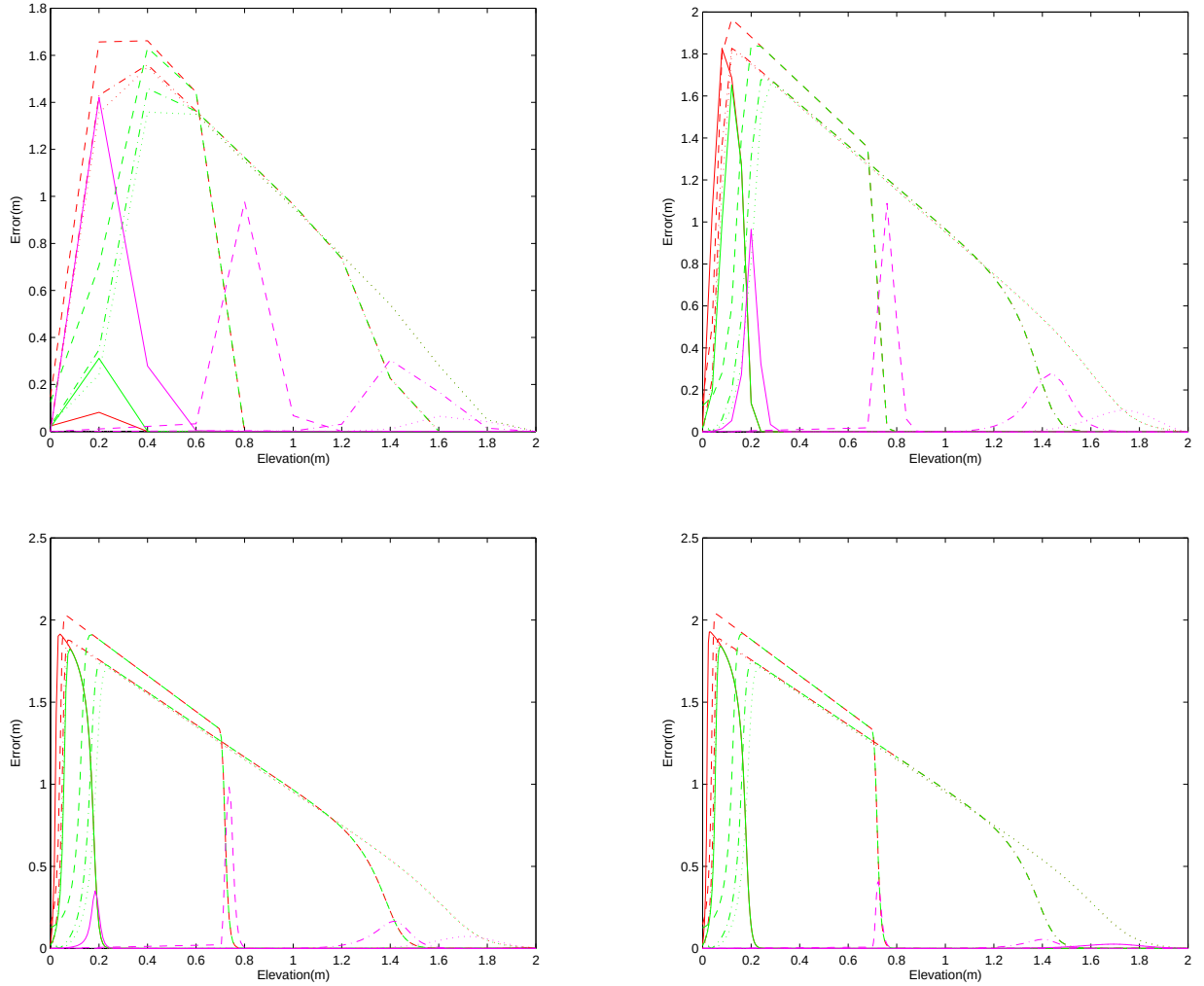


FIGURE 20. Error profile for 10, 50, 250, and 500 layers: nested Newton case for Test Problem 1. Red, green, and magenta lines: 10 s, 100 s, and 1000 s respectively. Solid, dash-dotted, dashed, and dotted lines are at times 35000 s, 155000 s, 240000 s, and 300000 s respectively.

The computed error graph for Picard, Newton, and nested Newton for all spatial and temporal discretizations is presented in Figure 21. Calculated RMSE for all cases and all schemes are presented in Tables 16, 17, 18 and 19.

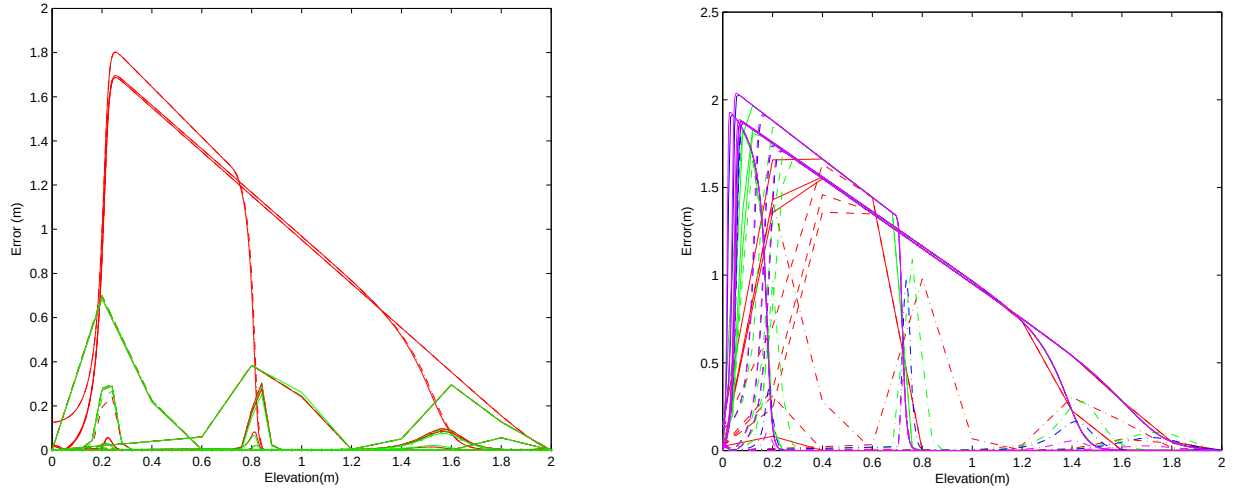


FIGURE 21. Error profile for Newton (red) and Picard (green) (left plot) and for nested Newton (right plot) for Test Problem 1. Red, green, blue, and magenta lines: 10, 50, 250, and 500 layers respectively for nested Newton. Solid, dash-dotted, dashed, and dotted lines are at times 35000 s, 155000 s, 240000 s, and 300000 s respectively.

TABLE 16. RMSE for 10 layers: Picard, Newton, and nested Newton: Test Problem 1.

Δt (s)	Method	35000 s	155000 s	240000 s	300000 s
1 s	Pic	0.2213	0.1393	9.83×10^{-2}	1.68×10^{-2}
1 s	New	0.2213	0.1393	9.83×10^{-2}	1.68×10^{-2}
1 s	Nes-New	—	—	—	—
10 s	Pic	0.2213	0.1392	9.83×10^{-2}	1.68×10^{-2}
10 s	New	0.2213	0.1392	9.83×10^{-2}	1.68×10^{-2}
10 s	Nes-New	2.55×10^{-2}	0.8319	0.9157	0.9162
100 s	Pic	0.2210	0.1398	9.83×10^{-2}	1.68×10^{-2}
100 s	New	0.2210	0.1388	9.82×10^{-2}	1.67×10^{-2}
100 s	Nes-New	9.40×10^{-2}	0.6915	0.7972	0.7917
1000 s	Pic	0.2174	0.1383	9.82×10^{-2}	1.67×10^{-2}
1000 s	New	0.2174	0.1416	9.80×10^{-2}	1.67×10^{-2}
1000 s	Nes-New	0.4366	0.2958	0.1053	2.35×10^{-2}

TABLE 17. RMSE for 50 layers: Picard, Newton, and nested Newton: Test Problem 1.

Δt (s)	Method	35000 s	155000 s	240000 s	300000 s
1 s	Pic	5.78×10^{-2}	4.95×10^{-2}	2.61×10^{-2}	9.33×10^{-4}
1 s	New	5.78×10^{-2}	4.95×10^{-2}	2.61×10^{-2}	9.33×10^{-4}
1 s	Nes-New	—	—	—	—
10 s	Pic	5.76×10^{-2}	4.93×10^{-2}	2.59×10^{-2}	9.33×10^{-4}
10 s	New	5.76×10^{-2}	4.94×10^{-2}	2.60×10^{-2}	9.32×10^{-4}
10 s	Nes-New	0.4186	0.9495	1.0239	1.0265
100 s	Pic	5.61×10^{-2}	4.98×10^{-2}	2.61×10^{-2}	9.37×10^{-4}
100 s	New	5.62×10^{-2}	4.73×10^{-2}	2.40×10^{-2}	9.19×10^{-4}
100 s	Nes-New	0.3250	0.8541	0.9266	0.9173
1000 s	Pic	4.38×10^{-2}	4.54×10^{-2}	2.31×10^{-2}	9.15×10^{-4}
1000 s	New	5.01×10^{-2}	4.12×10^{-2}	2.07×10^{-2}	9.05×10^{-4}
1000 s	Nes-New	0.1479	0.1877	7.47×10^{-2}	3.46×10^{-3}

TABLE 18. RMSE for 250 layers: Picard, Newton, and nested Newton: Test Problem 1.

Δt (s)	Method	35000 s	155000 s	240000 s	300000 s
1 s	Pic	4.50×10^{-3}	2.50×10^{-3}	8.68×10^{-4}	6.62×10^{-5}
1 s	New	4.50×10^{-3}	2.50×10^{-3}	8.89×10^{-4}	6.60×10^{-5}
1 s	Nes-New	—	—	—	—
10 s	Pic	4.20×10^{-3}	2.50×10^{-3}	8.39×10^{-4}	6.62×10^{-5}
10 s	New	4.20×10^{-3}	1.90×10^{-3}	5.61×10^{-4}	6.89×10^{-5}
10 s	Nes-New	0.4710	0.9943	1.0547	1.0578
100 s	Pic	1.50×10^{-3}	9.80×10^{-3}	2.50×10^{-4}	9.69×10^{-5}
100 s	New	3.20×10^{-3}	4.5×10^{-3}	3.50×10^{-3}	3.32×10^{-4}
100 s	Nes-New	0.3953	0.8919	0.9564	0.9461
1000 s	Pic	6.60×10^{-3}	1.00×10^{-3}	3.50×10^{-4}	5.98×10^{-4}
1000 s	New	3.37×10^{-3}	8.10×10^{-3}	5.20×10^{-3}	6.36×10^{-4}
1000 s	Nes-New	4.20×10^{-3}	0.1161	4.17×10^{-3}	2.44×10^{-3}

3.4.2. Test Problem 2.

In the CATHY code, there is a lookup table option to solve Richards' equation for layered soil. We implemented the lookup table option of CATHY for uniform distributions of points in the domain of the constitutive relationship curves. For the uniform distributions, we used equally spaced discretizations of moisture capacity, water saturation, and relative hydraulic conductivity. For our lookup table assessment we used four sets of lookup points (NLKP=6, 31, 151, 301) in the retention curves for this test problem. The Brooks-Corey soil moisture curves for the uniform distributions of lookup points are presented in Figure 22.

TABLE 19. RMSE for 500 layers: Picard, Newton, and nested Newton: Test Problem 1.

Δt (s)	Method	35000 s	155000 s	240000 s	300000 s
1 s	Pic	1.30×10^{-3}	7.30×10^{-4}	2.41×10^{-4}	1.70×10^{-5}
1 s	New	1.30×10^{-3}	7.94×10^{-4}	2.75×10^{-4}	1.69×10^{-5}
1 s	Nes-New	—	—	—	—
10 s	Pic	8.45×10^{-4}	0.8344	0.9367	0.9372
10 s	New	9.53×10^{-4}	2.58×10^{-4}	1.00×10^{-4}	3.85×10^{-5}
10 s	Nes-New	0.4787	0.9888	1.0585	1.0615
100 s	Pic	1.80×10^{-3}	0.8341	0.9366	0.9372
100 s	New	Div	Div	Div	Div
100 s	Nes-New	0.4045	0.8957	0.9594	0.9489
1000 s	Pic	6.80×10^{-3}	0.8328	0.9361	0.9371
1000 s	New	Div	Div	Div	Div
1000 s	Nes-New	1.29×10^{-2}	4.02×10^{-2}	1.34×10^{-2}	8.60×10^{-3}

We ran the CATHY model for this test problem on four different numbers of layers, i.e., 301, 151, 51, and 11 with three different time step sizes $\Delta t_{max} = 1000$ s, 100 s and 10 s per grid. The base case solution is made by the fine grid (301 nodes) with small time step size 1 s and the Picard method is used for this reference solution using a low tolerance of nonlinear convergence. We ran a total of 96 CATHY simulations (4 lookup points $\times$ 4 vertical discretizations $\times$ 3 time step sizes for each of the Picard and Newton options). For the nested Newton scheme we could not consider the 10 s time step size because the computational cost is very expensive, thus we ran 8 simulations (4 vertical discretizations at time step sizes of 1000 s and 100 s).

To obtain the numerical solution, we used dynamic time step control for iteration schemes for all the cases. Here we used the analytical differentiation of moisture curves. Lumped mass matrix is considered. Tolerance for nonlinear iteration is 10^{-3} . Maximum allowable nonlinear iteration is 10, which is denoted by ITER or ITUNS. There are also another two iteration indices ITUNS1=5 and ITUNS2=8. If $ITER < ITUNS1$, time step size is increased by the magnification factor $\Delta t_{mag} = 1.20$, if $ITUNS1 \leq ITER < ITUNS2$, time step size is not altered, if $ITUNS2 \leq ITER < ITUNS$, time step size is decreased with a reduction factor $\Delta t_{red} = 0.5$, if $ITER = ITUNS$, that is, convergence not achieved in ITUNS iteration, the solver back-steps unless time step size cannot be reduced any further. Back-stepping is also triggered

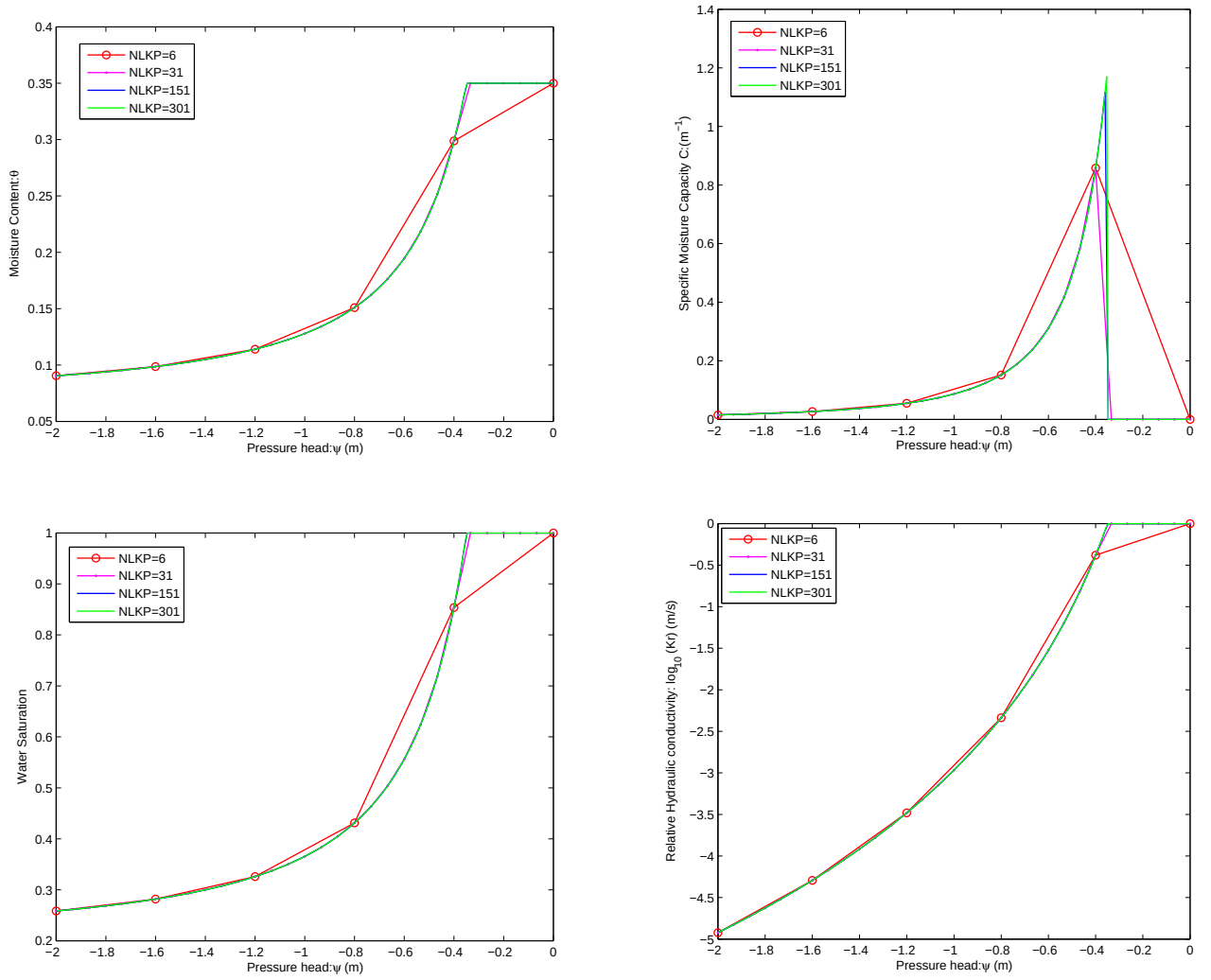


FIGURE 22. Soil 1 moisture curves for Test Problem 2.

if linear solver failed or if the convergence or residual errors become larger than maximum allowable convergence or residual error in the nonlinear solution. To solve the linear systems, we used BiCGSTAB, bi-conjugate gradients stabilized method with tolerance 10^{-10} and maximum iteration 1000.

The water saturations after $T_{max} = 1050000$ s for all the cases by CATHY and nested Newton are in excellent agreement with the published results [21, 82, 86]. Figure 24 shows the saturation prediction at a time of approximately 12 days. Figure 24 show that the solutions for 151 and 301 lookup table points coincide very well. This implies that for the soil moisture retention

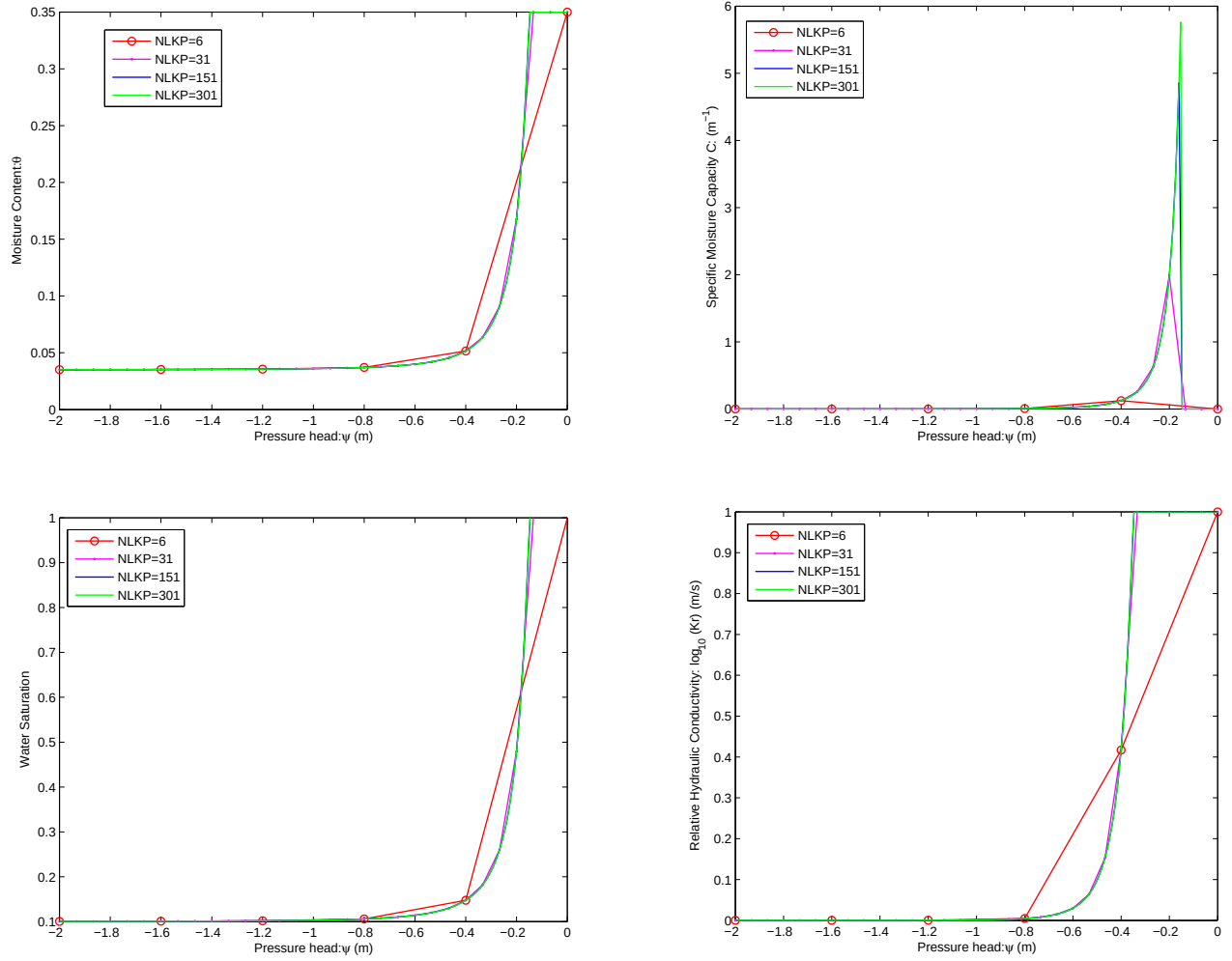


FIGURE 23. Soil 2 moisture curves for Test Problem 2.

curves, 151 lookup points are sufficient to get the good numerical solution.

The adaptive time stepping behaviors for the uniform distributions lookup table points are investigated by Picard and Newton methods. Adaptive time stepping included fail attempts and back-stepping. The similarities and differences are reported for every layer for each case of time step and lookup table points. Since the lookup table points assessment is very important in this section for the layered soil problem, so lookup table point wise time stepping behavior of the Newton scheme is illustrated in the Figure 25 for 6, 31, 151, and 301 lookup points cases. Figure 26 is the time stepping behavior for all layers, all time step sizes and all NLKP cases. Note that the 300 layer discretization of Newton scheme diverges for $\Delta t_{max} = 1000$ s with NLKP=6,

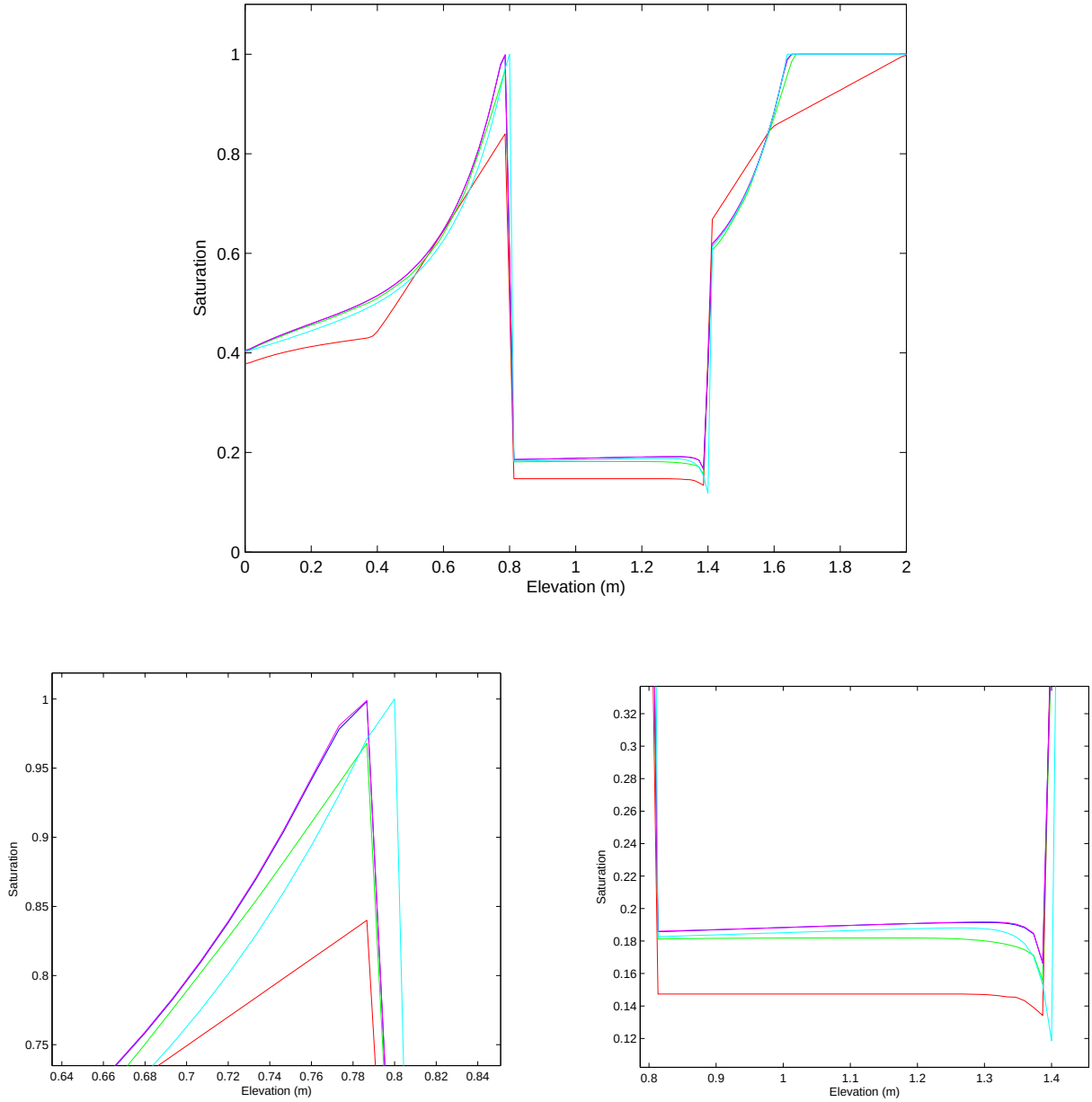


FIGURE 24. Saturation predictions after 12 days of Test Problem 2 (Red, green, blue, and magenta are for 6, 31, 151 and 301 lookup points and cyan is for nested Newton). The bottom two graphs are zooms on the sharp fronts shown in the top graph.

and NLKP=151, 301 with $\Delta t_{max} = 100$ s. From the first graph of Figure 25, it shows that after $T_{max} = 3.208e + 5$ s, 150 layer solution and after $T_{max} = 9.786e + 4$ s, 50 layer time stepping never achieved its maximum time step $\Delta t_{max} = 1000$ s. All other graphs give similar behavior. It is clear that for these cases, time stepping of Newton scheme varies from its maximum to

minimum step size. The corresponding Picard time stepping behavior is illustrated by the Figures 27 and 28. It is clear that Newton and Picard behavior are very different in the period of $2.32e+5$ s to the end of the simulation time. In this period the vertical discretizations of 50, 150, and 300 layers, Picard achieves smoothly its maximum time step sizes, whereas Newton shows fluctuation of time stepping. So this period of simulation is very difficult for the Newton scheme.

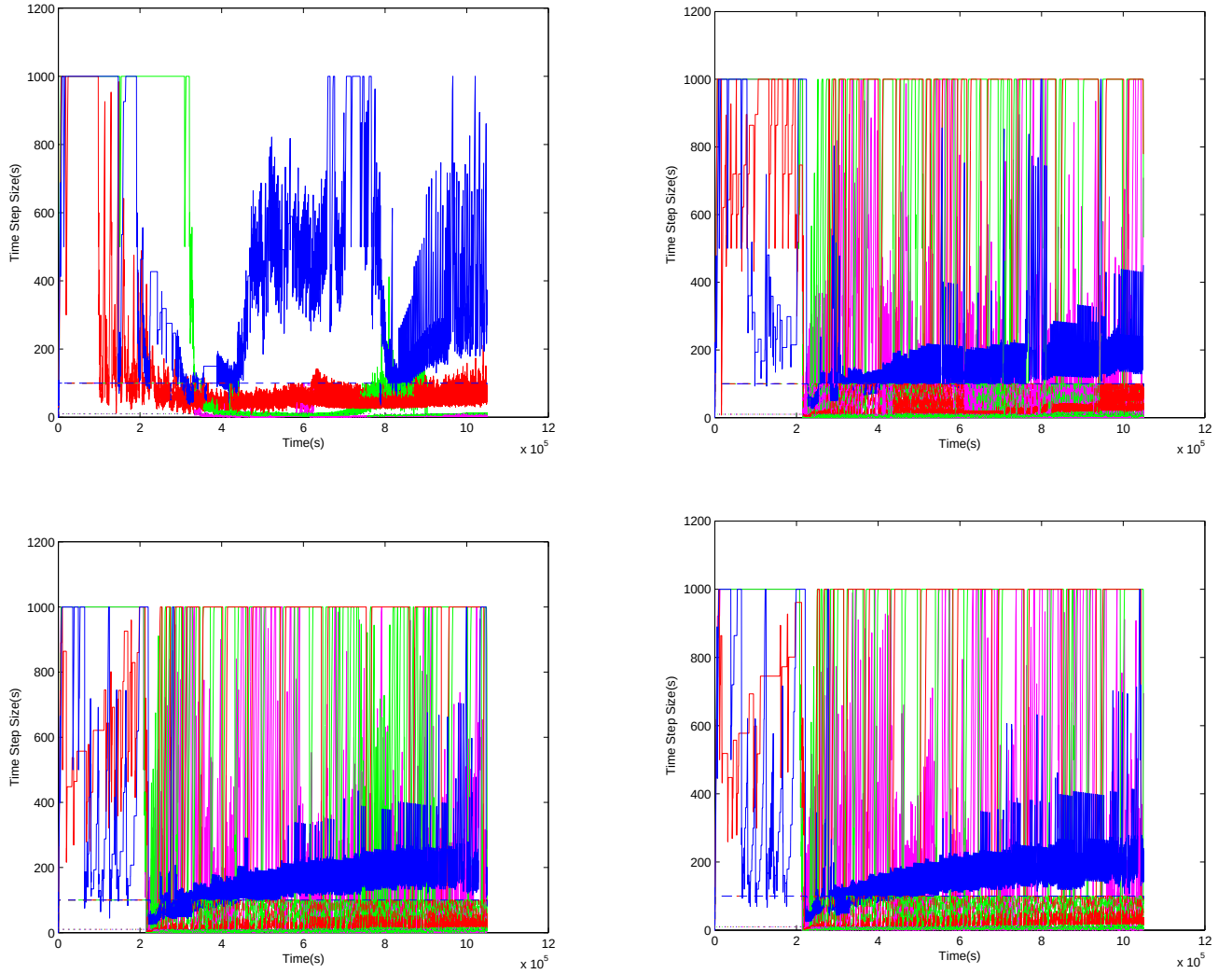


FIGURE 25. Time stepping behavior of Newton method for uniform distribution of 6, 31 (top two), 151 and 301 (bottom two) lookup points of Test Problem 2. Blue, red, green, and magenta lines: 10, 50, 150, and 300 layers respectively. Dotted, dashed, and solid lines: $\Delta t_{max} = 10$ s, 100 s, and 1000 s respectively.

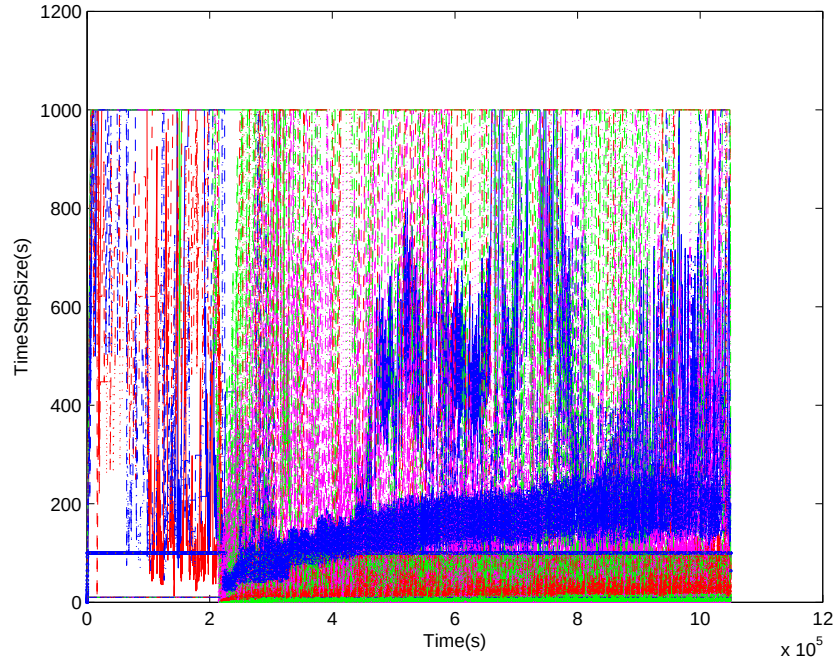


FIGURE 26. Time stepping behavior of Newton for Test Problem 2.

The nonlinear iterations per time step are graphically presented in Figures 29 and 30. Figure-29 clearly shows that Newton scheme needs to take maximum number of nonlinear iterations to achieve convergence for each of the vertical discretizations during the simulation. On the other hand, for 50, 150, and 300 layers discretizations, Picard scheme (Figure 30) needs less number of nonlinear iterations than Newton. Even though, for NLKP=31, 151, and 301 cases, it takes only 1 iteration per time step after 3.251×10^5 s, 3.069×10^5 s, and 2.887×10^5 s respectively for each layer. Also, note that Picard does not need maximum number of iterations in the whole period of simulation to get convergence. Newton and Picard nonlinear iterations behavior for all of the cases are shown in Figure 31.

Nested Newton scheme convergence behavior is shown in the Figure 32 individually for each vertical discretization. In the combined graphical representation illustrated in Figure 33, little similarity is found after 2×10^5 s for 50, 150, and 300 layers between nested Newton and Picard schemes.

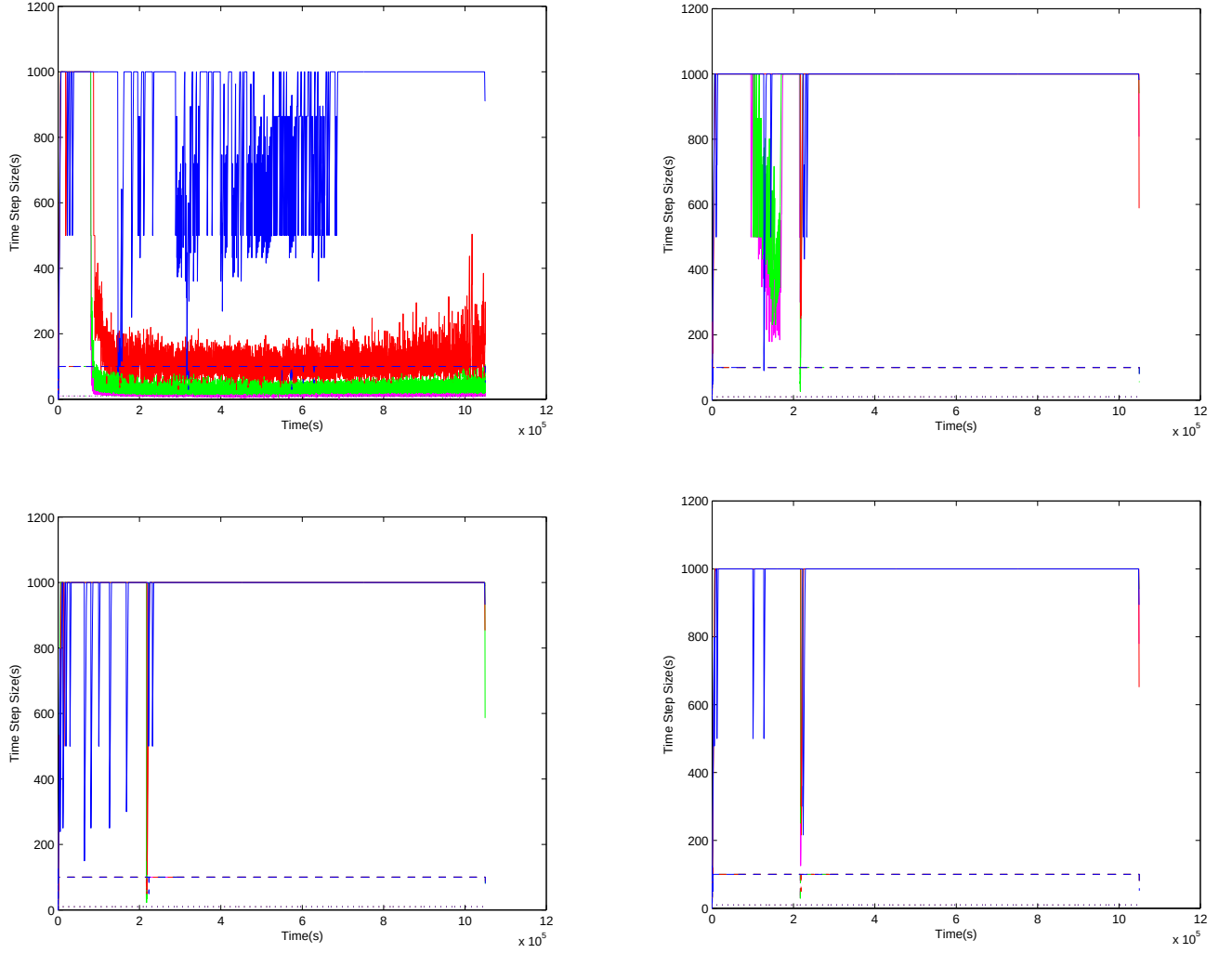


FIGURE 27. Time stepping behavior of Picard method for uniform distribution of 6, 31 (top two), 151 and 301 (bottom two) look up points of Test Problem 2. Blue, red, green, and magenta lines: 10, 50, 150, and 300 layers respectively. Dotted, dashed, and solid lines: $\Delta t_{max} = 10$ s, 100 s, and 1000 s respectively.

The cumulative mass balance errors are shown graphically in Figures 34 and 35 for the number of lookup table points for both the Newton and Picard schemes. Excellent mass balance errors are shown for all the cases. And for all different cases, the cumulative mass balance errors are shown in the Figure 36 for the Newton and Picard schemes. Both schemes show excellent mass balance results.

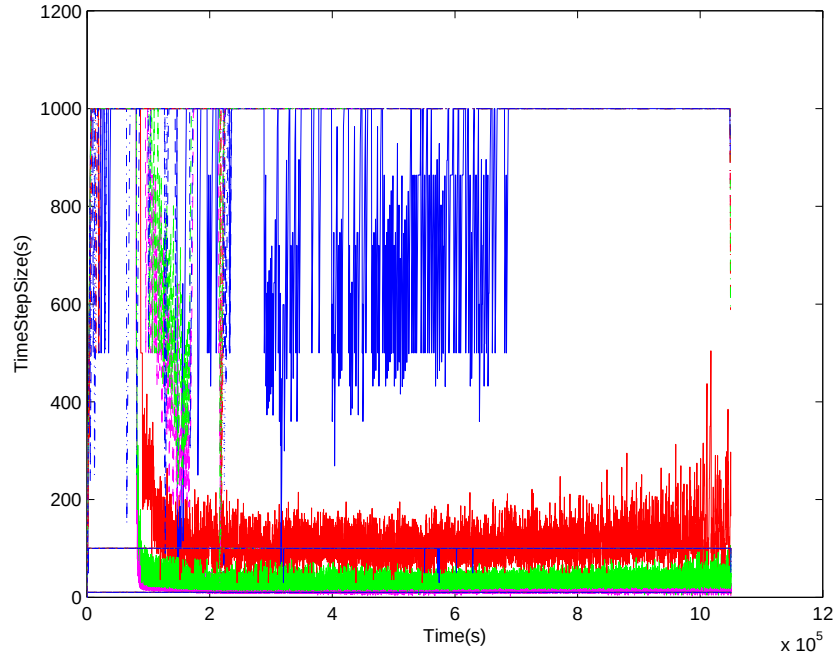


FIGURE 28. Time stepping behavior of Picard for Test Problem 2.

Important statistical data of CATHY model for Picard and Newton schemes for all the layers with all time step sizes for all uniform NLKP are summarized in Tables 20, 21, 22, and 23.

Fixed time step sizes are used for nested Newton scheme, so there is no back stepping. Thus, for every fixed time step, we get a fixed total number time steps. Besides the total number of outer iterations, the total number of inner iterations is also reported. The inner iterations directly represent the simulation performance. Also the average number of outer iterations per time step and the average number of inner iterations per outer iteration are indicated (Table 24).

The RMSE are calculated at the three different times, 250000 s, 550000 s and at the end of the simulation 1050000 s (approximately 12 days) using the L_2 norm for all cases by CATHY and nested Newton model. Numerical solutions of these two schemes with very dense grid spacing were considered as the exact solutions for determination of RMSE. Evaluated RMSE are acceptable for all the cases and are plotted on the basis of each set of NLKP for all layers with all time steps.

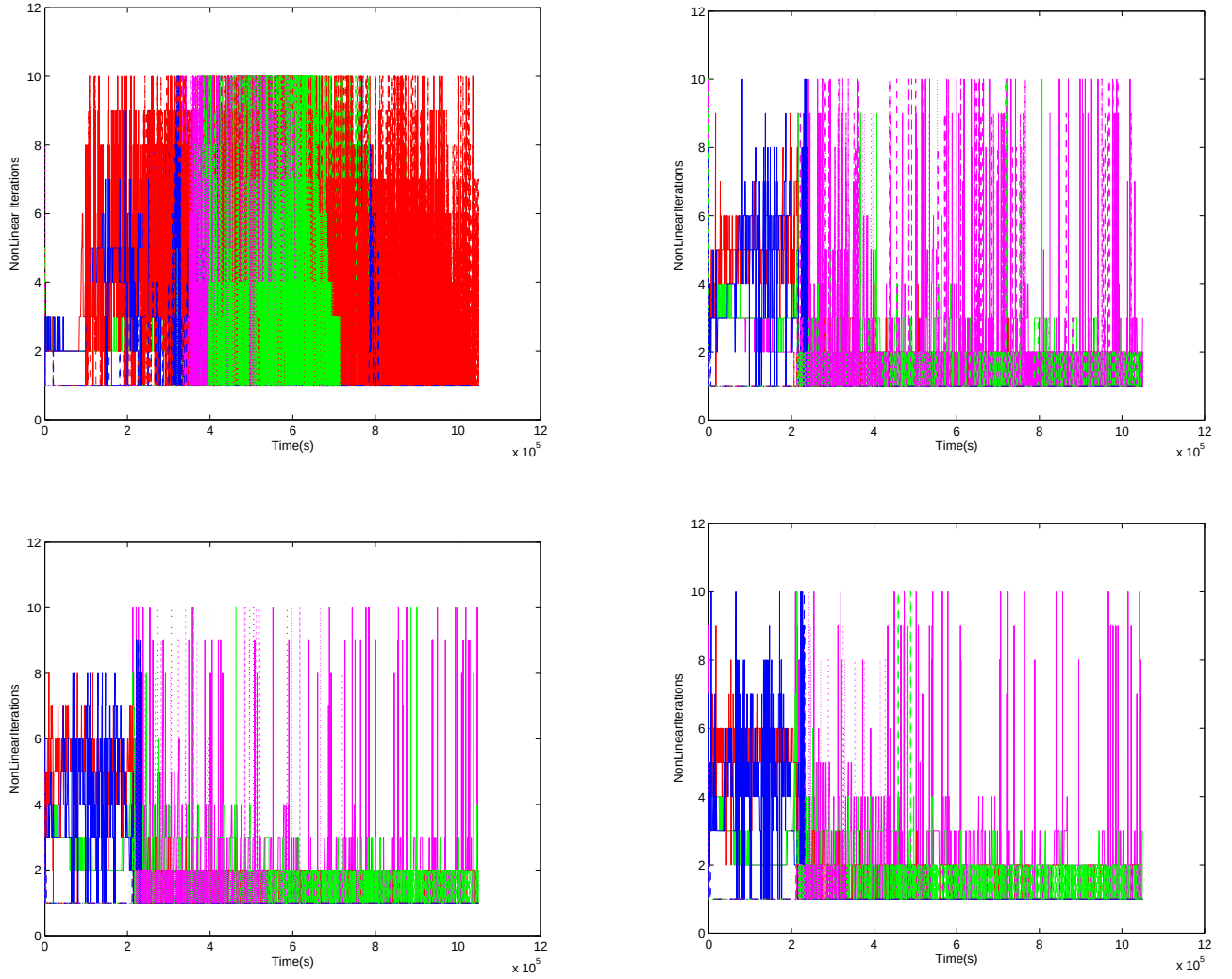


FIGURE 29. Convergence behavior of Newton method for uniform distribution of 6(top left), 31(top right), 151(bottom left), and 301(bottom right) lookup points. Blue, red, green, and magenta lines: 10, 50, 150, and 300 layers respectively. Dotted, dashed, and solid lines: $\Delta t_{max} = 10$ s, 100 s, and 1000 s respectively.

The RMSE graph for Newton and Picard are shown in Figures 37, 38, and 39 and for nested Newton in Figure 40.

The RMSE for all the vertical discretizations along with all the uniform distribution of lookup table points for all the time step sizes are presented in Table 25 for Picard and Newton schemes and in Table 26 for the nested Newton scheme.

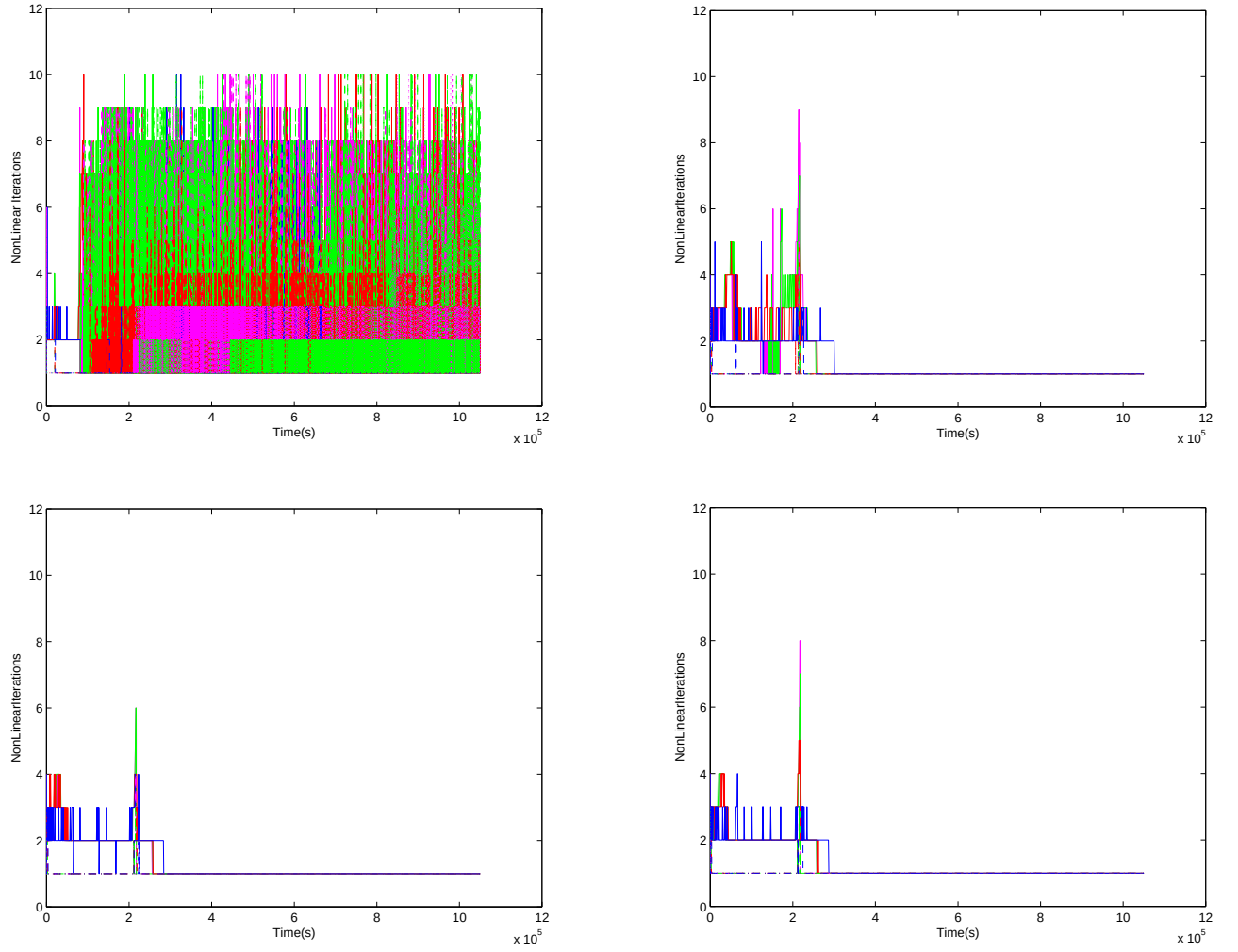


FIGURE 30. Convergence behavior of Picard method for uniform distribution of 6(top left), 31(top right), 151(bottom left), and 301(bottom right) lookup points. Blue, red, green, and magenta lines: 10, 50, 150, and 300 layers respectively. Dotted, dashed, and solid lines: $\Delta t_{max} = 10$ s, 100 s, and 1000 s respectively.

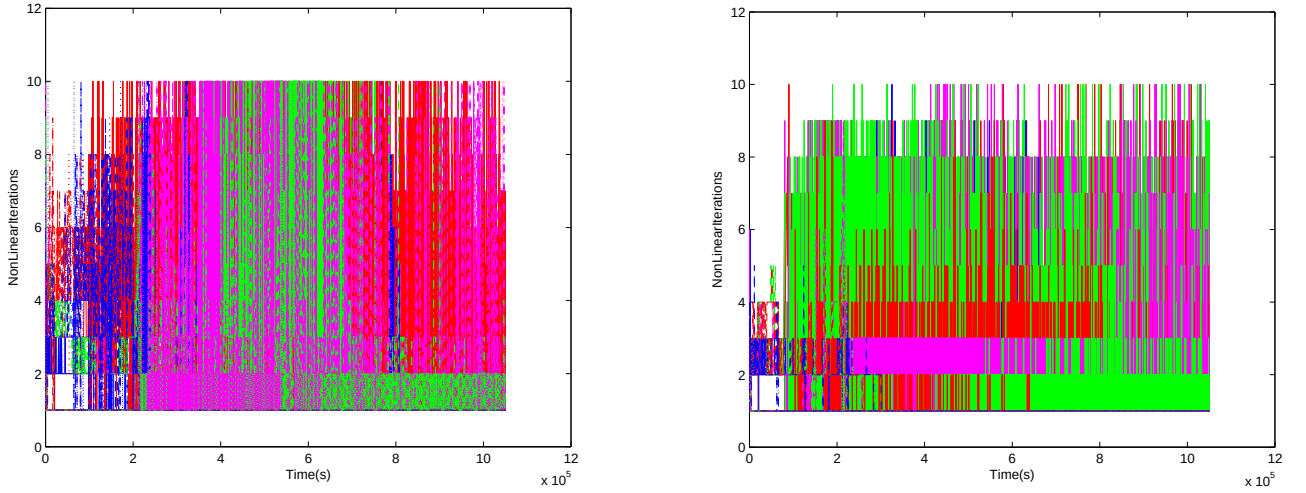


FIGURE 31. Convergence behavior of Newton (left) and Picard (right) methods of Test Problem 2 for all layers with all NLKP and all Δt .

TABLE 20. Computational performance of CATHY model: Picard and Newton schemes for 10 layers with $\Delta t_{max} = 10$ s, 100 s, and 1000 s for Test Problem 2.

–	$\Delta t(s)$	10	10	100	100	1000	1000
–	NLKP	Pic	New	Pic	New	Pic	New
MBE(m^3)	6	-8.75e-6	-8.39e-7	2.70e-5	1.43e-5	-4.98e-5	-5.27e-6
	31	3.76e-6	3.73e-6	1.10e-5	1.31e-5	-4.13e-6	3.62e-5
	151	7.23e-6	7.38e-6	1.87e-5	2.00e-5	2.60e-5	8.54e-5
	301	5.63e-5	4.13e-6	1.46e-5	1.49e-5	-2.23e-5	8.74e-5
MBE(perc.)	6	6.43e-2	6.13e-3	-1.99e-1	-1.04e-1	3.62e-1	3.81e-1
	31	-3.00e-2	-2.97e-2	-8.77e-2	-1.04e-1	3.28e-2	-2.90e-1
	151	-5.86e-2	-5.98e-2	-1.52e-1	-1.63e-1	-2.11e-1	-7.00e-1
	301	-4.56e-2	-3.35e-2	-1.19e-1	-1.21e-1	1.81e-1	-7.15e-1
No. of Time Steps	6	105061	105061	10609	10674	1412	3869
	31	105054	105054	10574	10884	1146	6638
	151	105050	105050	10565	11106	1169	6410
	301	105050	105058	10569	10980	1148	6459
Avg. $\Delta t(s)$	6	9.994	9.994	9.897e+1	9.837e+1	7.436e+2	2.714e+2
	31	9.995	9.995	9.930e+1	9.647e+1	9.162e+2	1.582e+2
	151	9.995	9.995	9.938e+1	9.454e+1	8.982e+2	1.638e+2
	301	9.995	9.994	9.935e+1	9.563e+1	9.146e+2	1.626e+2
NL Iter/ Time Step	6	1.00	1.00	1.21	1.45	3.15	4.36
	31	1.00	1.00	1.04	1.22	1.63	3.81
	151	1.00	1.00	1.04	1.36	1.72	3.87
	301	1.00	1.00	1.04	1.26	1.63	3.82
Lin Iter/ NL Iter	6	3.03	3.18	4.98	6.06	8.06	11.94
	31	5.28	5.16	6.38	8.86	9.85	22.03
	151	5.93	5.88	6.54	10.32	10.32	20.73
	301	5.93	5.86	6.55	10.09	10.07	19.93
No.of Back Steps	6	19	19	36	59	145	656
	31	16	16	22	160	31	1556
	151	15	15	19	307	42	14893
	301	15	17	21	244	31	1520
Solver Failures	6	0	0	0	3	0	4
	31	0	1	0	4	0	20
	151	0	3	0	3	0	19
	301	0	1	1	3	0	15

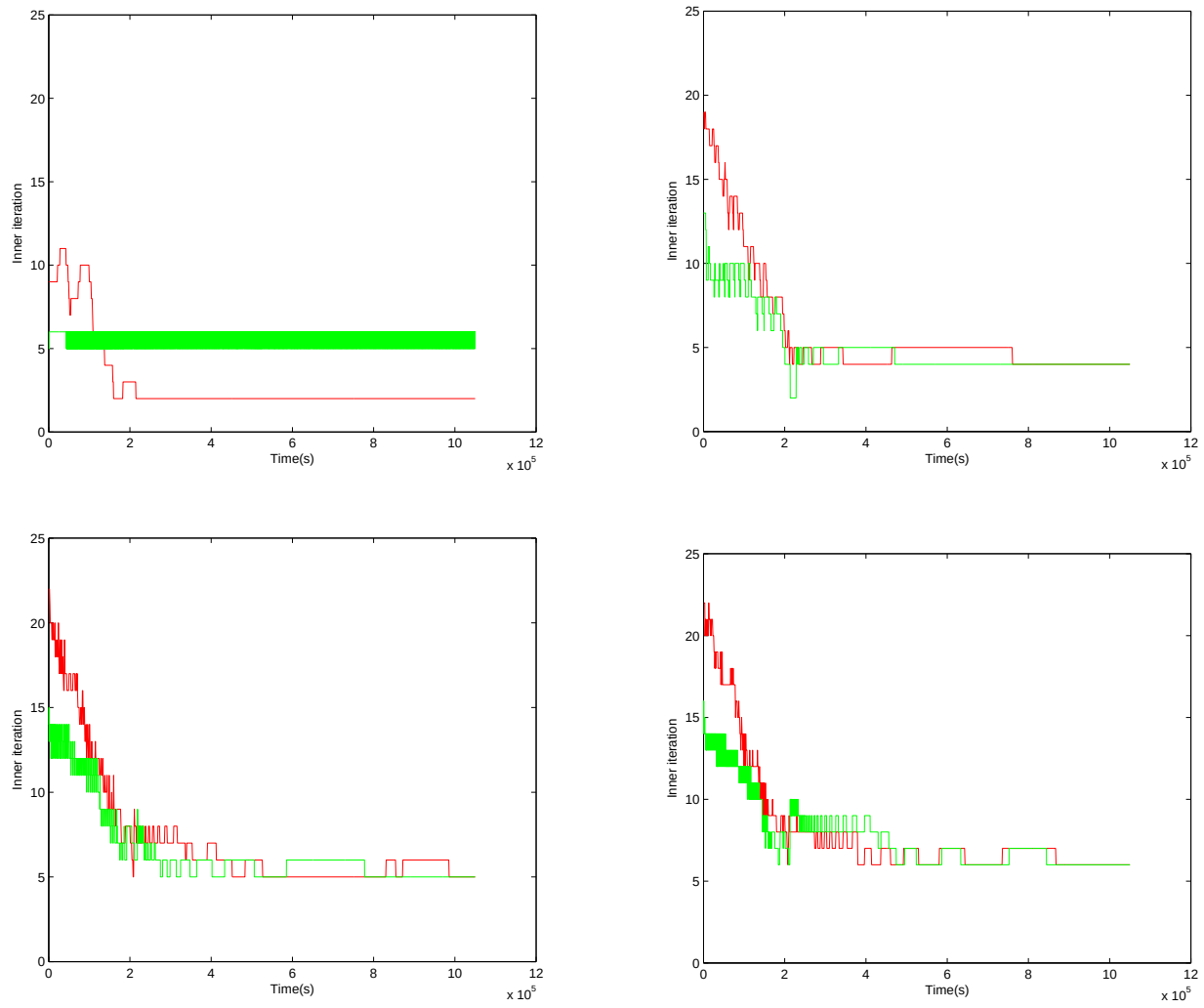


FIGURE 32. Convergence behavior of nested Newton for 10(top left), 50(top right), 150(bottom left), and 300(bottom right) layer discretizations of Test Problem 2. Red and green lines: $\Delta t_{max} = 1000$ s and 100 s respectively.

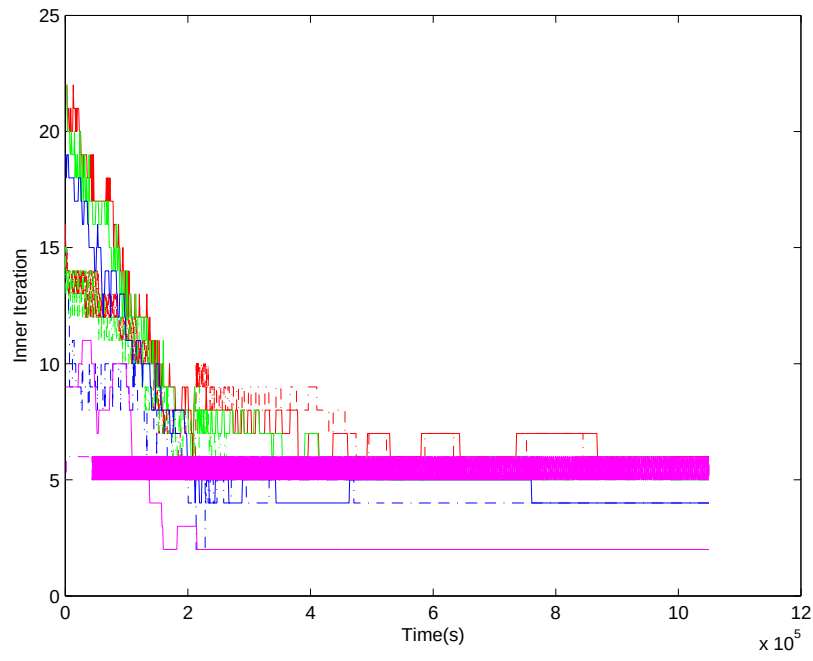


FIGURE 33. Convergence behavior of nested Newton scheme of Test Problem 2. Red, green, blue, and magenta lines: 300, 150, 50, and 10 layers respectively. Solid and dash-dotted lines: $\Delta t_{max}=1000$ s and 100 s respectively.

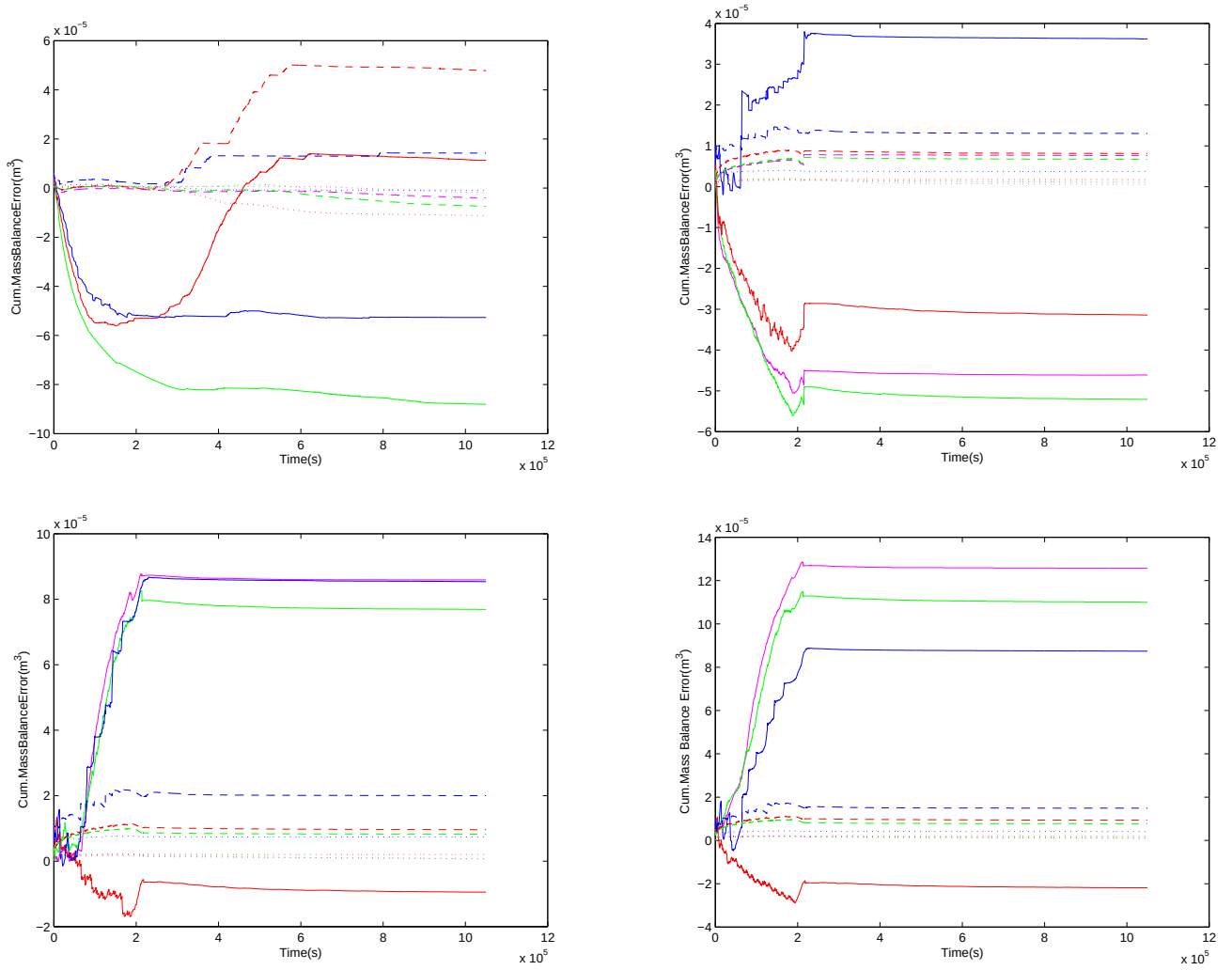


FIGURE 34. Cumulative mass balance error behavior of Newton method for uniform distribution 6(top left), 31(top right), 151(bottom left), and 301(bottom right) lookup points. Blue, red, green, and magenta lines: 10, 50, 150, and 300 layers, respectively. Dotted, dashed, and solid lines: $\Delta t_{max} = 10$ s, 100 s, and 1000 s respectively.

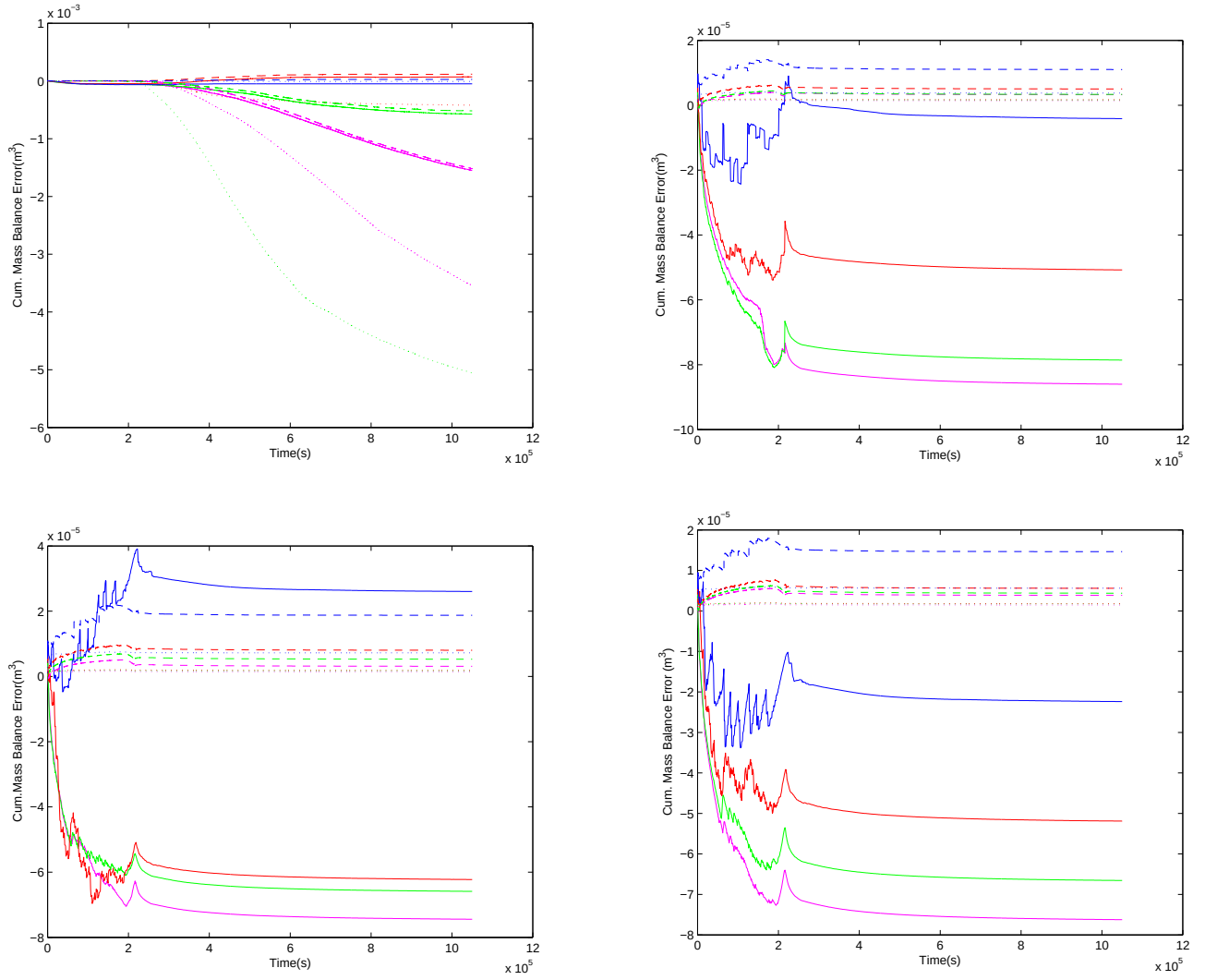


FIGURE 35. Cumulative mass balance error behavior of Picard method for uniform distribution of 6(top left), 31(top right), 151(bottom left), and 301(bottom right) lookup points. Blue, red, green, and magenta lines: 10, 50, 150, and 300 layers respectively. Dotted, dashed, and solid lines: $\Delta t_{max} = 10$ s, 100 s, and 1000 s respectively.

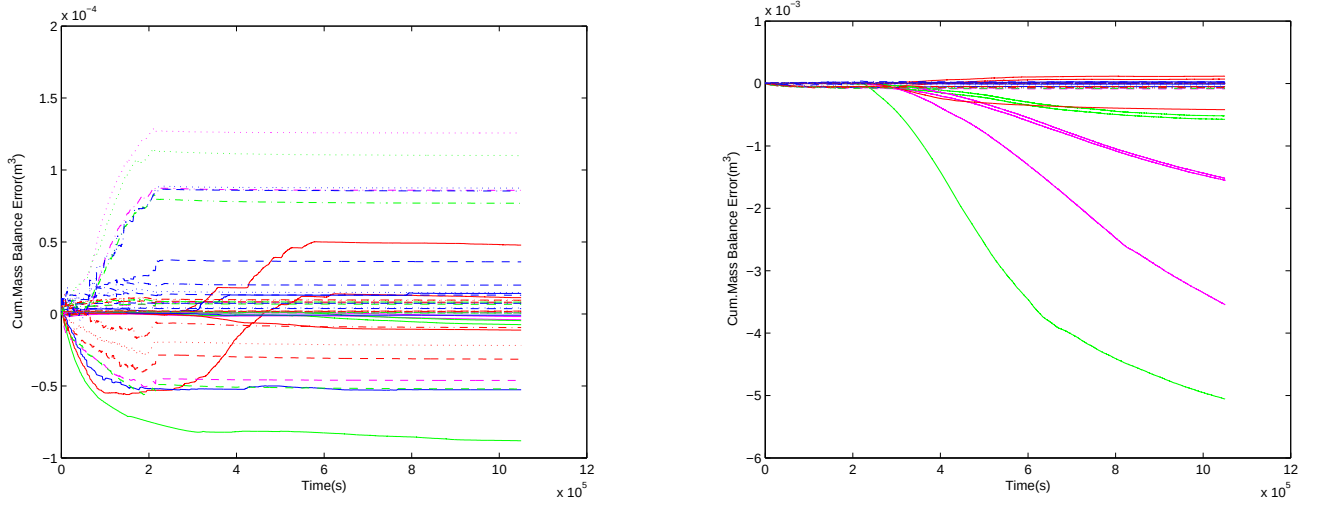


FIGURE 36. Cumulative mass balance error behavior for Newton (left) and Picard(right) methods of Test Problem 2 for all layers, for all NLKP and all Δt .

TABLE 21. Computational performance of CATHY model: Picard and Newton schemes for 50 layers with $\Delta t_{max} = 10$ s, 100 s, and 1000 s for Test Problem 2.

–	Δt (s)	10	10	100	100	1000	1000
–	NLKP	Pic	New	Pic	New	Pic	New
MBE (m ³)	6	-4.19e-4	-1.12e-5	1.17e-4	4.78e-5	7.10e-5	1.13e-5
	31	1.73e-6	1.76e-6	5.01e-6	8.15e-6	-5.08e-5	-3.14e-5
	151	1.88e-6	2.20e-6	8.03e-6	9.59e-6	-6.23e-5	-9.45e-6
	301	1.82e-6	1.89e-6	5.58e-6	9.33e-6	-5.19e-5	-2.18e-5
MBE(perc.)	6	2.99e0	8.25e-2	-8.71e-1	-3.54e-1	7.10e-5	-8.35e-2
	31	-1.37e-2	-1.39e-22	-3.98e-2	6.47e-2	4.01e-1	2.49e-1
	151	-1.52e-2	-1.63e-2	-6.56e-2	-7.72e-2	4.99e-1	7.60e-2
	301	-1.46e-2	-1.52e-2	-4.50e-2	-7.52e-2	4.15e-1	1.76e-1
No. of Time Steps	6	105061	105064	10700	18404	8913	15066
	31	105051	106735	10567	35081	1135	14534
	151	105051	106217	10566	29024	1146	11137
	301	105051	106366	10565	29102	1139	11151
Avg. Δt (s)	6	9.994	9.994	9.81e+1	5.705e+1	1.178e+2	6.969e+1
	31	9.995	9.837	9.937e+1	2.993e+1	9.251e+2	7.224e+1
	151	9.995	9.885	9.938e+1	3.618e+1	8.982e+2	9.428e+1
	301	9.995	9.872	9.938e+1	3.608e+1	9.219e+2	9.416e+1
NL Iter/ Time Step	6	1.01	1.01	1.91	3.78	4.58	4.36
	31	1.00	1.09	1.03	3.24	1.67	3.56
	151	1.00	1.06	1.04	3.05	1.62	3.55
	301	1.00	1.07	1.03	3.04	1.60	3.55
Lin Iter/ NL Iter	6	3.24	5.03	4.35	15.99	4.58	17.79
	31	6.55	8.29	7.73	24.57	10.23	22.86
	151	6.86	8.80	7.77	24.46	10.28	23.62
	301	6.86	9.18	7.75	23.23	10.22	22.22
No. of Back Steps	6	18	19	83	2722	2118	2210
	31	15	946	19	7898	25	3604
	151	15	663	20	5972	29	2682
	301	15	768	19	5971	26	2685
Solver Failures	6	0	2	0	47	0	69
	31	0	55	0	209	0	155
	151	0	99	0	191	0	146
	301	0	111	1	198	0	147

TABLE 22. Computational performance of CATHY model: Picard and Newton schemes for 150 layers with $\Delta t_{max} = 10$ s, 100 s, and 1000 s for Test Problem 2.

–	Δt (s)	10	10	100	100	1000	1000
–	NLKP	Pic	New	Pic	New	Pic	New
MBE (m^3)	6	-5.06e-3	-4.63e-6	-5.17e-4	-7.43e-6	-5.73e-4	-8.80e-5
	31	1.61e-6	5.56e-7	3.34e-6	6.71e-6	-7.86e-5	-5.21e-5
	151	1.72e-6	7.15e-7	5.28e-6	8.26e-6	6.59e-5	7.69e-5
	301	1.73e-6	1.02e-6	4.38e-6	7.73e-6	6.66e-5	1.10e-4
MBE(perc.)	6	2.73e+1	3.41e-2	3.68e0	5.47e-2	4.06e0	6.45e-1
	31	-1.28e-2	-4.41e-3	-1.28e-2	-5.33e-2	-2.65e-2	4.12e-1
	151	-1.38e-2	-5.76e-3	-1.38e-2	-6.65e-2	-4.26e-2	-6.24e-1
	301	-1.40e-2	-8.22e-3	-1.40e-2	-6.23e-2	-3.53e-2	-8.95e-1
No. of Time Steps	6	105067	133199	32545	78558	31682	76831
	31	105051	243071	10558	85175	1201	53079
	151	105051	240041	10562	79014	1147	43602
	301	105051	236084	10563	83710	1130	50552
Avg. Δt (s)	6	9.994	7.883	3.226e+1	1.337e+1	5.314e+2	1.367e+1
	31	9.995	4.320	9.945e+1	1.233e+1	8.743e+2	1.978e+1
	151	9.995	4.374	9.941e+1	1.329e+1	9.154e+2	2.408e+1
	301	9.995	4.448	9.940e+1	1.254e+1	9.292e+2	2.077e+1
NL Iter/ Time Step	6	1.09	2.35	4.19	3.62	4.26	3.74
	31	1.00	3.08	1.03	3.39	1.97	3.62
	151	1.00	3.07	1.03	3.38	1.61	3.62
	301	1.00	3.05	1.03	3.39	1.56	3.61
Lin Iter/ NL Iter	6	3.07	25.59	2.45	27.39	2.46	27.14
	31	6.54	20.99	7.55	16.78	9.80	13.51
	151	6.56	20.30	7.60	15.52	9.93	13.45
	301	6.60	20.14	7.59	15.18	9.96	11.43
No. of Back Steps	6	23	16215	7774	18499	2792	18953
	31	15	20523	17	20245	59	13753
	151	15	49640	19	18698	28	11287
	301	15	48475	19	19931	23	13084
Solver Failures	6	0	597	0	911	0	1142
	31	0	170	0	85	0	90
	151	0	320	0	113	0	127
	301	0	258	1	157	0	99

TABLE 23. Computational performance of CATHY model: Picard and Newton schemes for 300 layers with $\Delta t_{max} = 10$ s, 100 s, and 1000 s for Test Problem 2.

–	Δt (s)	10	10	100	100	1000	1000
–	NLKP	Pic	New	Pic	New	Pic	New
MBE (m ³)	6	-3.54e-3	-1.83e-6	-1.52e-3	-4.03e-6	-1.55e-3	div
	31	1.40e-6	1.10e-6	3.24e-6	7.63e-6	-8.60e-5	-4.61e-5
	151	1.43e-6	7.32e-7	3.11e-6	div	-7.44e-5	8.59e-5
	301	1.47e-6	1.04e-6	3.83e-6	div	-7.62e-5	1.16e-4
MBE(perc.)	6	2.07e+1	1.35e-2	1.01e-1	2.97e-2	1.03e+1	div
	31	-1.11e-2	-8.75e-3	-2.57e-2	-6.06e-2	6.78e-1	3.65e-1
	151	-1.15e-2	-5.89e-3	-2.50e-2	div	5.95e-1	-6.97e-1
	301	-1.18e-2	-8.44e-3	-3.09e-2	div	6.10e-1	-1.02e0
No. of Time Steps	6	105111	326937	593675	285181	58350	div
	31	105047	380698	10560	143872	1236	95730
	151	105051	371587	10556	div	1136	86856
	301	105051	380568	10560	div	1133	88445
Avg. Δt (s)	6	9.989	3.212	1.769e+1	3.682	1.799e+1	div
	31	9.996	2.758	9.949e+1	7.298	8.495e+2	1.097e+1
	151	9.995	2.826	9.947e+1	div	9.243e+2	1.209e+1
	301	9.995	2.759	9.943e+1	div	9.267e+2	1.187e+1
NL Iter/ Time Step	6	1.23	3.36	4.13	3.64	4.17	div
	31	1.00	3.13	1.03	3.53	2.02	3.65
	151	1.00	3.10	1.03	div	1.58	3.65
	301	1.00	3.14	1.03	div	1.56	3.64
Lin Iter/ NL Iter	6	2.45	26.44	2.02	26.65	1.99	div
	31	6.53	16.96	7.52	16.34	9.69	15.81
	151	6.57	14.33	7.56	div	9.91	13.81
	301	6.65	15.60	7.57	div	9.94	13.38
No. of Back Steps	6	33	75179	14864	72872	14787	div
	31	14	81169	17	36050	68	25014
	151	15	77980	16	div	25	22697
	301	15	81357	18	div	23	23098
Solver Failures	6	0	2340	0	24871	0	div
	31	0	301	0	2025	0	132
	151	0	177	0	div	0	83
	301	0	221	1	div	0	38

TABLE 24. Computational performance of nested Newton scheme: Test Problem 2.

	Δt_{max} (s)	1000	100
No. of Layers	No. of Time Steps	1050	10500
10	Tot. outer iterations	2241	31501
	Tot. inner iterations	3073	54385
	Avg. outer iterations	2.13	3.00
	Avg. inner iterations	1.37	1.73
50	Tot. outer iterations	4662	44074
	Tot. inner iterations	6214	52655
	Avg. outer iterations	4.40	4.20
	Avg. inner iterations	1.33	1.19
150	Tot. outer iterations	5391	57154
	Tot. inner iterations	7537	68352
	Avg. outer iterations	5.13	5.44
	Avg. inner iterations	1.40	1.20
300	Tot. outer iterations	5725	65013
	Tot. inner iterations	84790	80796
	Avg. outer iterations	5.45	6.19
	Avg. inner iterations	1.48	1.24

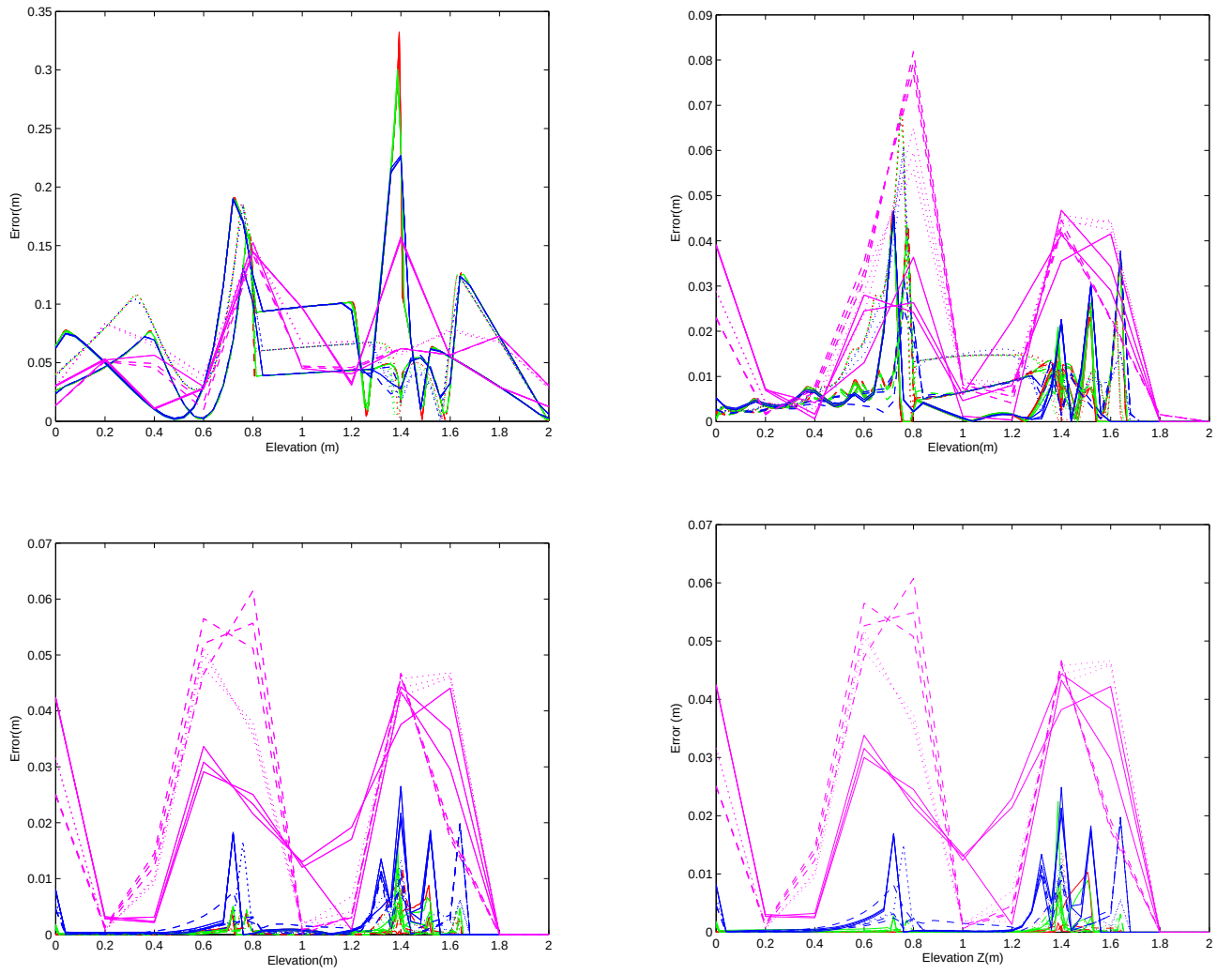


FIGURE 37. RMSE behavior of Newton method for uniform distribution of 6(top left), 31(top right), 151(bottom left), and 301(bottom right) lookup points. Solid, dotted, and dashed lines are at times 250000 s, 550000 s, and 1050000 s respectively.

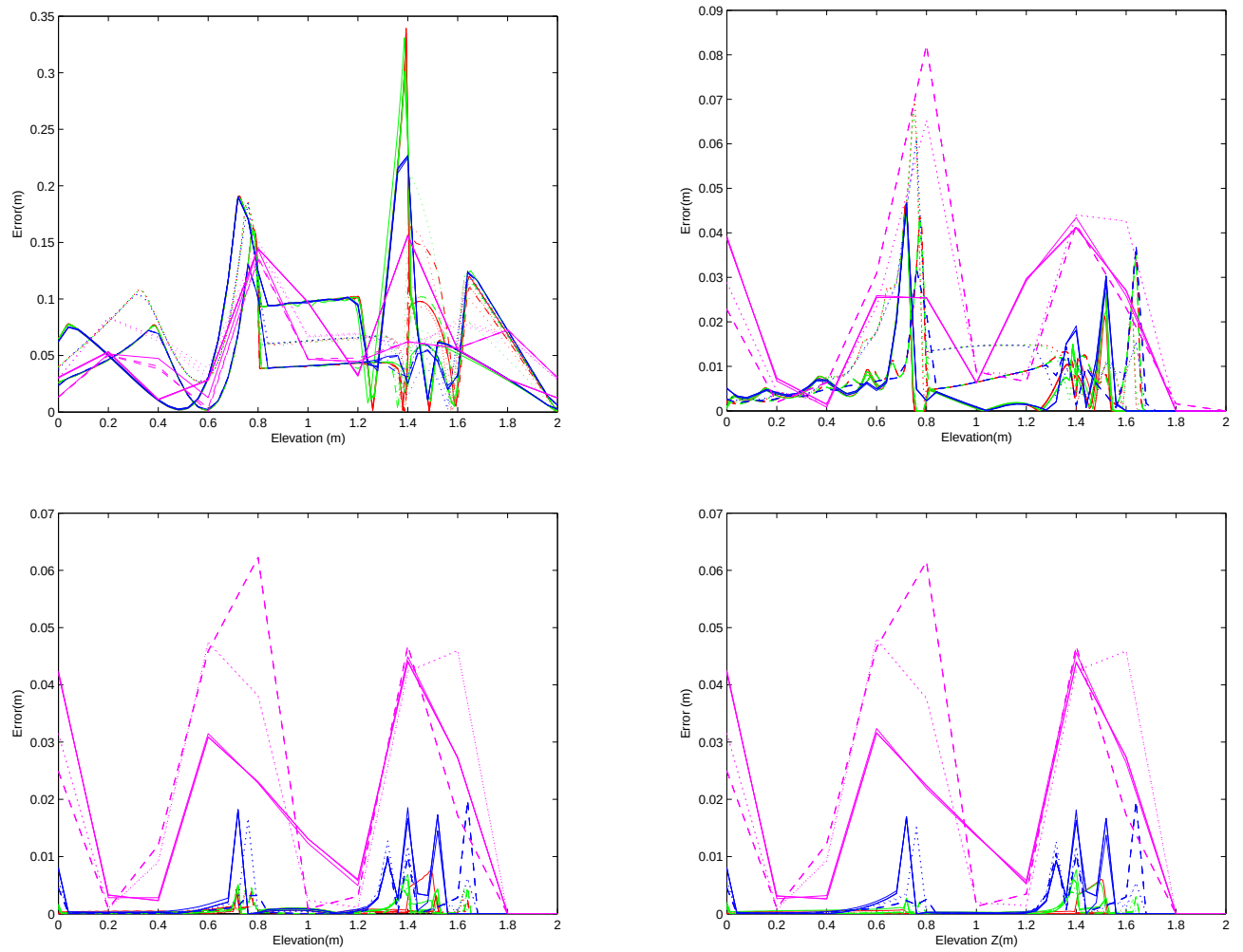


FIGURE 38. RMSE behavior of Picard method for uniform distribution of 6(top left), 31(top right), 151(bottom left), and 301(bottom right) lookup. Solid, dotted, and dashed lines are at times 250000 s, 550000 s, and 1050000 s respectively.

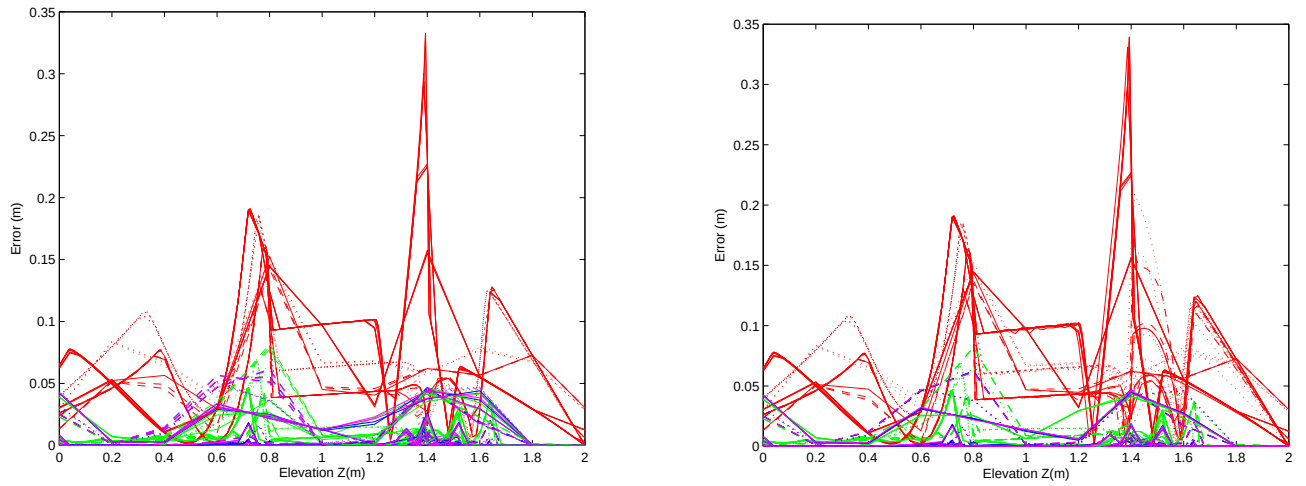


FIGURE 39. Combined (all layers and all NLKP with all Δt) RMSE behavior of Newton (left) and Picard (right) methods for uniform distribution of lookup points of Test Problem 2.

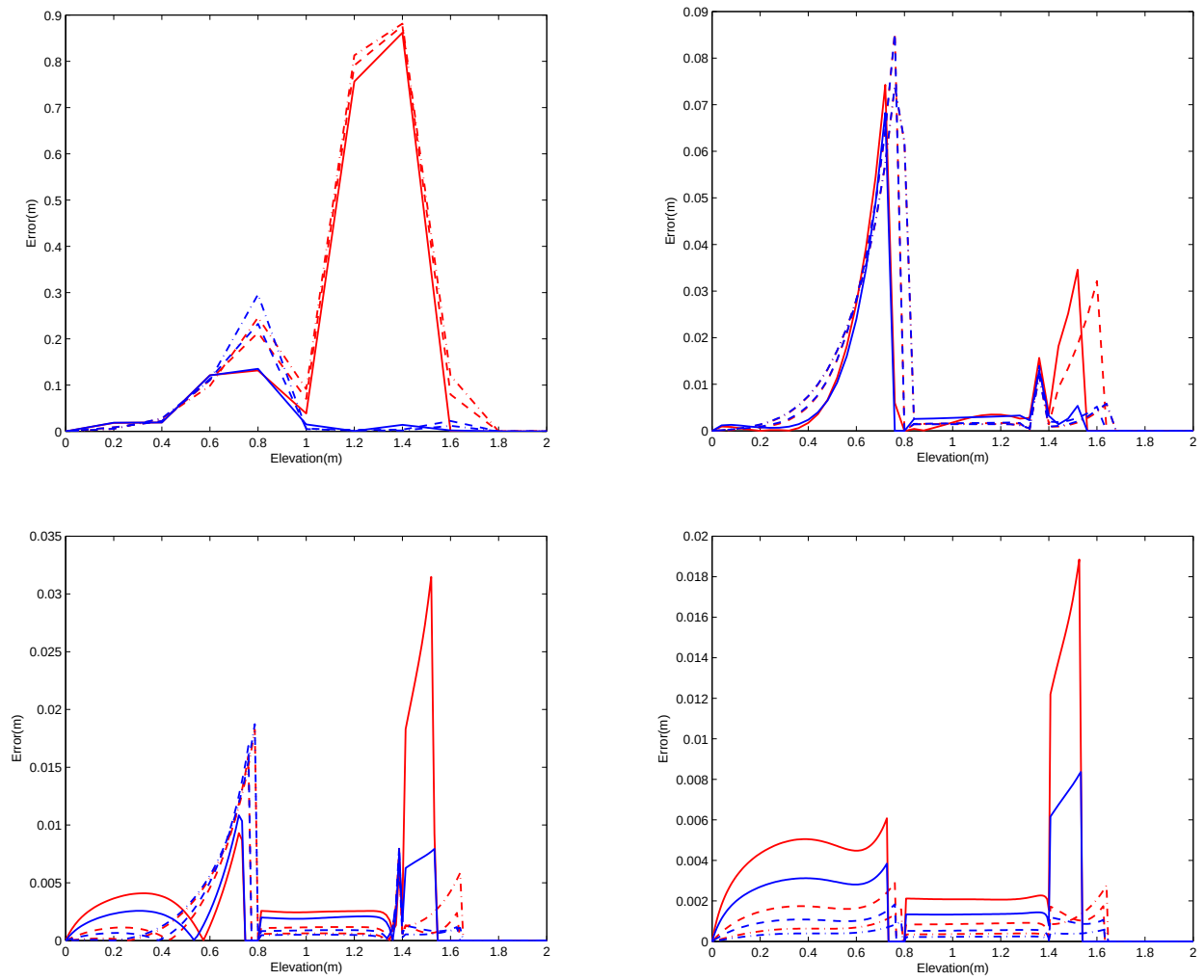


FIGURE 40. RMSE behavior of nested Newton scheme for 10(top left), 50(top right), 150(bottom left) and 300(bottom right) layer discretizations of Test Problem 2. Red and blue lines: $\Delta t_{max} = 100$ s and 1000 s respectively. Solid, dashed, and dotted lines are at times 250000 s, 550000 s, and 1050000 s respectively.

TABLE 25. RMSE of CATHY model: Picard and Newton schemes for all layers with all the time step sizes and all uniform NLKP cases for Test Problem 2.

—	—	Δt (s) $\rightarrow$	10	10	100	100	1000	1000
Layers	NLKP	Time	Pic	New	Pic	New	Pic	New
10	-	250000	7.65e-2	7.64e-2	7.65e-2	7.64e-2	7.66e-2	7.66e-2
	6	550000	7.29e-2	7.45e-2	7.31e-2	7.30e-2	7.43e-2	7.43e-2
	-	1050000	6.04e-2	6.24e-2	6.08e-2	6.33e-2	6.28e-2	6.55e-2
10	-	250000	2.38e-2	2.32e-2	2.37e-2	2.42e-2	2.40e-2	2.34e-2
	31	550000	2.95e-2	2.95e-2	2.95e-2	2.90e-2	2.95e-2	2.89e-2
	-	1050000	3.12e-2	3.11e-2	3.12e-2	3.09e-2	3.12e-2	3.07e-2
10	-	250000	2.37e-2	2.37e-2	2.36e-2	2.53e-2	2.39e-2	2.58e-2
	151	550000	2.81e-2	2.81e-2	2.81e-2	2.87e-2	2.81e-2	2.91e-2
	-	1050000	2.90e-2	2.89e-2	2.90e-2	2.87e-2	2.90e-2	2.89e-2
10	-	250000	2.37e-2	2.38e-2	2.37e-2	2.60e-2	2.40e-2	2.58e-2
	301	550000	2.81e-2	2.82e-2	2.81e-2	2.88e-2	2.82e-2	2.92e-2
	-	1050000	2.89e-2	2.89e-2	2.89e-2	2.87e-2	2.90e-2	2.88e-2
50	-	250000	8.44e-2	8.43e-2	8.42e-2	8.42e-2	8.45e-2	8.44e-2
	6	550000	7.25e-2	7.15e-2	7.28e-2	7.18e-2	7.15e-2	7.16e-2
	-	1050000	5.57e-2	5.58e-2	5.58e-2	5.53e-2	5.59e-2	5.54e-2
50	-	250000	9.60e-3	9.60e-3	9.60e-3	9.40e-3	9.40e-3	9.50e-3
	31	550000	1.50e-2	1.49e-2	1.50e-2	1.46e-2	1.49e-2	1.39e-2
	-	1050000	9.50e-3	9.40e-3	9.60e-3	9.20e-3	9.40e-3	8.60e-3
50	-	250000	4.70e-3	5.30e-3	4.70e-3	5.20e-3	4.60e-3	5.50e-3
	151	550000	3.70e-3	3.70e-3	3.70e-3	3.90e-3	3.70e-3	3.30e-3
	-	1050000	3.60e-3	3.60e-3	3.60e-3	3.80e-3	3.60e-3	3.70e-3
50	-	250000	4.50e-3	5.20e-3	4.50e-3	5.10e-3	4.40e-3	5.30e-3
	301	550000	3.50e-3	3.60e-3	3.50e-3	3.80e-3	3.60e-3	3.40e-3
	-	1050000	3.60e-3	3.70e-3	3.60e-3	3.80e-3	3.60e-3	3.80e-3
150	-	250000	8.90e-2	8.49e-2	8.53e-2	8.49e-2	8.45e-2	8.56e-2
	6	550000	8.14e-2	7.26e-2	7.33e-2	7.26e-2	7.15e-2	7.28e-2
	-	1050000	5.89e-2	5.64e-2	5.64e-2	5.64e-2	5.59e-2	5.64e-2
150	-	250000	8.10e-3	8.10e-3	8.10e-3	8.00e-3	9.40e-3	7.70e-3
	31	550000	1.50e-2	1.50e-2	1.50e-2	1.49e-2	1.49e-2	1.50e-2
	-	1050000	9.30e-3	9.30e-3	9.30e-3	9.20e-3	9.40e-3	9.30e-3
150	-	250000	1.10e-3	1.10e-3	1.10e-3	1.30e-3	4.60e-3	1.10e-3
	151	550000	1.00e-3	1.30e-3	1.00e-3	1.00e-3	3.70e-3	9.83e-4
	-	1050000	8.21e-4	8.95e-4	8.21e-4	7.72e-4	3.60e-3	8.08e-4
150	-	250000	8.72e-4	8.52e-4	8.81e-4	9.48e-4	4.40e-3	1.50e-3
	301	550000	8.03e-4	8.33e-4	8.03e-4	8.35e-4	3.60e-3	8.43e-4
	-	1050000	6.86e-4	8.57e-4	6.86e-4	6.38e-4	3.60e-3	6.94e-4
300	-	250000	8.60e-2	8.53e-2	8.57e-2	8.53e-2	8.60e-2	div
	6	550000	7.83e-2	7.30e-2	7.51e-2	7.30e-2	7.43e-2	div
	-	1050000	6.48e-2	5.66e-2	5.90e-2	5.66e-2	5.90e-2	div
300	-	250000	8.10e-3	8.00e-3	8.10e-3	7.90e-3	7.70e-3	7.80e-3
	31	550000	1.50e-2	1.50e-2	1.51e-2	1.51e-2	1.51e-2	1.51e-2
	-	1050000	9.40e-3	9.30e-3	9.20e-3	9.20e-3	9.30e-3	9.30e-3
300	-	250000	5.89e-4	5.75e-4	5.89e-4	div	1.50e-3	1.60e-3
	151	550000	5.03e-4	1.60e-3	5.03e-4	div	4.30e-4	5.09e-4
	-	1050000	4.56e-4	1.80e-3	4.57e-4	div	4.25e-4	5.16e-4
300	-	250000	1.84e-5	1.38e-4	5.99e-5	div	1.20e-3	2.00e-3
	301	550000	1.74e-6	1.70e-3	4.84e-6	div	1.85e-4	2.88e-4
	-	1050000	8.04e-7	3.35e-4	2.70e-6	div	5.73e-5	1.18e-4

TABLE 26. RMSE of nested Newton model: All layers with all time step sizes for Test Problem 2.

No. of Layers	Time (s)	$\Delta t_{max} = 100$ s	$\Delta t_{max} = 1000$ s
10	250000	0.2890	0.1442
	550000	0.3068	0.1091
	1050000	0.4238	0.2271
50	250000	8.01e-2	8.00e-2
	550000	7.50e-2	7.44e-2
	1050000	0.1593	0.1594
150	250000	4.85e-2	4.94e-2
	550000	4.35e-2	4.37e-2
	1050000	0.1146	0.1159
300	250000	3.78e-2	3.86e-2
	550000	3.22e-2	3.24e-2
	1050000	9.74e-2	9.78e-2

3.4.3. *Test Problem 3.*

We solved this test problem by the traditional iterative methods, that is, by the Picard and Newton methods with the help of CATHY model and by the nested Newton algorithm. To compare the accuracy of the results, we discretized the vertical column into 12, 60, 120 and 240 layers. CATHY generated reference solution is made by fine grid resolution with small time step size $\Delta t_{max} = 1$ s and strictly maintains the nonlinear convergence tolerance for the Picard and Newton schemes, and similar base solution is made by nested Newton algorithm. We used four time discretizations; these are 10 s, 100 s, 800 s, and 1600 s along with four sets of lookup points (6, 31, 151, and 301) for the soil retention curves.

To implement the CATHY model the analytical differentiation of moisture curves is considered with lumped mass matrix. The nonlinear tolerance is 10^{-3} . Maximum allowable nonlinear iterations is 10, which is denoted by ITER or ITUNS. Also ITUNS1=5 and ITUNS2=8 are used. The time step size is increased by the magnification factor $\Delta t_{mag} = 1.20$, and it is decreased with a reduction factor $\Delta t_{red} = 0.5$. If ITER=ITUNS, that is, convergence not achieved in ITUNS iterations, solver back-steps unless time step size cannot be reduced any further. Back-stepping is also triggered if linear solver failed or if the convergence or residual errors become larger than maximum allowable convergence or residual error in the nonlinear solution. We used BiCGSTAB, bi-conjugate gradients stabilized method with the tolerance 10^{-10} to solve the generated system of linear equations and maximum iteration is 1000. In total, we ran 128 simulations by the CATHY model for Picard and Newton and 16 simulations by nested Newton algorithm.

The van Genuchten soil retention curves are plotted in Figures 41 and 42 for the sand and clay respectively. The moisture curves are plotted for all the sets of look up table points and these points are taken equally spaced.

The computed water saturation after 1 day is illustrated in Figure 43. Picard, Newton, and nested Newton solution profiles. The three scheme shows very close behavior of water saturation prediction after 1 day. This water saturation is evaluated by 120 layers (with 151 points used

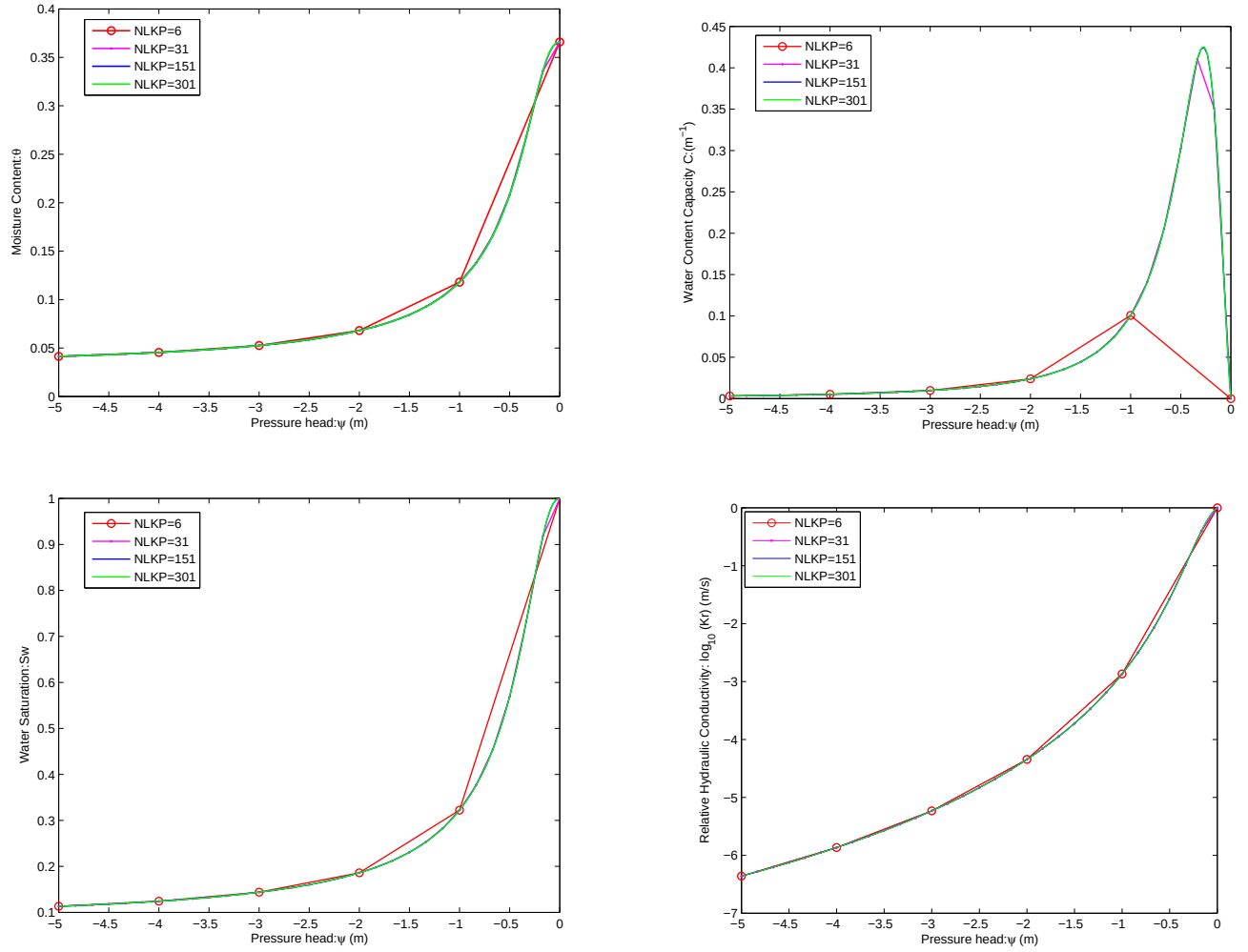


FIGURE 41. Moisture curves for sandy soil, Test Problem 3.

in the retention curves for Picard and Newton methods) along with maximum time step size $\Delta t_{max} = 10$ s and specified tolerance 10^{-3} .

To illustrate the time stepping behavior of Picard and Newton schemes, we show in Figure 44 the case of 240 layers with NLKP=31 and 151 for step sizes 10 s, 100 s, 800 s, and 1600 s. The time stepping behavior of 240 layers for Picard says that for the case of $\Delta t_{max} = 10$ s and 100 s, the solver almost achieved its maximum time step size during the full simulation for NLKP=151 and 301. At the beginning and at time=40000 s, for the NLKP=31 case, it needs to reduce the step size to get the convergence for both the step sizes $\Delta t_{max} = 10$ s and 100 s. For $\Delta t_{max} = 800$ s and 1600 s, the solver needs to widely negotiate to achieve convergence

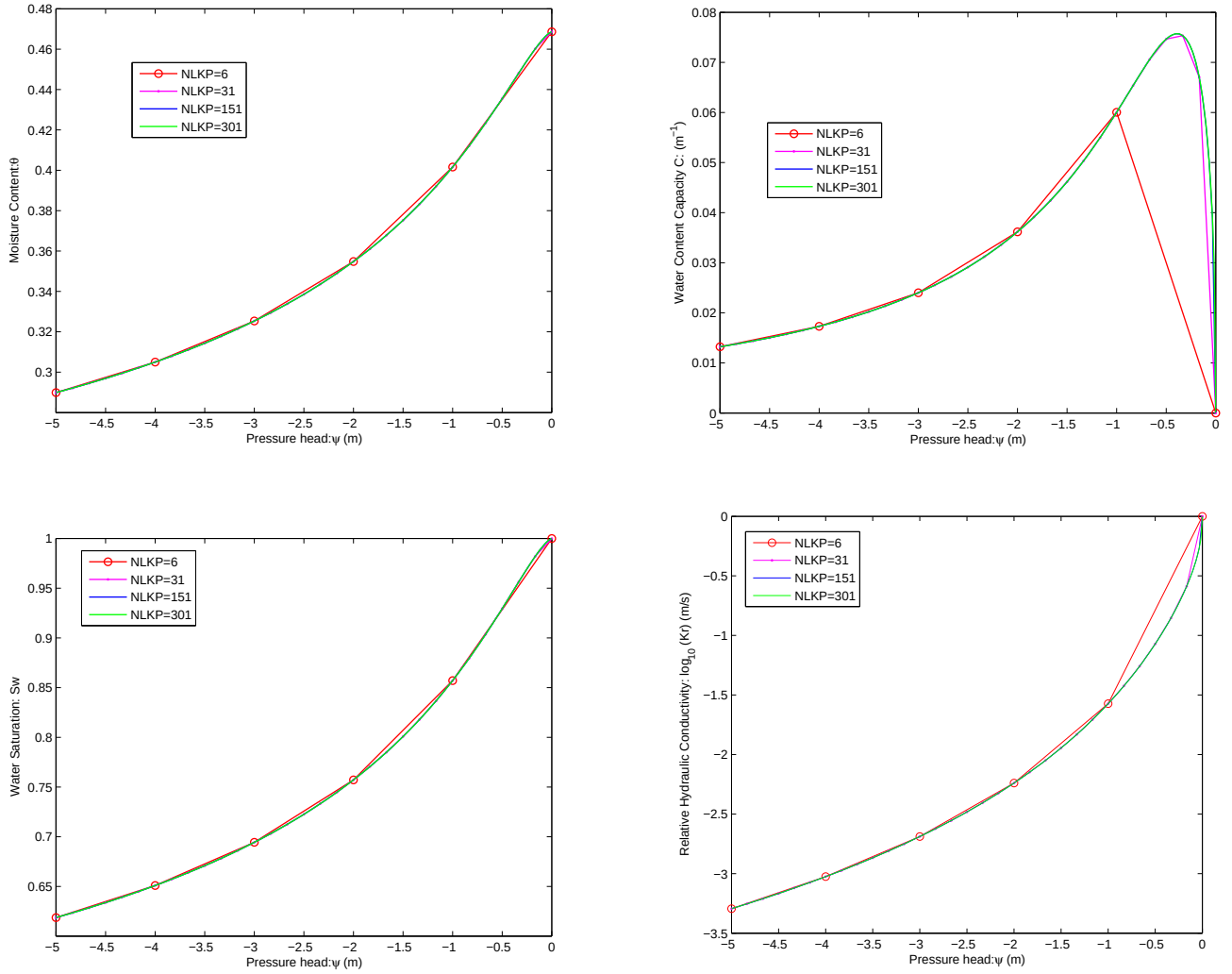


FIGURE 42. Moisture curves for clay soil, Test Problem 3.

with NLKP=31 and it faces more trouble than NLKP=151 and 301. Moreover, from the figure we see that the behaviors are very close for 151 and 301 points. We got expected results for NLKP=6 for all the vertical layer discretizations. The other two discretizations 60 and 120 behave very closely with the 240 layer case.

In the Newton case, at the very beginning of the simulation, solver needs to reduce its maximum step size 10 s for NLKP=31. For all the set of lookup points, from after time=8000 s to about 20000 s, to achieve convergence, the solver encounters some trouble, especially, in the interval 8000 s to 16000 s, where only about 2.50 s step size is used to complete the nonlinear

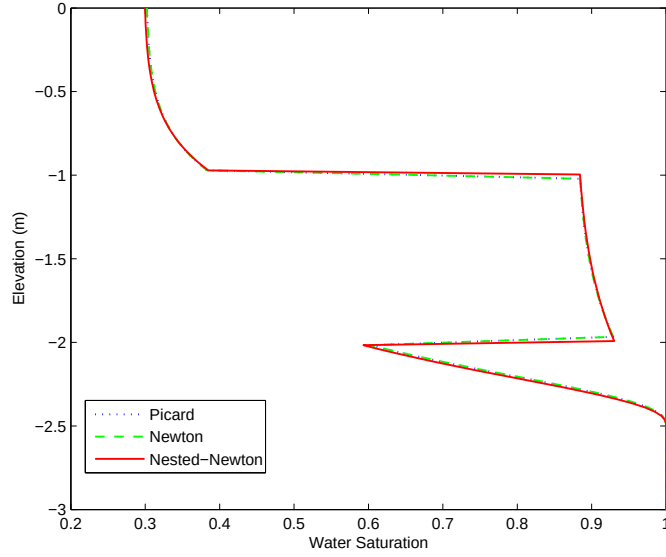


FIGURE 43. Water Saturation after 1 day for Test Problem 3

convergence. After time=20000 s, solver completes the simulation with maximum step size for all the cases. From the start of the simulation to 41000 s, it never achieves maximum step size $\Delta t_{max} = 100s$. All the NLKP cases, before time=40000 s solver is not able to obtain assigned maximum time step sizes $\Delta t_{max} = 800$ s or $\Delta t_{max} = 1600$ s. Even in this period, solver runs with maximum 100 s as a step size for all the set of lookup points.

Except 12 layers and NLKP=6 case, we have found very close time stepping behavior of 60, 120, and 240 layers with NLKP=31, 151, and 301 and for all the different time step sizes.

The complete figure of time stepping of Picard and Newton schemes is shown in Figure 45. From this figure we see that Picard and Newton schemes behave similarly after time=40000 s for $\Delta t_{max} = 100$ s and 800 s, and after 70000 s they show similar time stepping for $\Delta t_{max} = 1600$ s.

For simplicity, we analysed the 240 layer case with NLKP=31, 151, and 301 for all the time step sizes. The convergence behavior of Picard and Newton schemes of 240 layers are shown in Figure 46. At the beginning of the simulation, solver took 10 nonlinear iterations to obtain convergence for NLKP=301 with $\Delta t_{max} = 1600$ s and then almost it is complete within 5 to 6

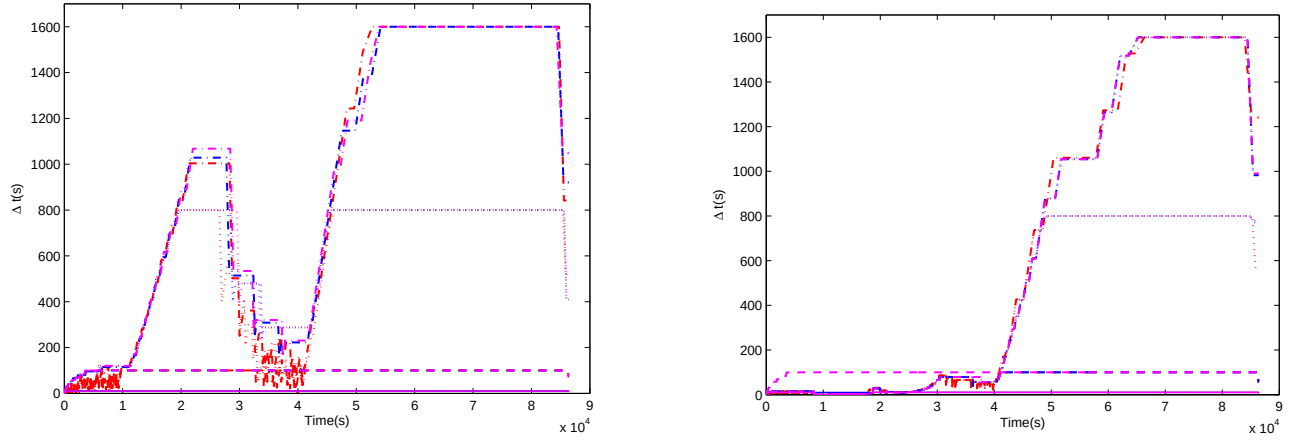


FIGURE 44. Time stepping behavior of Picard (left) and Newton(right): NLKP=31(red), 151(blue), and 301(magenta) for 240 layers with all the time step sizes 10 s(solid), 100 s(dashed), 800 s(dotted), and 1600 s(dot-dashed) respectively for Test Problem 3.

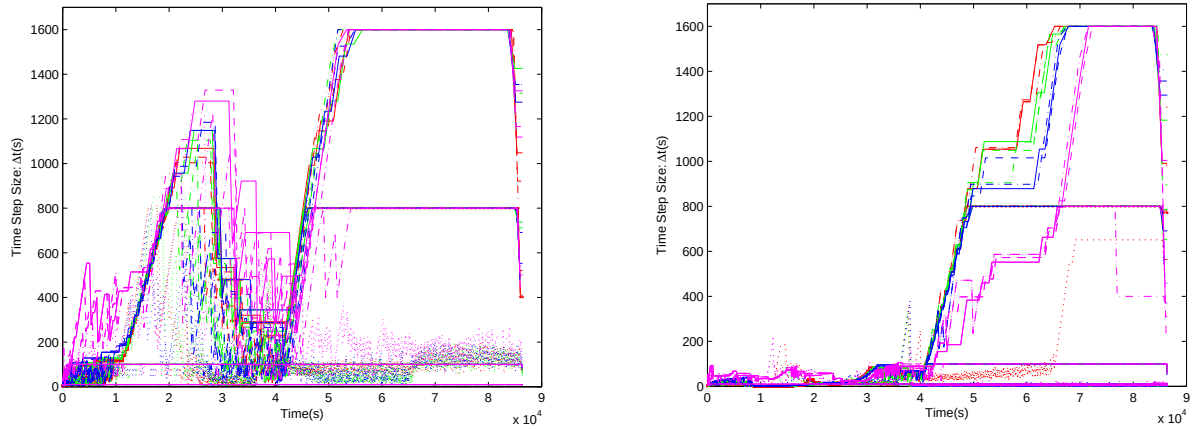


FIGURE 45. Complete time stepping behavior of Picard (left) and Newton(right) schemes of Test Problem 3. Red, green, blue, and magenta lines: 240, 120, 60, and 12 layers respectively. Dotted, dash-dotted, dashed, and solid lines: 6, 31, 151, and 301 lookup points respectively.

iterations. NLKP=151 has taken 3 times maximum 8 iterations and in the remaining part, it behaves same as the NLKP=301. For NLKP=31, maximum 10 iterations took once and then it does not need more than 8 iterations to complete the simulation. Similar behavior are found for the $\Delta t_{max} = 800$ s with NLKP=31, 151, and 301. After $T_{max} = 45000$ s, solver doesn't need more than 2 iterations for $\Delta t_{max} = 100$ s for each NLKP. For $\Delta t_{max} = 10$ s case, from $T_{max} = 10000$ s to $T_{max} = 45000$ s, only 2 iterations are spent and then it is taken only one

iteration for NLKP=151 and 301. Almost same thing happened for NLKP=31 case. Expected behavior is shown for 12 layers and NLKP=6. For all the other vertical soil layer cases similar behavior applies. Complete convergence behavior of Picard and Newton schemes is presented by the Figure 47.

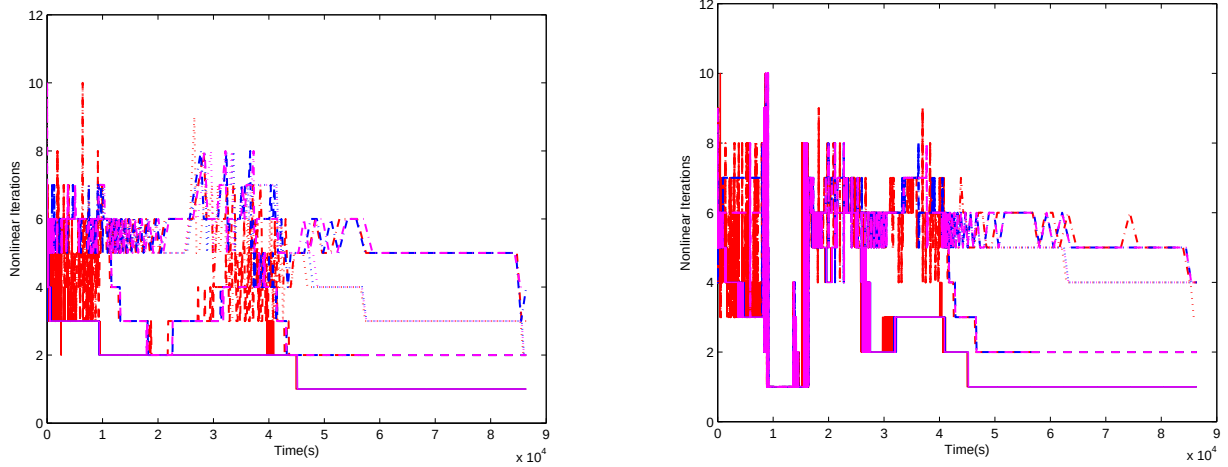


FIGURE 46. Convergence behavior of Picard (left) and Newton(right): NLKP=31(red), 151(blue), and 301(magenta) for 240 layers with all the time step sizes 10 s(solid), 100 s(dashed), 800 s(dotted), and 1600 s(dot-dashed) for Test Problem 3.

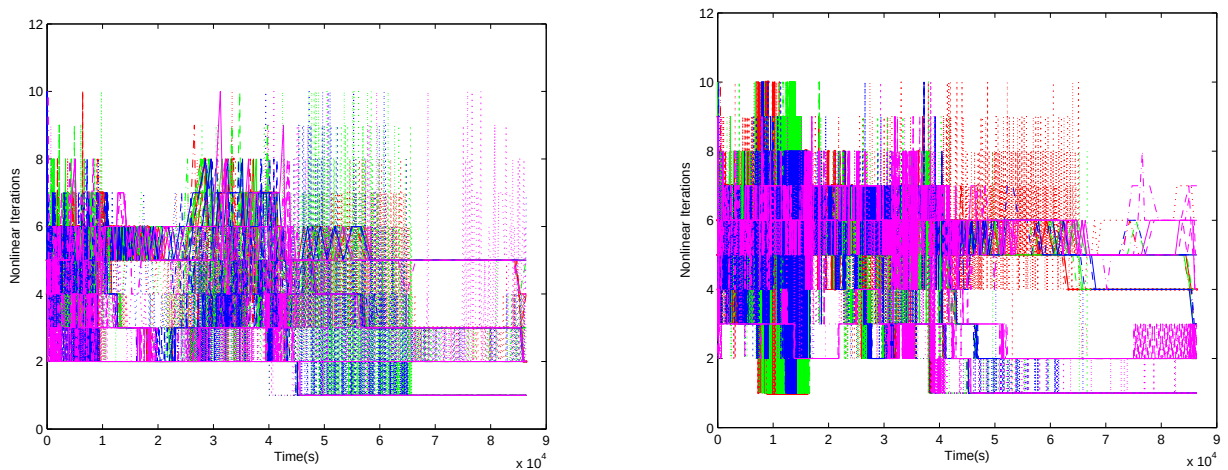


FIGURE 47. Convergence behavior of Picard (left) and Newton(right) schemes of Test Problem 3. Red, green, blue, and magenta lines: 240, 120, 60, and 12 layers respectively. Dotted, dash-dotted, dashed, and solid lines: 6, 31, 151, and 301 lookup points respectively.

In the nested Newton scheme, inner iterations indicate the overall performance of the solver. The 1st graph of Figure 48 is the 240 layers case. Clearly from the figure, the inner iterations behavior of 1600 s and 800 s are same. After 30000 s and 40000 s, solver needs only 2 inner iterations until completion of the simulation for 800 s and 1600 s cases respectively. On the other hand, after 10000 s, 3 inner iterations are needed per outer iteration to achieve convergence. The 2nd graph of Figure 48 represents the complete inner iterations behavior for all the cases.

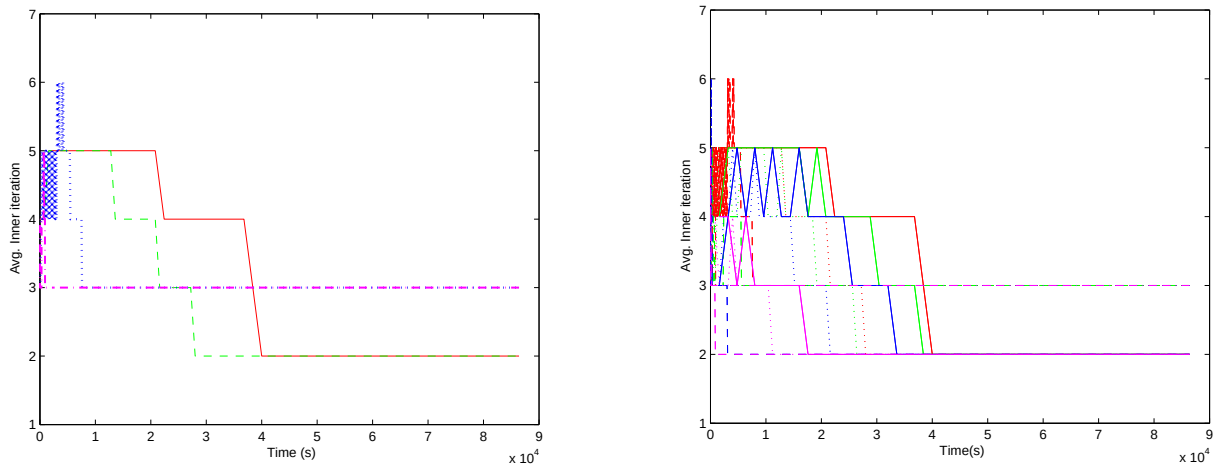


FIGURE 48. Convergence behavior of nested Newton scheme for 240 layers (left with red, green, blue, and magenta lines: $\Delta t_{max} = 1600$ s, 800 s, 100 s, and 10 s respectively) and for all the layers with all time step sizes (right with red, green, blue, and magenta lines: 240, 120, 60, and 12 layers respectively and solid, dotted, dashed, and dash-dotted lines: $\Delta t_{max} = 1600$ s, 800 s, 100 s, and 10 s respectively) for Test Problem 3.

To investigate the behavior of cumulative mass balance error for Problem 3, we consider only 240 layer case. We illustrate here the graph of 240 layer case with NLKP=31, 151, and 301 for the case of $\Delta t_{max} = 10$ s, 100 s, 800 s and 1600 s (Figure 49). For all the cases of 240 layers, excellent mass balance error are shown and it is less than 6×10^{-4} for Picard scheme and 1.8×10^{-4} for Newton scheme. Combined mass balance error (all layers with all NLKP and all time step sizes) for Picard and Newton are shown in Figure 50.

The computational performance of CATHY model for Picard and Newton schemes is presented in Tables 27, 28, 29, 30, 31, 32, 33, and 34 where we give summary statistics for the

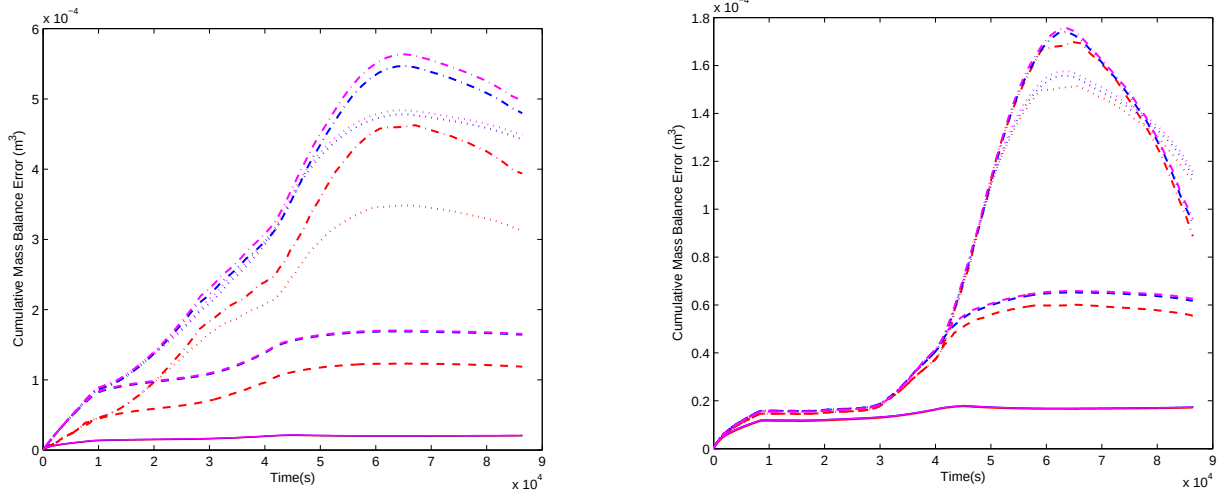


FIGURE 49. Cumulative mass balance error behavior of Picard (left) and Newton(right): NLKP=31(red), 151(blue), and 301(magenta) for 240 layers with all the time step sizes 10 s(solid), 100 s(dashed), 800 s(dotted), and 1600 s(dash-dotted) for Test Problem 3.

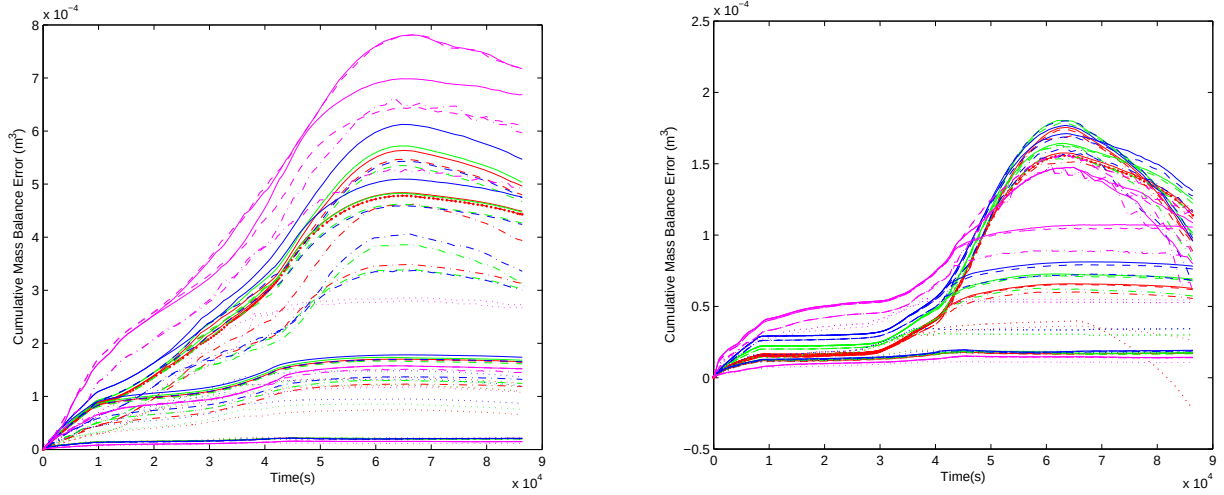


FIGURE 50. Cumulative mass balance error behavior of Picard (left) and Newton(right): Test Problem 3.

Picard and Newton schemes run over a range of mesh discretizations (10, 60, 120, and 240 layers) and maximum time step sizes (1600 s, 800 s, 10 s, and 1 s). The 8 performance indicators are: total volumetric and percentage mass balance error, total number of time steps and average step size, the average number of Newton or Picard iterations taken at each time step, the average number of iterations needed to solve the linear algebraic system at each Picard or Newton iteration, the number of back-stepping occurrences, and the number of linear solver

failures.

TABLE 27. Computational performance of CATHY model: Picard and Newton schemes for 12 layers with $\Delta t_{max}=10$ s and 100 s for Test Problem 3.

–	Δt_{max} (s) $\rightarrow$	10	10	100	100
–	NLKP	Pic	New	Pic	New
MBE (m ³)	6	1.16e-5	1.07e-5	1.08e-4	5.45e-5
	31	1.48e-5	1.40e-5	1.45e-4	8.48e-5
	151	1.48e-5	1.45e-5	1.52e-4	1.04e-4
	301	1.48e-5	1.44e-5	1.52e-4	1.06e-4
MBE (perc.)	6	5.79e-2	5.36e-2	5.40e-1	2.73e-1
	31	7.41e-2	6.99e-2	7.26e-1	4.24e-1
	151	7.41e-2	7.08e-2	7.60e-1	5.18e-1
	301	7.41e-2	7.18e-2	7.60e-1	5.28e-1
No. of Time . Steps	6	8693	15171	950	11877
	31	8650	8652	910	1418
	151	8642	8644	878	1330
	301	8642	8640	876	1336
Avg. Δt (s)	6	9.939	5.695	9.095e+1	7.275e+0
	31	9.988	9.986e+0	9.495e+1	6.093e+1
	151	9.998	5.695	9.841e+1	7.275e+0
	301	9.998	9.986	9.863e+1	6.093e+0
NL Iter/ Time Steps	6	1.57	3.41	3.36	3.87
	31	1.55	1.95	2.87	4.97
	151	1.54	1.95	2.62	5.06
	301	1.54	1.95	2.58	4.97
Lin Iter/ NL Iter	6	7.17	20.03	11.91	22.84
	31	5.90	4.60	10.06	6.51
	151	5.86	4.55	10.40	6.60
	301	5.86	4.55	10.41	6.59
No. of Back Steps	6	36	2867	45	2886
	31	7	8	27	24
	151	1	2	8	7
	301	1	0	6	3
Solver Failures	6	0	27	0	17
	31	0	0	0	0
	151	0	0	0	0
	301	0	0	0	0

Fixed time step sizes are used for nested Newton scheme, so there is no back stepping. Thus, for every fixed time step, we get fixed total number time steps. Besides, the total number of outer iterations, the total number of inner iterations is also reported. The inner iterations directly represent the simulation performance. Also the average number of outer iterations per time step and the average number of inner iterations per outer iteration are indicated (Table 35).

We calculated the root mean squared error at three different times (32000 s, 56000 s, and 86400 s) for all the cases using the base solution. There are two base solutions, one for Picard and Newton and the other for nested Newton. For the CATHY model, we used 240 layers with

TABLE 28. Computational performance of CATHY model: Picard and Newton schemes for 12 layers with $\Delta t_{max}=800$ s and 1600 s for Test Problem 3.

–	Δt_{max} (s) $\rightarrow$	800	800	1600	1600
–	NLKP	Pic	New	Pic	New
MBE (m ³)	6	2.66e-4	5.28e-5	2.73e-4	5.28e-5
	31	4.93e-4	1.16e-4	5.96e-4	6.06e-5
	151	6.11e-4	1.16e-4	7.19e-4	8.56e-5
	301	6.69e-4	1.09e-4	7.18e-4	7.98e-5
MBE (perc.)	6	1.33e+0	2.64e-1	1.37e+0	2.64e-1
	31	2.46e+0	5.79e-1	2.98e+0	3.03e-1
	151	3.05e+0	5.78e-1	3.59e+0	4.28e-1
	301	3.34e+0	5.43e-1	3.59e+0	3.99e-1
No. of Time s Steps	6	488	11934	502	11934
	31	217	1072	179	1049
	151	165	974	132	962
	301	162	988	138	976
Avg. Δt (s)	6	7.436e+2	7.240e+0	1.721e+2	7.240e+0
	31	3.982e+2	8.060e+1	4.827e+2	8.236e+1
	151	5.236e+2	7.240e+0	6.545e+2	7.240e+0
	301	5.333e+2	8.060e+1	6.261e+2	8.236e+1
NL Iter/ Time Steps	6	5.86	3.86	5.91	3.87
	31	5.69	6.18	6.35	6.21
	151	5.37	6.40	6.27	6.44
	301	5.40	6.27	6.41	6.30
Lin Iter/ NL Iter	6	15.74	23.15	15.29	23.17
	31	12.28	6.61	12.31	6.59
	151	13.58	6.71	13.62	6.81
	301	12.92	6.64	12.93	6.60
No. of Back Steps	6	97	2912	100	2913
	31	33	32	30	33
	151	12	9	12	11
	301	12	6	16	7
Solver Failures	6	0	22	0	22
	31	0	0	0	0
	151	0	0	0	1
	301	0	0	0	0

NLKP=301 and $\Delta t_{max} = 1$ s for the base solution to calculate the root mean squared error of Picard and Newton schemes. For the nested Newton case, reference solution is made by the same vertical discretization with same time step size. The RMSE are presented by the Tables 36, 37, 38, 39, and 40.

The error behavior of Picard and Newton is shown in Figure 51 for 240 layers with all set of lookup points for $\Delta t_{max} = 10$ s. Figure 52, shows the Picard and Newton error behavior for all the vertical discretizations along with all NLKP and all time step sizes. The 240 layers and complete error behavior of nested Newton method are shown in Figure 53. From these tables and graphs, all schemes appear to show low errors for all the cases.

TABLE 29. Computational performance of CATHY model: Picard and Newton schemes for 60 layers with $\Delta t_{max}=10$ s and 100 s for Test Problem 3.

–	Δt_{max} (s) $\rightarrow$	10	10	100	100
–	NLKP	Pic	New	Pic	New
MBE (m ³)	6	1.99e-5	1.82e-5	8.67e-4	3.44e-5
	31	2.05e-5	1.87e-5	1.32e-4	6.80e-5
	151	2.11e-5	1.91e-5	1.65e-4	7.63e-5
	301	2.10e-5	1.93e-5	1.74e-4	7.82e-5
MBE (perc.)	6	9.98e-2	9.09e-2	4.34e-1	1.72e-1
	31	1.03e-1	9.33e-2	6.61e-1	3.40e-1
	151	1.06e-1	9.54e-2	8.27e-1	3.81e-1
	301	1.05e-1	9.64e-2	8.68e-1	3.91e-1
No. of Time Steps	6	8806	18654	1584	17741
	31	8677	11084	1047	5145
	151	8643	11094	918	5275
	301	8646	11163	894	5132
Avg. Δt (s)	6	9.811	4.632	5.455e+1	4.870e+0
	31	9.957	7.795e+0	8.252e+1	1.679e+1
	151	9.997	7.788	9.412e+1	1.638e+1
	301	9.993	7.740	9.664e+1	1.684e+1
NL Iter/ Time Steps	6	1.80	3.86	4.90	4.11
	31	1.66	3.39	3.73	5.96
	151	1.61	3.41	3.16	5.81
	301	1.62	3.40	3.01	5.90
Lin Iter/ NL Iter	6	6.21	31.52	8.54	39.41
	31	5.39	3.78	7.71	3.69
	151	5.44	3.74	8.69	3.62
	301	5.44	3.73	9.05	3.69
No. of Back Steps	6	111	3543	267	3852
	31	26	12	81	52
	151	2	0	18	7
	301	3	0	7	5
Solver Failures	6	0	273	0	398
	31	0	0	0	1
	151	0	0	0	0
	301	0	0	0	0

TABLE 30. Computational performance of CATHY model: Picard and Newton schemes for 60 layers with $\Delta t_{max}=800$ s and 1600 s for Test Problem 3.

–	Δt_{max} (s) $\rightarrow$	800	800	1600	1600
–	NLKP	Pic	New	Pic	New
MBE (m ³)	6	1.37e-4	3.44e-5	1.20e-4	3.44e-5
	31	3.00e-4	1.17e-4	3.36e-4	6.50e-5
	151	4.24e-4	1.27e-4	4.74e-4	9.76e-5
	301	4.75e-4	1.31e-4	5.47e-4	9.56e-5
MBE (perc.)	6	6.83e-1	1.72e-1	6.00e-1	1.72e-1
	31	1.50e+0	5.83e-1	1.68e+0	3.25e-1
	151	2.12e+0	6.37e-1	2.37e+0	4.88e-1
	301	2.38e+0	6.55e-1	2.73e+0	4.78e-1
No. of Time Steps	6	1300	17769	1412	17769
	31	475	4765	433	4748
	151	298	4894	270	4876
	301	247	4750	216	4734
Avg. Δt (s)	6	6.646e+1	4.862e+0	6.119e+1	4.862e+0
	31	1.819e+2	1.813e+1	1.995e+2	1.820e+1
	151	2.899e+2	1.765e+1	3.200e+2	1.772e+1
	301	3.498e+2	1.819e+1	4.00e+2	1.825e+1
NL Iter/ Time Steps	6	5.83	4.12	5.75	4.12
	31	6.09	6.31	6.44	6.32
	151	5.86	6.41	6.32	6.15
	301	5.67	6.25	6.26	6.26
Lin Iter/ NL Iter	6	9.89	38.61	9.58	38.62
	31	7.64	3.82	7.77	3.83
	151	9.14	3.64	9.05	3.66
	301	10.18	3.72	10.19	3.75
No. of Back Steps	6	310	3868	341	3869
	31	94	57	91	58
	151	28	10	28	11
	301	10	8	10	9
Solver Failures	6	0	345	0	346
	31	0	4	0	5
	151	0	0	0	4
	301	0	3	0	4

TABLE 31. Computational performance of CATHY model: Picard and Newton schemes for 120 layers with $\Delta t_{max} = 10$ s and 100 s for Test Problem 3.

–	Δt_{max} (s) $\rightarrow$	10	10	100	100
–	NLKP	Pic	New	Pic	New
MBE (m ³)	6	2.04e-5	1.84e-5	7.53e-5	3.01e-5
	31	2.01e-5	1.68e-5	1.25e-4	5.73e-5
	151	2.05e-5	1.72e-5	1.65e-4	6.81e-5
	301	2.02e-5	1.77e-5	1.68e-4	6.91e-5
MBE (perc.)	6	1.02e-1	9.20e-2	3.76e-1	1.51e-1
	31	1.01e-1	8.42e-2	6.23e-1	2.87e-1
	151	1.02e-1	8.62e-2	8.07e-1	3.40e-1
	301	1.01e-1	8.83e-2	8.40e-1	3.46e-1
No. of Time Steps	6	8929	25916	1914	24437
	31	8672	16644	1098	10917
	151	8644	16835	926	10887
	301	8651	16839	907	10925
Avg. Δt (s)	6	9.676	3.334	4.514e+1	3.536e+0
	31	9.963	5.191e+0	7.869e+1	7.914e+0
	151	9.995	5.132e+0	9.330e+1	7.936e+0
	301	9.987	5.131e+0	9.526e+1	7.908e+0
NL Iter/ Time Steps	6	1.95	4.18	5.03	4.33
	31	1.67	4.07	3.89	5.59
	151	1.64	4.06	3.20	5.73
	301	1.64	4.06	3.09	5.72
Lin Iter/ NL Iter	6	5.74	41.22	7.39	42.23
	31	5.28	3.42	7.08	3.39
	151	5.28	3.38	8.45	3.34
	301	5.26	3.38	8.68	3.33
No. of Back Steps	6	188	4635	336	4695
	31	22	225	90	300
	151	1	201	11	207
	301	3	203	5	212
Solver Failures	6	0	1417	0	1423
	31	0	0	0	2
	151	0	0	0	2
	301	0	0	0	2

TABLE 32. Computational performance of CATHY model: Picard and Newton schemes for 120 layers with $\Delta t_{max} = 800$ s and 1600 s for Test Problem 3.

–	Δt_{max} (s) $\rightarrow$	800	800	1600	1600
–	NLKP	Pic	New	Pic	New
MBE (m ³)	6	1.09e-4	3.00e-5	1.19e-4	3.00e-5
	31	3.02e-4	1.14e-4	3.13e-4	8.13e-5
	151	4.24e-4	1.22e-4	4.67e-4	1.02e-5
	301	4.47e-4	1.25e-5	5.03e-4	9.98e-5
MBE (perc.)	6	6.80e-1	1.50e-1	5.97e-1	1.50e-1
	31	1.51e+0	5.69e-1	1.57e+0	4.07e-1
	151	2.13e+0	6.11e-1	2.33e+0	5.08e-1
	301	2.23e+0	6.25e-1	2.52e+0	4.99e-1
No. of Time Steps	6	1767	24428	1702	24428
	31	511	10530	518	10512
	151	305	10503	279	10485
	301	278	10542	250	10523
Avg. Δt (s)	6	4.890e+1	3.537e+0	5.076e+1	3.537e+0
	31	1.691e+2	8.205e+0	1.668e+2	8.219e+0
	151	2.833e+2	8.226e+0	3.097e+2	8.240e+0
	301	3.108e+2	8.196e+0	3.456e+2	8.211e+0
NL Iter/ Time Steps	6	5.75	4.33	5.75	4.33
	31	6.18	5.73	6.46	5.74
	151	5.77	5.88	6.22	5.88
	301	5.69	5.87	6.18	5.88
Lin Iter/ NL Iter	6	8.03	41.22	8.23	41.23
	31	6.88	3.41	6.77	3.42
	151	8.82	3.36	8.78	3.39
	301	9.28	3.38	9.24	3.39
No. of Back Steps	6	412	4706	387	4707
	31	97	302	110	303
	151	15	210	16	211
	301	8	215	9	216
Solver Failures	6	0	1395	0	1396
	31	0	5	0	6
	151	0	5	0	6
	301	0	5	0	6

TABLE 33. Computational performance of CATHY model: Picard and Newton schemes for 240 layers with $\Delta t_{max} = 10$ s and 100 s for Test Problem 3.

–	Δt_{max} (s) $\rightarrow$	10	10	100	100
–	NLKP	Pic	New	Pic	New
MBE (m ³)	6	2.28e-5	1.91e-5	6.56e-5	2.63e-5
	31	2.03e-5	1.71e-5	1.19e-4	5.55e-5
	151	2.07e-5	1.74e-5	1.64e-4	6.17e-5
	301	2.09e-5	1.73e-5	1.65e-4	6.26e-5
MBE (perc.)	6	1.14e-1	9.57e-2	3.28e-1	1.31e-1
	31	1.02e-1	8.53e-2	5.93e-1	2.78e-1
	151	1.04e-1	8.70e-2	8.22e-1	3.09e-1
	301	1.04e-1	8.66e-2	8.27e-1	3.13e-1
No. of Time Steps	6	9067	20100	2025	14654
	31	8688	23903	1161	18384
	151	8668	24058	925	18404
	301	8654	24074	916	18419
Avg. Δt (s)	6	9.529	4.299	4.267e+1	5.896e+0
	31	9.945	3.615e+0	7.442e+1	4.725e+0
	151	9.968	3.591e+0	9.341e+1	4.695e+0
	301	9.984	3.589e+0	9.432e+1	4.691e+0
NL Iter/ Time Steps	6	2.09	3.57	5.43	4.56
	31	1.69	3.32	4.02	4.02
	151	1.66	3.30	3.22	4.02
	301	1.65	3.30	3.16	3.99
Lin Iter/ NL Iter	6	5.34	4.36	5.89	5.11
	31	5.15	4.92	6.55	4.17
	151	5.17	4.35	8.20	4.34
	301	5.20	4.25	8.42	4.34
No. of Back Steps	6	258	2381	359	2460
	31	29	3806	105	3836
	151	9	3859	9	3868
	301	4	3858	4	3862
Solver Failures	6	0	7	0	38
	31	0	13	0	11
	151	0	16	0	14
	301	0	9	0	14

TABLE 34. Computational performance of CATHY model: Picard and Newton schemes for 240 layers with $\Delta t_{max} = 800$ s and 1600 s for Test Problem 3.

–	Δt_{max} (s) $\rightarrow$	800	800	1600	1600
–	NLKP	Pic	New	Pic	New
MBE (m ³)	6	1.10e-4	-2.16e-5	1.24e-4	-2.16e-5
	31	3.13e-4	1.12e-4	3.94e-4	8.87e-5
	151	4.43e-4	1.14e-4	4.80e-4	9.41e-5
	301	4.49e-4	1.16e-4	5.03e-4	9.60e-4
MBE (perc.)	6	5.49e-1	-1.08e-1	6.22e-1	-1.08e-1
	31	1.57e+0	5.58e-1	1.97e+0	4.44e-1
	151	2.21e+0	5.69e-1	2.40e+0	4.71e-1
	301	2.25e+0	5.79e-1	2.48e+0	4.80e-1
No. of Time Steps	6	1746	14412	1688	14412
	31	573	17898	508	17878
	151	300	18020	280	18001
	301	288	18035	265	18016
Avg. Δt (s)	6	4.948e+1	5.995e+0	5.118e+1	5.995e+0
	31	1.508e+2	4.827e+0	1.701e+2	4.833e+0
	151	2.880e+2	4.795e+0	3.086e+2	4.800e+0
	301	3.000e+2	4.791e+0	3.260e+2	4.796e+0
NL Iter/ Time Step	6	6.18	4.60	6.22	4.60
	31	6.21	4.07	6.49	4.07
	151	5.83	4.07	6.24	4.07
	301	5.74	4.04	6.16	4.04
Lin Iter/ NL Iter	6	7.03	4.95	7.05	4.98
	31	6.18	4.17	6.20	4.18
	151	8.55	4.36	8.40	4.37
	301	8.92	4.35	8.78	4.37
No. of Back Steps	6	406	2452	391	2453
	31	111	3839	101	3840
	151	12	3871	13	3872
	301	7	3865	8	3866
Solver Failures	6	0	35	0	36
	31	0	14	0	15
	151	0	17	0	18
	301	0	17	0	18

TABLE 35. Computational performance of nested Newton scheme: Test Problem 3.

	Δt_{max} (s) $\rightarrow$	1600	800	100	10
No. of Layers	No. of Time Steps	54	108	864	8640
12	Tot. outer iterations	108	216	1728	25915
	Tot. inner iterations	121	231	1737	25932
	Avg. outer iterations	2.00	2.00	2.00	3.00
	Avg. inner iterations	1.12	1.07	1.00	1.00
60	Tot. outer iterations	108	216	1728	25914
	Tot. inner iterations	146	260	1760	25957
	Avg. outer iterations	2.00	2.00	2.00	3.00
	Avg. inner iterations	1.35	1.20	1.02	1.00
120	Tot. outer iterations	108	216	2569	25906
	Tot. inner iterations	159	280	2630	25969
	Avg. outer iterations	2.00	2.00	2.97	3.00
	Avg. inner iterations	1.47	1.30	1.02	1.00
240	Tot. outer iterations	108	216	2562	25890
	Tot. inner iterations	168	292	2709	25997
	Avg. outer iterations	2.00	2.00	2.96	3.00
	Avg. inner iterations	1.569	1.35	1.06	1.00

TABLE 36. RMSE of CATHY model: Picard and Newton schemes for 12 layers for Test Problem 3.

–	Δt_{max} (s) $\rightarrow$	10	10	100	100	800	800	1600	1600
NLKP	Time (s)	Pic	New	Pic	New	Pic	New	Pic	New
6	32000	2.10e-2	2.14e-2	1.94e-2	2.07e-2	1.85e-2	2.07e-2	1.82e-2	2.07e-2
	56000	3.80e-2	3.81e-2	3.75e-2	3.78e-2	3.75e-2	3.78e-2	3.75e-2	3.78e-2
	86400	3.54e-2	3.54e-2	3.32e-2	3.45e-2	3.04e-2	3.45e-2	3.01e-2	3.45e-2
31	32000	6.50e-3	6.00e-3	7.60e-3	6.40e-3	1.14e-2	6.40e-3	9.30e-3	6.40e-3
	56000	3.06e-2	3.05e-2	3.45e-2	3.22e-2	4.56e-2	3.24e-2	4.55e-2	3.24e-2
	86400	1.49e-2	1.49e-2	1.58e-2	1.52e-2	2.53e-2	1.53e-2	2.83e-2	1.49e-2
151	32000	7.10e-3	6.60e-3	8.60e-3	7.00e-3	1.19e-2	7.00e-3	1.42e-2	7.00e-3
	56000	3.13e-2	3.12e-2	3.56e-2	3.34e-2	4.98e-2	3.15e-2	5.24e-2	3.15e-2
	86400	1.34e-2	1.34e-2	1.50e-2	1.41e-2	2.96e-2	1.42e-2	3.41e-2	1.40e-2
301	32000	7.10e-3	6.60e-3	8.60e-3	6.90e-3	1.27e-2	6.90e-3	1.10e-2	6.90e-3
	56000	3.13e-2	3.13e-2	3.60e-2	3.35e-2	5.36e-2	3.38e-2	5.69e-2	3.38e-2
	86400	1.33e-2	1.33e-2	1.50e-2	1.42e-2	3.20e-2	1.43e-2	3.36e-2	1.39e-2

TABLE 37. RMSE of CATHY model: Picard and Newton schemes for 60 layers for Test Problem 3.

–	Δt_{max} (s) $\rightarrow$	10	10	100	100	800	800	1600	1600
NLKP	Time (s)	Pic	New	Pic	New	Pic	New	Pic	New
6	32000	2.78e-2	2.78e-2	2.64e-2	2.76e-2	2.50e-2	2.76e-2	2.56e-2	2.76e-2
	56000	3.09e-2	3.10e-2	2.90e-2	3.04e-2	3.76e-2	3.04e-2	2.81e-2	3.04e-2
	86400	3.92e-2	3.93e-2	3.69e-2	3.87e-2	3.52e-2	3.87e-2	3.58e-2	3.87e-2
31	32000	1.10e-3	1.10e-3	2.70e-3	1.20e-3	5.30e-3	1.20e-3	4.60e-3	1.20e-3
	56000	4.20e-3	4.20e-3	4.80e-3	3.70e-3	6.50e-3	4.40e-3	1.06e-2	4.80e-3
	86400	4.70e-3	4.80e-3	4.90e-3	4.00e-3	1.13e-2	4.40e-3	1.25e-2	4.10e-3
151	32000	1.10e-3	9.35e-4	4.10e-3	1.20e-3	6.50e-3	1.20e-3	7.30e-3	1.20e-3
	56000	2.60e-3	2.60e-3	7.40e-3	3.40e-3	1.83e-2	2.80e-3	1.86e-2	4.20e-3
	86400	1.10e-3	1.20e-3	6.40e-3	2.10e-3	1.87e-2	4.70e-3	2.16e-2	3.00e-3
301	32000	4.40e-3	1.30e-3	4.40e-3	1.30e-3	6.10e-3	1.30e-3	9.10e-2	1.30e-3
	56000	7.60e-3	3.00e-3	7.60e-3	3.00e-3	1.80e-3	4.80e-3	2.04e-2	6.70e-3
	86400	6.90e-3	2.30e-3	6.90e-3	2.30e-3	2.15e-2	4.80e-3	2.50e-2	3.10e-3

TABLE 38. RMSE of CATHY model: Picard and Newton schemes for 120 layers for Test Problem 3.

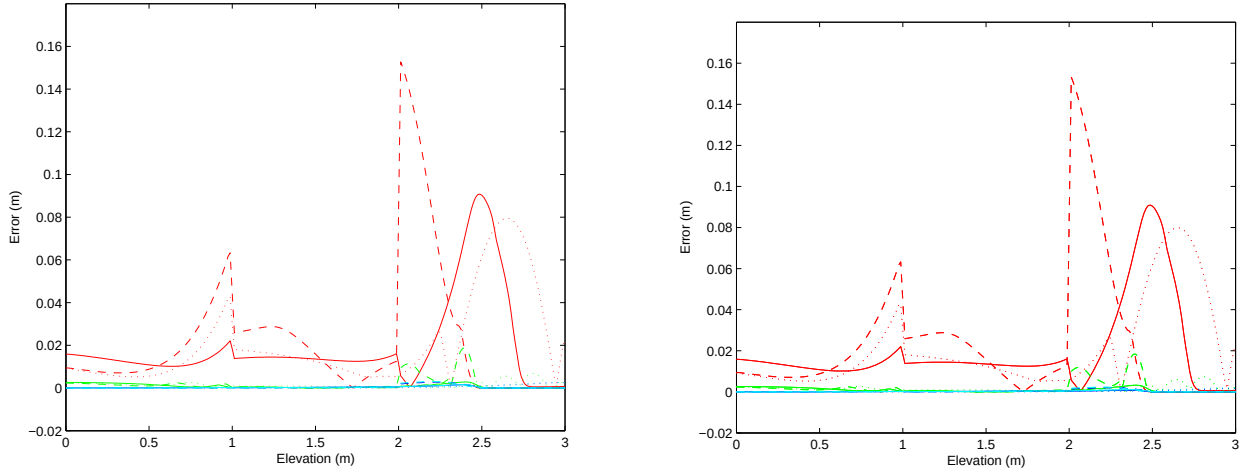
–	Δt_{max} (s) $\rightarrow$	10	10	100	100	800	800	1600	1600
NLKP	Time (s)	Pic	New	Pic	New	Pic	New	Pic	New
6	32000	2.91e-2	2.91e-2	2.80e-2	2.90e-2	2.71e-2	2.90e-2	2.69e-2	2.90e-2
	56000	2.72e-2	2.72e-2	2.55e-2	2.69e-2	2.46e-2	2.69e-2	2.42e-2	2.69e-2
	86400	3.58e-2	3.59e-2	3.42e-2	3.56e-2	3.31e-2	3.56e-2	3.28e-2	3.56e-2
31	32000	2.10e-3	2.20e-3	1.20e-3	2.00e-3	3.30e-3	2.00e-3	3.00e-3	2.00e-3
	56000	3.20e-3	3.00e-3	6.90e-3	4.80e-3	1.50e-3	8.10e-3	1.26e-2	7.00e-3
	86400	4.90e-3	4.80e-3	8.90e-3	6.10e-3	1.72e-2	8.10e-3	1.76e-2	6.80e-3
151	32000	6.29e-4	7.87e-4	2.20e-3	6.92e-4	3.50e-3	6.92e-4	4.10e-3	6.92e-4
	56000	4.60e-3	4.40e-3	1.03e-2	5.90e-3	2.00e-3	1.03e-3	1.78e-2	1.40e-3
	86400	4.90e-3	4.70e-3	1.18e-2	7.20e-3	2.47e-2	9.90e-3	2.65e-2	8.70e-3
301	32000	6.63e-4	7.54e-4	2.30e-3	3.40e-4	5.90e-3	3.40e-4	5.70e-3	3.40e-4
	56000	4.60e-3	4.40e-3	1.08e-2	6.30e-4	2.42e-2	7.50e-3	2.53e-2	7.60e-3
	86400	5.00e-3	4.80e-3	1.22e-2	7.30e-3	2.57e-2	9.90e-3	2.84e-2	8.70e-3

TABLE 39. RMSE of CATHY model: Picard and Newton schemes for 240 layers for Test Problem 3.

–	Δt_{max} (s) $\rightarrow$	10	10	100	100	800	800	1600	1600
NLKP	Time (s)	Pic	New	Pic	New	Pic	New	Pic	New
6	32000	2.83e-2	2.84e-2	2.74e-2	2.82e-2	2.65e-2	2.81e-2	2.61e-2	2.81e-2
	56000	2.92e-2	2.94e-2	2.79e-2	2.88e-2	2.64e-2	2.88e-2	2.60e-2	2.88e-2
	86400	3.88e-2	3.89e-2	3.73e-2	3.87e-2	3.58e-2	4.02e-2	3.53e-2	4.02e-2
31	32000	1.30e-3	1.30e-3	1.60e-3	1.20e-3	3.90e-3	1.20e-3	4.60e-3	1.20e-3
	56000	2.00e-3	2.10e-3	3.70e-3	1.80e-3	7.90e-3	1.80e-3	3.30e-2	3.30e-3
	86400	4.00e-3	4.00e-3	5.30e-3	3.90e-3	1.35e-2	5.10e-3	1.75e-2	4.50e-3
151	32000	4.82e-4	2.93e-4	3.60e-3	4.95e-4	6.00e-3	4.95e-4	5.10e-3	4.95e-4
	56000	8.07e-4	5.11e-4	7.50e-3	1.80e-3	1.34e-2	5.90e-3	1.00e-2	3.50e-3
	86400	8.98e-4	6.74e-4	8.00e-3	2.90e-3	2.17e-2	5.40e-3	2.35e-2	4.30e-3
301	32000	4.85e-4	3.66e-4	3.40e-3	1.50e-4	5.00e-3	1.50e-4	6.90e-3	1.50e-4
	56000	8.25e-4	6.26e-4	7.20e-3	2.10e-4	1.39e-2	6.30e-3	1.35e-2	3.30e-3
	86400	9.63e-4	7.24e-4	8.10e-3	3.00e-3	2.20e-2	5.60e-3	2.43e-2	4.30e-3

TABLE 40. RMSE of nested Newton model: All layers with all time step sizes for Test Problem 3.

No. of Layers	Time (s)	$\Delta t_{max} = 10$ s	$\Delta t_{max} = 100$ s	$\Delta t_{max} = 800$ s	$\Delta t_{max} = 1600$ s
12	32000	0.4826	0.4826	0.4826	0.4826
	56000	0.2711	0.2711	0.2711	0.2711
	86400	0.2003	0.2003	0.2003	0.2003
60	32000	0.4610	0.4610	0.4609	0.4602
	56000	0.2641	0.2641	0.2641	0.2641
	86400	9.77e-2	9.80e-2	9.77e-2	9.77e-2
120	32000	0.4578	0.4578	0.4576	0.4619
	56000	0.2626	0.2627	0.2627	0.2627
	86400	7.65e-2	7.66e-2	7.66e-2	7.66e-2
240	32000	0.4562	0.4562	0.4558	0.4669
	56000	0.2619	0.2619	0.2619	0.2619
	86400	6.35e-2	6.35e-2	6.35e-2	6.35e-2

FIGURE 51. RMSE behavior of 240 layers for $\Delta t_{max} = 10$ s with all NLKP: Picard (left) and Newton (right) of Test Problem 3. Red, green, blue, and cyan lines: 6, 31, 151, and 301 lookup points respectively. Solid, dotted, and dashed lines are at times 32000 s, 56000 s, and 86400 s respectively.

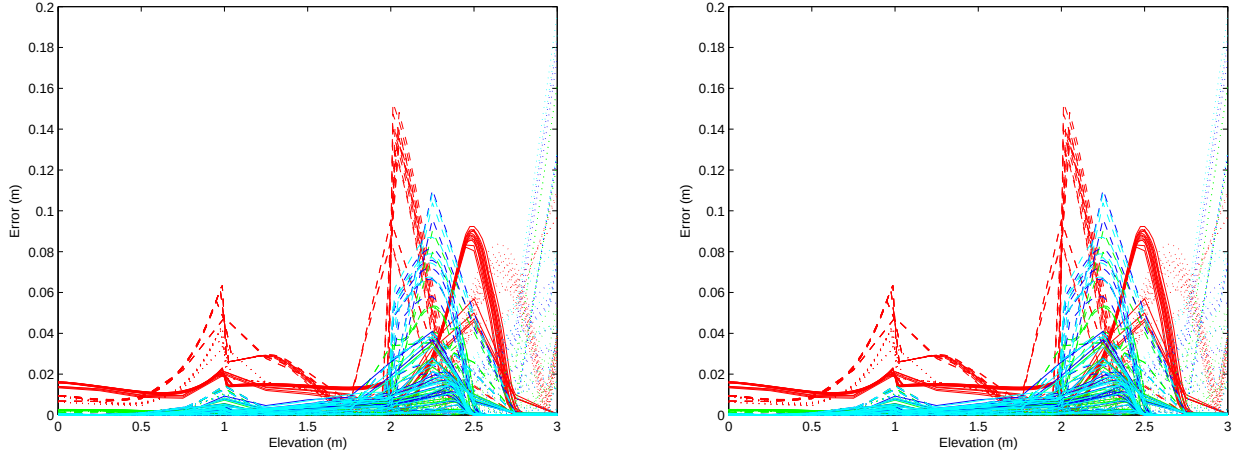
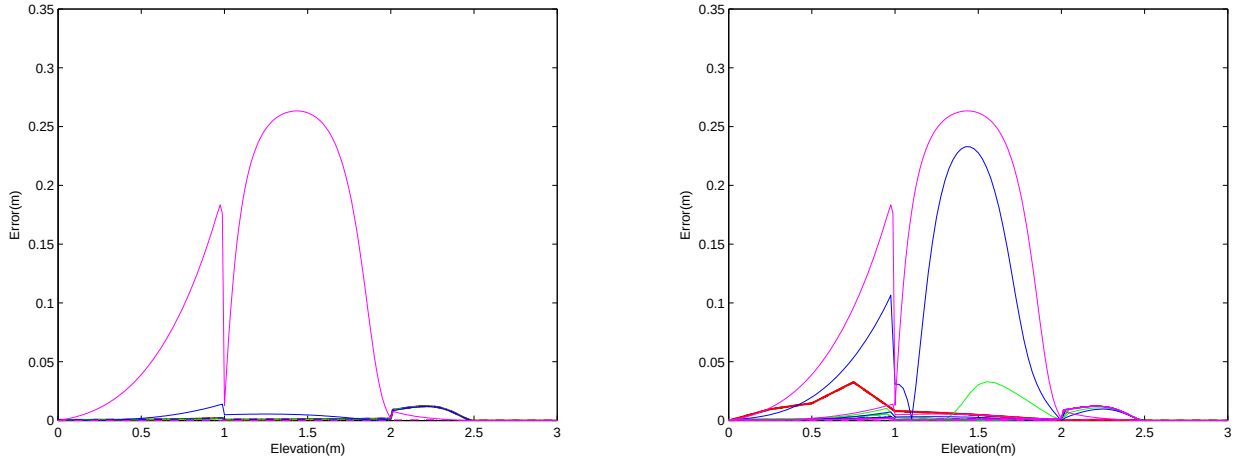


FIGURE 52. RMSE behavior of Picard (left) and Newton (right) schemes of Test Problem 3. Red, green, blue, and cyan lines: 6, 31, 151, and 301 lookup points respectively. Solid, dotted, and dashed lines are at times 32000 s, 56000 s, and 86400 s respectively.



1

FIGURE 53. RMSE behavior of nested Newton (left graph (red, green, blue, and magenta lines: $\Delta t_{max} = 10$ s, 100 s, 800 s, and 1600 s respectively and solid, dotted, and dashed lines are at times 32000 s, 56000 s, and 86400 s respectively) for 240 layers and right graph (red, green, blue, and magenta lines are at times 12, 60, 120, and 240 layers respectively and solid, dotted, and dashed lines: 32000 s, 56000 s, and 86400 s respectively) for all layers) scheme of Test Problem 3.

3.5. Conclusions.

Richards' equation is a parabolic partial differential equation for flow in variably saturated porous media, with strong nonlinearities due to pressure head dependencies in the soil moisture capacity and hydraulic conductivity terms. It is necessary to use some numerical approximation method to solve the Richards equation for its nature, where the spatial domain is divided into discrete elements and nodal points and the solution is obtained by marching through time in discrete steps, starting with a known solution at time zero. Implicit two-level time discretization is often adopted in solving the equation numerically. As a result the stability of the overall scheme is ensured. The nonlinear nature of the equation, however, requires that the implicit scheme be solved iteratively, unless the nonlinear components are linearized in some manner. Newton and Picard iteration are the most common numerical methods for solving Richards' equation. In this work we have described in detail the Newton scheme, Picard scheme and a nested Newton-type linearization algorithm. For implementing the iterative techniques, we can mention that Newton method is quadratically convergent whereas the Picard scheme is convergent linearly, the iterative Picard preserves symmetry, while the iterative Newton approach results in nonsymmetric system matrices, and dynamic time stepping can be easily handled for the iterative Newton and Picard schemes. On the other hand, fixed time stepping is used in the nested Newton-type linearization scheme.

Three one-dimensional test problems, a sharp moisture front that infiltrates into the soil column, flow into a layered soil with variable initial conditions, and flow into dry heterogeneous soil, were used to evaluate the performance of the three schemes. Time stepping, nonlinear iterations, and RMSE plots were produced to illustrate the behavior of the different schemes. Convergence behavior plots showed theoretically expected rates of convergence for each of the time discretization strategies. Moreover all schemes were also observed to be stable for all of the test problems.

We can also conclude, under general assumptions on the soil properties, that the iterates are well defined and monotonically converge to the exact solution. Mass conservation both local and

global is always assured at each Picard iteration within a small number of inner and outer iterations. The simple numerical tests have confirmed the robustness, efficiency, and convenience of the proposed algorithm for solving the mixed form of Richards' equation under different flow conditions and for any time step size.

4. USING LOOKUP TABLES FOR HETEROGENEOUS SOILS

4.1. **Introduction.**

The one-dimensional θ -based Richards equation has been widely adopted for soil hydrology modules in land surface parameterization models instead of using ψ -based or mixed forms of the equation. For coarse grids, the θ -based formulation is appealing because this form has better mass conservation performance regardless of the grid size. Also, the expression of hydraulic conductivity $K(\theta)$ is generally more nonlinear than the expression of hydraulic diffusivity $D(\theta)$. So, when evaluating the internodal average parameters (i.e., D and K) with the same grid size, the former gives less error [146]. Therefore, taking water content as the primary variable is helpful for model calibration, which is a significant advantage of θ -based models.

However, the θ -based form has limitations on its applicability. Since water content cannot reflect the hydraulic gradient when the soil is saturated, it is restricted only to unsaturated flow problems [59]. To solve Richards' equation efficiently the water content in the unsaturated zone and the pressure head in the saturated zone can be used [75], although this particular scheme was explicit in time and suffered from severe mass balance error at the transition between the saturated and unsaturated zone [40]. Nevertheless, the θ -based form can still be utilized as an unsaturated module in coupled subsurface water movement models, to simulate subsurface flow in the vadose zone.

Some authors have reasoned that it is not desirable to simulate flow in heterogeneous soils by θ -based formulations because water content is not continuous across boundaries between materials with different hydraulic properties. Only a few papers have studied how to handle the discontinuity of water content in θ -based codes in heterogeneous soils. Two ghost nodes (above and below the interface, respectively) were introduced to describe the water content discontinuity at the material interface for the analysis of infiltration into layered soil [59]. In addition, a generalized θ -based formulation is proposed which considers the influence of soil heterogeneity [59]. Using the method of lines, the extension is made of the θ -based Richards equation to layered soil profiles [85]. The method of lines technique can handle the water content

discontinuity since it considers the flow dynamics within each soil layer separately. By using the main wetting curve, the water content discontinuity is dealt with by means of expressions that satisfy the continuity of matric head and Darcian flux at the interface.

Although there are some successes with the θ -based Richards equation in dealing with heterogeneous media, a few problems remain to be addressed. The algorithm is easy to implement in a non-iterative model, but its performance in iterative models has not been verified [59]. Thus, the approximate solution of the jump condition may produce significant error [59]. In addition, the method requires solving each homogenous layer with interrelated boundary conditions separately, but the assumption of flux continuity requires that no water storage can take place in the control volume of nodes at the interface, thus it may introduce considerable error in the storage term [85]. In this chapter, two cases of layered soil problems are considered to investigate the efficiency, accuracy, and numerical behavior of a lookup point strategy for computing the soil moisture curves.

4.2. Implementation.

To investigate the performance of the lookup table option of the CATHY model, we consider two one-dimensional numerical test problems, one of them involving vertical drainage through a layered soil from initially saturated conditions and another involving a one-dimensional flow into an initially very dry layered soil of sand and clay. These test problems are described in detail in the previous chapter, denoted by Test Problem 2 and Test Problem 3. There is a sharp region produced in the moisture capacity and relative hydraulic conductivity curves for these test problems. We examined the performance of the lookup table scheme in two ways, uniform and nonuniform distributions of lookup points in the domain of the constitutive relationship curves, and for both the Newton and Picard schemes. Simple equally spaced discretization of the moisture capacity, water saturation, relative hydraulic conductivity, and other retention curves is defined for the uniform distributions of lookup table points. We have taken many points where the retention curves are very sharp and fewer points are used where the curves are

varying less for the nonuniform distribution.

For both test problems, we used dynamic time stepping strategies that can be easily incorporated into iterative techniques such as the Newton and Picard schemes. The time step size can be increased by the factor $\Delta t_{mag} = 1.20$ if convergence at the current time level is achieved in very few iterations, and decreased by a reduction factor $\Delta t_{red} = 0.5$ if the solution converged slowly. A small time step size improves the initial solution estimate used in the iteration procedure. If convergence is not attained, that is, if some specified maximum number of iterations (ITUNS=10) is exceeded, the solution at the current time level can be recomputed using a smaller time step size. Also we set the nonlinear tolerance, $tol=10^{-3}$, and for solving the linear systems, we used BiCGSTAB (bi-conjugate gradients stabilized method) with tolerance 10^{-10} and maximum iterations 1000.

The comparisons are made in terms of: total volumetric (MBE (m^3)) and percentage mass balance error (MBE (perc.)), total number of time steps and average step size, the average number of nonlinear iterations taken at each time step, the average number of iterations needed to solve the linear algebraic system at each nonlinear iteration, the number of back-stepping occurrences, the number of linear solver failures (only relevant for the Newton scheme), and RMSE. The discussions are illustrated for the Picard and Newton schemes separately for both Test Problem 2 and Test Problem 3. To compare with the nonuniform distribution case, the numerical results of the uniform distribution case of test Problems 2 and 3 are taken from the previous chapter.

4.3. Results.

4.3.1. Test Problem 2.

To compare the performance between uniform and nonuniform distributions, two cases of grid discretizations (51 and 151 nodes) with two time steps ($\Delta t_{mag} = 100$ s and 1000 s) and two values for the number of lookup table points (NLKP=31 and 151) are considered. There are 16

runs in total for each of the iteration schemes (Picard and Newton).

The soil moisture curves for the uniform and nonuniform distribution of lookup points for the Brooks-Corey model are presented in Figures 54 and 55 for Soil 1 and Soil 2 respectively.

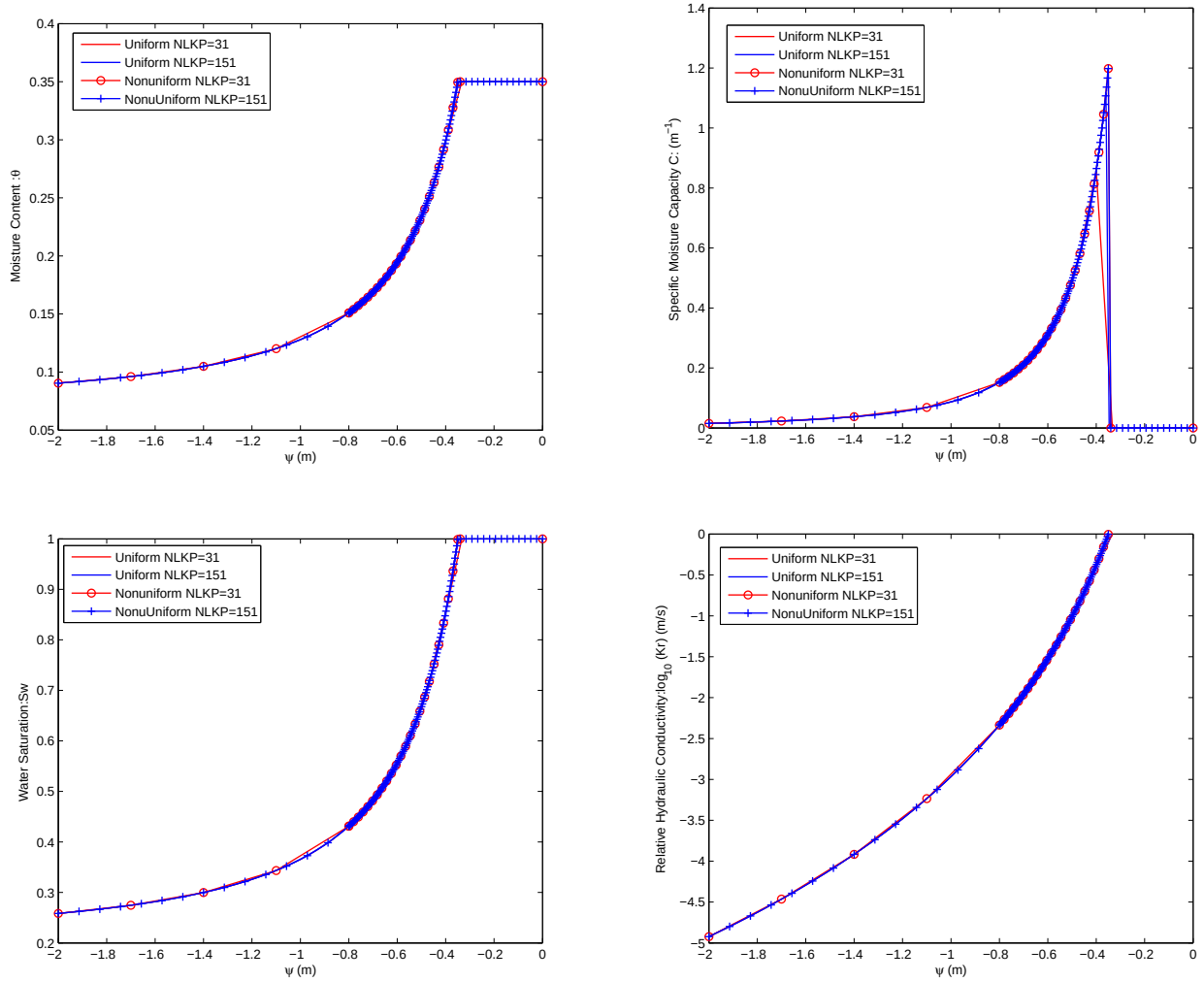


FIGURE 54. Soil 1 moisture curves for the uniform and nonuniform lookup table points cases.

The time stepping, nonlinear convergence, and cumulative mass balance error behavior of uniform and nonuniform NLKP are illustrated in the Figures 56, 58, and 60 respectively.

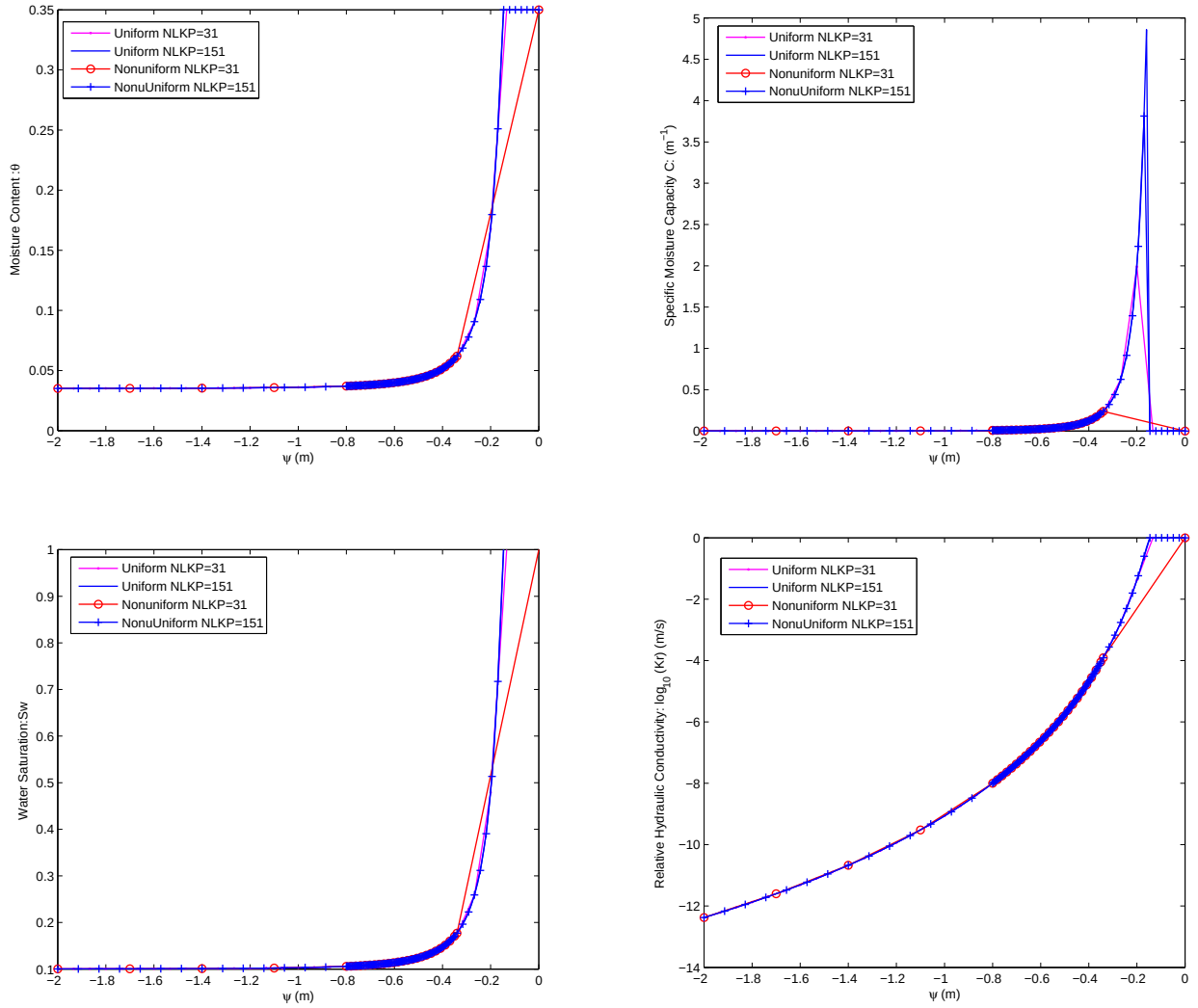


FIGURE 55. Soil 2 moisture curves for the uniform and nonuniform lookup table points cases.

The graphical representations of time stepping (Figure 56) for the Picard method shows that the uniform and nonuniform cases both achieved maximum step size $\Delta t_{max} = 100$ s for all the vertical layer discretizations. For NLKP=31, except at the beginning and ending time, the nonuniform case never achieved the maximum time step size 1000 s for 50 and 150 layers, whereas for the uniform distribution, the simulation completed with the maximum step size 1000 s except at the time near about $T_{max} = 2 \times 10^5$ s for 50 layers. For 150 layers, the uniform distribution is not able to achieve its maximum step size 1000 s in the period $T_{max} = 1.0 \times 10^5$ s to $T_{max} = 2.0 \times 10^5$ s. For NLKP=151, both uniform and nonuniform cases achieved maximum

step size 1000 s in the whole simulation for both the 50 and 150 layer cases.

For the Newton scheme (Figure 57), after $T_{max} = 2.122 \times 10^5 s$, the uniform and nonuniform cases for all the vertical layers with NLKP=31, was unable to achieve maximum step size $\Delta t_{max} = 100$ s for the whole simulation. The step size needed to be reduced to achieve convergence. But for the 1000 s case with NLKP=31 of 50 and 150 layers, the uniform case performs better. For NLKP=151, the time stepping behavior of the uniform and nonuniform cases is almost same.

In Figure 58 showing nonlinear iterations per time step of Picard, the nonuniform distribution faced trouble to get convergence for 50 and 150 layers with NLKP=31, whereas the uniform distribution needed only one iteration per time step for both time step sizes $\Delta t_{max} = 100$ s and $\Delta t_{max} = 1000$ s. For 50 and 150 layers with NLKP=151, both the uniform and nonuniform give almost the same behavior.

The Newton scheme (Figure 59) shows more or less the same behavior of nonlinear iterations per time step as we found in the Picard scheme. Also, we can say that in this case, for NLKP=31 the uniform distribution performs better but not for NLKP=151.

Figures 60 and 61 shows that for most of the runs the uniform case gives less total volumetric mass balance error ($MBE(m^3)$) for all vertical layers with NLKP=31 and 151 and for both the Picard and Newton schemes.

The comparison of the computational performance of the lookup table tests are summarised in Tables 41 and 42 for the Picard and Newton schemes respectively.

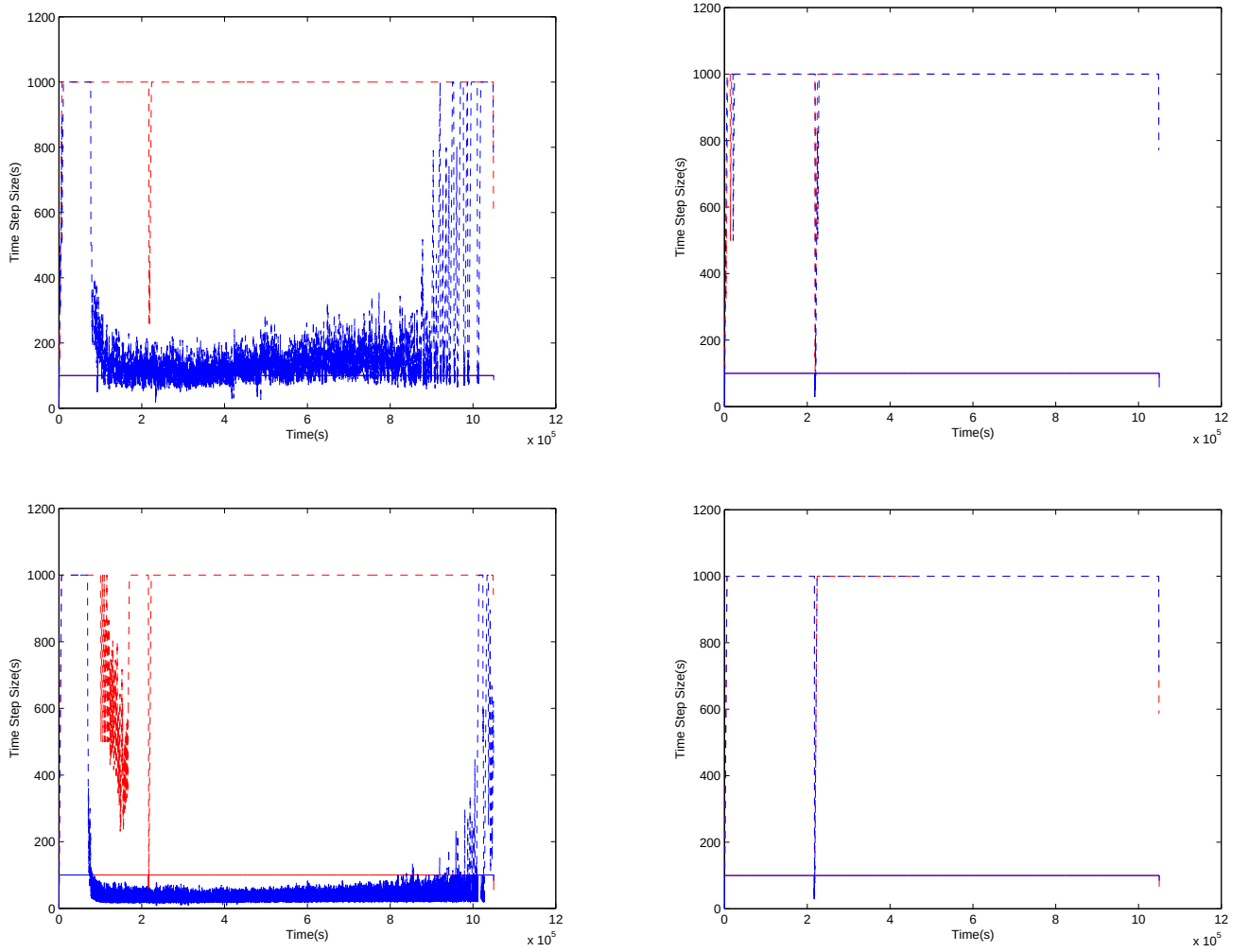


FIGURE 56. Comparison of time stepping behavior of Picard scheme for uniform (red color) and nonuniform (blue color) distribution of lookup points for 50 and 150 layers (the sequence of figures are 1st 2 for 50 layers of 31 and 151 points respectively and 2nd 2 for 150 layers of 31 and 151 points respectively).

The 8 performance indicators are discussed one by one for the Picard and Newton schemes as follows:

For the Picard scheme our findings are: For 50 layers, uniform distributions give better results with $\Delta t_{max} = 100$ s for both sets (31 and 151) of lookup points but for the $\Delta t_{max} = 1000$ s case, the nonuniform distribution gives good results on the basis of total volumetric mass balance error. For 150 layers with NLKP=31, for total volumetric mass balance the uniform distribution performs better than the nonuniform distribution. On the other hand, for 151 lookup points,

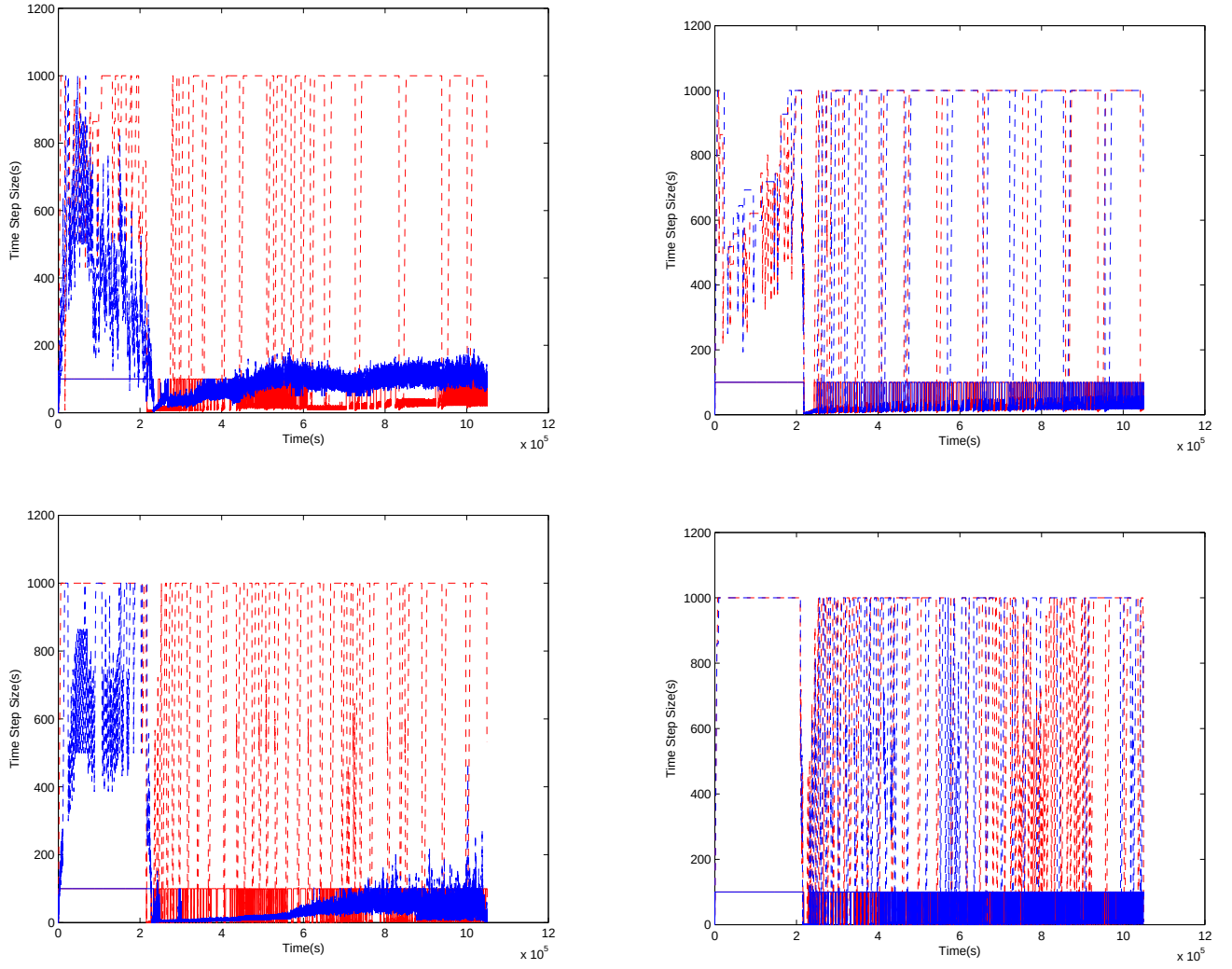


FIGURE 57. Comparison of time stepping behavior of Newton scheme for uniform (red color) and nonuniform (blue color) distribution of lookup points for 50 and 150 layers (the sequence of figures are 1st 2 for 50 layers of 31 and 151 points respectively and 2nd 2 for 150 layers of 31 and 151 points respectively).

nonuniform is preferable to uniform for both time step sizes. For 50 layers and NLKP=31, in terms of mass balance in percentage error, uniform performs better than nonuniform for the 100 s time step size but when $\Delta t_{max} = 1000$ s, the performance is reversed. Nonuniform performs better than uniform for both time step sizes with NLKP=151. For the 150 layers case, uniform distribution is the better strategy for all the investigated cases ($\Delta t_{max} = 100$ s and 1000 s and NLKP=31 and 151). For both the 50 and 150 layer cases, when $\Delta t_{max} = 100$ s is considered, the uniform distribution takes less time steps for every set of NLKP. For 150 layers with

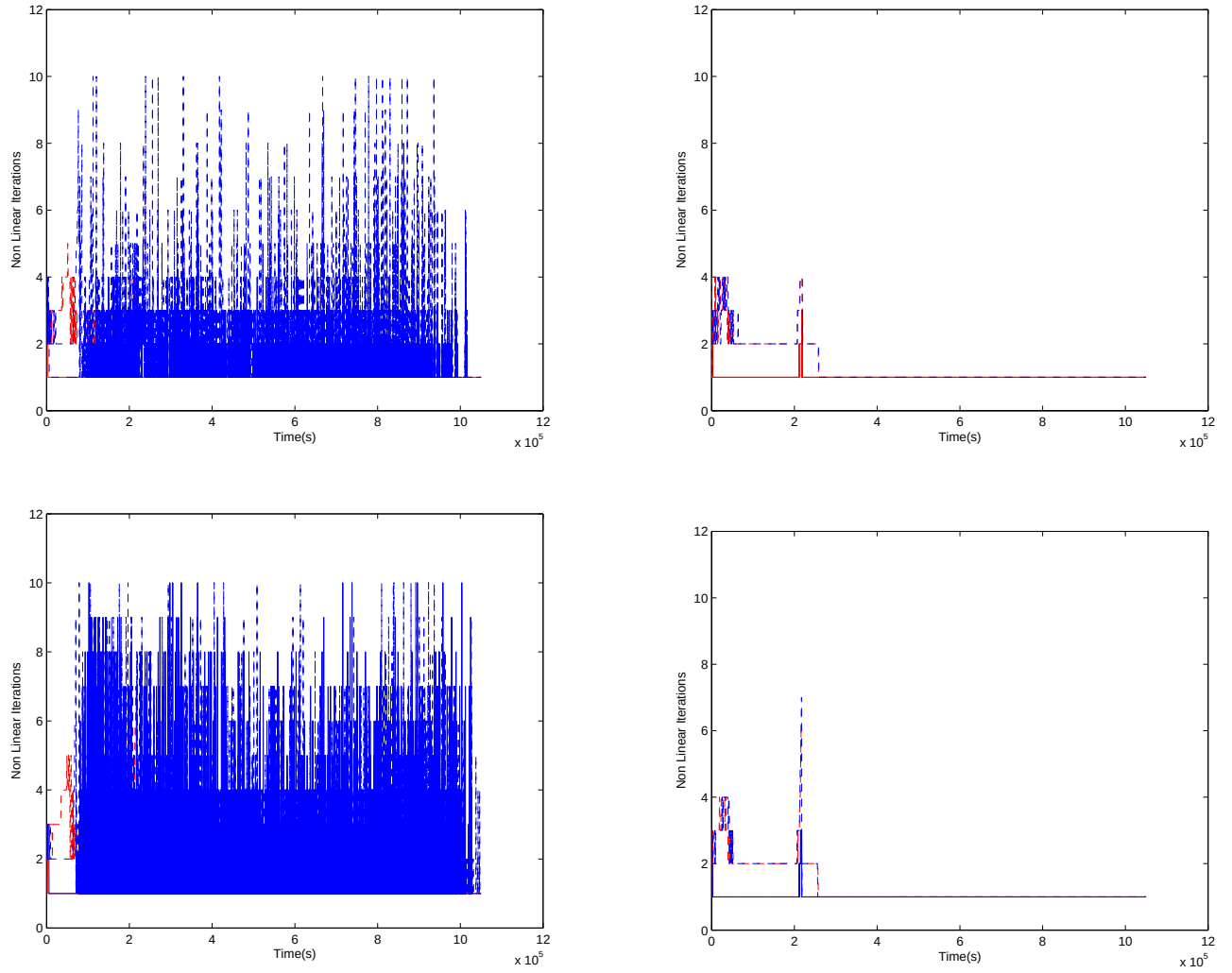


FIGURE 58. Comparison of convergence behavior of Picard scheme for uniform (red color) and nonuniform (blue color) distribution of lookup points for 50 and 150 layers (the sequence of figures are 1st 2 for 50 layers of 31 and 151 points respectively and 2nd 2 for 150 layers of 31 and 151 points respectively).

NLKP=31, uniform needs only 10558 time steps to complete the simulation whereas nonuniform look up distributions takes many more time steps (28699). For both layers discretizations with NLKP=151, uniform and nonuniform cases take a comparable number of time steps for the time step size $\Delta t_{max} = 1000$ s. But for the 31 lookup point case (with $\Delta t_{max} = 100$ s) uniform is much better than nonuniform. Uniform distribution is better at achieving the maximum time step size for $\Delta t_{max} = 100$ s for both vertical layers with 31 and 151 NLKP. For $\Delta t_{max} = 1000$ s and NLKP=151, nonuniform distribution case is better than uniform distribution. On the overall assessment of this case, the uniform distribution points need fewer iterations to achieve

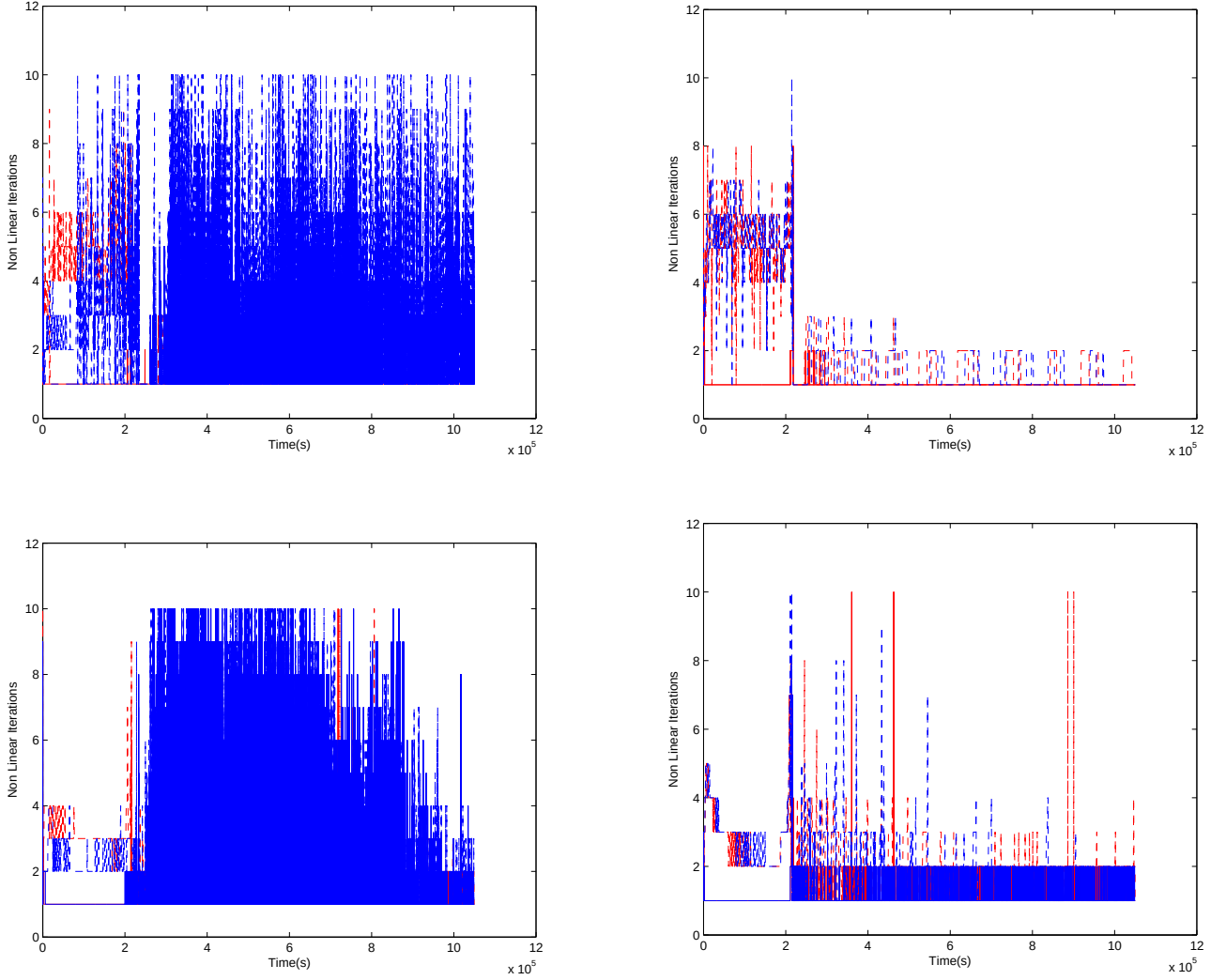


FIGURE 59. Comparison of convergence behavior of Newton scheme for uniform (red color) and nonuniform (blue color) distribution of lookup points for 50 and 150 layers (the sequence of figures are 1st 2 for 50 layers of 31 and 151 points respectively and 2nd 2 for 150 layers of 31 and 151 points respectively).

convergence for all the cases. The results show that the uniform distribution case needs less linear iterations per non linear iteration to satisfy the termination criteria except for the case NLKP=151 with $\Delta t_{max} = 1000$ s of 150 layers. For 150 layers with NLKP=31, very little back stepping (only 17) occurs in the case of uniform distribution but for the nonuniform case this happened 6969 times. On the basis of back stepping, uniform distributions are preferable.

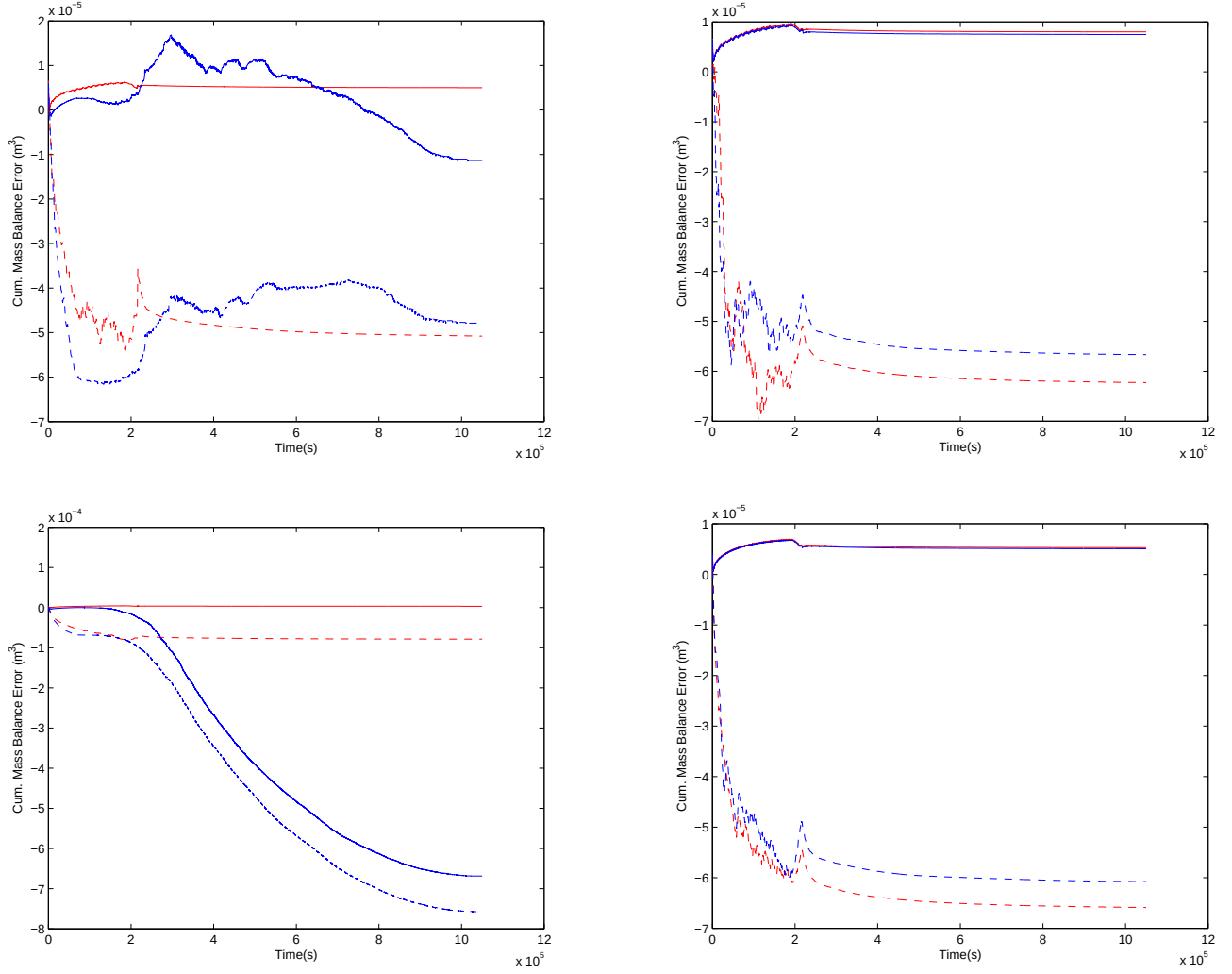


FIGURE 60. Comparison of cumulative mass balance behavior of Picard scheme for uniform (red color) and nonuniform (blue color) distribution of lookup points for 50 and 150 layers (the sequence of figures are 1st 2 for 50 layers of 31 and 151 points respectively and 2nd 2 for 150 layers of 31 and 151 points respectively).

For the Newton scheme our findings are: For the $\Delta t_{max} = 100$ s case, at 50 layers the nonuniform distribution gives better results than uniform distribution for NLKP=31 for both cumulative mass balance error in m^3 and in percent, but completely opposite results are found for NLKP=151. Uniform distributions of 150 layers clearly show better performance for both NLKP with $\Delta t_{max} = 100$ s. For the $\Delta t_{max} = 1000$ s case, it is the nonuniform distributions that performs better. For the NLKP=151 case, uniform is better than non uniform for both vertical layer discretizations but for NLKP=31, nonuniform takes fewer time steps than uniform distribution for $\Delta t_{max} = 100$ s. Except for NLKP=31 of 50 layers for $\Delta t_{max} = 1000$ s case, uniform

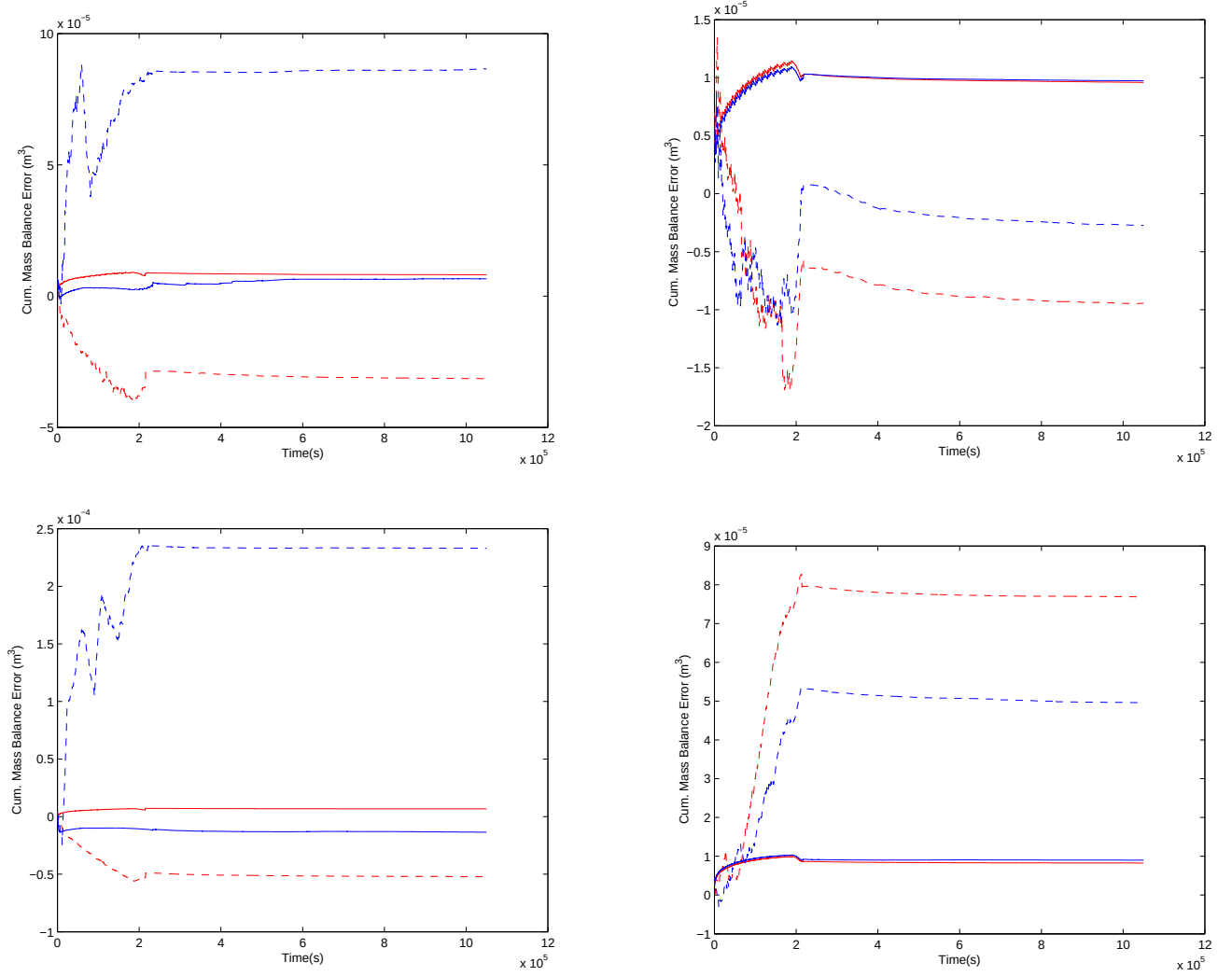


FIGURE 61. Comparison of cumulative mass balance behavior of Newton scheme for uniform (red color) and nonuniform (blue color) distribution of look up points for 50 and 150 layers (the sequence of figures are 1st 2 for 50 layers of 31 and 151 points respectively and 2nd 2 for 150 layers of 31 and 151 points respectively).

needs fewer time steps than nonuniform. The uniform distribution with 151 points and with 50 and 150 layers achieved bigger average time step sizes for $\Delta t_{max} = 100$ s and $\Delta t_{max} = 1000$ s but for 31 points nonuniform achieves a larger average time step size. For all the cases, uniform distributions take fewer nonlinear iterations per time step to achieve convergence. For the 50 layer case, nonuniform needs fewer linear iterations per non linear iteration to satisfy the termination criteria for all the cases. For the 150 layers case, uniform distribution leads to superior performance except the NLKP=151 with $\Delta t_{max} = 100$ s. For 50 layers, uniform

TABLE 41. Test Problem 2, Picard scheme: comparison of computational performance of lookup points (31 and 151) for uniform and nonuniform case, 50 and 150 layers, and $\Delta t_{max} = 100$ s and 1000 s.

–	–	$\Delta t(s) \rightarrow$	100	100	1000	1000
–	Layers	NLKP	Uni	Non	Uni	Non
MBE(m^3)	50	31	5.01e-6	-1.13e-5	-5.08e-5	-4.79e-5
	50	151	8.03e-6	7.51e-5	-6.23e-5	-5.67e-5
	150	31	3.34e-6	-6.69e-4	-7.86e-5	-7.58e-4
	150	151	5.28e-6	5.06e-6	6.59e-5	-6.08e-5
MBE(perc.)	50	31	-3.98e-2	8.93e-2	4.01e-1	3.77e-1
	50	151	-6.56e-2	-6.04e-2	4.99e-1	4.53e-1
	150	31	-1.28e-2	5.01e0	-2.65e-2	5.64e0
	150	151	-1.38e-2	-4.07e-2	-4.26e-2	4.87e-1
No. of Time Steps	50	31	10567	10583	1135	7025
	50	151	10566	10584	1146	1145
	150	31	10558	28699	1201	27745
	150	151	10562	10573	1147	1139
Avg. $\Delta t(s)$	50	31	9.937e+1	8.71e+1	9.251e+2	1.495e+2
	50	151	9.938e+1	8.956e+1	8.982e+2	9.170e+2
	150	31	9.945e+1	3.659e+1	8.743e+2	3.784e+2
	150	151	9.941e+1	9.931e+1	9.154e+2	9.219e+2
NL Iter/ Time Step	50	31	1.03	1.49	1.67	4.30
	50	151	1.04	1.04	1.62	1.62
	150	31	1.03	4.00	1.97	4.13
	150	151	1.03	1.03	1.61	1.60
Lin Iter/ NL Iter	50	31	7.73	6.86	10.23	5.51
	50	151	7.77	7.76	10.28	10.18
	150	31	7.55	3.97	9.80	3.95
	150	151	7.60	7.57	9.93	9.99
No. of Back Steps	50	31	19	27	25	1702
	50	151	20	25	29	29
	150	31	17	6969	59	7066
	150	151	19	22	28	26
Solver Failures	50	31	0	0	0	0
	50	151	0	0	0	0
	150	31	0	0	0	0
	150	151	0	0	0	0

distribution of lookup points does more back stepping than nonuniform case for NLKP=31 but when NLKP=151 it does less back stepping for both step sizes. For 150 layers with NLKP=151, uniform distribution does less back stepping than nonuniform but with 31 points the opposite occurs. The solver fails less for all the cases of uniform distributions with 150 layers but with 50 layers the opposite occurs.

The RMSE behavior for the lookup tests under Picard and Newton iteration are shown in Figures 62 and 63 for the case $\Delta t_{max} = 100$ s and in Figures 64 and 65 in a comparison of the $\Delta t_{max} = 100$ s and 1000 s cases, and the results are summarized in Tables 43 and 44. The RMSE are evaluated using the CATHY generated reference solution (301 nodes in the vertical

TABLE 42. Test Problem 2, Newton scheme: comparison of computational performance of lookup points (31 and 151) for uniform and nonuniform case, 50 and 150 layers and $\Delta t_{max} = 100$ s and 1000 s.

–	–	$\Delta t(s) \rightarrow$	100	100	1000	1000
–	Layers	NLKP	Uni	Non	Uni	Non
MBE(m^3)	50	31	8.15e-6	6.60e-6	-3.14e-5	8.65e-5
	50	151	9.59e-6	9.73e-6	-9.45e-6	-2.73e-6
	150	31	6.71e-6	-1.35e-5	-5.21e-5	2.33e-4
	150	151	8.26e-6	9.00e-6	7.69e-5	4.96e-5
MBE(perc.)	50	31	6.47e-2	-5.21e-2	2.49e-1	-6.88e-1
	50	151	-7.72e-2	-7.84e-2	7.60e-2	2.20e-2
	150	31	-5.33e-2	1.07e-1	4.12e-1	-1.87e0
	150	151	-6.65e-2	-7.25e-2	-6.24e-1	-4.01e-1
No. of Time Steps	50	31	35081	14074	14534	12057
	50	151	29024	29993	11137	11724
	150	31	85175	61544	53079	60754
	150	151	79014	84283	43602	49883
Avg. $\Delta t(s)$	50	31	2.993e+1	7.461e+1	7.224e+1	8.710e+1
	50	151	3.618e+1	3.508e+1	9.428e+1	8.956e+1
	150	31	1.233e+1	1.706e+1	1.978e+1	1.728e+1
	150	151	1.329e+1	1.246e+1	2.408e+1	2.105e+1
NL Iter/ Time Step	50	31	3.24	2.98	3.56	4.29
	50	151	3.05	3.08	3.55	3.55
	150	31	3.39	3.82	3.62	3.97
	150	151	3.38	3.39	3.62	3.62
Lin Iter/ NL Iter	50	31	24.57	17.74	22.86	21.81
	50	151	24.46	22.20	23.62	19.57
	150	31	15.52	32.90	13.45	34.40
	150	151	15.18	14.15	11.43	12.21
No. of Back Steps	50	31	7898	1290	3604	2518
	50	151	5972	6226	2682	2837
	150	31	20245	13863	13753	14319
	150	151	18698	20093	11287	12916
Solver Failures	50	31	209	62	155	91
	50	151	191	145	146	86
	150	31	85	1594	90	1883
	150	151	113	134	127	131

soil column, 301 lookup points, $\Delta t_{max} = 1$ s, and specified nonlinear tolerance 10^{-3}). The results from these figures show that the uniform distribution of lookup points outperforms the nonuniform distribution in all cases.

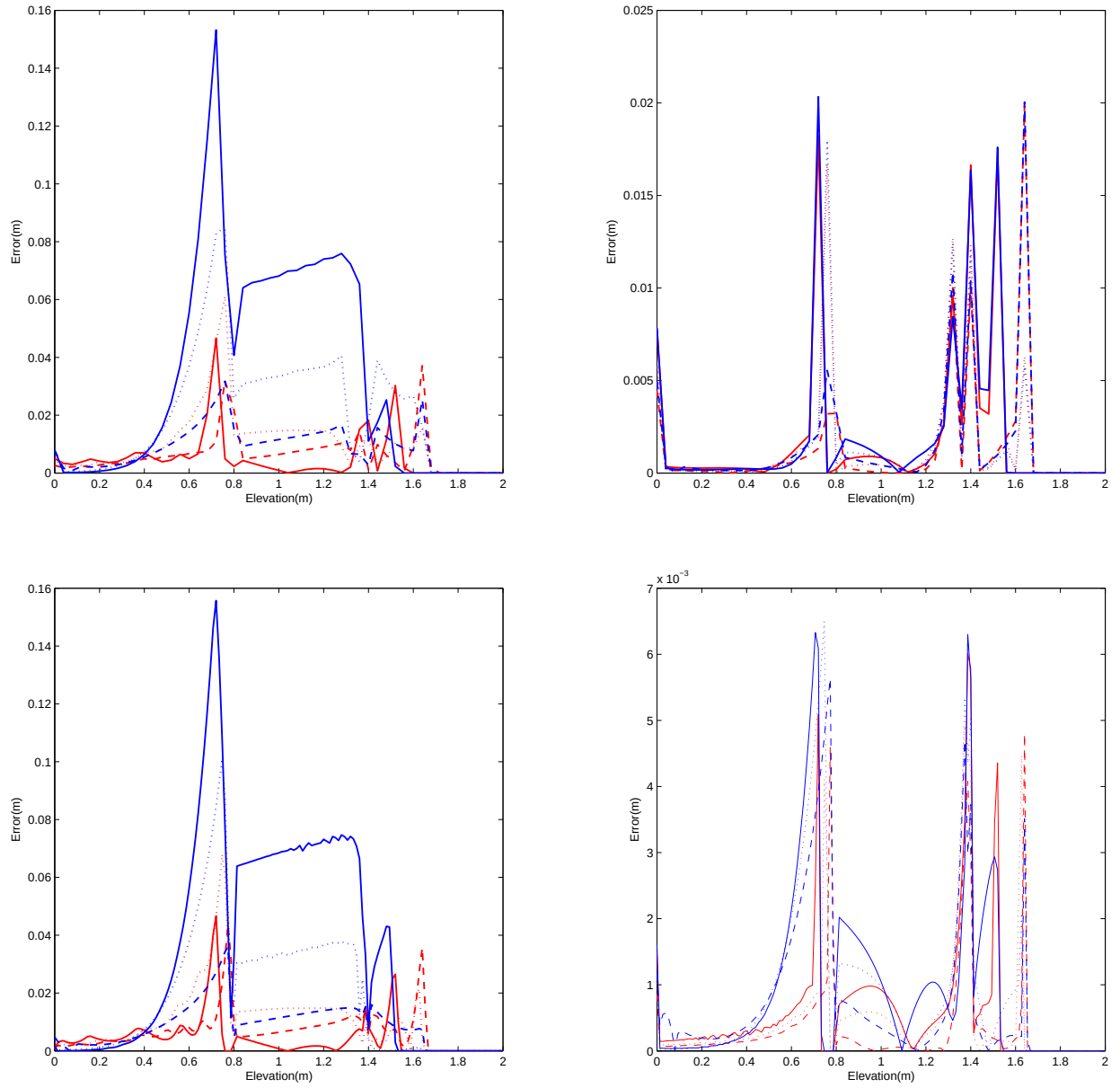


FIGURE 62. Comparison of RMSE behavior of Picard scheme for uniform (red color) and nonuniform (blue color) distribution of lookup points for 50 and 150 layers (the sequence of figures are 1st 2 for 50 layers of 31 and 151 points respectively and 2nd 2 for 150 layers of 31 and 151 points respectively; the solid, dotted, and dashed lines are the errors at 250000 s, 550000 s, and 1050000 s respectively) and $\Delta t_{max} = 100$ s case of Test Problem 2.

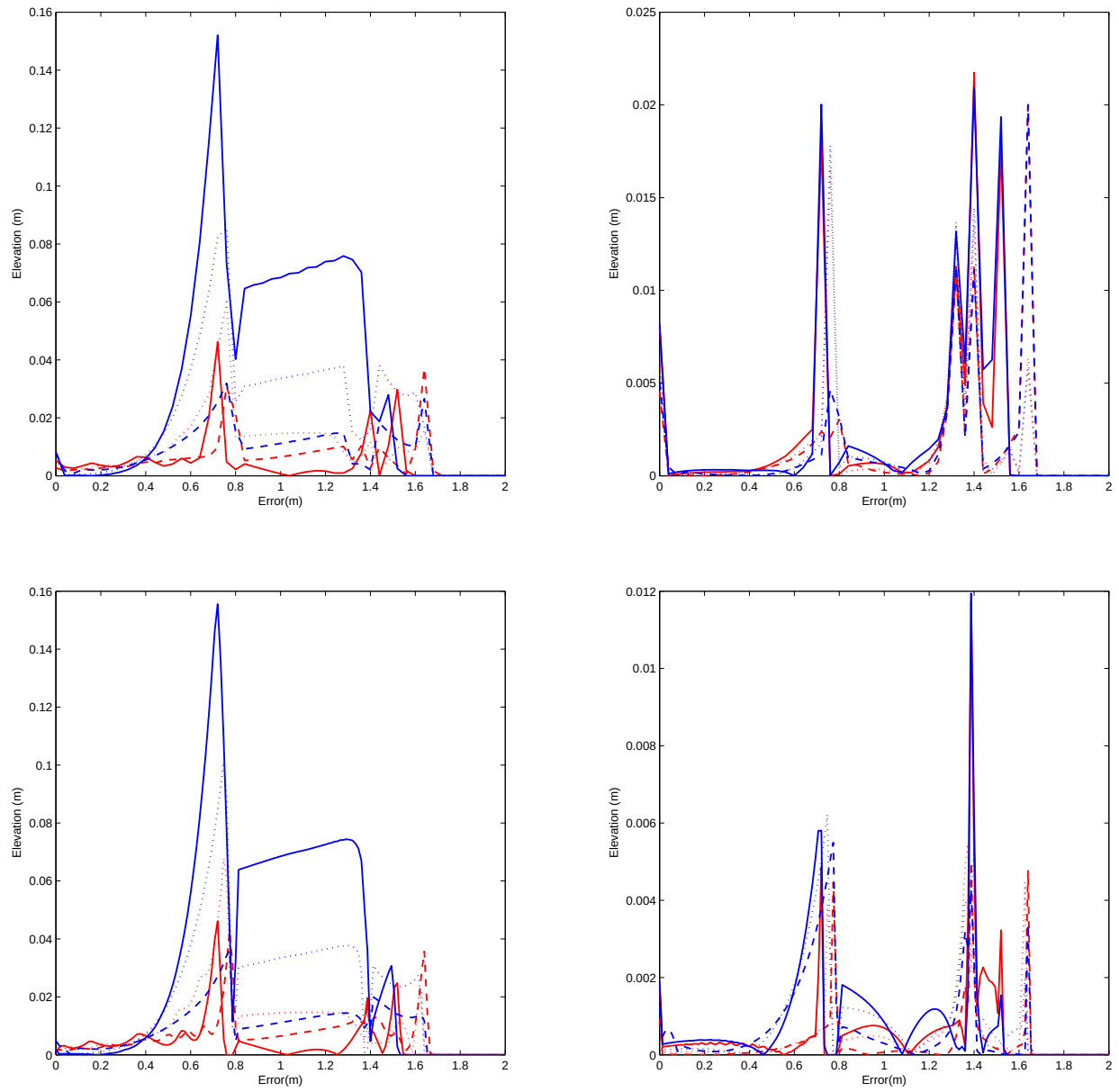


FIGURE 63. Comparison of RMSE behavior of Newton scheme for uniform (red color) and nonuniform (blue color) distribution of lookup points for 50 and 150 layers (the sequence of figures are 1st 2 for 50 layers of 31 and 151 points respectively and 2nd 2 for 150 layers of 31 and 151 points respectively; the solid, dotted, and dashed lines are the errors at 250000 s, 550000 s, and 1050000 s respectively) and $\Delta t_{max} = 100$ s case of Test Problem 2.

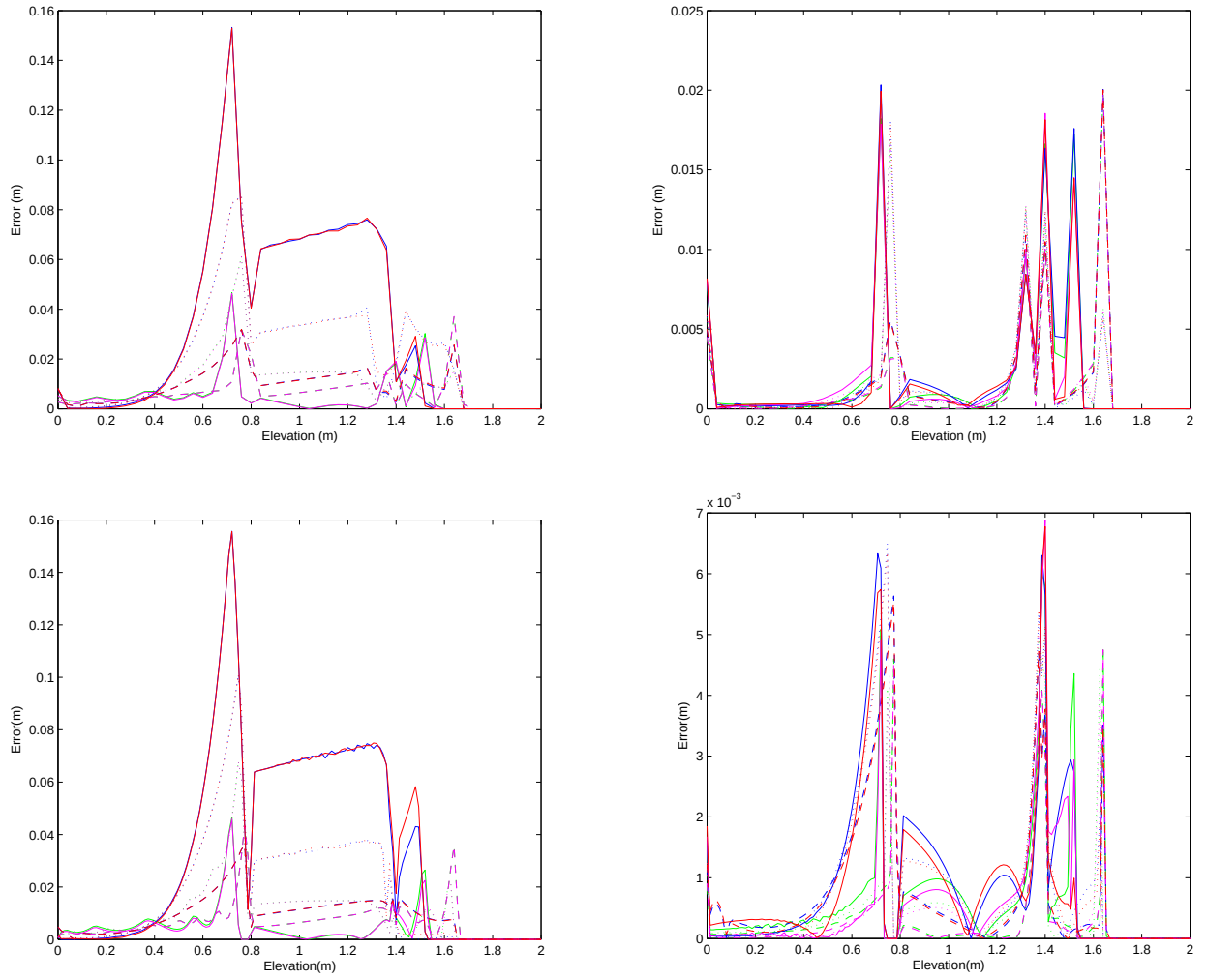


FIGURE 64. Comparison of RMSE behavior of Picard scheme for uniform and nonuniform distribution of lookup points for 50 and 150 layers (the sequence of figures are 1st 2 for 50 layers of 31 and 151 points respectively and 2nd 2 for 150 layers of 31 and 151 points respectively) for $\Delta t_{max} = 100$ s and 1000 s cases of Test Problem 2. Green and magenta for uniform and blue and red for nonuniform distribution. Also, solid, dotted, and dashed lines are the errors at 250000 s, 550000 s, and 1050000 s respectively.

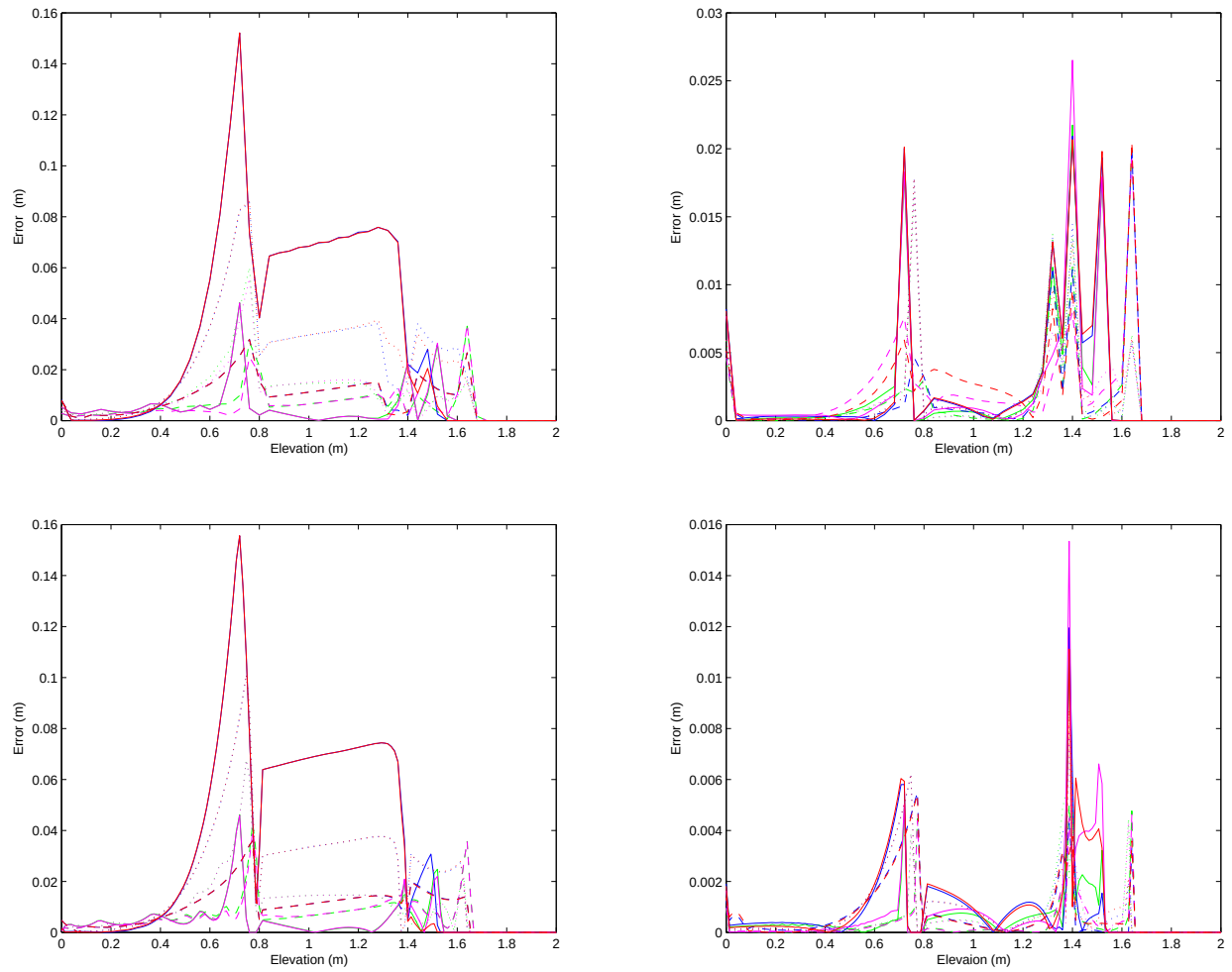


FIGURE 65. Comparison of RMSE behavior of Newton scheme for uniform and nonuniform distribution of lookup points for 50 and 150 layers (the sequence of figures are 1st 2 for 50 layers of 31 and 151 points respectively and 2nd 2 for 150 layers of 31 and 151 points respectively) for $\Delta t_{max} = 100$ s and 1000 s cases of Test Problem 2. Green and magenta for uniform and blue and red for nonuniform distribution. Also, solid, dotted, and dashed lines are the errors at 250000 s, 550000 s, and 1050000 s respectively.

TABLE 43. RMSE of CATHY model (uniform and nonuniform NLKP): Picard scheme for 50 and 150 layers with 31 and 151 NLKP and time step sizes $\Delta t_{max} = 100$ s and $\Delta t_{max} = 1000$ s for Test Problem 2.

—	—	$\Delta t_{max}(s)$	100	100	1000	1000
Layers	NLKP	Time	Uni	Non	Uni	Non
50	-	250000	9.60e-3	4.96e-2	9.40e-3	4.95e-2
	31	550000	1.50e-2	2.94e-2	1.49e-2	2.93e-2
	-	1050000	9.60e-3	1.14e-2	9.40e-3	1.15e-2
50	-	250000	4.70e-3	4.90e-2	4.60e-3	4.70e-2
	151	550000	3.70e-3	3.80e-2	3.70e-3	3.80e-2
	-	1050000	3.60e-3	3.80e-2	3.60e-3	3.80e-2
150	-	250000	8.10e-3	5.02e-2	7.70e-3	5.08e-2
	31	550000	1.50e-2	2.84e-2	1.50e-2	2.84e-2
	-	1050000	9.30e-3	1.14e-2	9.30e-3	1.13e-2
150	-	250000	1.10e-3	1.60e-2	1.10e-3	2.70e-2
	151	550000	1.00e-3	1.60e-2	9.83e-4	2.20e-2
	-	1050000	8.21e-4	1.40e-2	8.08e-4	2.20e-2

TABLE 44. RMSE of CATHY model (uniform and nonuniform NLKP): Newton scheme for 50 and 150 layers with 31 and 151 NLKP and time step sizes $\Delta t_{max} = 100$ s and $\Delta t_{max} = 1000$ s for Test Problem 2.

—	—	$\Delta t_{max}(s)$	100	100	1000	1000
Layers	NLKP	Time	Uni	Non	Uni	Non
50	-	250000	9.43e-3	4.97e-2	9.45e-3	4.96e-2
	31	550000	1.46e-2	2.94e-2	1.38e-2	2.95e-2
	-	1050000	9.17e-3	1.15e-2	8.63e-3	1.15e-2
50	-	250000	5.21e-3	5.59e-3	5.46e-3	5.63e-3
	151	550000	3.89e-3	4.01e-3	3.26e-3	3.75e-3
	-	1050000	3.76e-3	3.81e-3	3.71e-3	3.90e-3
150	-	250000	8.04e-3	5.00e-2	7.89e-3	4.96e-2
	31	550000	1.49e-2	2.97e-2	1.50e-2	2.97e-2
	-	1050000	9.24e-3	1.19e-2	9.03e-3	1.19e-2
150	-	250000	1.32e-3	1.64e-3	1.83e-3	1.88e-3
	151	550000	1.04e-3	1.48e-3	9.54e-4	1.56e-3
	-	1050000	7.72e-4	1.29e-3	7.82e-4	1.28e-3

4.3.2. *Test Problem 3.*

To further investigate the behavior of lookup table points to solve Richards' equation, we considered two vertical discretizations of 60 and 120 layers with three different time step sizes $\Delta t_{max} = 10$ s, 800 s, and 1600 s and two set of lookup points (31 and 151) in the soil retention curves. The lookup points are concentrated in the sharp region of the moisture curves for the nonuniform distribution case. There are 24 runs in total for each of the iteration schemes (Picard and Newton).

The van Genuchten soil moisture curves for the uniform and nonuniform distribution of lookup points are presented in Figures 66 and 67.

The time stepping, nonlinear convergence, and cumulative mass balance error behavior of uniform and nonuniform NLKP are presented in Figures 68, 70, and 72 respectively for the Picard scheme and in Figures 69, 71, and 73 respectively for the Newton scheme.

From the Picard time stepping graph (Figure 68) the uniform distribution takes bigger time steps for all the vertical layers with both NLKP 31 and 151 for $\Delta t_{max} = 800$ s and 1600 s up to time=40000 s, after which there is no large difference between the behavior of uniform and nonuniform distributions. For $\Delta t_{max} = 10$ s, both uniform and non uniform cases run at the maximum step size.

For the Newton's case (Figure 69), after time=40000 s, nonuniform performs better for all the cases with $\Delta t_{max} = 1600$ s. Before this time, uniform and nonuniform behave comparably for all cases.

For the nonlinear iterations, Picard case, Figure 70 shows that nonuniform needs fewer nonlinear iterations per time step than uniform distribution for all the vertical layers with step sizes 800 s and 1600 s for each NLKP. But for the $\Delta t_{max} = 10$ s case, uniform performs better. On

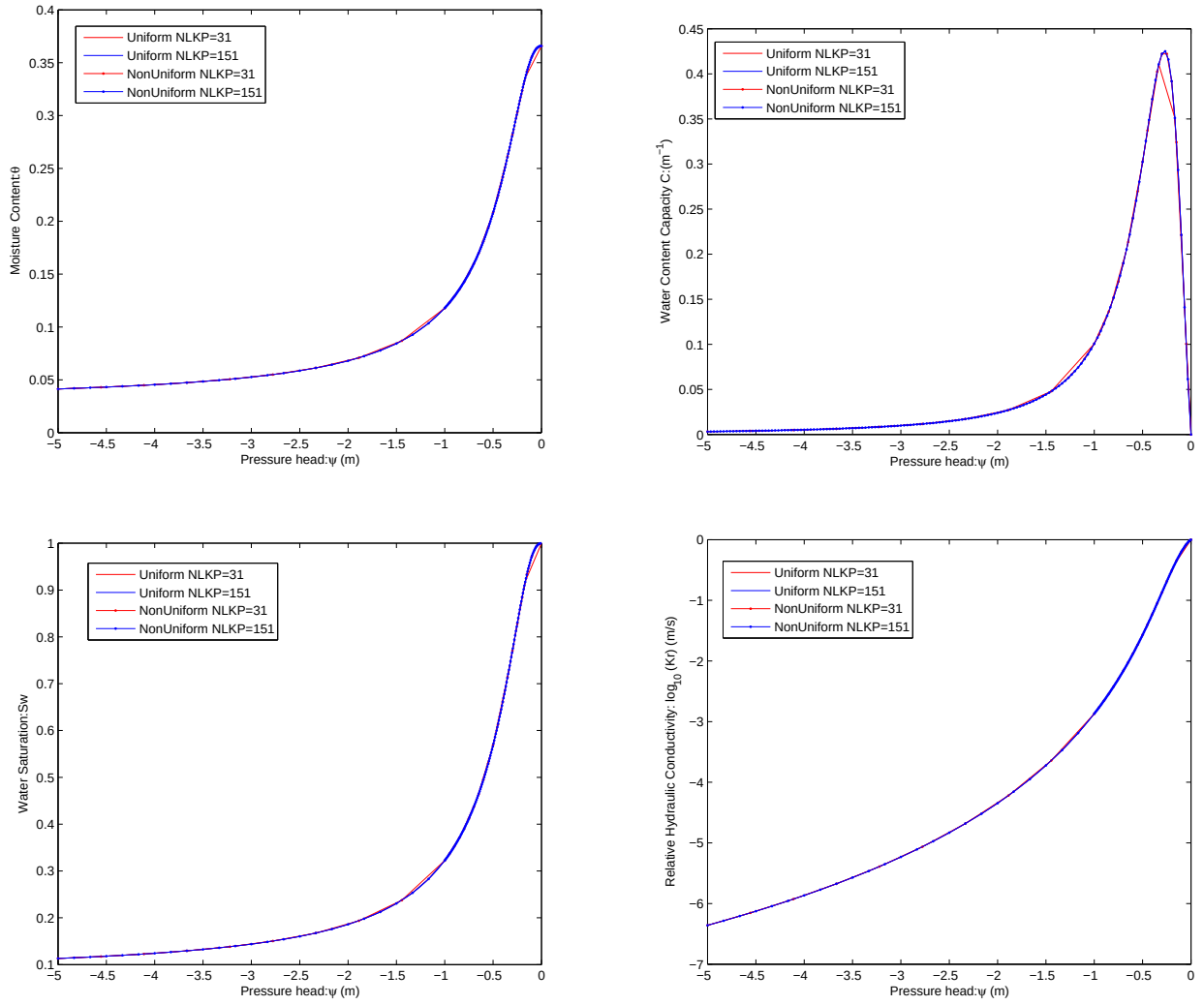


FIGURE 66. Sandy layer moisture curves for the uniform and nonuniform lookup table point cases.

the other hand, the results for the Newton case (Figure 71) are the reverse.

The cumulative mass balance error graphs for Picard (Figure 72) and Newton (Figure 73) show that Picard performs better with uniformly distributed lookup points while Newton does better in the nonuniform case.

The comparison of computational statistics of lookup table points for CATHY are summarized in Tables 45 and 46 for Picard and Newton schemes respectively.

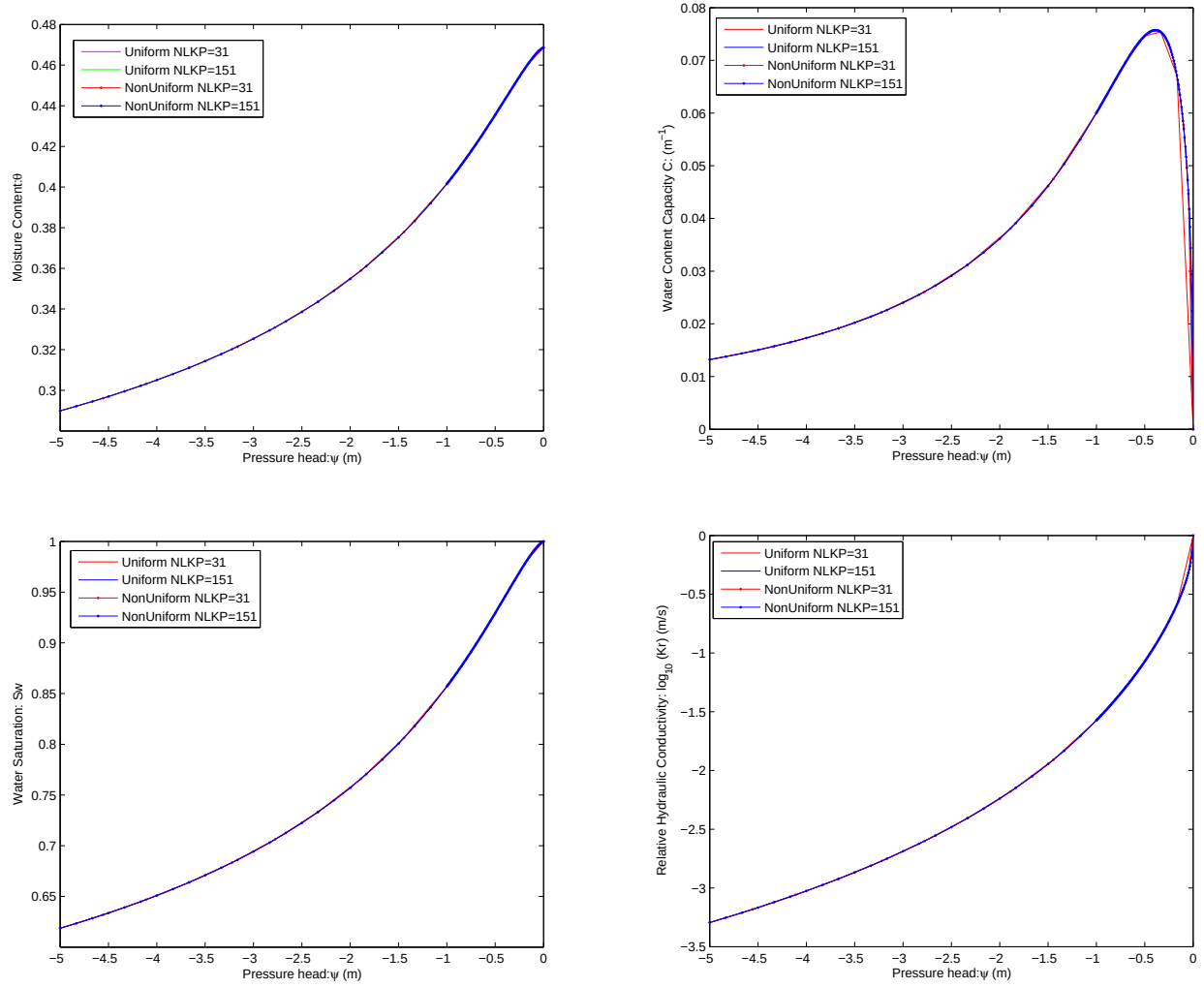


FIGURE 67. Clay layer moisture curves for the uniform and nonuniform lookup table points cases.

The 8 performance indicators are discussed one by one for the Picard and Newton schemes as follows:

For Picard the following observations can be made: Both sets of nonuniform distributions of lookup points in the retention curves gives smaller volumetric mass balance than the uniform case for all layer and Δt_{max} cases. On the basis of percentage mass balance error, the nonuniform case again performs better. For all NLKP and step sizes, uniform distribution needs fewer time steps than nonuniform case to complete the simulation. On the basis of average time step size per time step, for all cases uniform distribution achieves a larger value than nonuniform

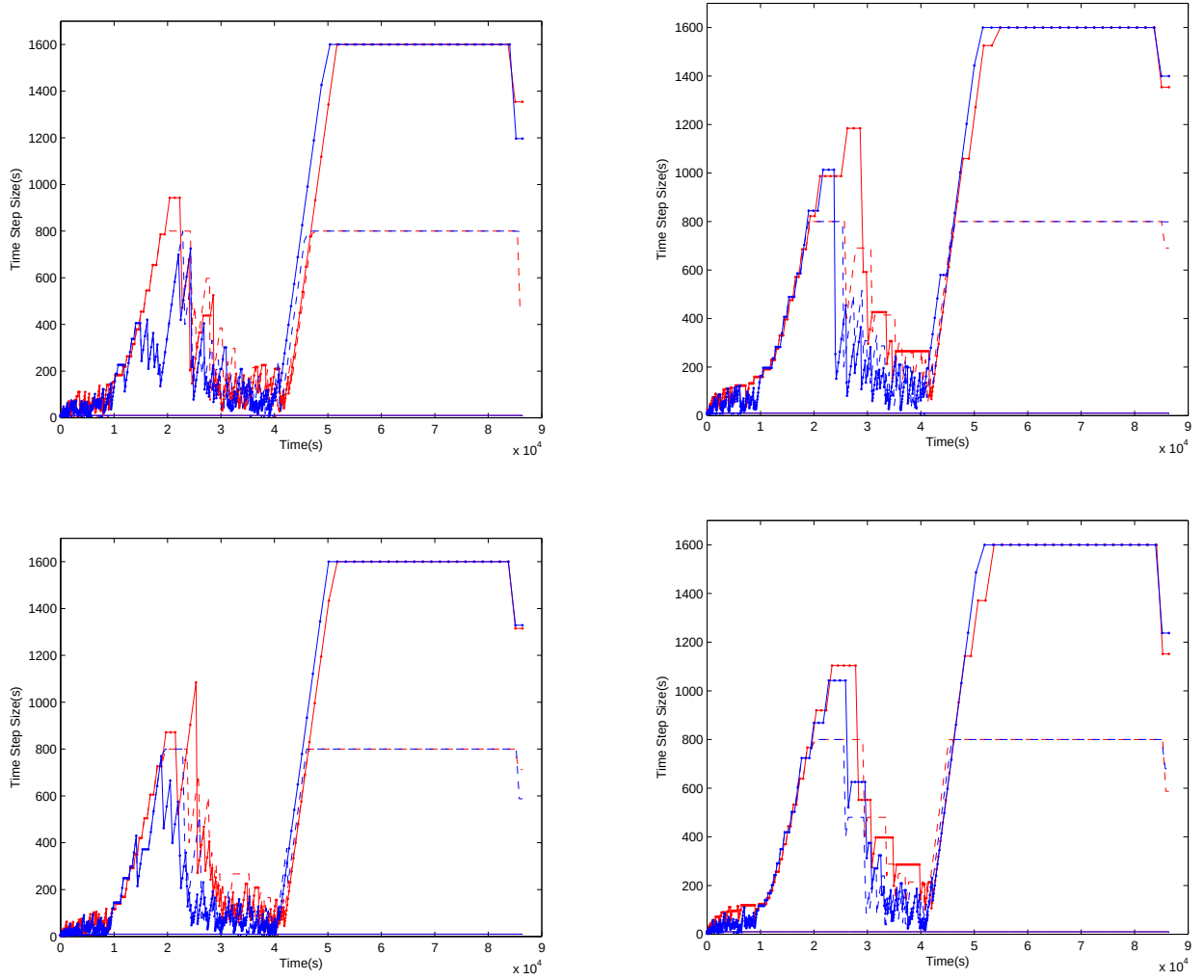


FIGURE 68. Comparison of time stepping behavior of Picard scheme for uniform (red color) and nonuniform (blue color) distribution of lookup points for 60 and 120 layers (the sequence of figures are 1st two for 60 layers of 31 and 151 points respectively and 2nd two for 120 layers of 31 and 151 points respectively). $\Delta t_{max} = 10\text{s}$, 800 s , and 1600 s are marked by solid, dashed, and dot-dashed lines respectively.

case. Except for the time step size 1600 s case, nonuniform distribution needs fewer nonlinear iterations per time step to converge and fewer linear iterations per nonlinear iteration except for the case $\Delta t_{max} = 1600\text{ s}$. For each of the cases of NLKP with all the time step sizes, back stepping occurs less for the uniform case than the nonuniform case.

For the Newton scheme, our findings are: Uniform distribution of lookup points gives smaller values of volumetric mass balance errors than nonuniform case for $\Delta t_{max} = 800\text{ s}$ and 1600

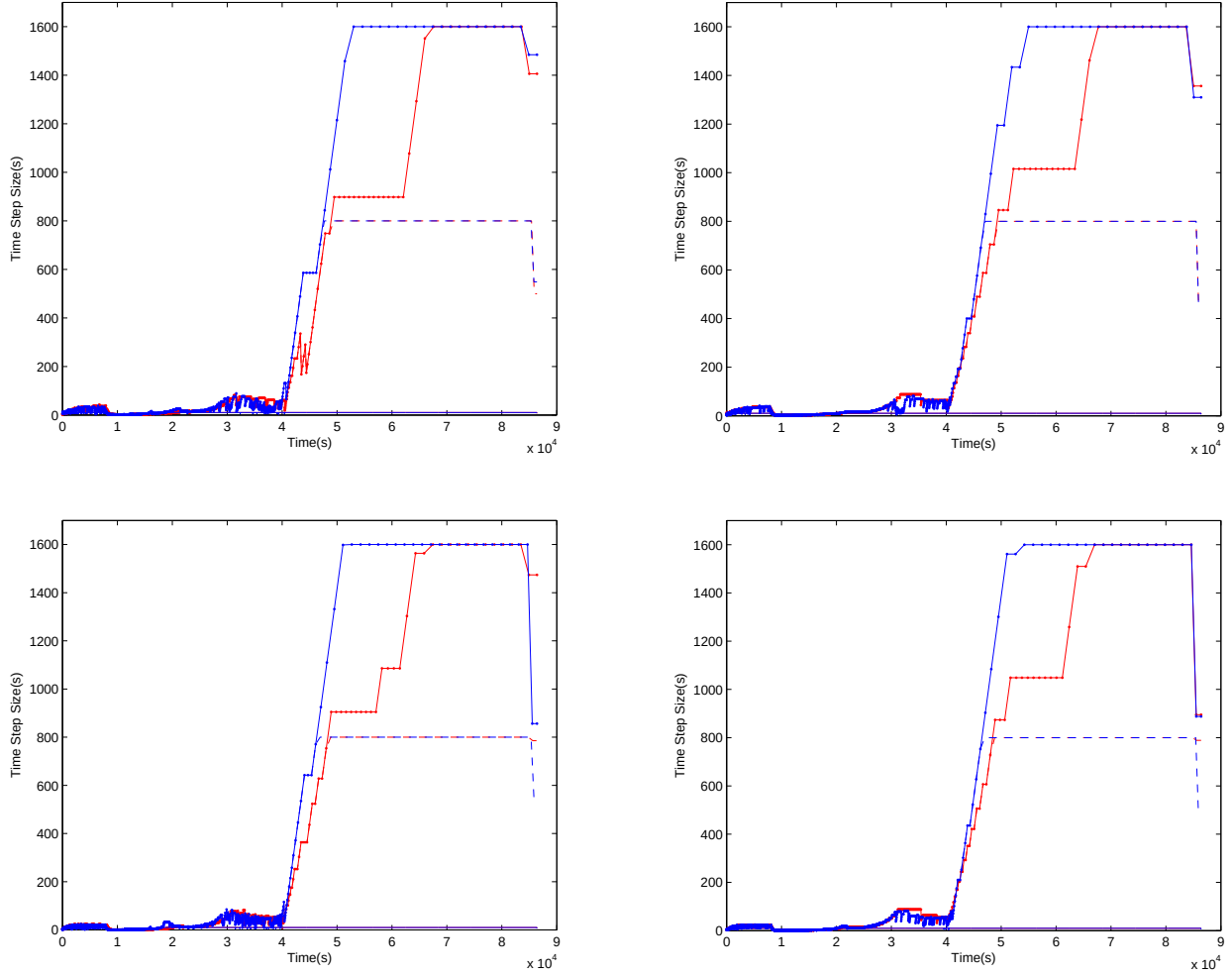


FIGURE 69. Comparison of time stepping behavior of Newton scheme for uniform (red color) and nonuniform (blue color) distribution of lookup points for 60 and 120 layers (the sequence of figures are 1st two for 60 layers of 31 and 151 points respectively and 2nd two for 120 layers of 31 and 151 points respectively). $\Delta t_{max} = 10$ s, 800 s, and 1600 s are marked by solid, dashed, and dot-dashed lines respectively.

s and for both settings of NLKP and vertical layers discretizations. On the other hand, for $\Delta t_{max} = 10$ s, uniform and nonuniform give very close values. For the percentage error of volumetric mass balance, the same behavior is found for uniform and nonuniform cases as we saw for total volumetric mass balance error. For all the cases the uniform distribution needs many more time steps to complete the simulation, except for the NLKP=151 with time step size $\Delta t_{max} = 800$ s and 1600 s cases of 120 layer, for which uniform distribution takes fewer steps than nonuniform. For NLKP=31 of 60 layers, the average time step for uniform distributions is bigger than nonuniform in the case of $\Delta t_{max} = 10$ s and 800 s but for the 1600 s case nonuniform

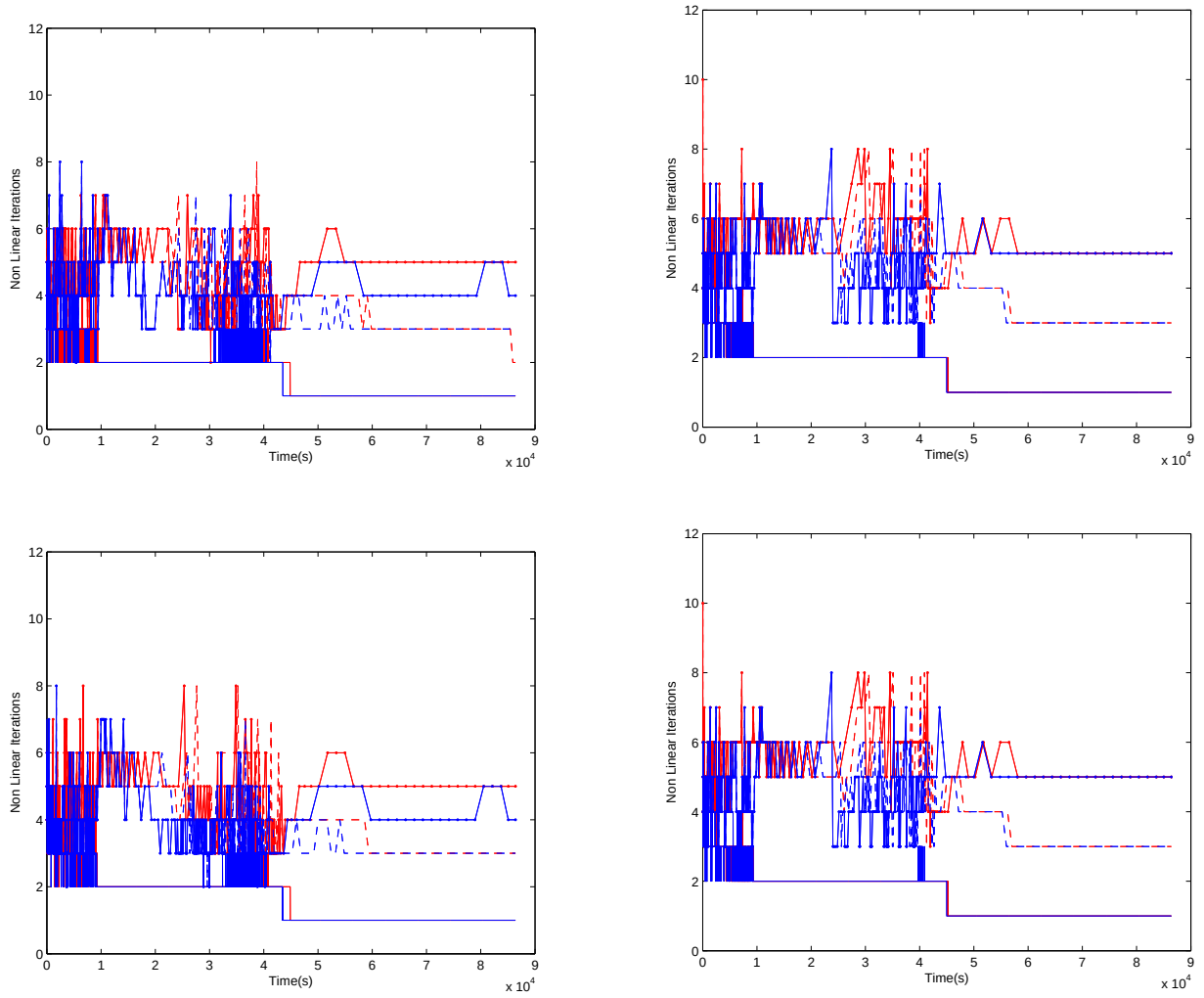


FIGURE 70. Comparison of convergence behavior of Picard scheme for uniform (red color) nonuniform (blue color) distribution of lookup points for 60 and 120 layers (the sequence of figures are 1st two for 60 layers of 31 and 151 points respectively and 2nd two for 120 layers of 31 and 151 points respectively). $\Delta t_{max} = 10$ s, 800 s, and 1600 s are marked by solid, dashed, and dot-dashed respectively.

is bigger. For NLKP=31 of 120 layers, nonuniform takes bigger step size for $\Delta t_{max} = 10$ s and 800 s cases but not for 1600 s case. For 151 points of 120 layers, $\Delta t_{max} = 800$ s and 1600 s cases, uniform distributions perform better but not for $\Delta t_{max} = 10$ s case. For the 60 layers case nonuniform takes fewer nonlinear iterations per time step except for the $\Delta t_{max} = 1600$ s case. For $\Delta t_{max} = 10$ s with NLKP=151 of 120 layers, uniform and nonuniform take very close number of nonlinear iterations (4.06 and 4.07 respectively). Fewer back steps occur for all the cases of uniform distributions compared to non uniform distributions of lookup points. There

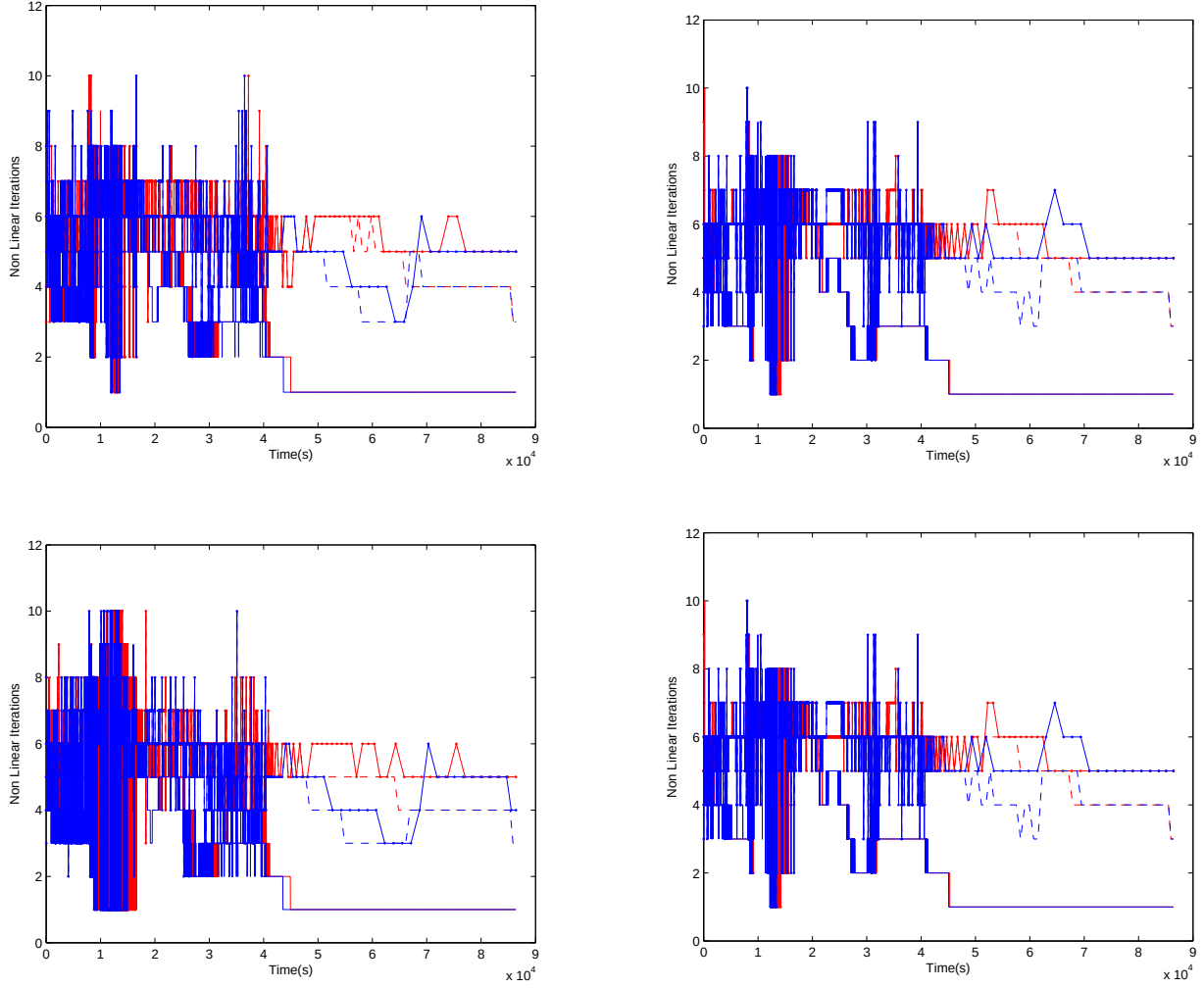


FIGURE 71. Comparison of convergence behavior of Newton scheme for uniform (red color) nonuniform (blue color) distribution of lookup points for 60 and 120 layers (the sequence of figures are 1st two for 60 layers of 31 and 151 points respectively and 2nd two for 120 layers of 31 and 151 points respectively). $\Delta t_{max} = 10$ s, 800 s, and 1600 s are marked by solid, dashed, and dot-dashed lines respectively.

is little difference between uniform and nonuniform distributions in terms of linear solver failures.

The RMSE behavior for uniform and nonuniform distribution of lookup point shown in Figure 74 for the Picard (top 2) and Newton (bottom 2) schemes. The CATHY-generated base solution used 240 vertical layers, NLKP=301, time step size is 1 s, tolerance is 10^{-3} . The comparison of calculated RMSE at three different times (32000 s, 56000 s, and 86400 s) for uniform and nonuniform lookup point distributions is presented in Tables 47 and 48. For all vertical layer

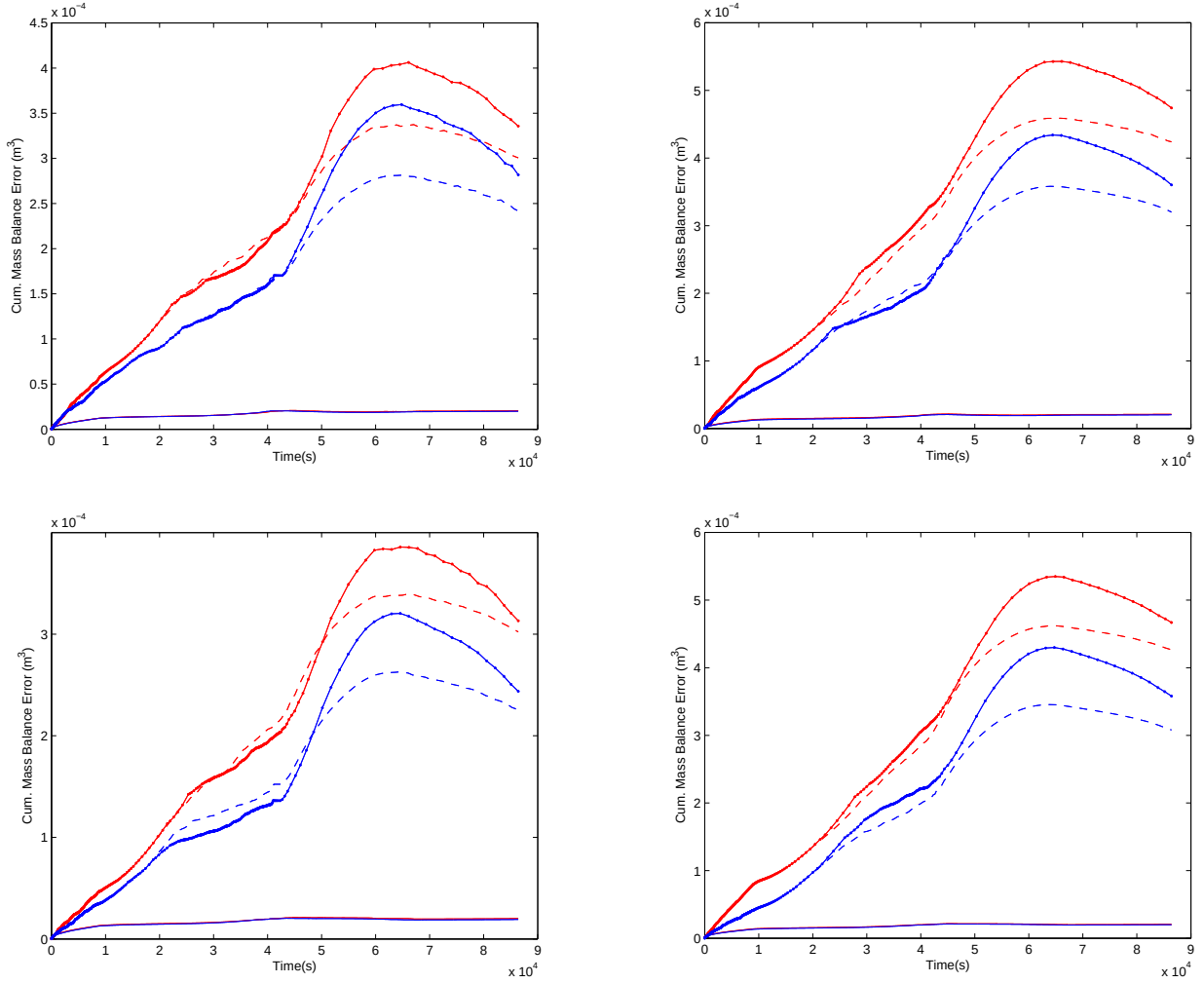


FIGURE 72. Comparison of cumulative mass balance behavior of Picard scheme for uniform (red color) nonuniform (blue color) distribution of lookup points for 60 and 120 layers (the sequence of figures are 1st two for 60 layers of 31 and 151 points respectively and 2nd two for 120 layers of 31 and 151 points respectively). $\Delta t_{max} = 10$ s, 800 s, and 1600 s are marked by solid, dashed, and dot-dashed lines respectively.

discretizations and time step sizes with NLKP=31 and 151, the error graphs for the Picard and Newton methods are shown in Figures 75 and 76 respectively.

From the RMSE table for Newton, we see that the calculated root mean squared error values at three different times for the uniform distribution are smaller than for the nonuniform distribution for all cases except $\Delta t_{max} = 10$ s. For the Picard method, for NLKP=31 with $\Delta t_{max} = 10$ s, uniform shows smaller root mean squared error only at time=32000 s, while at

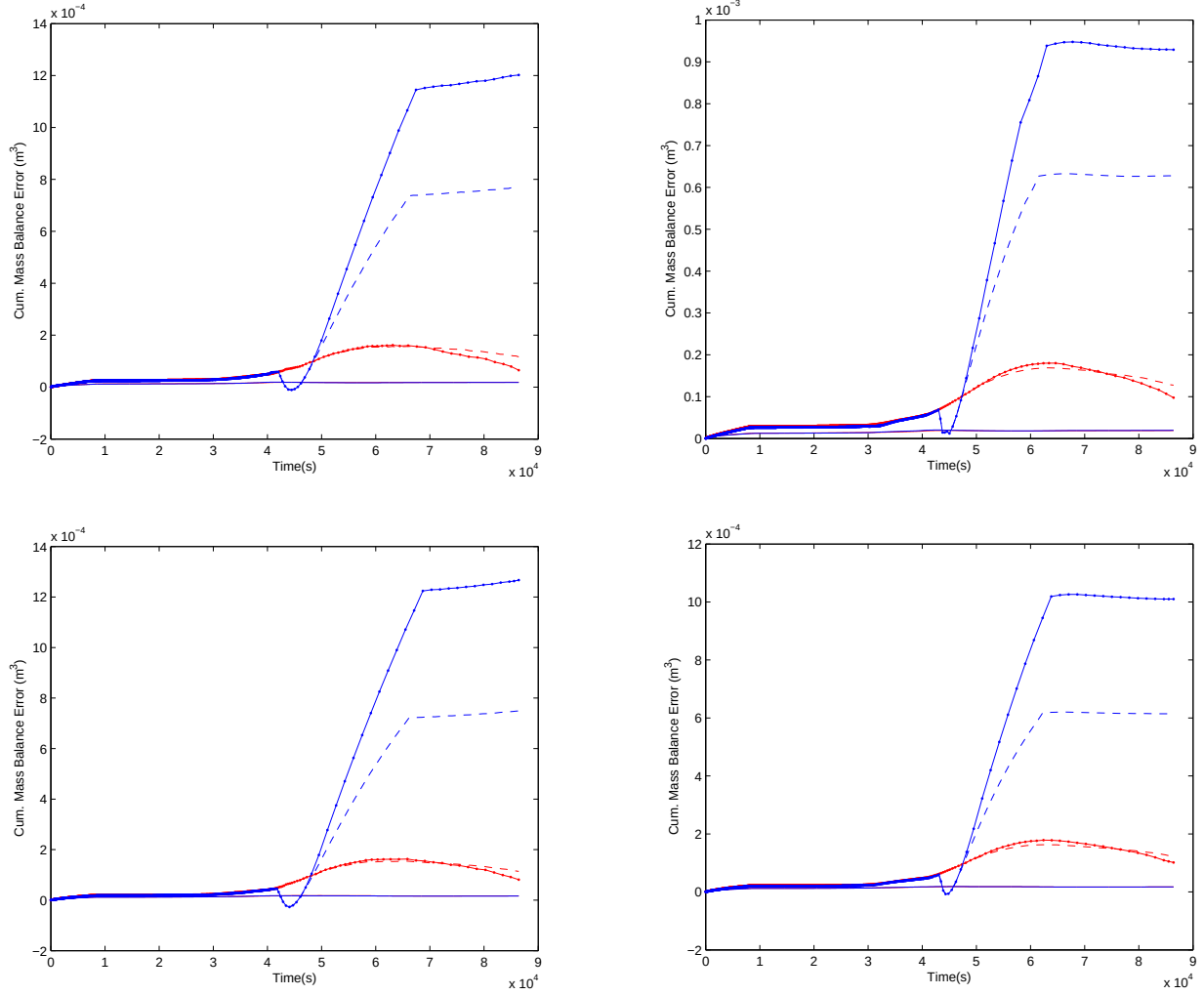


FIGURE 73. Comparison of cumulative mass balance behavior of Newton scheme for uniform (red color) nonuniform (blue color) distribution of lookup points for 60 and 120 layers (the sequence of figures are 1st two for 60 layers of 31 and 151 points respectively and 2nd two for 120 layers of 31 and 151 points respectively). $\Delta t_{max} = 10$ s, 800 s, and 1600 s are marked by solid, dashed, and dot-dashed lines respectively.

times= 56000 s and 86400 s, nonuniform does better. For $\Delta t_{max} = 800$ s and 1600 s, non uniform gives smaller values than uniform for both layers except at time=56000 s. For NLKP=151 and 60 layers, uniform shows smaller root mean squared errors than nonuniform but for 120 layers the values are same at the three time levels for $\Delta t_{max} = 10$ s. For $\Delta t_{max} = 800$ s and 1600 s, the nonuniform distribution performs better for each of the layers at the three time levels.

TABLE 45. Test Problem 3, Picards scheme: comparison of computational performance of lookup points (31 and 151) for uniform and nonuniform case, 60 and 120 layers, and Δt_{max} = 10 s, 800 s, and 1600 s.

–	–	$\Delta t(s) \rightarrow$	10	10	800	800	1600	1600
–	L	NLKP	Uni	Non	Uni	Non	Uni	Non
MBE(m^3)	60	31	2.05e-5	2.05e-5	3.00e-4	2.42e-4	3.36e-4	2.82e-4
	60	151	2.11e-5	2.03e-5	3.24e-4	3.20e-4	4.74e-4	3.60e-4
	120	31	2.01e-5	1.92e-5	3.02e-4	2.25e-4	3.13e-4	2.44e-4
	120	151	2.05e-5	2.00e-5	4.24e-4	3.08e-4	4.67e-4	3.58e-4
MBE(perc.)	60	31	1.03e-1	1.00e-1	1.50e0	1.21e0	1.68e0	1.41e0
	60	151	1.06e-1	1.02e-1	2.12e0	1.60e0	2.37e0	1.80e0
	120	31	1.01e-1	9.60e-2	1.51e0	1.12e0	1.57e0	1.22e0
	120	151	1.02e-1	9.98e-2	2.13e0	1.54e0	2.33e0	1.79e0
No. of Time Steps	60	31	8677	8713	475	570	433	546
	60	151	8643	8678	298	448	270	431
	120	31	8672	8785	511	819	518	808
	120	151	8644	8671	305	545	279	528
Avg. $\Delta t(s)$	60	31	9.957	9.916	1.819e+2	1.516e+2	1.995e+2	1.582e+2
	60	151	9.997	9.956	2.899e+2	1.929e+2	3.200e+2	2.005e+2
	120	31	9.963	9.835	1.691e+2	1.055e+2	1.668e+2	1.069e+2
	120	151	9.995	9.964	2.833e+2	1.585e+2	3.097e+2	1.636e+2
NL Iter/ Time Step	60	31	1.66	1.70	6.02	6.05	6.44	6.28
	60	151	1.61	1.66	5.86	6.19	6.32	6.50
	120	31	1.67	1.77	6.18	5.98	6.46	6.13
	120	151	1.64	1.67	5.77	6.14	6.22	6.38
Lin Iter/ NL Iter	60	31	5.39	5.37	7.64	7.36	7.77	7.20
	60	151	5.44	5.33	9.14	7.78	9.05	7.75
	120	31	5.28	5.08	6.88	5.79	6.77	7.71
	120	151	5.28	5.22	8.82	6.63	7.78	6.47
No. of Back Steps	60	31	26	50	94	124	91	126
	60	151	2	27	28	88	28	92
	120	31	22	96	97	190	110	196
	120	151	1	21	15	108	16	111
Solver Failures	60	31	0	0	0	0	0	0
	60	151	0	0	0	0	0	0
	120	31	0	0	0	0	0	0
	120	151	0	0	0	0	0	0

TABLE 46. Test Problem 3, Newton scheme: comparison of computational performance of lookup points (31 and 151) for uniform and nonuniform case, 60 and 120 layers, and $\Delta t_{max}=10$ s, 800 s, and 1600 s.

—	—	$\Delta t(s) \rightarrow$	10	10	800	800	1600	1600
—	L	NLKP	Uni	Non	Uni	Non	Uni	Non
MBE(m^3)	60	31	1.87e-5	1.80e-5	1.73e-4	7.70e-4	6.50e-4	1.20e-3
	60	151	1.91e-5	1.95e-5	1.27e-4	6.28e-4	9.76e-4	9.29e-4
	120	31	1.68e-5	1.62e-5	1.14e-4	7.49e-4	8.13e-5	1.27e-3
	120	151	1.72e-5	1.73e-5	1.22e-4	6.15e-4	1.02e-5	1.01e-3
MBE(perc.)	60	31	9.33e-2	9.02e-2	5.83e-1	3.85e0	3.25e-1	6.01e0
	60	151	9.54e-2	9.94e-2	6.37e-1	3.14e0	4.88e-1	4.65e0
	120	31	8.42e-2	8.08e-2	5.69e-1	3.74e0	4.07e-1	6.34e0
	120	151	8.62e-2	8.63e-2	6.11e-1	3.07e0	5.08e-1	5.05e0
No. of Time Steps	60	31	11084	10887	4765	4560	4748	4536
	60	151	11094	11091	4894	4829	4876	4805
	120	31	16644	15978	10530	9786	10512	9762
	120	151	16835	16651	10503	10548	10485	10524
Avg. $\Delta t(s)$	60	31	7.795	7.936	1.813e+1	1.895e+1	1.820e+1	1.905e+1
	60	151	7.778	7.790	1.765e+1	1.789e+1	1.772e+1	1.789e+1
	120	31	5.191	5.407	8.205e0	8.829e0	8.219e0	8.851e0
	120	151	5.132	5.189	8.226e0	8.191e0	8.240e0	8.210e0
NL Iter/ Time Step	60	31	3.39	3.28	6.31	6.20	6.32	6.21
	60	151	3.41	3.39	6.41	6.25	6.15	6.27
	120	31	4.07	3.90	5.73	5.64	5.74	5.64
	120	151	4.06	4.07	5.88	6.72	5.88	5.73
Lin Iter/ NL Iter	60	31	3.78	4.26	3.82	4.45	3.83	4.46
	60	151	3.74	3.97	3.64	4.23	3.66	4.26
	120	31	3.42	3.79	3.41	3.67	3.42	3.69
	120	151	3.38	3.57	3.36	3.45	3.39	3.47
No. of Back Steps	60	31	12	55	57	106	58	107
	60	151	0	13	10	66	11	67
	120	31	225	392	302	451	303	452
	120	151	201	232	210	305	211	306
Solver Failures	60	31	0	0	4	6	5	7
	60	151	0	0	0	6	4	7
	120	31	0	0	5	5	6	6
	120	151	0	0	5	4	6	5

TABLE 47. RMSE of CATHY model (uniform and nonuniform NLKP): Picard scheme for 60 and 120 layers with NLKP=31 and 151 and time step sizes $\Delta t_{max}=10$ s, 800 s, and 1600 s for Test Problem 3.

—	—	$\Delta t_{max}(s)$	10	10	800	800	1600	1600
Layers	NLKP	Time	Uni	Non	Uni	Non	Uni	Non
60	-	32000	1.10e-3	6.70e-3	5.30e-3	5.00e-3	4.60e-3	5.00e-3
	31	56000	4.20e-3	3.80e-3	6.50e-3	9.90e-3	1.06e-2	4.80e-3
	-	86400	4.70e-3	1.90e-3	1.13e-2	9.10e-3	1.25e-2	1.11e-2
60	-	32000	1.10e-3	1.10e-3	6.50e-3	4.90e-3	7.30e-3	4.90e-3
	151	56000	2.60e-3	2.80e-3	1.83e-2	1.51e-2	1.86e-2	1.40e-2
	-	86400	1.10e-3	1.40e-3	1.87e-2	1.37e-2	2.16e-2	1.59e-2
120	-	32000	2.10e-3	8.10e-3	3.30e-3	5.90e-3	3.00e-3	5.90e-3
	31	56000	3.20e-3	2.70e-3	1.50e-2	8.70e-3	1.26e-2	9.50e-3
	-	86400	4.90e-3	4.30e-3	1.72e-2	1.45e-2	1.76e-2	1.48e-2
120	-	32000	2.10e-3	2.10e-3	3.50e-3	2.80e-3	4.10e-3	3.00e-3
	151	56000	4.00e-3	4.00e-3	1.78e-2	1.58e-2	1.78e-2	1.40e-2
	-	86400	4.70e-3	4.70e-3	1.47e-2	1.86e-2	2.65e-2	2.10e-2

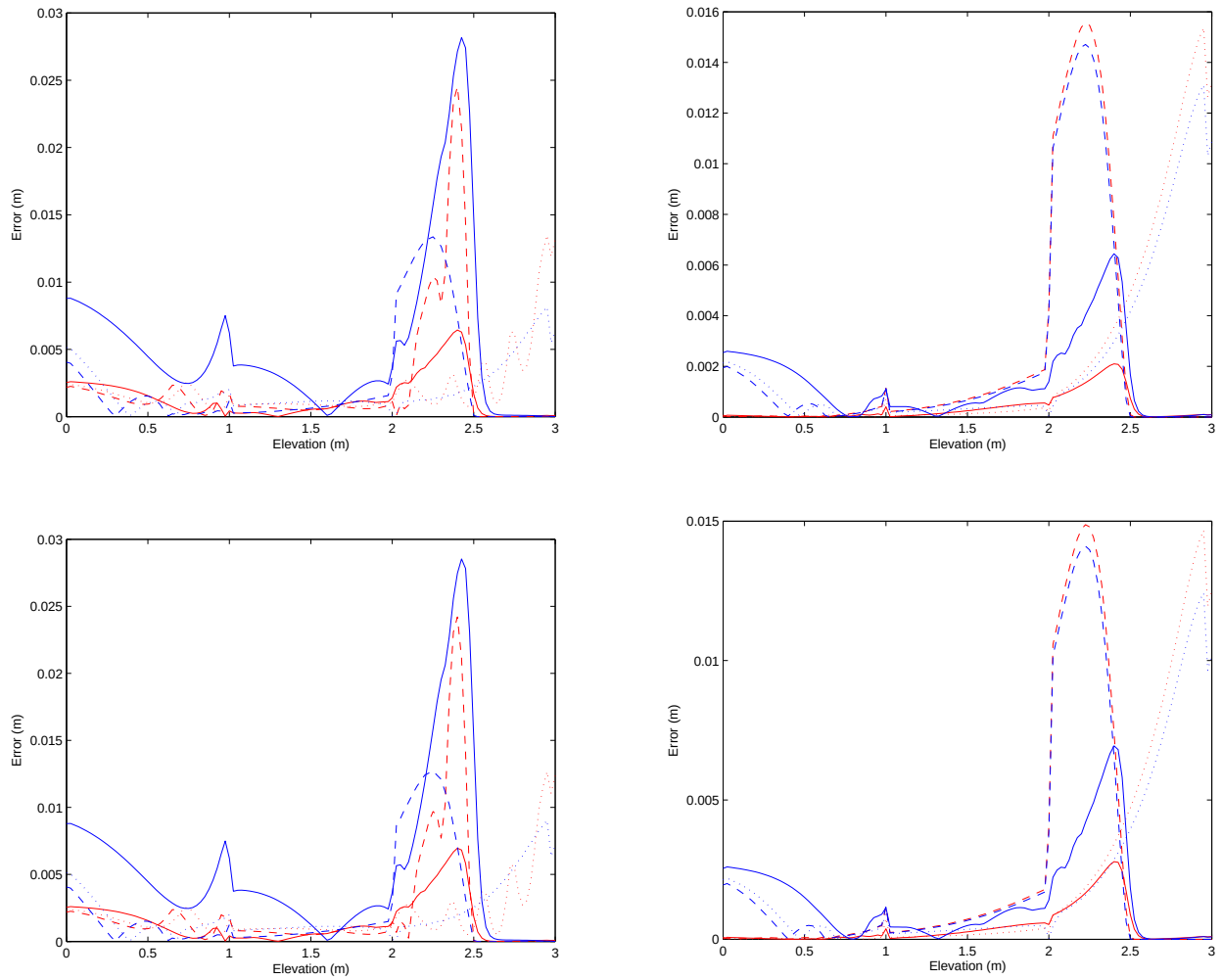


FIGURE 74. Comparison of RMSE behavior for Picard (top 2 graphs) and Newton (bottom 2 graphs) with uniform (red) and nonuniform (blue) distributions of lookup points. Solid, dotted, and dashed lines are at times 32000 s, 56000 s, and 86400 s respectively.

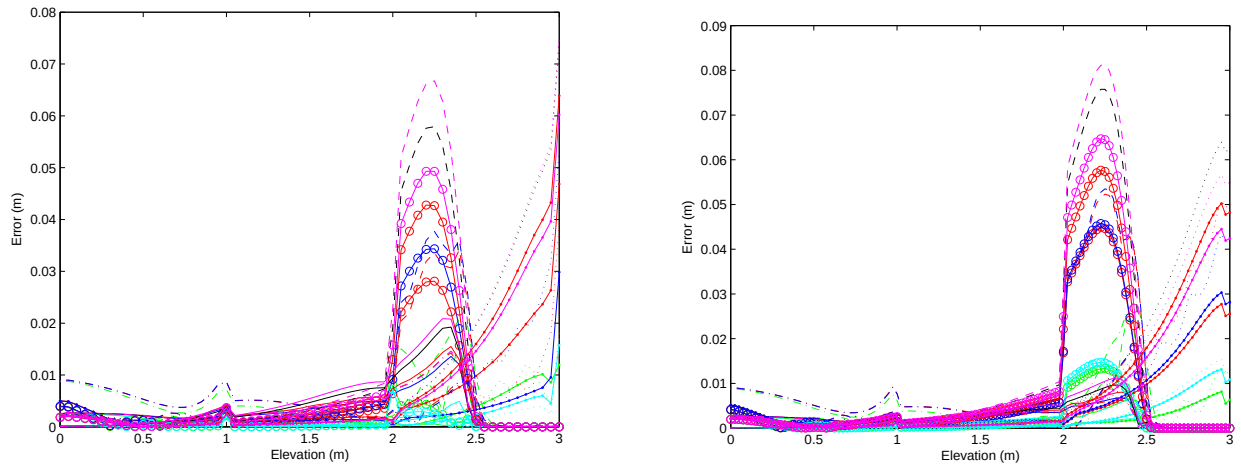


FIGURE 75. Comparison of RMSE behavior of Picard Scheme with 60 (left) and 120 (right) layers (NLKP=31 (red: $\Delta t_{max}=10$ s, green: $\Delta t_{max}=800$ s, and blue: $\Delta t_{max}=1600$ s) and NLKP=151 (cyan: $\Delta t_{max}=10$ s, black: $\Delta t_{max}=800$ s, and magenta: $\Delta t_{max}=1600$ s)).

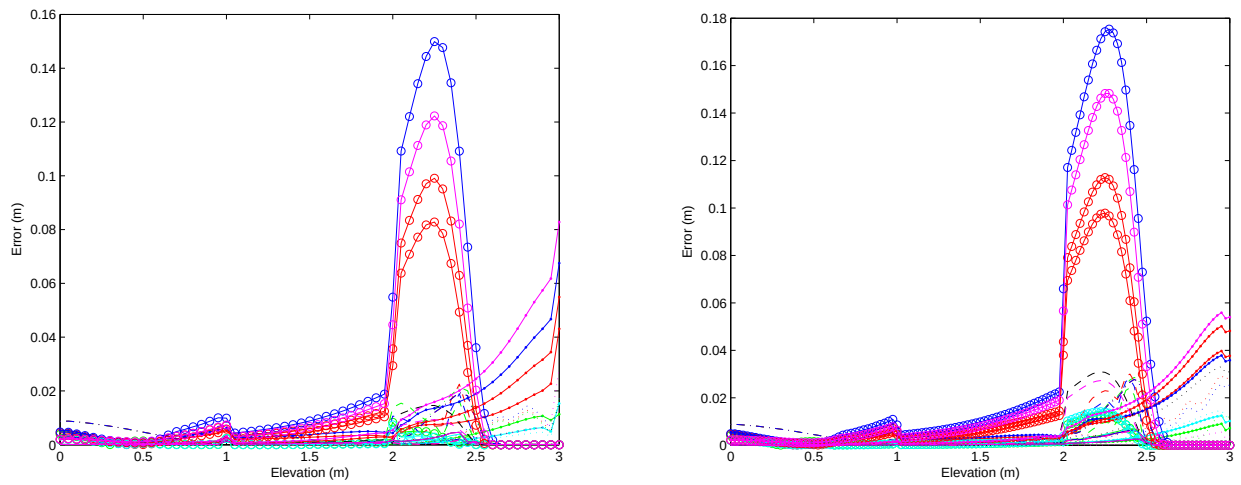


FIGURE 76. Comparison of RMSE behavior of Newton Scheme with 60 (left) and 120 (right) layers (NLKP=31 (red: $\Delta t_{max}=10$ s, green: $\Delta t_{max}=800$ s, and blue: $\Delta t_{max}=1600$ s) and NLKP=151 (cyan: $\Delta t_{max}=10$ s, black: $\Delta t_{max}=800$ s, and magenta: $\Delta t_{max}=1600$ s)).

TABLE 48. RMSE of CATHY model (uniform and nonuniform NLKP): Newton scheme for 60 and 120 layers with NLKP=31 and 151 and time step sizes $\Delta t_{max}=10$ s, 800 s, and 1600 s for Test Problem 3.

—	—	$\Delta t_{max}(s)$	10	10	800	800	1600	1600
Layers	NLKP	Time	Uni	Non	Uni	Non	Uni	Non
60	-	32000	1.10e-3	6.80e-3	1.20e-3	6.48e-3	1.20e-3	6.40e-3
	31	56000	4.20e-3	3.90e-3	4.40e-3	9.20e-3	4.80e-3	1.70e-2
	-	86400	4.80e-3	2.00e-3	4.40e-3	3.24e-2	4.10e-3	5.00e-2
60	-	32000	3.95e-4	1.10e-3	1.20e-3	1.20e-3	1.20e-3	1.20e-3
	151	56000	2.60e-3	2.80e-3	2.80e-3	1.27e-2	4.20e-3	2.16e-2
	-	86400	1.20e-3	1.50e-3	4.70e-3	2.69e-2	3.03e-3	4.02e-2
120	-	32000	2.20e-3	8.20e-3	2.02e-3	8.00e-3	2.00e-3	8.00e-3
	31	56000	3.00e-3	2.90e-3	8.10e-3	1.30e-2	7.00e-3	1.27e-2
	-	86400	4.80e-3	4.10e-3	8.10e-3	3.73e-2	6.80e-3	5.92e-2
120	-	32000	2.20e-3	2.20e-3	6.92e-4	1.90e-3	6.92e-4	1.90e-3
	151	56000	3.70e-3	3.70e-3	1.03e-2	1.61e-2	1.40e-3	1.81e-2
	-	86400	4.50e-3	4.50e-3	9.90e-3	3.21e-2	8.70e-3	4.96e-2

4.4. Conclusions.

The comparative performance between the uniform and nonuniform distribution options for the lookup table points depends on the indicators being examined. If we consider 150 layers with NLKP=151, and if we focus on the number of time steps, average time step size, nonlinear iterations per time step, linear iterations per nonlinear iteration, back stepping, and solver failures, then we can say that the uniform distribution is the better strategy. In terms of total volumetric and percentage mass balance errors the two options give similar results. In terms of RMSE the uniform option again appears to have an edge over the non uniform choice. For other configurations of layers, NLKP, and other parameters, the relative performances vary and it is difficult to draw a general conclusion concerning the best choice between the uniform and nonuniform distributions.

5. OVERALL CONCLUSIONS

In the first chapter of this work, we formulated an approach for a one-dimensional finite difference solution of Richards' equation and the method can be successfully implemented in a method of lines framework along with Matlab code. It is a straightforward approach for applying sophisticated adaptive temporal integration methods to PDE models of flow in porous media. We have demonstrated that the nonlinear models of one-dimensional flow can be solved efficiently in the context of method of lines. For our two test problems, tables of computational statistics show that the number of function evaluations, the number of Jacobian evaluations, and the number of steps taken were at the acceptable level. High accuracy can be achieved with a substantial savings in computational effort, and with excellent RMSE and mass-conservation properties. Further research could examine the performance of the scheme in more complex flow problems, e.g., 2D and 3D systems.

The numerical solution of large-scale nonlinear problems is computationally expensive and requires highly efficient and robust algorithms. Optimization of CPU is ensured by efficiency and storage resources to attain a desired level of solution accuracy. Robustness means that a given algorithm exhibits acceptable convergence behavior across a wide spectrum of simulation scenarios. The two most commonly used iterative procedures, Picard and Newton, and a nested Newton-type linearization algorithm for solving Richards' equation, have been tested in a series of simulations of flow in variably saturated porous media. Experiments featuring a sharp moisture front that infiltrates into the soil column, drainage, and flow into dry heterogeneous soil in one-dimensional soil media were conducted. We have investigated the various factors that are affecting the numerical techniques. In many cases the Picard scheme converges well, and in these cases, for linearizing Richards' equation, the Picard scheme is a simple and efficient method. There are some difficulties encountered with complex time-varying boundary conditions, strongly nonlinear characteristic equations, and saturated/unsaturated interfaces. However, there are some cases where the Newton scheme also fails to converge, although Newton is generally more robust and faster converging than Picard according to the nature of the hydraulic soil properties. Evaluating the various schemes for two- and three-dimensional flow

problems is important area for future work.

The objectives of the last phase of our modeling research programme included the development and implementation of a numerical procedure for the effective simulation of flow through porous media under variably saturated conditions within complex geometries, using uniform and nonuniform distributions of lookup table points for evaluating the soil hydraulic characteristics and the derivatives of these strongly nonlinear relationships. This contribution describes the implementation, testing, and evaluation of an effective procedure for the simulation of variably saturated flow in porous media with spatially varying properties, e.g., by taking many points in the sharp region of soil moisture curves. We have solved accurately and with computational efficiency some discriminating tests cases involving relatively extreme conditions with regard to vertical drainage through a layered soil from initially saturated conditions and sharp boundaries between the unsaturated and saturated conditions. The various affecting factors of Picard and Newton schemes are illustrated and summarized by figures and tables. We have shown that uniform distribution is the better strategy to solve the Richards equation for drainage problems. while the non uniform discretizations can be chosen for layered soil problems. Further research will investigate 2D and 3D flow domains.

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