A quadrature-based scheme for numerical solutions to Kirchhoff transformed Richards' equation

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Motivation

The study of water dynamics in the subsoil is of primary importance for understanding phenomena in Earth's critical zone, i.e. in heterogeneous, near surface environment in which complex interactions involving rock, soil, water, air, and living organisms regulate the natural habitat and determine the availability of life-sustaining resources. In particular, movement through unsaturated soils is crucial for managing many human activities, such as

- agriculture and irrigation issues;
- environmental engineering (stormwater infiltration trench, landfills management, . . .);
- geotechnical engineering (slope stability);
- . . .

1D Richards' Equation

In a 1D domain, water infiltration in the unsaturated zone can be described by Richards' equation in the water content θ and pressure head ψ:

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left(K_z k_r(\psi)\left(\frac{\partial \psi}{\partial z} - 1\right)\right), \; t \in [0, T], \; z \in [0, Z],$$

endowed with initial and boundary conditions

$$\begin{aligned}
\theta(0, z) &= \theta^0(z), \quad z \in [0, Z], \\
\theta(t, 0) &= \theta_0(t), \quad t \in [0, T], \\
\theta(t, Z) &= \theta_Z(t), \quad t \in [0, T],
\end{aligned}$$

where K_z is the saturated conductivity tensor and $k_r(\psi)$ the relative permeability scalar function.

Gardner's constitutive relations

Here, we assume that water retention function and relative permeability function are defined as

$$\theta(\psi) = \begin{cases} \theta_r + (\theta_S - \theta_r)e^{\lambda\psi}, & \text{for } \psi \leq 0, \\ 0, & \text{for } \psi > 0, \end{cases}$$

and

$$k_r(\psi) := \begin{cases} e^{\lambda\psi}, & \text{for } \psi \leq 0, \\ 1, & \text{for } \psi > 0, \end{cases}$$

respectively, where λ is a soil index parameter (L^{-1}) related to the pore-sized distribution.

Kirchhoff transform

Because of the high-nonlinearity of Richards' equation, an increasingly widespread approach is to operate a change of variables, in order to obtain a fully linearized equation, easier to handle with. In particular we define the following Kirchhoff integral transformation:

$$\mu(\psi) := \int_{-\infty}^{\psi} k_r(s)\,\mathrm{d}s,$$

which we plug into the boundary value problem to better deal with nonlinearities and make the problem less stiff than it originally appears. Within Gardner's framework we then have, for the unsaturated zone,

$$\mu(\psi) = \frac{1}{\lambda} e^{\lambda\psi}, \quad k_r(\psi) = \lambda\mu(\psi).$$

Mass balance condition

One measure of a numerical simulator is its ability to conserve global mass over the domain of interest. Adequate conservation of global mass is a necessary but not sufficient condition for acceptability of a numerical simulator. To measure the ability of the simulator to conserve mass, let a mass balance measure be defined as follows [Celia et al.(1990)]:

$$MB(t) = \frac{\text{total additional mass in the domain}}{\text{total net flux into the domain}}.$$

Exploiting mass balance condition

Usually, one uses finite differences to discretize both temporal and spatial operators on a spatial mesh $\{z_0, \ldots, z_K\}$ and a temporal mesh $\{t_0, \ldots, t_N\}$, and then solves the resulting numerical problem.

Idea

Leverage mass balance condition by integrating both sides of Richards' equation with respect to time and depth over $[t_n, t_{n+1}] \times [z_k, z_{k+1}]$:

$$\int_{z_k}^{z_{k+1}} \int_{t_n}^{t_{n+1}} \frac{\partial \theta}{\partial t} \,\mathrm{d}t\,\mathrm{d}z = \int_{z_k}^{z_{k+1}} \int_{t_n}^{t_{n+1}} \frac{\partial}{\partial z} \left(K_z k_r(\psi) \left(\frac{\partial \psi}{\partial z} - 1 \right) \right) \mathrm{d}t\,\mathrm{d}z.$$

Exploiting mass balance condition

Usually, one uses finite differences to discretize both temporal and spatial operators on a spatial mesh $\{z_0, \dots, z_K\}$ and a temporal mesh $\{t_0, \dots, t_N\}$, and then solves the resulting numerical problem.

Idea: applying Kirchhoff transform

Leverage mass balance condition by integrating both sides of Richards' equation with respect to time and depth over $[t_n, t_{n+1}] \times [z_k, z_{k+1}]$:

$$(\theta_S - \theta_r)\lambda \int_{z_k}^{z_{k+1}} \int_{t_n}^{t_{n+1}} \frac{\partial \mu}{\partial t} \,\mathrm{d}t \,\mathrm{d}z = K_z \int_{z_k}^{z_{k+1}} \int_{t_n}^{t_{n+1}} \frac{\partial}{\partial z} \left(\frac{\partial \mu}{\partial z} - \lambda \mu \right) \mathrm{d}t \,\mathrm{d}z.$$

From mass balance condition...

Thus, defining

$$\nu := \frac{\partial \mu}{\partial z}$$

and reducing double integrals, we can write

$$\begin{aligned}(\theta_S - \theta_r)\lambda \int_{z_k}^{z_{k+1}} \mu(t_{n+1}, z) - \mu(t_n, z)\,\mathrm{d}z \\ = K_S \int_{t_n}^{t_{n+1}} \nu(t, z_{k+1}) - \lambda\mu(t, z_{k+1}) \\ - \nu(t, z_k) + \lambda\mu(t, z_k)\,\mathrm{d}t,\end{aligned}$$

... to the quadrature-based numerical scheme

from which

$$
\begin{aligned}
&\int_{t_n}^{t_{n+1}} \nu(t, z_{k+1}) - \nu(t, z_k)\,\mathrm{d}t \\
&= \frac{\theta_S - \theta_r}{K_S}\lambda \int_{z_k}^{z_{k+1}} \mu(t_{n+1}, z) - \mu(t_n, z)\,\mathrm{d}z \\
&\quad + \lambda \int_{t_n}^{t_{n+1}} \mu(t, z_{k+1}) - \mu(t, z_k)\,\mathrm{d}t.
\end{aligned}
$$

Apply the trapezoidal rule to discretize above integrals:

$$
\begin{aligned}
(\nu_{k+1}^{n+1} - \nu_k^{n+1} + \nu_{k+1}^n - \nu_k^n)\Delta t &= \frac{\theta_S - \theta_r}{K_S}\lambda(\mu_{k+1}^{n+1} - \mu_{k+1}^n + \mu_k^{n+1} - \mu_k^n)\Delta z \\
&\quad + \lambda(\mu_{k+1}^{n+1} - \mu_k^{n+1} + \mu_{k+1}^n - \mu_k^n)\Delta t.
\end{aligned}
$$

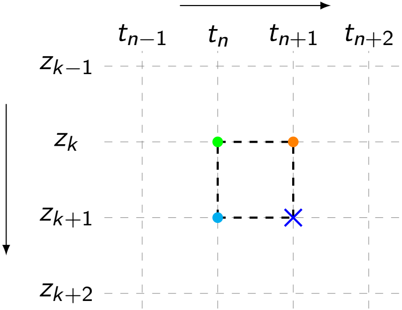
From a linear ODE to the scheme

We can rearrange and get

$$\nu_{k+1}^{n+1} - (1+\alpha)\lambda\mu_{k+1}^{n+1} = F_k^{n+1}, \quad \alpha := \frac{\theta_S - \theta_r}{K_S}\frac{\Delta z}{\Delta t},$$

where

$$F_k^{n+1} := \nu_k^{n+1} - (1-\alpha)\lambda\mu_k^{n+1} - \nu_{k+1}^{n} + (1-\alpha)\lambda\mu_{k+1}^{n} + \nu_k^{n} - (1+\alpha)\lambda\mu_k^{n}.$$



Quadrature-based numerical scheme

Therefore, we need to solve the initial value problem

$$\begin{cases} \frac{\mathrm{d}\mu}{\mathrm{d}z}(z)\Big|_{t_{n+1}} - (1+\alpha)\lambda\mu(z)\Big|_{t_{k+1}} = F_k^{n+1}, \quad z \in [z_k, z_{k+1}] \\ \mu(t_{n+1}, z_k) = \mu_k^{n+1}, \end{cases}$$

We then compute the exact solution to previous IVP at z_{k+1} and get

Quadrature-based numerical scheme

$$\mu_{k+1}^{n+1} = \varepsilon\mu_k^{n+1} + \frac{\varepsilon - 1}{(1+\alpha)\lambda}F_k^{n+1}, \quad \varepsilon := e^{(1+\alpha)\lambda\Delta z},$$
$$\nu_{k+1}^{n+1} = (1+\alpha)\lambda\mu_{k+1}^{n+1} + F_k^{n+1},$$

which represents the required step to compute the numerical solution at the mesh point corresponding to (t_{n+1}, z_{k+1}).

Quadrature-based numerical scheme

Alternatively, the numerical scheme can be formulated as

$$\nu_{k+1}^{n+1} = \left((1+\alpha)\lambda\mu_k^{n+1} + F_k^{n+1}\right)\varepsilon,$$
$$\mu_{k+1}^{n+1} = \mu_k^{n+1} + \frac{\varepsilon - 1}{\varepsilon(1+\alpha)\lambda}\nu_{k+1}^{n+1}.$$

It then follows that the solution μ_{k+1}^{n+1} can be also computed by

$$\mu_{k+1}^{n+1} = \mu_0^{n+1} + \frac{\varepsilon^{k+1} - 1}{(1+\alpha)\lambda}\nu_0^{n+1} + \frac{\varepsilon - 1}{(1+\alpha)\lambda}\sum_{j=0}^{k}\varepsilon^j F_{k-j}^{n+1},$$
$$F_k^{n+1} = F_{k-1}^n + F_{k-1}^{n+1} - F_k^n + 2\alpha\lambda(\mu_k^{n+1} - \mu_{k+1}^n),$$

with $F_k^0 := \nu_k^0 - (1+\alpha)\lambda\mu_k^0$.

Quadrature-based numerical scheme

Remark

Let us highlight here that the quadrature-based numerical scheme relies on the knowledge, at each time t_{n+1}, of ν_0^{n+1}. This value has to be precisely determined by means of a zero finding routine, in such a way that $\mu_K^{n+1} = \mu(t_{n+1}, Z)$. This approach resembles a shooting method, since we need to determine a specific initial value for $\frac{\mathrm{d}\mu}{\mathrm{d}z}$ at $z = z_0$ in order to fulfill the assigned Dirichlet boundary conditions at $z = Z$ for the Kirchhoff transformed equation.

Theoretical results

Proposition (Boundedness)

Let us assume that $|\mu_0^n|,\ |\nu_0^n|$ *are uniformly bounded for* $n = 0, \dots, N$. *Then* μ_k^n, ν_k^n *are uniformly bounded for* $n = 1, \dots, N,\ k = 1, \dots, K$.

Proposition (Stability)

If $\frac{\varepsilon-1}{(1+\alpha)\lambda}$, *with* $\varepsilon := e^{(1+\alpha)\lambda\Delta z}$, *is sufficiently small then the numerical scheme*

$$\mu_{k+1}^{n+1} = \varepsilon\mu_k^{n+1} + \frac{\varepsilon - 1}{(1+\alpha)\lambda} F_k^{n+1},$$
$$\nu_{k+1}^{n+1} = (1+\alpha)\lambda\mu_{k+1}^{n+1} + F_k^{n+1},$$

is l^2*-stable.*

Theoretical results

Proof.

Computing the Fourier transform of μ_{k+1}^{n+1} we obtain

$$
\begin{aligned}
e^{\imath\xi}\hat{\mu}^{n+1} &= e^{(1+\alpha)\lambda\Delta z}\hat{\mu}^{n+1} \\
&\quad + \frac{\varepsilon-1}{(1+\alpha)\lambda}\Big(\imath\xi\hat{\mu}^{n+1} - (1-\alpha)\lambda\hat{\mu}^{n+1} - \imath\xi e^{\imath\xi}\hat{\mu}^{n} \implies \hat{\mu}^{n+1} = \rho(\xi)\hat{\mu}^{n}, \\
&\quad + \imath\xi\hat{\mu}^{n} + (1-\alpha)\lambda e^{\imath\xi}\hat{\mu}^{n} - (1+\alpha)\lambda\hat{\mu}^{n}\Big),
\end{aligned}
$$

where the Fourier symbol is

$$
\rho(\xi) := \frac{\imath\xi e^{\imath\xi} - (1-\alpha)\lambda e^{\imath\xi} + (1+\alpha)\lambda - \imath\xi}{e^{(1+\alpha)\lambda\Delta z} + \imath\xi\varepsilon - (1-\alpha)\lambda\varepsilon - e^{\imath\xi}}\,\frac{\varepsilon-1}{(1+\alpha)\lambda}.
$$

According to the assumptions $|\rho(\xi)|^2 \leq 1$ for all $\xi \in [-\pi, \pi]$, and this proves the claim. □

Theoretical results

Next result provides order of convergence for the quadrature-based numerical scheme.

Theorem (Consistency)

The quadrature-based numerical scheme is consistent with the Kirchhoff-transformed Richards' equation and the local truncation error of order is $O(\Delta t \Delta z^2 + \Delta t^2 \Delta z)$. *Moreover, if* $\Delta t = M \Delta z$ *for some* $M > 0$ *then local truncation errors are* $O(\Delta z^3)$ *in space and* $O(\Delta t^3)$ *in time.*

Theoretical results

Proof...

Let $\overline{\mu}$ be the exact solution to the original IVP, which we can rewrite in a more compact form, skipping boundary and initial conditions, as

$$\nu_z(t,z) - \lambda\nu(t,z) - c\lambda\mu_t(t,z) = 0, \tag{1}$$

where $c := \frac{(\theta_S - \theta_r)}{K_S}$ and $\nu_z(t,z) = \frac{\partial \nu}{\partial z}(t,z)$. If we now evaluate

$$\begin{aligned}(\nu_{k+1}^{n+1} - \nu_k^{n+1} + \nu_{k+1}^{n} - \nu_k^{n})\Delta t = \frac{\theta_S - \theta_r}{K_S}\lambda(\mu_{k+1}^{n+1} - \mu_{k+1}^{n} + \mu_k^{n+1} - \mu_k^{n})\Delta z \\ + \lambda(\mu_{k+1}^{n+1} - \mu_k^{n+1} + \mu_{k+1}^{n} - \mu_k^{n})\Delta t.\end{aligned}$$

at the exact solution to (1) and resort to first order Taylor expansions, letting $\mu_{t,i}^{j} := \mu(t_j, z_i)$ and $\nu_i^j := \nu(t_j, z_i)$ and $\nu_{z,i}^{j} := \nu_z(t_j, z_i)$ for suitable i, j, we get that

Theoretical results

...continued...

$$
\begin{aligned}
&\left(\nu_{k+1}^{n+1} - \nu_k^{n+1} + \nu_{k+1}^n - \nu_k^n\right)\Delta t - c\lambda\left(\mu_{k+1}^{n+1} - \mu_{k+1}^n + \mu_k^{n+1} - \mu_k^n\right)\Delta z \\
&\quad - \lambda\left(\mu_{k+1}^{n+1} - \mu_k^{n+1} + \mu_{k+1}^n - \mu_k^n\right)\Delta t \\
&= \left(\nu_{z,k+1}^{n+1}\,\Delta z + \nu_{z,k}^n\,\Delta z + O(\Delta z^2)\right)\Delta t \\
&\quad - c\lambda\left(\mu_{t,k+1}^{n+1}\,\Delta t + \mu_{t,k}^n\,\Delta t + O(\Delta t^2)\right)\Delta z \\
&\quad - \lambda\left(\nu_{k+1}^{n+1}\,\Delta z + \nu_k^n\,\Delta z + O(\Delta z^2)\right)\Delta t \\
&= \Delta t\Delta z\left(\nu_{z,k+1}^{n+1} - \lambda\nu_{k+1}^{n+1} - c\lambda\mu_{t,k+1}^{n+1}\right) + \Delta t\Delta z\left(\nu_{z,k}^n - \lambda\nu_k^n - c\lambda\mu_{t,k}^n\right) \\
&\quad + O(\Delta t\Delta z^2) + O(\Delta t^2\Delta z) \\
&= O(\Delta t\Delta z^2 + \Delta t^2\Delta z),
\end{aligned}
$$

Theoretical results

...continued.

where last step follows from (1), and proves consistency. Moreover, if we now assume that $\Delta t = M\Delta z$ for some $M > 0$ then last equality yields that local truncation error is third order both in space and in time, and this proves the claim.

Corollary

The numerical solution of the quadrature-based scheme converges to the exact solution to Kirchhoff transformed Richards' equation with global order 2 *both in space and in time.*

Example 1

We consider a sandy loam with the following hydraulic parameters

$$\theta_r = 0.065, \quad \theta_S = 0.45, \quad K_S = 299.5\,\mathrm{cm/d}, \quad \lambda = 0.1,$$

referring to a soil collected in an experimental site near Simcoe (Southwestern Ontario). The top boundary condition decreases linearly with respect to time:

$$\theta(t,0) = \frac{2T - t}{2T}\theta_{top}, \quad t \in [0, T],$$

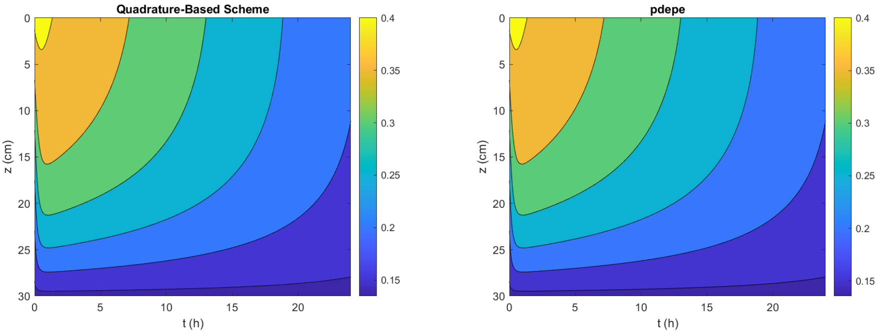
where

$$\theta_{top} = 0.1 \cdot \theta_r + 0.9 \cdot \theta_S,$$

whereas the boundary condition at the bottom is defined as

$$\theta(t,Z) = 0.7 \cdot \theta_r + 0.2 \cdot \theta_S, \quad t \in [0, T].$$

Example 1


Quadrature-Based Scheme
pdepe
z (cm)
t (h)
0
5
10
15
20
25
30
0.4
0.35
0.3
0.25
0.2
0.15

Example 1

Numerical orders of convergence with $\Delta z = 3.75 \cdot 10^{-3}$ cm and $\Delta t = 3.125 \cdot 10^{-4}$ days, providing a mass balance of 99.82%

Step-sizes for θ_{ref}	Numerical order
	$O^z_{\mathrm{num}}(32\Delta t, 32\Delta z) = 1.2054$
	$O^z_{\mathrm{num}}(16\Delta t, 16\Delta z) = 1.1423$
$\Delta t, \quad \Delta z$	$O^z_{\mathrm{num}}(8\Delta t, 8\Delta z) = 1.1492$
	$O^z_{\mathrm{num}}(4\Delta t, 4\Delta z) = 1.2508$
	$O^z_{\mathrm{num}}(2\Delta t, 2\Delta z) = 1.6130$

Example 2

Here we consider the same soil as in previous example, with same hydraulic parameters. Letting

$$\theta_{top} := 0.3 \cdot \theta_r + 0.7 \cdot \theta_S, \quad \theta_{bottom} := 0.6 \cdot \theta_r + 0.3 \cdot \theta_S,$$

we consider the following time dependent top boundary condition

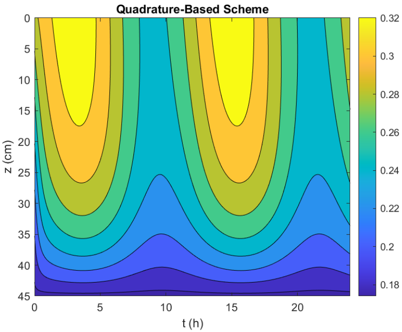
$$\theta(t, 0) = \frac{3\theta_{top} + \theta_{bottom}}{4} + \frac{\theta_{top} - \theta_{bottom}}{2} \sin\left(4\pi \frac{t}{T}\right),$$

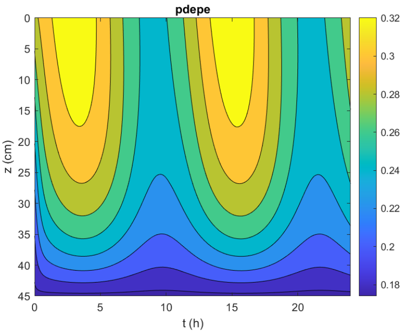
with $T = 1$ day, and a constant bottom boundary condition

$$\theta(t, Z) = \theta_{bottom},$$

with $Z = 45$ cm.

Example 2


Quadrature-Based Scheme
z (cm)
t (h)
0
5
10
15
20
25
30
35
40
45
0
5
10
15
20
0.32
0.3
0.28
0.26
0.24
0.22
0.2
0.18


pdepe
z (cm)
t (h)
0
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25
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35
40
45
0
5
10
15
20
0.32
0.3
0.28
0.26
0.24
0.22
0.2
0.18

Example 2

Numerical orders of convergence with $\Delta z = 0.1406$ cm and $\Delta t = 0.001$ days, providing a mass balance of 100.65%

Step-sizes for θ_{ref}	Numerical order
	$O^z_{\mathrm{num}}(32\Delta t, 32\Delta z) = 1.4027$
	$O^z_{\mathrm{num}}(16\Delta t, 16\Delta z) = 1.1968$
$\Delta t, \quad \Delta z$	$O^z_{\mathrm{num}}(8\Delta t, 8\Delta z) = 1.1744$
	$O^z_{\mathrm{num}}(4\Delta t, 4\Delta z) = 1.2595$
	$O^z_{\mathrm{num}}(2\Delta t, 2\Delta z) = 1.6032$

Example 3

We consider a clay soil in the Ottawa region, with Gardner's hydraulic parameters

$$\theta_r = 0, \quad \theta_S = 0.48, \quad K_S = 175.4\,\mathrm{cm/d}, \quad \lambda = 0.1.$$

Letting

$$\theta_{top} := 0.1 \cdot \theta_r + 0.9 \cdot \theta_S, \quad \theta_{bottom} := 0.6 \cdot \theta_r + 0.4 \cdot \theta_S,$$

we consider the following time dependent top boundary condition

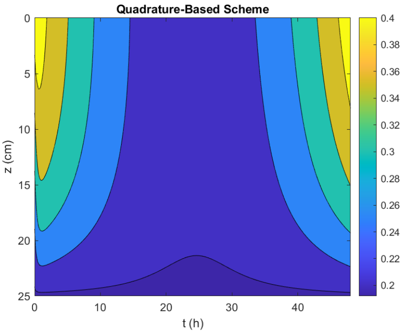
$$\theta(t,0) = \frac{1}{2}\left(\left(\frac{2t}{T} - 1\right)^2 + 1\right)\theta_{top},$$

with $T = 2$ days, and a constant bottom boundary condition

$$\theta(t,Z) = \theta_{bottom},$$

with $Z = 25$ cm.

Example 3


Quadrature-Based Scheme
pdepe
z (cm)
t (h)
0
5
10
15
20
25
0
10
20
30
40
0.4
0.38
0.36
0.34
0.32
0.3
0.28
0.26
0.24
0.22
0.2

Example 3

Numerical orders of convergence with $\Delta z = 0.0026$ cm and $\Delta t = 0.0063$ days, providing a mass balance of 100.71%

Step-sizes for θ_{ref}	Numerical order
	$O^z_{\mathrm{num}}(32\Delta t, 32\Delta z) = 3.8094$
	$O^z_{\mathrm{num}}(16\Delta t, 16\Delta z) = 2.0037$
$\Delta t, \quad \Delta z$	$O^z_{\mathrm{num}}(8\Delta t, 8\Delta z) = 1.0801$
	$O^z_{\mathrm{num}}(4\Delta t, 4\Delta z) = 1.3516$
	$O^z_{\mathrm{num}}(2\Delta t, 2\Delta z) = 1.6497$

Example 4

We consider two layered soils: an upper clay soil with parameters

$$\theta_{r,1} = 0, \quad \theta_{S,1} = 0.48, \quad K_{S,1} = 175.4\,\mathrm{cm/d}, \quad \lambda = 0.01,$$

and, after a depth of $b_1 = 25$ cm, a silty loam soil, with parameters

$$\theta_{r,2} = 0.0102, \quad \theta_{S,2} = 0.40, \quad K_{S,2} = 100.1\,\mathrm{cm/d}, \quad \lambda = 0.01,$$

which extends to a depth of 70 cm, so that the whole soil column has a total depth of 95 cm. The time dependent top boundary condition is

$$\theta(t,0) = \frac{2T - t}{2T}\theta_t, \quad t \in [0, T],$$

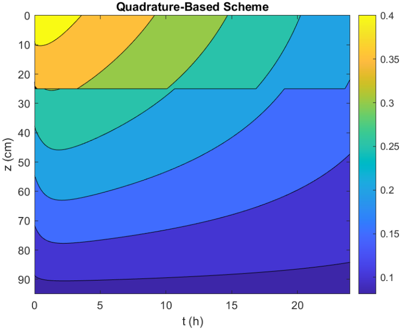
where

$$\theta_t = 0.1 \cdot \theta_{r,1} + 0.9 \cdot \theta_{S,1},$$

whereas the boundary condition at the bottom is the constant value

$$\theta(t,Z) = 0.7 \cdot \theta_{r,2} + 0.2 \cdot \theta_{S,2}, \quad t \in [0, T].$$

Example 4


Quadrature-Based Scheme
z (cm)
t (h)
0
10
20
30
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50
60
70
80
90
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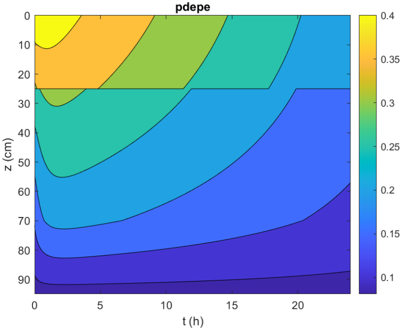
5
10
15
20
0.4
0.35
0.3
0.25
0.2
0.15
0.1


pdepe
z (cm)
t (h)
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0.3
0.25
0.2
0.15
0.1

Conclusions

- Second order finite difference method in space and time for Richards' equation
- Zero-finding routine at each iteration
- Easy to implement
- Mass conservation property
- Suitable for layered soils
- Managing root water uptake models...

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