



Ross scheme, Newton-Raphson iterative methods and time-stepping strategies for solving the mixed-form of Richards' equation

Hassane^{1,2} Mamadou Maina F. Z., Ackerer^{1,*} P.

¹Laboratoire d'Hydrologie et de Géochimie de Strasbourg,
Univ. Strasbourg/EOST - CNRS
1 rue Blessig, 67084 Strasbourg,
France

²CEA-Laboratoire de Modélisation des Transferts dans l'Environnement,
Bât. 225, F-13108 Saint Paul lez Durance cedex,
France

*Corresponding author: ackerer@unistra.fr

ABSTRACT

1 The solution of the mathematical model for flow in variably saturated porous media described
2 by Richards equation (RE) is subject to heavy numerical difficulties due to its highly non-
3 linear properties and remains very challenging. Two different algorithms are used in this work
4 to solve the mixed-form of RE: the traditional iterative algorithm and a time-adaptive
5 algorithm consisting of changing the time step magnitude within the iteration procedure while
6 the state variable is kept constant. The Ross method is an example of this type of scheme, and
7 we show that it is equivalent to the Newton-Raphson method with a time-adaptive algorithm.
8 Both algorithms are coupled to different time stepping strategies: the standard heuristic
9 approach based on the number of iterations and two strategies based on the time truncation
10 error or on the change of water saturation. Three different test cases are used to evaluate the
11 efficiency of these algorithms.



12 The numerical results highlight the necessity of implementing two types of errors: the
13 iterative convergence error (maximum difference of the state variable between two iterations)
14 and an estimate of the time truncation errors. The algorithms using these two types of errors
15 together were found to be the most efficient when highly accurate results are required.

16

17 **Key words:** Unsaturated flow, Newton-Raphson, Time stepping



18 1. Introduction

19 Water movement in soils is one of the key processes in the water cycle since it contributes to
20 the renewal of groundwater resources through recharge, to vegetation growth through
21 transpiration, to soil fertility through salinization/alteration and to atmospheric humidity
22 through evaporation and transpiration. Water movement is usually modeled using the
23 Richards equation (Richards, 1931), which is now commonly adopted for many studies in soil
24 science and/or hydrology, including the use of physically based hydrological models applied
25 to large-scale catchments and for long time simulations (e.g., for climate change studies).
26 However, this equation is highly nonlinear and despite numerous efforts over the last 40
27 years, its numerical solution requires much computational time.

28 Assuming a rigid solid matrix, the Richards equation (RE) is given by,

$$29 \begin{cases} \frac{\partial \theta}{\partial t} + S_w s_0 \frac{\partial \psi}{\partial t} + \nabla \cdot \mathbf{q} = f \\ \mathbf{q} = -k_r(\psi) \mathbf{K} [\nabla \psi + \nabla z] \end{cases} \quad (1)$$

30 where θ is the volumetric water content [L^3/L^3], S_w is the water saturation [-], s_0 is the specific
31 storage coefficient [L^{-1}], ψ is the pressure head [L], \mathbf{q} is the water flux based on the extended
32 Darcy's law [L/T], t is the time [T], z is the vertical coordinate (positive upward) [L], f is the
33 sink/source term [T^{-1}], \mathbf{K} is the saturated hydraulic conductivity tensor [L/T] and $k_r(\psi)$ is the
34 relative hydraulic conductivity [-]. The model includes initial and boundary conditions of the
35 Dirichlet (prescribed pressure head) or Neumann (prescribed flux) type.

36 Equation (1) is also called the mixed form of RE. Two alternative formulations exist for RE.

37 The pressure form is defined by:

$$38 \begin{cases} [C(\psi) + S_w s_0] \frac{\partial \psi}{\partial t} + \nabla \cdot \mathbf{q} = f \\ \mathbf{q} = -k_r(\psi) \mathbf{K} [\nabla \psi + \nabla z] \end{cases} \quad (2)$$



39 where $C(\psi) = \frac{\partial \theta}{\partial \psi}$ is the specific moisture capacity [L^{-1}], and the soil moisture form that is

40 restricted to unsaturated conditions is defined by:

$$41 \quad \begin{cases} \frac{\partial \theta}{\partial t} + \nabla \cdot \mathbf{q} = f \\ \mathbf{q} = -(\mathbf{D}(\theta)\nabla\theta + k_r(\theta)\mathbf{K}\nabla z) \end{cases} \quad (3)$$

42 where $\mathbf{D}(\theta) = k_r(\theta)\mathbf{K} \frac{d\psi}{d\theta}$ is the pore water diffusivity [L^2/T].

43 Constitutive relations are required to solve RE. For the pressure-water content relationship,

44 the most common model is the Van Genuchten model (van Genuchten, 1980):

$$45 \quad S_w(\psi) = \frac{\theta(\psi) - \theta_r}{\theta_s - \theta_r} = \begin{cases} \left(1 + |\alpha\psi|^\eta\right)^{-m} & \psi < 0 \\ 1 & \psi \geq 0 \end{cases} \quad (4)$$

46 where $m = 1 - 1/\eta$, S_w is the effective saturation, θ_r and θ_s are the residual and saturated

47 volumetric water content respectively, α and η are experimentally estimated coefficients.

48 This model is usually associated with Mualem model (Mualem, 1976) for the relative

49 permeability of the aqueous phase:

$$50 \quad k_r(S_w) = \begin{cases} S_w^{1/2} \left[1 - (1 - S_w^{1/m})^m\right]^2 & \psi < 0 \\ 1.0 & \psi \geq 0 \end{cases} \quad (5)$$

51 A summary of the most popular relations can be found in Belfort et al. (2013).

52 Due to the strong heterogeneities of the unsaturated zone and nonlinearities in the constitutive

53 relations (Eq. (4) and (5)), analytical solution of RE does not exist except in special cases

54 (Celia et al., 1990; van Dam and Feddes, 2000). Therefore, numerical methods such as finite

55 difference (Feddes et al., 1988; Romano et al., 1998; van Dam and Feddes, 2000), finite



56 element (Gottardi and Venutelli, 2001), and mixed finite element (Bause and Knabner, 2004;
57 Bergamaschi and Putti, 1999; Fahs et al., 2009; Farthing et al., 2003) are used to solve RE.

58 Iterative methods based on the Picard (fixed point) or Newton-Raphson approach (Lehmann
59 and Ackerer, 1998; Paniconi and Putti, 1994) are the most popular techniques for solving this
60 highly nonlinear equation. Alternative iterative methods are based on transform formulations
61 (Crevoisier et al., 2009; Ross and Bristow, 1990; Williams et al., 2000; Zha et al., 2013) or
62 the method of lines (Fahs et al., 2009; Matthews et al., 2004; Miller et al., 1998; Tocci et al.,
63 1997). Additionally, very few non-iterative schemes have been developed (Kavetski and
64 Binning, 2004, 2002a; Paniconi et al., 1991).

65

66 Despite the many existing numerical methods, solution of the RE is still a challenging
67 research topic with many remaining questions about reduction of the computational time,
68 treatment of nonlinearities, and improvement of the accuracy of these methods for difficult
69 problems such as infiltration in very dry soils (Diersch and Perrochet, 1999; Forsyth et al.,
70 1995; R. G. Hills, 1989).

71 In this study, we analyzed the performance of different algorithms based on the Newton-
72 Raphson method since the classical Picard scheme has been found less efficient (Lehmann
73 and Ackerer, 1998). Applied to the soil moisture form of the RE equation, we demonstrate
74 that the recently developed Ross method (Ross, 2003; Crevoisier et al., 2009; Zha et al., 2013)
75 is equivalent to Newton-Raphson method (section 2). A detailed presentation of the Newton-
76 Raphson method applied to the mixed form or RE is given in section 3. The standard Newton-
77 Raphson algorithm is based on the computation of the corresponding matrices in an iterative
78 way by updating the parameters until convergence. An alternative algorithm has been
79 suggested more recently where the parameters are kept unchanged within one time step and



80 the time step is adapted to reach convergence. This algorithm has been applied to the
 81 pressure-based form of RE by Kavetski and Binning (2002a) and to the soil moisture form by
 82 Crevoisier et al. (2009), Ross (2003), Zha et al. (2013). Although this algorithm is called “non
 83 iterative” because the parameters are not updated during the calculation, iterations may be
 84 necessary to adapt the magnitude of the time step. Therefore, in the following, we will refer to
 85 the usual algorithm as “iterative” and to the alternative algorithm as “time-adaptive”. To our
 86 knowledge, this alternative algorithm has never been applied to the mixed form of RE.
 87 Section 4 is dedicated to both algorithms and to the time stepping strategy used for solving
 88 RE. Finally, in section 5, the numerical accuracy and robustness of the algorithms applied to
 89 the mixed-form of RE are evaluated using three different test cases.

90

91 2. The Ross method and the Newton-Raphson method

92 The moisture-based formulation is applicable in unsaturated conditions only and is prone to
 93 numerical difficulties in the case of heterogeneous soils, explaining the reduced attention
 94 directed to this formulation. However, discontinuous water content can be handled by adapted
 95 schemes and moisture-based formulation appears to be very accurate for initially dry
 96 conditions (Zha et al., 2013, 2015).

97 Ross (2003) suggested a non-iterative formulation that has been recently extended to different
 98 soil conditions (Crevoisier et al., 2009; Varado et al., 2006a) and to two and three dimensions
 99 (Zha et al., 2013).

100 In its initial one-dimensional finite-volume formulation and for a volume (cell) i , the Ross
 101 method (Ross, 2003) is based on the following set of equations:

$$102 \quad \frac{\Delta z}{\Delta t} (\theta_i^{n+1} - \theta_i^n) = \frac{\Delta z}{\Delta t} (\theta_{s,i} - \theta_{r,i}) (S_i^{n+1} - S_i^n) = q_+^\sigma - q_-^\sigma \quad (6)$$

103 with:

$$104 \quad \begin{cases} q_+^\sigma = q_+^n + \sigma \left[\left(\frac{\partial q_i^n}{\partial S_i^n} \right) (S_i^{n+1} - S_i^n) + \left(\frac{\partial q_i^n}{\partial S_{i+1}^n} \right) (S_{i+1}^{n+1} - S_{i+1}^n) \right] \\ q_-^\sigma = q_-^n + \sigma \left[\left(\frac{\partial q_i^n}{\partial S_i^n} \right) (S_i^{n+1} - S_i^n) + \left(\frac{\partial q_i^n}{\partial S_{i-1}^n} \right) (S_{i-1}^{n+1} - S_{i-1}^n) \right] \end{cases} \quad (7)$$



105 where S_i^{n+1} is the water saturation at cell/node i at time $(n+1)$, q_-^σ (resp. q_+^σ) is the water flux
 106 between cell i and $(i-1)$ (resp. $i+1$) at time $t = t^n + \sigma \Delta t$, $\sigma \in [0,1]$ and Δz is the size of the
 107 cell i . $\theta_{s,i}$ is the saturated water content and $\theta_{r,i}$ is the residual water content. For simplicity,
 108 we assume here that all cells are of the same size.

109 The previous mass balance equation (6) leads to the following equation for cell i :

$$110 \quad -\left(\frac{\partial q_-^n}{\partial S_{i-1}^n}\right)(S_{i-1}^{n+1} - S_{i-1}^n) + \left[\frac{\Delta z}{\sigma \Delta t}(\theta_{s,i} - \theta_{r,i}) - \left(\left(\frac{\partial q_-^n}{\partial S_i^n}\right) - \left(\frac{\partial q_+^n}{\partial S_i^n}\right)\right)\right](S_i^{n+1} - S_i^n) \quad (8)$$

$$+ \left(\frac{\partial q_+^n}{\partial S_{i+1}^n}\right)(S_{i+1}^{n+1} - S_{i+1}^n) = q_-^n - q_+^n$$

111

112 The Newton-Raphson method was initially developed as a root-finding algorithm of an
 113 arbitrary equation that has been generalized for solving a system of non-linear equations.
 114 Applied to the soil moisture form of the RE and using an implicit scheme, the NR consists in
 115 defining a residual based on the mass balance equation (Eq. (6)) at iteration k for time step
 116 $n+1$ and for cell i written as:

$$117 \quad R_i^{n+1,k} = \frac{\Delta z}{\Delta t}(\theta_{s,i} - \theta_{r,i})(S_i^{n+1,k} - S_i^n) + q_+^{n+1,k} - q_-^{n+1,k} \quad (9)$$

118 where $R_i^{n+1,k}$ is called the residual.

119 The NR consists in computing the solution at iteration $k+1$ by estimating the residual of the
 120 next iteration $R_i^{n+1,k+1}$ using a first order Taylor development and setting it equal to zero as:

$$121 \quad \frac{R_i^{n+1,k}}{\partial S_{i+1}^{n+1,k}}(S_i^{n+1,k+1} - S_i^{n+1,k}) + R_i^{n+1,k} = 0 \quad (10)$$

122

123 The derivatives of this residual are:

$$124 \quad \begin{cases} \frac{\partial R_i^{n+1,k}}{\partial S_{i-1}^{n+1,k}} = -\frac{\partial q_-^{n+1,k}}{\partial S_{i-1}^{n+1,k}} \\ \frac{\partial R_i^{n+1,k}}{\partial S_i^{n+1,k}} = \frac{\Delta z}{\Delta t}(\theta_{s,i} - \theta_{r,i}) + \frac{\partial q_+^{n+1,k}}{\partial S_i^{n+1,k}} - \frac{\partial q_-^{n+1,k}}{\partial S_i^{n+1,k}} \\ \frac{\partial R_i^{n+1,k}}{\partial S_{i+1}^{n+1,k}} = \frac{\partial q_+^{n+1,k}}{\partial S_{i+1}^{n+1,k}} \end{cases} \quad (11)$$



125

126 which leads to the following set of linear equations:

$$\begin{aligned}
 127 \quad & -\frac{\partial q_-^{n+1,k}}{\partial S_{i-1}^{n+1,k}}(S_{i-1}^{n+1,k+1} - S_{i-1}^{n+1,k}) + \left[\frac{\Delta z}{\Delta t}(\theta_{s,i} - \theta_{r,i}) + \frac{\partial q_+^{n+1,k}}{\partial S_i^{n+1,k}} - \frac{\partial q_-^{n+1,k}}{\partial S_i^{n+1,k}} \right] (S_i^{n+1,k+1} - S_i^{n+1,k}) \\
 & + \frac{\partial q_+^{n+1,k}}{\partial S_{i+1}^{n+1,k}}(S_{i+1}^{n+1,k+1} - S_{i+1}^{n+1,k}) = \frac{\Delta z}{\Delta t}(\theta_{s,i} - \theta_{r,i})(S_i^{n+1,k} - S_i^n) + q_+^{n+1,k} - q_-^{n+1,k}
 \end{aligned} \tag{12}$$

128

129 For the first iteration, we have $S_i^{n+1,k+1} = S_i^{n+1}$ and $S_i^{n+1,k} = S_i^n$, and therefore :

$$\begin{aligned}
 130 \quad & -\frac{\partial q_-^n}{\partial S_{i-1}^n}(S_{i-1}^{n+1} - S_{i-1}^n) + \left[\frac{\Delta z}{\Delta t}(\theta_{s,i} - \theta_{r,i}) + \frac{\partial q_+^n}{\partial S_i^n} - \frac{\partial q_-^n}{\partial S_i^n} \right] (S_i^{n+1} - S_i^n) \\
 & + \frac{\partial q_+^n}{\partial S_{i+1}^n}(S_{i+1}^{n+1} - S_{i+1}^n) = q_+^{n,k} - q_-^{n,k}
 \end{aligned} \tag{13}$$

131

132 Whatever the formulation of the fluxes q (as a function of the pressure or the water content,
 133 expressed by Kirchhoff transform as in Ross (2003) or not), the implicit Ross method (eq. (8)
 134 with $\sigma = 1$) is equivalent to the first iteration of the Newton-Raphson method (eq. (13)).

135

136 3. Newton Raphson method for the mixed form Richards' equation

137 Because the pressure-based formulation does not ensure mass conservation - except for the
 138 approximation provided by Rathfelder and Abriola (1994) - and due to the limitations of the
 139 moisture-based formulation (see previous section), the mixed formulation has been widely
 140 used since the work of Celia et al. (1990).

141 The mixed form of the Richards equation given by equation (1) is rewritten as:

$$142 \quad \frac{\partial \theta}{\partial t} + S_w S_0 \frac{\partial \psi}{\partial t} = \nabla \cdot k_r(\psi) \mathbf{K} [\nabla \psi + \nabla z] + f \tag{14}$$

143 and is discretized by:

$$144 \quad \mathbf{A}^{n+1,k} \boldsymbol{\Psi}^{n+1,k+1} + \mathbf{B}^{n+1,k} \frac{\boldsymbol{\Psi}^{n+1,k+1} - \boldsymbol{\Psi}^n}{\Delta t^{n+1}} + \mathbf{E} \frac{\boldsymbol{\theta}^{n+1,k+1} - \boldsymbol{\theta}^n}{\Delta t^{n+1}} = \mathbf{F}^{n+1,k} \tag{15}$$



145 where \mathbf{A} is the discretized form of the divergence term, \mathbf{B} and \mathbf{E} are the discretized forms of
 146 the storage terms and \mathbf{F} is the discretized form of the sink/source term and the boundary
 147 conditions, n is the time step and k the iteration counter. Δt^{n+1} is the time step magnitude
 148 defined by $\Delta t^{n+1} = t^{n+1} - t^n$. Matrices \mathbf{A} , \mathbf{B} , \mathbf{E} and vector \mathbf{F} depend on the numerical scheme
 149 used for the spatial discretization. The implicit scheme is applied for the spatial discretization.
 150 For the Newton-Raphson method, the residual is defined now by:

$$151 \quad \mathbf{R}(\psi^{n+1,k}) = \mathbf{A}^{n+1,k} \psi^{n+1,k} + \mathbf{B}^{n+1,k} \frac{\psi^{n+1,k} - \psi^n}{\Delta t^{n+1}} + \mathbf{E} \frac{\theta^{n+1,k} - \theta^n}{\Delta t^{n+1}} - \mathbf{F}^{n+1,k} \quad (16)$$

152 and its derivatives are:

$$153 \quad \mathbf{R}'(\psi^{n+1,k}) = \mathbf{A}^{n+1,k} + \frac{\partial \mathbf{A}^{n+1,k}}{\partial \psi^{n+1,k}} \psi^{n+1,k} + \frac{\mathbf{B}^{n+1,k}}{\Delta t^{n+1}} + \frac{\partial \mathbf{B}^{n+1,k}}{\partial \psi^{n+1,k}} \frac{\psi^{n+1,k} - \psi^n}{\Delta t^{n+1}} \\ + \frac{\mathbf{E}}{\Delta t^{n+1}} \frac{\partial \theta^{n+1,k}}{\partial \psi^{n+1,k}} - \frac{\partial \mathbf{F}^{n+1,k}}{\partial \psi^{n+1,k}} \quad (17)$$

154 Looking for $\psi^{n+1,k+1}$ such as $\mathbf{R}(\psi^{n+1,k+1}) = 0$, the system to solve is similar to Eq. (10):

$$155 \quad \mathbf{R}'(\psi^{n+1,k}) \Delta \psi^{n+1,k+1} = -\mathbf{R}(\psi^{n+1,k}) \quad (18)$$

156 with $\Delta \psi^{n+1,k+1} = \psi^{n+1,k+1} - \psi^{n+1,k}$.

157

158 The NR formulation is also used for the non-iterative scheme by applying only one NR step
 159 per time step, with $\psi^{n+1} = \psi^{n+1,1}$ where $\psi^{n+1,0} = \psi^n$ (Paniconi et al., 1991; Zha et al., 2015).

160

161 4. Algorithms and time stepping strategy

162 The usual algorithm used to solve RE consists in defining a time step that remains constant
 163 and to iteratively compute the parameters and variables in the following way:

164 *For a given time step n*

165 - Define the time step length Δt^{n+1} depending on the time stepping strategy.



166 - Initialization of the iterative process by setting $\boldsymbol{\psi}^{n+1,1} = \boldsymbol{\psi}^n$.
 167 *do k=1, maxit*
 168 1. Computation of the variable $\boldsymbol{\theta}^{n+1,k}$, the parameter $\mathbf{K}^{n+1,k}$ and their derivatives
 169 $\frac{d\boldsymbol{\theta}^{n+1,k}}{d\boldsymbol{\psi}^{n+1,k}}, \frac{\partial \mathbf{K}^{n+1,k}}{\partial \boldsymbol{\psi}^{n+1,k}}$ using $\boldsymbol{\psi}^{n+1,k}$.
 170 2. Computation of the system matrix \mathbf{R}' and the residual \mathbf{R} .
 171 3. Computation of the system solution $\boldsymbol{\psi}^{n+1,k+1}$.
 172 4. Check convergence. If convergence is achieved, exit.
 173 *enddo*

174 **Next time step**

175 where k is the iteration counter and *maxit* the maximum number of iterations.

176

177 The time-adaptive algorithm consists of keeping the pressure head constant and changing the
 178 time step length. The algorithm is described by the following:

179

180 **For a given time step n**

181 - Computation of the variable $\boldsymbol{\theta}^n$, the parameter \mathbf{K}^n and their derivatives $\frac{d\boldsymbol{\theta}^n}{d\boldsymbol{\psi}^n}, \frac{\partial \mathbf{K}^n}{\partial \boldsymbol{\psi}^n}$
 182 using $\boldsymbol{\psi}^n$.

183 *do k=1, maxit*

184 1. Define a time step $\Delta t^{n+1,k}$ depending on the time stepping strategy.
 185 2. Computation of the system matrix \mathbf{R}' and the residual \mathbf{R} .
 186 3. Computation of the system solution $\boldsymbol{\psi}^{n+1,k+1}$.
 187 4. Check convergence. If convergence is achieved, exit.

188 *enddo*

189 **Next time step**

190

191 The main advantage of the alternative algorithm is its avoidance of the computation of the
 192 variable $\boldsymbol{\theta}$, the parameter \mathbf{K} and their derivatives $\frac{d\boldsymbol{\theta}}{d\boldsymbol{\psi}}$ and $\frac{\partial \mathbf{K}}{\partial \boldsymbol{\psi}}$ during the iterations. Due to



193 the highly nonlinear relations between θ , \mathbf{K} , $\frac{d\theta}{d\psi}$, $\frac{\partial \mathbf{K}}{\partial \psi}$ and the pressure, this computation

194 may require significant CPU time.

195

196 The most popular time step management during the simulation is that of the heuristic type

197 (Miller et al., 2006). The time step Δt^{n+1} is computed depending on Δt^n and the number of

198 iterations k necessary to reach convergence in the following way:

$$199 \quad \begin{cases} \text{if } k \leq m_1 & \Delta t^{n+1} = k_1 \Delta t^n & k_1 > 1.0 \\ \text{if } m_1 \leq k \leq m_2 & \Delta t^{n+1} = \Delta t^n \\ \text{if } m_2 \leq k & \Delta t^{n+1} = k_2 \Delta t^n & k_2 < 1.0 \end{cases} \quad (19)$$

200

201 where k_1 , k_2 , m_1 , m_2 are user-defined constants.

202 Other heuristic time step management procedures have been suggested by Kirkland et al.,

203 (1992) based on the water volumes exchanged between the adjacent cells of the grid and by

204 Ross (2003), where the time step size is controlled by the maximum allowed change in the

205 saturation.

206 For the Ross method, the fluxes are computed first and the time step magnitude is calculated

207 accordingly using

$$208 \quad \Delta t^{n+1} = \frac{\Delta S_{max}}{\max_i \left(\frac{|q_{-i}^n - q_{+i}^n|}{\Delta z_i (\theta_{s,i} - \theta_{r,i})} \right)} \quad (20)$$

209 where ΔS_{max} is the user-defined maximum saturation change. After the computation of the

210 actual change in the saturation, the time step is modified if the maximum of the actual change

211 exceeds $(1 + \lambda) \max_i (|\Delta S_i|)$ where λ is a user-defined value, according to:

$$212 \quad \Delta t^{n+1,k} = \frac{\Delta S_{max}}{\max_i (|\Delta S_i|)} \Delta t^{n+1,k-1} \quad (21)$$

213 and the system of equations is solved again. More details about handling the fluxes at

214 boundaries and saturated conditions can be found in Crevoisier et al. (2009), Ross (2003) and

215 Varado et al. (2006b).

216

217 Adaptive time stepping strategies based on time truncation error control were found to be

218 superior to others approaches (Hirthe and Graf, 2012; Kavetski et al., 2001; Tocci et al.,



219 1997). The Method of Lines using the DASPDK integrator was applied to the Richards'
 220 equation by Matthews et al. (2004), Miller et al. (1998), Tocci et al. (1997) among others. The
 221 Method of Lines consists of discretization of the spatial part of the PDE only, leading to a
 222 system of ordinary differential equations. It has been found to be significantly more efficient
 223 than other temporal discretizations (Miller et al., 2006). However, Kavetski and Binning
 224 (2002b) reported difficulties in obtaining convergence for the DASPDK solver associated with
 225 an arithmetic mean of inter-block conductivities for the most difficult problem addressed by
 226 Miller et al. (1998).

227 The adaptive scheme used in this work evaluates the time steps through truncation error due
 228 to the temporal discretization as proposed by Thomas and Gladwell (1988). This scheme was
 229 already applied to the pressure-based formulation by Kavetski et al. (2001) and to the
 230 moisture-based formulation by Kavetski and Binning (2004).

231 The difference between the first-order and second-order time approximations can be
 232 considered as an estimate of the local truncation error of the first-order scheme. The first-
 233 order approximation is given by:

$$234 \quad \Psi_{(1)}^{n+1} = \Psi^n + \Delta t^{n+1} \frac{\partial \Psi^n}{\partial t} \quad (22)$$

235 The second-order approximation is:

$$236 \quad \begin{aligned} \Psi_{(2)}^{n+1} &= \Psi^n + \Delta t^{n+1} \frac{\partial \Psi^n}{\partial t} + \frac{1}{2} (\Delta t^{n+1})^2 \frac{\partial^2 \Psi^n}{\partial t^2} \\ &= \Psi^n + \frac{1}{2} (\Delta t^{n+1}) \left[\frac{\partial \Psi^{n+1}}{\partial t} + \frac{\partial \Psi^n}{\partial t} \right] \end{aligned} \quad (23)$$

$$237 \quad \text{using } \frac{\partial \Psi^{n+1}}{\partial t} = \frac{\partial \Psi^n}{\partial t} + \Delta t^{n+1} \frac{\partial^2 \Psi^n}{\partial t^2} .$$

238 This truncation error is given by:



$$\begin{aligned} \varepsilon_i^{n+1} &= \max_i \left| \psi_{(2),i}^{n+1} - \psi_{(1),i}^{n+1} \right| = \frac{1}{2} \Delta t^{n+1} \max_i \left| \frac{\partial \psi_i^{n+1}}{\partial t} - \frac{\partial \psi_i^n}{\partial t} \right| \\ &\approx \frac{1}{2} \Delta t^{n+1} \max_i \left| \frac{\psi_i^{n+1} - \psi_i^n}{\Delta t^{n+1}} - \frac{\psi_i^n - \psi_i^{n-1}}{\Delta t^n} \right| \end{aligned} \quad (24)$$

240 When the truncation error is smaller than γ , the temporal truncation error tolerance defined by
 241 the user, the size of the next time step is calculated by:

$$\Delta t^{n+1} = \Delta t^n \min \left(s \sqrt{\frac{\gamma}{\max(\varepsilon_i^{n+1}, EPS)}}, r_{\max} \right) \quad (25)$$

243 When the truncation error is superior to γ , the computation is repeated with a reduced time
 244 step defined as following:

$$\Delta t^n = \Delta t^n \max \left(s \sqrt{\frac{\gamma}{\max(\varepsilon_i^{n+1}, EPS)}}, r_{\min} \right) \quad (26)$$

246 where r_{\max} and r_{\min} are user-defined constants used to avoid too drastic changes of the time
 247 step. s is considered to be a safety factor that ensures that the time step changes are
 248 reasonable. EPS is used to avoid floating point errors when the truncation error becomes too
 249 small.

250

251 5. Evaluation of the algorithms' performance

252 We applied the NR method to the mixed form of RE using the standard iterative algorithm
 253 and the time-adaptive algorithm. Implicit standard finite volumes have been used to solve the
 254 partial differential equation and arithmetic means are used to compute the inter-block
 255 hydraulic conductivity. The detailed discretizations of the matrix $\mathbf{R}'(\boldsymbol{\psi}^{n+1,k})$ and the vector
 256 $\mathbf{R}(\boldsymbol{\psi}^{n+1,k})$ (see Eq. (18)) are given in Appendix 1. The time-adaptive algorithms have been



257 applied as described by the authors: Ross (2003) for the time stepping based on the saturation
258 changes and Kavetski et al. (2001) for the time stepping based on the truncation errors.

259 For the standard iterative algorithm, we defined two types of errors to check the convergence:
260 the error based on the maximum change of the state variables between two iterations defined
261 by $\varepsilon_\psi = \max_i |\psi_i^{n+1,k+1} - \psi_i^{n+1,k}|$ and the truncation error ε_t defined by Eq. (24). Convergence is
262 assumed to be achieved when:

$$263 \quad \varepsilon_\psi < \tau_a + \tau_r \left| \psi_{imax}^{n+1,k+1} \right| \quad (27)$$

264 where τ_a and τ_r are the absolute and relative user-defined tolerances and $\psi_{imax}^{n+1,k+1}$ is the
265 pressure corresponding to ε_ψ and when:

$$266 \quad \varepsilon_t < \tau_a + \tau_r \left| \psi_{imax}^{n+1,k+1} \right| \quad (28)$$

267 where the parameters have the same meaning as those for the previous criterion but $\psi_{imax}^{n+1,k+1}$
268 represents the pressure value corresponding to ε_t .

269 The tested algorithms are summarized in Table 1. Computations of all possible combinations
270 for the standard iterative scheme have been performed. We present only the four most
271 efficient algorithms.

272 We investigated three one-dimensional problems with various initial and boundary conditions
273 and hydraulic functions to assess the accuracy, efficiency and computational costs of the
274 different algorithms. The selected test cases represent a range of difficult infiltration problems
275 widely analyzed in the literature:

- 276 - TC1: infiltration in a homogeneous initially dry soil with constant prescribed pressure
277 at the surface and prescribed pressure at the bottom (Celia et al., 1990);



278 - TC2: infiltration in a homogeneous soil initially at hydrostatic equilibrium with a
279 prescribed constant flux at the soil surface and prescribed pressure at the bottom
280 (Miller et al., 1998);

281 - TC3: infiltration/evaporation in an initially dry heterogeneous soil, with variable
282 positive and negative fluxes at the surface and free drainage at the base of the soil
283 column (Lehmann and Ackerer, 1998).

284 For the three test cases, the soil hydraulic functions were described by Mualem-Van
285 Genuchten models (Mualem, 1976; van Genuchten, 1980), see Eq. (4) and (5).

286 The required parameters, boundary conditions and initial conditions are summarized in Table
287 2. The evolution of the relative hydraulic conductivity, the water saturation and the specific
288 moisture capacity with respect to the pressure values are shown in Figures 1, 2 and 3,
289 respectively. For TC1, the pressure will vary from -1000 cm to -75 cm only due to the
290 specific conditions of this test case. Therefore, the parameter variations are smaller than those
291 for the other test cases. Since the parameters' variations are more abrupt for test cases 2 and 3,
292 their solutions are more challenging.

293 Preliminary tests were performed to define the optimal spatial discretization. We assume that
294 the errors are only originated from the time step size and the linearization.

295 The following criteria were used for the time stepping strategy:

296 - $k_1=0.80$, $k_2=1.20$, $m_1=5$, $m_2=10$, which are the usual values for the heuristic strategy
297 defined by Eq. (19);

298 - $r_{min}=0.10$, $r_{max}=4.0$, $s=0.9$, $EPS=10^{-10}$, which are the standard values for the time
299 stepping scheme based on time discretization error defined by Eq. (26) (Kavetski et
300 al., 2001);



301 - the maximum change in saturation has been evaluated using the maximum change in
302 the pressure according to the following relationship:

$$303 \quad \Delta S_{max} \approx \frac{1}{(\theta_{s,imax} - \theta_{r,imax})} \left. \frac{d\theta}{d\psi} \right|_{imax}^n (\tau_a + \tau_r |\psi_{imax}^{n+1,k+1}|) \quad (29)$$

304 The simulations have been performed using different values of τ_r and with $\tau_a = 0.0$.

305

306 We used several criteria to evaluate the performance of these codes. A typical error used in
307 solving RE is the global cumulative mass balance error defined by:

$$308 \quad MB(t^{n+1}) = \frac{\sum_{i=1}^M \Delta z_i (\theta_i^{n+1} - \theta_i^0)}{\sum_{k=1}^{n+1} (q_{in}^k - q_{out}^k) \Delta t^k} \quad (30)$$

309 where Δz_i is the size of the cell/element i , θ_i^{n+1} is its water content at time t^{n+1} , θ_i^0 is the
310 initial water content, and q_{in}^k and q_{out}^k are the inflow and outflow, respectively, at the domain
311 boundaries at time t^k . M is the number of cells/elements. The fluxes at the boundaries are
312 defined by $q^k = \frac{1}{2}(q^k + q^{k-1})$. The mass balance errors were checked for each runs but were
313 found to be negligible since we solved the mass-conserving RE form.

314 While it is necessary to satisfy the global mass balance for an accurate numerical scheme, a
315 low mass balance error is not sufficient to ensure the accuracy of the solution. Therefore,
316 solutions have also been compared with the reference solution obtained using a very fine
317 temporal discretization and the iterative Newton-Raphson method. This comparison is based
318 on the average relative error defined by:



$$\varepsilon_k = \left[\frac{1}{M} \sum_i \frac{|\psi_i^{ref} - \hat{\psi}_i|^k}{|\psi_i^{ref}|^k} \right]^{1/k} \quad (31)$$

319 where M is the number of cells, ψ^{ref} is the reference solution and $\hat{\psi}$ is the tested numerical
 320 solution. ε_1 represents the average absolute relative error (called L₁-norm in the following),
 321 ε_2 is the average quadratic error (L₂-norm) and ε_∞ is the highest local relative difference
 322 between the numerical and the reference solutions (L_∞-norm).
 323

324 Since the time-adaptive algorithm does not require the computation of the parameters and
 325 their derivatives during the iterative procedure, we use N_{sol} to denote the number of times
 326 where the system of equations is solved and N_{param} to denote the number of times where the
 327 parameters are computed. Of course, these counters are equal to each other for the standard
 328 algorithm and N_{param} is less than N_{sol} for the time-adaptive algorithm. For comparison
 329 purposes, the computational costs are estimated by N_{sol} for the standard algorithm and by $(N_{sol}$
 330 $+N_{param})/2$ for the time-adaptive algorithm. The efficiency of the algorithms have been
 331 evaluated by comparing the computational costs for a given relative tolerance τ_r . The errors
 332 are presented in the tables and the figures. The figures show some additional results not listed
 333 in the tables that already contains much information.

334

335 *TC1: Infiltration in a homogenous soil with constant boundary conditions*

336 This test case simulates an infiltration into a homogeneous porous medium. This problem is
 337 addressed here because it has been widely analyzed previously by many authors like
 338 Bouchemella et al. (2015), Celia et al. (1990), El Kadi and Ling (1993), Rathfelder and
 339 Abriola, (1994), Tocci et al. (1997), among others. The computations were performed with a



340 spatial discretization of 0.1 cm. The initial time step size was set to $1.0 \cdot 10^{-5}$ s, and the
341 maximum time step size was set to 400 s.

342 The results for the iterative and time-adaptive algorithms are presented in Tables 3 and 4,
343 respectively. When both convergence criteria are used (algorithms SH $_{\Delta\psi_{\Delta t}}$ and
344 SS $_{\Delta\psi_{\Delta t}}$), N_{trunc} represents the number of times where the truncation error is the most
345 restrictive condition. For the heuristic time stepping schemes, the convergence is mostly
346 linked to the truncation error (N_{trunc} is close to N_{sol}), whereas when the saturation time
347 stepping scheme is used, the most restrictive criterion is the maximum difference in the
348 pressure.

349 When the time stepping scheme is based on saturation, for both iterative and time-adaptive
350 algorithms, the number of iterations required to solve the problem is proportional to the
351 relative tolerance. Therefore, highly accurate solutions incur high computational costs.

352 For the time-adaptive scheme, the number of parameter changes N_{param} is close to the number
353 of iterations for low tolerance values. Small tolerance values lead to small time steps,
354 avoiding time step adjustments. This is not the case for larger tolerance values that lead to
355 larger time steps and therefore to additional iterations (see for example TA_T for the
356 tolerance of $\tau_r = 10^{-2}$ – Table 4).

357 The three types of errors provide the same information. The best solution for one type of error
358 is also the best solution for the two others.

359 On average, the iterative algorithm is faster than the time-adaptive algorithm that requires
360 more iterations for a given error. This is also shown in Figure 4 that presents the convergence
361 rate of the L_2 -norm with respect to the computational costs, *i.e.*, the number of iterations or
362 number of iterations and number of parameter changes. The time-adaptive algorithm with
363 time stepping based on the truncation errors performs quite poorly compared to the other



364 algorithms. Irrespective of the tolerance, this algorithm leads to a wetting front moving faster
365 (Fig. 5).

366 When the relative tolerance is set to a very low value ($\tau_r=10^{-5}$), the iterative scheme with
367 time stepping based on the saturation changes shows behavior that is different from that found
368 for the less restrictive tolerance. The criterion based on truncation errors is no longer
369 significant ($N_{\text{trunc}}=252$), possibly explaining why the accuracy of the scheme remains
370 constant. This also indicates that errors due to time discretization have to be handled, either in
371 the convergence criterion or in the time stepping strategy.

372 For this test case, the most efficient algorithms are the iterative algorithms using the time
373 stepping strategy based on truncation error ($ST_{\Delta\psi}$) or based on the saturation changes
374 ($SS_{\Delta\psi_{\Delta t}}$), except for the case of very high precision where $ST_{\Delta\psi}$ outperforms the other
375 algorithms.

376

377 *TC2: Infiltration in a homogenous soil with hydrostatic initial conditions*

378 This test case models an infiltration in a 200 cm vertical column of unconsolidated clay loam
379 with non-uniform grain size distribution and was considered by Miller et al. (1998) to be a
380 very challenging test. This problem was found to be more challenging from the numerical
381 point of view compared to TC1 due to the relative permeability function that enhances the
382 non-linear behavior of Richards' equation (Fig. 1, 2, 3). The cell size has been set to 0.125
383 cm, the initial time step to 10^{-5} s and the maximum time step magnitude to 1000 s.

384 The different norms for the iterative and the time-adaptive schemes are given in Tables 5 and
385 6.

386 Investigation of this test case leads to similar qualitative conclusions when the time stepping
387 scheme is based on the saturation differences ($SS_{\Delta\psi_{\Delta t}}$ and TA_S). The standard scheme



388 SH $\Delta\psi$ fails to provide an accurate solution within a reasonable number of iterations (less
389 than 10^7).

390 The most efficient methods are the schemes using the time stepping strategy based on
391 truncation errors (Fig. 6). However, as found for TC1, the adaptive time algorithm failed to
392 provide highly accurate results (L_2 -norm error less than approximately $4.5 \cdot 10^{-4}$).

393 Figure 7 shows the time step magnitudes for approximately equal L_2 -norms for the two time-
394 adaptive algorithms and for the iterative algorithm using truncation errors for time stepping
395 ($4.254 \cdot 10^{-4}$ within 3503 iterations for ST $\Delta\psi$, $4.563 \cdot 10^{-4}$ within 3094 iterations for TA $_T$ and
396 $4.844 \cdot 10^{-4}$ within 113583 iterations for TA $_S$). The increase in the time step length after 10 s
397 is the same, irrespective of the algorithm. For a smaller time, both truncation time stepping
398 strategies differ for the estimate of the first time step only. The scheme using the saturation
399 based time stepping is penalized by the poor estimate of the first maximum allowed saturation
400 change. This leads to the estimate of the first time step magnitude that was too long for
401 reaching convergence.

402

403 *TC3: Infiltration/evaporation in a heterogeneous soil*

404 This case study simulates infiltration in an initially dry heterogeneous soil with a succession
405 of rainfall and evaporations as upper boundary conditions during 35 days. This problem
406 differs from the two previous cases by the soil heterogeneity and also by the non-monotonic
407 boundary conditions at the soil surface. It is expected that non-monotonic discontinuous
408 boundary conditions will increase the difficulty of finding accurate solutions. The soil profile
409 consists of three 60 cm thick layers. The layers are discretized using cells with the size of 0.10
410 cm. The maximum time step magnitude is chosen as 0.20 days to avoid a too rough
411 discretization of the upper boundary conditions. The initial time step is set to 10^{-5} day.



412 The relative errors estimated by the iterative algorithms and the time-adaptive algorithms are
413 presented in Tables 7 and 8, respectively, and are plotted in Figure 8.

414 The standard iterative scheme fails to converge within the maximum number of iterations
415 (10^7) when the tolerance is not sufficiently restrictive. The detailed analyses of the
416 computation showed that the time step size was quite large compared to the more restrictive
417 conditions until day 28.0 where the infiltration fluxes were equal to 1.50 cm/day and where
418 the conditions were near saturation due to the previous infiltration period. This led to a
419 decrease of the time step to close to the minimum value (10^{-8} s), causing the procedure to
420 stop. More restrictive conditions lead to smaller time steps from the beginning of the
421 simulation and a better approximation of the solutions during the entire simulation.

422 The iterative scheme coupled with the truncation based time step strategy showed a
423 surprisingly unstable behavior for $\tau_r=10^{-3}$. The scheme did not converge for
424 $\tau_r \in [0.96 \cdot 10^{-3}; 1.04 \cdot 10^{-3}]$. The results presented in Table 7 and Figure 8 are obtained for
425 $\tau_r = 0.90 \cdot 10^{-3}$. At this stage of our work, we were not able to provide a meaningful
426 explanation for this effect.

427 The time-adaptive algorithm with the saturation based time stepping scheme is the most
428 efficient for an L_2 -norm greater than 10^{-4} . For more accurate results, the iterative method with
429 the time stepping strategy using the truncation error must be preferred. The impact of the time
430 stepping strategy for these two algorithms is shown in Figure 9 for approximately the same
431 L_2 -norm ($2.051 \cdot 10^{-3}$ within 1283 iterations for TA_S and $1.517 \cdot 10^{-3}$ within 6504 iterations for
432 ST_Δψ). The time step changes is related to the boundary conditions variations as expected.
433 The strategy based on the saturation variation leads to a longer time step than the strategy
434 using the time truncation error. This difference can be quite important (see the simulation



435 between days 25 and 30). The consequences of this difference are a reduced number of
436 iterations but also a less accurate computation, irrespective of the error norm.

437

438 **6. Summary and conclusions**

439 The solution of RE is complex and very time consuming due to its highly non-linear
440 properties. Several algorithms have been tested for the mixed-form of Richards equation,
441 including time-adaptive methods. Based on the numerical examples that differ in their
442 parameters (level of non-linearity) and in their initial and boundary conditions, the
443 conclusions and recommendations are:

- 444 1. Our numerical developments showed that the method suggested by Ross (2003) in its
445 implicit formulation can be considered as a Newton-Raphson method with a time-
446 adaptive algorithm.
- 447 2. The different algorithms have different convergence rates (accuracy improvement of
448 the scheme as a function of the computational costs). Therefore, an algorithm can be
449 very efficient for a given accuracy and less efficient for another level of precision.
- 450 3. The mass balance is not a good criterion for the evaluation of the results because the
451 mixed-form preserves the mass balance, irrespective of the pressure distribution
452 within the profile.
- 453 4. The use of both criteria (ε_{ψ} , the maximum variable difference between two iterations,
454 ε_t the time truncation error) should be implemented in the iterative procedure. The use
455 of ε_{ψ} only, which is the case in many numerical codes, does not provide any
456 information about the accuracy of the time derivative approximation.
- 457 5. Our 1-dimensional examples did not show a significant advantage of the time-adaptive
458 algorithm that avoids the computation of the parameters for each iteration. However,



459 this may depend on the number of elements used for the spatial discretization, and this
460 conclusion may be different for 2D or 3D domains.

461

462 Depending on the type of the problem that must be solved (parameters behavior with respect
463 to the pressure, time variations of the boundary conditions), the time truncation errors may be
464 predominant compared to the error corresponding to the pressure changes between two
465 iterations. Therefore, we recommend the use of both types of errors by implementing the
466 truncation errors either in the convergence procedure (convergence reached if ε_p and ε_t are
467 smaller than a user's defined tolerance) or in the time stepping strategy as defined by
468 Kavetski et al. (2001).

469

470



References

- Bause, M., Knabner, P., 2004. Computation of variably saturated subsurface flow by adaptive mixed hybrid finite element methods. *Adv. Water Resour.* 27, 565–581. doi:10.1016/j.advwatres.2004.03.005
- Belfort, B., Younes, A., Fahs, M., Lehmann, F., 2013. On equivalent hydraulic conductivity for oscillation-free solutions of Richard's equation. *J. Hydrol.* 505, 202–217. doi:10.1016/j.jhydrol.2013.09.047
- Bergamaschi, L., Putti, M., 1999. Mixed finite elements and Newton-type linearizations for the solution of Richards' equation. *Int. J. Numer. Methods Eng.* 45, 1025–1046. doi:10.1002/(SICI)1097-0207(19990720)45
- Bouchemella, S., Seridi, A., Alimi-Ichola, I., 2015. Numerical simulation of water flow in unsaturated soils: comparative study of different forms of Richards's equation. *Eur. J. Environ. Civ. Eng.* 19, 1–26. doi:10.1080/19648189.2014.926294
- Celia, M.A., Bouloutas, E.T., Zarba, R.L., 1990. A general mass-conservative numerical solution for the unsaturated flow equation. *Water Resour. Res.* 26, 1483–1496. doi:10.1029/WR026i007p01483
- Crevoisier, D., Chanzy, A., Voltz, M., 2009. Evaluation of the Ross fast solution of Richards' equation in unfavourable conditions for standard finite element methods. *Adv. Water Resour.* 32, 936–947. doi:10.1016/j.advwatres.2009.03.008
- Diersch, H.-J.G., Perrochet, P., 1999. On the primary variable switching technique for simulating unsaturated-saturated flows. *Adv. Water Resour.* 23, 271–301. doi:10.1016/S0309-1708(98)00057-8
- El Kadi, A.I., Ling, G., 1993. The Courant and Peclet Number criteria for the numerical solution of the Richards Equation. *Water Resour. Res.* 29. doi:10.1029/93WR00929
- Fahs, M., Younes, A., Lehmann, F., 2009. An easy and efficient combination of the Mixed Finite Element Method and the Method of Lines for the resolution of Richards' Equation. *Environ. Model. Softw.* 24, 1122–1126. doi:10.1016/j.envsoft.2009.02.010
- Farthing, M.W., Kees, C.E., Miller, C.T., 2003. Mixed finite element methods and higher order temporal approximations for variably saturated groundwater flow. *Adv. Water Resour.* 26, 373–394. doi:10.1016/S0309-1708(02)00187-2
- Feddes, R.A., Kabat, P., Van Bakel, P.J.T., Bronswijk, J.J.B., Halbertsma, J., 1988. Modelling soil water dynamics in the unsaturated zone — State of the art. *J. Hydrol.* 100, 69–111. doi:10.1016/0022-1694(88)90182-5
- Forsyth, P.A., Wu, Y.S., Pruess, K., 1995. Robust numerical methods for saturated-unsaturated flow with dry initial conditions in heterogeneous media. *Adv. Water Resour.* 18, 25–38. doi:10.1016/0309-1708(95)00020-J
- Gottardi, G., Venutelli, M., 2001. UPF: two-dimensional finite-element groundwater flow model for saturated-unsaturated soils. *Comput. Geosci.* 27, 179–189. doi:10.1016/S0098-3004(00)00082-0
- Hirthe, E.M., Graf, T., 2012. Non-iterative adaptive time-stepping scheme with temporal truncation error control for simulating variable-density flow. *Adv. Water Resour.* 49, 46–55. doi:10.1016/j.advwatres.2012.07.021
- Kavetski, D., Binning, P., 2004. Truncation error and stability analysis of iterative and non-iterative Thomas-Gladwell methods for first-order non-linear differential equations. *Int. J. Numer. Methods Eng.* 60, 2031–2043. doi:10.1002/nme.1035
- Kavetski, D., Binning, P., 2002a. Adaptive backward Euler time stepping with truncation error control for numerical modelling of unsaturated fluid flow. *Int. J. Numer. Methods Eng.* 53, 1301–1322. doi:10.1002/nme.329



- Kavetski, D., Binning, P., 2002b. Noniterative time stepping schemes with adaptive truncation error control for the solution of Richards equation. *Water Resour. Res.* 38. doi:10.1029/2001WR000720
- Kavetski, D., Binning, P., Sloan, S.W., 2001. Adaptive time stepping and error control in a mass conservative numerical solution of the mixed form of Richards equation. *Adv. Water Resour.* 24, 595–605. doi:10.1016/S0309-1708(00)00076-2
- Kirkland, M.R., Hills, R.G., Wierenga, P.J., 1992. Algorithms for solving Richards' equation for variably saturated soils. *Water Resour. Res.* 28, 2049–2058.
- Lehmann, F., Ackerer, P., 1998. Comparison of Iterative Methods for Improved Solutions of the Fluid Flow Equation in Partially Saturated Porous Media. *Transp. Porous Media* 31, 275–292. doi:10.1023/A:1006555107450
- Matthews, C.J., Braddock, R.D., Sander, G.C., 2004. Modeling flow through a one-dimensional multi-layered soil profile using the Method of Lines. *Environ. Model. Assess.* 9, 103–113.
- Miller, C.T., Abhishek, C., Farthing, M.W., 2006. A spatially and temporally adaptive solution of Richards' equation. *Adv. Water Resour.* 29, 525–545. doi:10.1016/j.advwatres.2005.06.008
- Miller, C.T., Williams, G.A., Kelley, C.T., Tocci, M.D., 1998. Robust solution of Richards' equation for nonuniform porous media. *Water Resour. Res.* 34, 2599–2610. doi:10.1029/98WR01673
- Mualem, Y., 1976. A new model for predicting the hydraulic conductivity of unsaturated porous media. *Water Resour. Res.* 12, 513–522. doi:10.1029/WR012i003p00513
- Paniconi, C., Aldama, A.A., Wood, E.F., 1991. Numerical evaluation of iterative and noniterative methods for the solution of the nonlinear Richards equation. *Water Resour. Res.* 27, 1147–1163.
- Paniconi, C., Putti, M., 1994. A comparison of Picard and Newton iteration in the numerical solution of multidimensional variably saturated flow problems. *Water Resour. Res.* 30, 3357–3374. doi:10.1029/94WR02046
- R. G. Hills, I.P., 1989. Modeling one-dimensional infiltration into very dry soils: 1. Model development and evaluation. *Water Resour. Res.* 25. doi:10.1029/WR025i006p01259
- Rathfelder, K., Abriola, L.M., 1994. Mass conservative numerical solutions of the head-based Richards equation. *Water Resour. Res.* 30, 2579–2586. doi:10.1029/94WR01302
- Richards, L.A., 1931. Capillary conduction of liquids through porous medium. *J. Appl. Phys.* 1, 318–333. doi:10.1063/1.1745010
- Romano, N., Brunone, B., Santini, A., 1998. Numerical analysis of one-dimensional unsaturated flow in layered soils. *Adv. Water Resour.* 21, 315–324. doi:10.1016/S0309-1708(96)00059-0
- Ross, P.J., 2003. Modeling Soil Water and Solute Transport—Fast, Simplified Numerical Solutions. *Agron. J.* 95, 1352. doi:10.2134/agronj2003.1352
- Ross, P.J., Bristow, K.L., 1990. Simulating Water Movement in Layered and Gradational Soils Using the Kirchhoff Transform. *Soil Sci. Soc. Am. J.* 54, 1519. doi:10.2136/sssaj1990.03615995005400060002x
- Thomas, R.M., Gladwell, I., 1988. Variable-order variable-step algorithms for second-order systems. Part 1: The methods. *Int. J. Numer. Methods Eng.* 26, 39–53.
- Tocci, M.D., Kelley, C.T., Miller, C.T., 1997. Accurate and economical solution of the pressure-head form of Richards' equation by the method of lines. *Adv. Water Resour.* 20, 1–14. doi:10.1016/S0309-1708(96)00008-5
- van Dam, J.C., Feddes, R.A., 2000. Numerical simulation of infiltration, evaporation and shallow groundwater levels with the Richards equation. *J. Hydrol.* 233, 72–85. doi:10.1016/S0022-1694(00)00227-4



- van Genuchten, M.T., 1980. A Closed-form Equation for Predicting the Hydraulic Conductivity of Unsaturated Soils¹. *Soil Sci. Soc. Am. J.* 44, 892. doi:10.2136/sssaj1980.03615995004400050002x
- Varado, N., Braud, I., Ross, P.J., 2006a. Development and assessment of an efficient vadose zone module solving the 1D Richards' equation and including root extraction by plants. *J. Hydrol.* 323, 258–275. doi:10.1016/j.jhydrol.2005.09.015
- Varado, N., Braud, I., Ross, P.J., Haverkamp, R., 2006b. Assessment of an efficient numerical solution of the 1D Richards' equation on bare soil. *J. Hydrol.* 323, 244–257. doi:10.1016/j.jhydrol.2005.07.052
- Williams, G.A., Miller, C.T., Kelley, C.T., 2000. Transformation approaches for simulating flow in variably saturated porous media. *Water Resour. Res.* 36, 923–934. doi:10.1029/1999WR900349
- Zha, Y., Shi, L., Ye, M., Yang, J., 2013. A generalized Ross method for two- and three-dimensional variably saturated flow. *Adv. Water Resour.* 54, 67–77. doi:10.1016/j.advwatres.2013.01.002
- Zha, Y., Tso, M.C.-H., Shi, L., Yang, J., 2015. Comparison of Non iterative Algorithms Based on Different Forms of Richards' Equation. *Environ. Model. Assess.* 21, 357–370. doi:10.1007/s10666-015-9467-1



1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23
24
25
26

APPENDIX 1.

The numerical method used in the paper is implicit standard finite difference. For a cell i of the grid, the unsaturated flow equation (4) can be discretized in the following way:

$$\begin{cases} \frac{\theta_i^{n+1} - \theta_i^n}{\Delta t} + S_w s_0 \frac{\psi_i^{n+1} - \psi_i^n}{\Delta t} + \frac{q_{i+}^{n+1} - q_{i-}^{n+1}}{\Delta z_i} = f_i \\ q_{i-}^{n+1} = -K_{i-} \left(\frac{\psi_i^{n+1} - \psi_{i-1}^{n+1}}{\Delta z_{i-}} - 1 \right) \\ q_{i+}^{n+1} = -K_{i+} \left(\frac{\psi_{i+1}^{n+1} - \psi_i^{n+1}}{\Delta z_{i+}} - 1 \right) \end{cases} \quad (\text{A32})$$

where n is the time step, K_{i-} is the inter-block conductivity between cell i and $(i-1)$ defined by $K_{i-} = \frac{\Delta z_{i-1} K(\psi_{i-1}) + \Delta z_i K(\psi_i)}{\Delta z_{i-1} + \Delta z_i}$, K_{i+} is the inter-block conductivity between cell i and $(i+1)$ defined by $K_{i+} = \frac{\Delta z_i K(\psi_i) + \Delta z_{i+1} K(\psi_{i+1})}{\Delta z_i + \Delta z_{i+1}}$. $\Delta z_{i-} = \frac{1}{2}(\Delta z_{i-1} + \Delta z_i)$ is the distance between the center of cell $(i-1)$ and i . $\Delta z_{i+} = \frac{1}{2}(\Delta z_i + \Delta z_{i+1})$ is the distance between the center of cell i and $(i+1)$.

The residual is:

$$R(\psi_i^{n+1,k}) = \Delta z_i (\theta_i^{n+1,k} - \theta_i^n) + \Delta z_i S_w s_0 (\psi_i^{n+1,k} - \psi_i^n) + \Delta t (q_{i+}^{n+1,k} - q_{i-}^{n+1,k}) - \Delta t \Delta z_i f_i \quad (\text{A33})$$

where k is the iteration counter.

The residual derivatives are:

$$\begin{aligned} \frac{\partial R(\psi_i^{n+1,k})}{\partial \psi_{i-1}^{n+1,k}} &= -\Delta t \frac{\partial q_{i-}^{n+1,k}}{\partial \psi_{i-1}^{n+1,k}} \\ \frac{\partial R(\psi_i^{n+1,k})}{\partial \psi_i^{n+1,k}} &= \Delta z_i \frac{d\theta_i^{n+1,k}}{d\psi_i^{n+1,k}} + \Delta z_i S_w s_0 + \Delta t \left(\frac{\partial q_{i+}^{n+1,k}}{\partial \psi_i^{n+1,k}} - \frac{\partial q_{i-}^{n+1,k}}{\partial \psi_i^{n+1,k}} \right) \\ \frac{\partial R(\psi_i^{n+1,k})}{\partial \psi_{i+1}^{n+1,k}} &= \Delta t \frac{\partial q_{i+}^{n+1,k}}{\partial \psi_{i+1}^{n+1,k}} \end{aligned} \quad (\text{A34})$$

Therefore, the system to solve is:



$$\begin{aligned}
 & -\Delta t \frac{\partial q_{i-}^{n+1,k}}{\partial \psi_{i-1}^{n+1,k}} \Delta \psi_{i-1}^{n+1,k+1} + \\
 27 \quad & \left[\Delta z_i \frac{d\theta_i^{n+1,k}}{d\psi_i^{n+1,k}} + \Delta z_i S_w s_0 + \Delta t \left(\frac{\partial q_{i+}^{n+1,k}}{\partial \psi_i^{n+1,k}} - \frac{\partial q_{i-}^{n+1,k}}{\partial \psi_i^{n+1,k}} \right) \right] \Delta \psi_i^{n+1,k+1} + \\
 & \Delta t \frac{\partial q_{i+}^{n+1,k}}{\partial \psi_{i+1}^{n+1,k}} \Delta \psi_{i+1}^{n+1,k+1} = \\
 & -\Delta z_i (\theta_i^{n+1,k} - \theta_i^n) - \Delta z_i S_w s_0 (\psi_i^{n+1,k} - \psi_i^n) - \Delta t (q_{i+}^{n+1,k} - q_{i-}^{n+1,k}) + \Delta t \Delta z_i f_i
 \end{aligned} \tag{A35}$$

28
 29

30 With the following derivatives of the fluxes $q_{i-}^{n+1,k}$

$$\begin{aligned}
 31 \quad & \left\{ \begin{aligned}
 32 \quad & \frac{\partial q_{i-}^{n+1,k}}{\partial \psi_{i-1}^{n+1,k}} = -\frac{\partial K_{i-}^{n+1,k}}{\partial \psi_{i-1}^{n+1,k}} \left(\frac{\psi_i^{n+1,k} - \psi_{i-1}^{n+1,k}}{\Delta z_{i-}} - 1 \right) + \frac{K_{i-}^{n+1,k}}{\Delta z_{i-}} \\
 & \frac{\partial q_{i-}^{n+1,k}}{\partial \psi_i^{n+1,k}} = -\frac{\partial K_{i-}^{n+1,k}}{\partial \psi_i^{n+1,k}} \left(\frac{\psi_i^{n+1,k} - \psi_{i-1}^{n+1,k}}{\Delta z_{i-}} - 1 \right) - \frac{K_{i-}^{n+1,k}}{\Delta z_{i-}}
 \end{aligned} \right. \tag{A36}
 \end{aligned}$$

33
 34 and $q_{i+}^{n+1,k}$:

$$\begin{aligned}
 35 \quad & \left\{ \begin{aligned}
 36 \quad & \frac{\partial q_{i+}^{n+1,k}}{\partial \psi_i^{n+1,k}} = -\frac{\partial K_{i+}^{n+1,k}}{\partial \psi_i^{n+1,k}} \left(\frac{\psi_{i+1}^{n+1,k} - \psi_i^{n+1,k}}{\Delta z_{i+}} - 1 \right) + \frac{K_{i+}^{n+1,k}}{\Delta z_{i+}} \\
 & \frac{\partial q_{i+}^{n+1,k}}{\partial \psi_{i+1}^{n+1,k}} = -\frac{\partial K_{i+}^{n+1,k}}{\partial \psi_{i+1}^{n+1,k}} \left(\frac{\psi_{i+1}^{n+1,k} - \psi_i^{n+1,k}}{\Delta z_{i+}} - 1 \right) - \frac{K_{i+}^{n+1,k}}{\Delta z_{i+}}
 \end{aligned} \right. \tag{A37}
 \end{aligned}$$

37
 38 The component of the vector of the residuals \mathbf{R} is given by equation (A33) and the
 39 coefficients of the matrix \mathbf{R}' for cell i are:
 40

$$\begin{aligned}
 41 \quad & R'_{i-1,i} = \Delta t \left[\frac{\partial K_{i-}^{n+1,k}}{\partial \psi_{i-1}^{n+1,k}} \left(\frac{\psi_i^{n+1,k} - \psi_{i-1}^{n+1,k}}{\Delta z_{i-}} - 1 \right) - \frac{K_{i-}^{n+1,k}}{\Delta z_{i-}} \right] \\
 & R'_{i,i} = \Delta z_i \left[\frac{d\theta_i^{n+1,k}}{d\psi_i^{n+1,k}} + S_w s_0 \right] - \Delta t \left[\frac{\partial K_{i+}^{n+1,k}}{\partial \psi_i^{n+1,k}} \left(\frac{\psi_{i+1}^{n+1,k} - \psi_i^{n+1,k}}{\Delta z_{i+}} - 1 \right) - \frac{K_{i+}^{n+1,k}}{\Delta z_{i+}} \right] \\
 & + \Delta t \left[\frac{\partial K_{i-}^{n+1,k}}{\partial \psi_i^{n+1,k}} \left(\frac{\psi_i^{n+1,k} - \psi_{i-1}^{n+1,k}}{\Delta z_{i-}} - 1 \right) + \frac{K_{i-}^{n+1,k}}{\Delta z_{i-}} \right] \\
 42 \quad & R'_{i,i+1} = -\Delta t \left[\frac{\partial K_{i+}^{n+1,k}}{\partial \psi_{i+1}^{n+1,k}} \left(\frac{\psi_{i+1}^{n+1,k} - \psi_i^{n+1,k}}{\Delta z_{i+}} - 1 \right) + \frac{K_{i+}^{n+1,k}}{\Delta z_{i+}} \right]
 \end{aligned} \tag{A38}$$

43 In case of prescribed flux at the upper boundary, the residual is written as:
 44



$$45 \quad R_1(\psi_1^{n+1,k}) = \Delta z_1 \left[(\theta_1^{n+1,k} - \theta_1^n) + S_w s_0 (\psi_1^{n+1,k} - \psi_1^n) \right] + \Delta t (q_{1+}^{n+1} - q_{BC}) - \Delta t \Delta z_1 f_1 \quad (A39)$$

46

47 Using the derivatives as defined in (A36) and (A37), the matrix coefficients are changed as
 48 follow:

49

$$50 \quad R'_{1,1} = \Delta z_1 \left(\frac{d\theta_1^{n+1,k}}{d\psi_1^{n+1,k}} + S_w s_0 \right) - \Delta t \left[\frac{\partial K_{1+}^{n+1,k}}{\partial \psi_1^{n+1,k}} \left(\frac{\psi_2^{n+1,k} - \psi_1^{n+1,k}}{\Delta z_{1+}} - 1 \right) - \frac{K_{1+}^{n+1,k}}{\Delta z_{1+}} \right] \quad (A40)$$

$$R'_{1,2} = -\Delta t \left[\frac{\partial K_{1+}^{n+1,k}}{\partial \psi_2^{n+1,k}} \left(\frac{\psi_2^{n+1,k} - \psi_1^{n+1,k}}{\Delta z_{1+}} - 1 \right) + \frac{K_{1+}^{n+1,k}}{\Delta z_{1+}} \right]$$

51

52 If the flux is applied at the bottom of the profile, similar developments lead to the residual:

53

$$54 \quad R_N = \Delta z_N \left[(\theta_N^{n+1,k} - \theta_N^n) + S_w s_0 (\psi_N^{n+1,k} - \psi_N^n) \right] + \Delta t (q_{BC} - q_{N-}^{n+1,k}) - \Delta t \Delta z_N f_N \quad (A41)$$

55

56 and its derivatives

57

$$58 \quad R'_{N-1,N} = \Delta t \left[\frac{\partial K_{N-}^{n+1,k}}{\partial \psi_{N-1}^{n+1,k}} \left(\frac{\psi_N^{n+1,k} - \psi_{N-1}^{n+1,k}}{\Delta z_{N-}} - 1 \right) - \frac{K_{N-}^{n+1,k}}{\Delta z_{N-}} \right] \quad (A42)$$

$$R'_{N,N} = \Delta z_N \left(\frac{d\theta_N^{n+1,k}}{d\psi_N^{n+1,k}} + S_w s_0 \right) + \Delta t \left[\frac{\partial K_{N-}^{n+1,k}}{\partial \psi_N^{n+1,k}} \left(\frac{\psi_N^{n+1,k} - \psi_{N-1}^{n+1,k}}{\Delta z_{N-}} - 1 \right) + \frac{K_{N-}^{n+1,k}}{\Delta z_{N-}} \right]$$

59

60 If the pressure is described at the top of the soil, the corresponding flux is defined by:

61

$$62 \quad q_{1-}^{n+1,k} = -K_{1-} \left(\frac{\psi_1^{n+1,k} - \psi_{BC}}{\Delta z_1 / 2} - 1 \right) \quad (A43)$$

63

64 And the derivative is:

65

$$66 \quad \frac{\partial q_{1-}^{n+1,k}}{\partial \psi_1^{n+1,k}} = -\frac{\partial K_{1-}^{n+1,k}}{\partial \psi_1^{n+1,k}} \left(\frac{\psi_1^{n+1,k} - \psi_{BC}}{\Delta z_1 / 2} - 1 \right) - \frac{K_{1-}^{n+1,k}}{\Delta z_1 / 2} \quad (A44)$$

67

68 The corresponding residual and the matrix coefficients are:



$$69 \quad R_1 = \Delta z_1 \left[(\theta_1^{n+1,k} - \theta_1^n) + S_w s_0 (\psi_1^{n+1,k} - \psi_1^n) \right] + \Delta t (q_{1+}^{n+1,k} - q_{1-}^{n+1,k}) - \Delta t \Delta z_1 f_1 \quad (A45)$$

70 and

$$71 \quad R'_{1,1} = \Delta z_1 \left(\frac{d\theta_1^{n+1,k}}{d\psi_1^{n+1,k}} + S_w s_0 \right) - \Delta t \left[\frac{\partial K_{1+}^{n+1,k}}{\partial \psi_1^{n+1,k}} \left(\frac{\psi_2^{n+1,k} - \psi_1^{n+1,k}}{\Delta z_{1+}} - 1 \right) - \frac{K_{1+}^{n+1,k}}{\Delta z_{1+}} \right]$$

$$+ \Delta t \left[\frac{\partial K_{1-}^{n+1,k}}{\partial \psi_1^{n+1,k}} \left(\frac{\psi_1^{n+1,k} - \psi_{BC}}{\Delta z_1 / 2} - 1 \right) + \frac{K_{1-}^{n+1,k}}{\Delta z_1 / 2} \right] \quad (A46)$$

$$R'_{1,2} = -\Delta t \left[\frac{\partial K_{1+}^{n+1,k}}{\partial \psi_2^{n+1,k}} \left(\frac{\psi_2^{n+1,k} - \psi_1^{n+1,k}}{\Delta z_{1+}} - 1 \right) + \frac{K_{1+}^{n+1,k}}{\Delta z_{1+}} \right]$$

72

73 Similarly, if the pressure is prescribed at the soils column's bottom, we have:

74

$$75 \quad R_N = \Delta z_N \left[(\theta_N^{n+1,k} - \theta_N^n) + S_w s_0 (\psi_N^{n+1,k} - \psi_N^n) \right] + \Delta t (q_{N+}^{n+1,k} - q_{N-}^{n+1,k}) - \Delta t \Delta z_N f_N \quad (A47)$$

76 and

$$R'_{N-1,N} = \Delta t \left[\frac{\partial K_{N-}^{n+1,k}}{\partial \psi_{N-1}^{n+1,k}} \left(\frac{\psi_N^{n+1,k} - \psi_{N-1}^{n+1,k}}{\Delta z_{N-}} - 1 \right) - \frac{K_{N-}^{n+1,k}}{\Delta z_{N-}} \right]$$

$$77 \quad R'_{N,N} = \Delta z_N \left(\frac{d\theta_N^{n+1,k}}{d\psi_N^{n+1,k}} + S_w s_0 \right) - \Delta t \left[\frac{\partial K_{N+}^{n+1,k}}{\partial \psi_N^{n+1,k}} \left(\frac{\psi_{BC} - \psi_N^{n+1,k}}{\Delta z_N / 2} - 1 \right) - \frac{K_{N+}^{n+1,k}}{\Delta z_N / 2} \right]$$

$$+ \Delta t \left[\frac{\partial K_{N-}^{n+1,k}}{\partial \psi_N^{n+1,k}} \left(\frac{\psi_N^{n+1,k} - \psi_{N-1}^{n+1,k}}{\Delta z_{N-}} - 1 \right) + \frac{K_{N-}^{n+1,k}}{\Delta z_{N-}} \right]$$

78

79 The numerical code is written in FORTRAN 90 and is available upon request.



List of Tables

Table 1. Different options of the tested algorithms. Reference to the corresponding equation in parenthesis.

Table 2: Domain size (L), initial conditions (IC), boundary conditions at the soil surface (BC_u) and at the soil bottom (BC_l), saturated hydraulic conductivity (K_s), residual and saturated water contents (θ_r, θ_s) and shape parameters (α, n) for the different test cases. Length and time units are centimeters and seconds.

Table 3: Relative errors and number of iterations obtained for the iterative algorithm depending on different convergence criteria for TC1.

Table 4: Relative errors and number of iterations obtained for the time-adaptive algorithm depending on different convergence criteria for TC1.

Table 5: Relative errors and number of iterations obtained for the iterative algorithm depending on different convergence criteria for TC2 (n.c.: non convergence in less than 10^7 iterations).

Table 6: Relative errors and number of iterations obtained for the time-adaptive algorithm depending on different convergence criteria for TC2.

Table 7: Relative errors and number of iterations obtained for the iterative algorithm depending on different convergence criteria for TC3 (n.c.: non convergence in less than 10^7 iterations, * convergence failed for 10^{-3} , $\tau_r = 0.90 \cdot 10^{-3}$).

Table 8: Relative errors and number of iterations obtained for the time-adaptive algorithm depending on different convergence criteria for TC3.



	Standard iterative algorithm						Time-adaptive algorithm			
	Heuristic (19)	Time stepping			Stopping criterion		Truncation (25) (26)	Saturation (20) (21)		
		Truncation (25)	Truncation (26)	Saturation (20)	Pressure (27)	Truncation (28)		Truncation (25) (26)	Saturation (20) (21)	
SH_Δψ	x					x				
SH_Δψ_Δt	x					x		x		
ST_Δψ		x				x				
SS_Δψ_Δt				x		x		x		
TA_T								x		
TA_S									x	

Table 1: Different options of the tested algorithms. Reference to the corresponding equation in parenthesis.

	L	IC	BC_u	BC_l	K_s	θ_r	θ_s	α	η
TC1	30	-1000.0	$\psi = -75$	$\psi = -1000$	$9.22 \cdot 10^{-3}$	0.102	0.368	0.0335	2.0
TC2	200	z-200	$q=3.7 \cdot 10^{-5}$	$\psi = 0$	$7.18 \cdot 10^{-5}$	0.095	0.410	0.019	1.31
TC3	60	-100.0	q(t)	q(t)= $K_M(t)$	$6.26 \cdot 10^{-3}$	0.0286	0.366	0.028	2.239
	60	-100.0			$1.51 \cdot 10^{-4}$	0.106	0.469	0.0104	1.395
	60	-100.0			$6.26 \cdot 10^{-3}$	0.0286	0.366	0.028	2.239

Table 2: Domain size (L), initial conditions (IC), boundary conditions at the soil surface (BC_u) and at the soil bottom (BC_l), saturated hydraulic conductivity (K_s), residual and saturated water contents (θ_r, θ_s) and shape parameters (α, η) for the different test cases.

$K_M(t)$ is the hydraulic conductivity of the last grid cell.

Length and time units are centimeters and seconds respectively.



Tol.	Algorithm	L_1	L_2	L_∞	N_{trunc}	N_{sol}
10^{-5}	SH_Δψ	$1.918 \cdot 10^{-3}$	$8.829 \cdot 10^{-3}$	0.106		2177
	SH_Δψ_Δt	$8.391 \cdot 10^{-6}$	$6.459 \cdot 10^{-5}$	$8.782 \cdot 10^{-4}$	542371	615880
	ST_Δψ	$3.968 \cdot 10^{-4}$	$1.045 \cdot 10^{-3}$	$3.512 \cdot 10^{-3}$		6160
	SS_Δψ_Δt	$1.136 \cdot 10^{-5}$	$3.406 \cdot 10^{-5}$	$2.817 \cdot 10^{-4}$	252	3920446
10^{-4}	SH_Δψ	$2.557 \cdot 10^{-3}$	$1.375 \cdot 10^{-2}$	0.168		1701
	SH_Δψ_Δt	$7.818 \cdot 10^{-5}$	$2.259 \cdot 10^{-4}$	$1.593 \cdot 10^{-3}$	170438	194420
	ST_Δψ	$1.331 \cdot 10^{-3}$	$1.316 \cdot 10^{-3}$	$1.181 \cdot 10^{-2}$		1950
	SS_Δψ_Δt	$8.607 \cdot 10^{-6}$	$3.525 \cdot 10^{-5}$	$3.899 \cdot 10^{-4}$	154597	392041
10^{-3}	SH_Δψ	$3.956 \cdot 10^{-3}$	$1.166 \cdot 10^{-2}$	0.125		1312
	SH_Δψ_Δt	$2.320 \cdot 10^{-4}$	$7.553 \cdot 10^{-4}$	$7.883 \cdot 10^{-3}$	52723	60303
	ST_Δψ	$2.241 \cdot 10^{-3}$	$5.702 \cdot 10^{-3}$	$1.792 \cdot 10^{-2}$		620
	SS_Δψ_Δt	$6.567 \cdot 10^{-5}$	$1.585 \cdot 10^{-4}$	$1.453 \cdot 10^{-3}$	9895	39110
10^{-2}	SH_Δψ	$6.559 \cdot 10^{-3}$	$1.716 \cdot 10^{-2}$	0.119		1018
	SH_Δψ_Δt	$2.224 \cdot 10^{-3}$	$7.923 \cdot 10^{-3}$	$7.111 \cdot 10^{-2}$	15540	17888
	ST_Δψ	$9.954 \cdot 10^{-3}$	$2.630 \cdot 10^{-2}$	$8.727 \cdot 10^{-2}$		243
	SS_Δψ_Δt	$8.283 \cdot 10^{-4}$	$2.271 \cdot 10^{-3}$	$1.478 \cdot 10^{-2}$	862	3804

Table 3: Relative errors and number of iterations obtained for the iterative algorithm depending on different convergence criteria for TC1.



Tol.	Algorithm	L₁	L₂	L_∞	N_{param}	N_{sol}
10 ⁻⁵	TA_T	5.016 10 ⁻³	2.376 10 ⁻²	0.269	32197	35938
	TA_S	6.152 10 ⁻⁶	2.429 10 ⁻⁵	2.561 10 ⁻⁴	9316700	9322946
10 ⁻⁴	TA_T	5.598 10 ⁻³	2.580 10 ⁻²	0.284	10169	11520
	TA_S	2.839 10 ⁻⁵	1.363 10 ⁻⁴	1.654 10 ⁻³	931616	938144
10 ⁻³	TA_T	1.524 10 ⁻²	7.085 10 ⁻²	0.822	3231	4032
	TA_S	2.537 10 ⁻⁴	1.271 10 ⁻³	1.568 10 ⁻²	93114	100898
10 ⁻²	TA_T	6.241 10 ⁻²	0.274	2.459	1023	1402
	TA_S	2.519 10 ⁻³	1.224 10 ⁻²	0.142	9267	18292

Table 4: Relative errors and number of iterations obtained for the time-adaptive algorithm depending on different convergence criteria for TC1.



Tol.	Algorithm	L₁	L₂	L_∞	N_{trunc}	N_{sol}
10 ⁻⁵	SH_Δψ	6.966 10 ⁻³	1.818 10 ⁻²	5.878 10 ⁻²		573
	SH_Δψ_Δt	3.697 10 ⁻⁴	9.766 10 ⁻⁴	3.332 10 ⁻³	53769	59643
	ST_Δψ	1.578 10 ⁻⁴	4.254 10 ⁻⁴	2.451 10 ⁻³		3503
	SS_Δψ_Δt	-	-	-	-	n. c.
10 ⁻⁴	SH_Δψ	6.966 10 ⁻³	1.818 10 ⁻²	5.878 10 ⁻²		509
	SH_Δψ_Δt	6.968 10 ⁻⁴	1.979 10 ⁻³	5.726 10 ⁻³	16557	18428
	ST_Δψ	5.814 10 ⁻⁴	1.492 10 ⁻³	6.711 10 ⁻³		1033
	SS_Δψ_Δt	3.279 10 ⁻⁶	1.239 10 ⁻⁵	8.603 10 ⁻⁵	0	2474120
10 ⁻³	SH_Δψ	6.966 10 ⁻³	1.818 10 ⁻²	5.878 10 ⁻²		410
	SH_Δψ_Δt	3.699 10 ⁻³	9.761 10 ⁻³	3.275 10 ⁻²	4830	5444
	ST_Δψ	1.553 10 ⁻³	4.226 10 ⁻³	2.457 10 ⁻²		317
	SS_Δψ_Δt	2.355 10 ⁻⁵	6.230 10 ⁻⁵	2.341 10 ⁻⁴	0	247426
10 ⁻²	SH_Δψ	6.892 10 ⁻³	1.800 10 ⁻²	5.780 10 ⁻²		309
	SH_Δψ_Δt	9.135 10 ⁻³	2.409 10 ⁻²	7.925 10 ⁻²	376	580
	ST_Δψ	2.756 10 ⁻³	1.134 10 ⁻²	7.715 10 ⁻²		180
	SS_Δψ_Δt	2.973 10 ⁻⁴	7.884 10 ⁻⁴	3.252 10 ⁻³	0	24757

Table 5: Relative errors and number of iterations obtained for the iterative algorithm depending on different convergence criteria for TC2 (n.c.: non convergence in less than 10⁷ iterations).



Tol.	Algorithm	L₁	L₂	L_∞	N_{param}	N_{sol}
10 ⁻⁵	TA_T	1.230 · 10 ⁻⁴	4.563 · 10 ⁻⁴	3.346 · 10 ⁻³	3089	3098
	TA_S	8.741 · 10 ⁻⁶	2.308 · 10 ⁻⁵	7.905 · 10 ⁻⁵	1136193	1136199
10 ⁻⁴	TA_T	1.572 · 10 ⁻³	4.497 · 10 ⁻³	2.404 · 10 ⁻²	986	987
	TA_S	2.701 · 10 ⁻⁵	7.219 · 10 ⁻⁵	3.095 · 10 ⁻⁴	113616	113616
10 ⁻³	TA_T	4.707 · 10 ⁻³	1.346 · 10 ⁻²	7.169 · 10 ⁻²	323	323
	TA_S	1.754 · 10 ⁻⁴	4.844 · 10 ⁻⁴	2.391 · 10 ⁻³	11358	11358
10 ⁻²	TA_T	5.220 · 10 ⁻³	1.683 · 10 ⁻²	0.101	135	135
	TA_S	1.596 · 10 ⁻³	4.444 · 10 ⁻³	2.243 · 10 ⁻²	1132	1132

Table 6: Relative errors and number of iterations obtained for the time-adaptive algorithm depending on different convergence criteria for TC2.



Tol.	Algorithm	L_1	L_2	L_∞	N_{trunc}	N_{sol}
10^{-5}	SH_Δψ	$9.994 \cdot 10^{-3}$	$1.119 \cdot 10^{-2}$	$1.554 \cdot 10^{-2}$		1644
	SH_Δψ_Δt	$6.612 \cdot 10^{-4}$	$7.346 \cdot 10^{-4}$	$1.116 \cdot 10^{-3}$	171636	190588
	ST_Δψ	$6.830 \cdot 10^{-4}$	$7.775 \cdot 10^{-4}$	$1.648 \cdot 10^{-3}$		16984
	SS_Δψ_Δt	$7.185 \cdot 10^{-5}$	$7.935 \cdot 10^{-5}$	$1.297 \cdot 10^{-4}$	197481	1646346
10^{-4}	SH_Δψ	$6.664 \cdot 10^{-3}$	$7.280 \cdot 10^{-3}$	$1.033 \cdot 10^{-2}$		1734
	SH_Δψ_Δt	$3.512 \cdot 10^{-3}$	$3.898 \cdot 10^{-3}$	$5.811 \cdot 10^{-3}$	57312	63956
	ST_Δψ	$1.300 \cdot 10^{-3}$	$1.517 \cdot 10^{-3}$	$2.412 \cdot 10^{-3}$		6504
	SS_Δψ_Δt	$5.380 \cdot 10^{-5}$	$6.536 \cdot 10^{-5}$	$1.010 \cdot 10^{-4}$	41073	186351
10^{-3}	SH_Δψ	-	-	-		n.c.
	SH_Δψ_Δt	$2.625 \cdot 10^{-3}$	$2.899 \cdot 10^{-3}$	$4.971 \cdot 10^{-3}$	22047	24779
	ST_Δψ	$4.730 \cdot 10^{-3}$	$5.422 \cdot 10^{-3}$	$1.036 \cdot 10^{-2}$		1297*
	SS_Δψ_Δt	$7.569 \cdot 10^{-4}$	$8.820 \cdot 10^{-4}$	$1.402 \cdot 10^{-3}$	16474	31276
10^{-2}	SH_Δψ	-	-	-		n.c.
	SH_Δψ_Δt	$5.493 \cdot 10^{-3}$	$6.306 \cdot 10^{-3}$	$1.171 \cdot 10^{-3}$	7438	8812
	ST_Δψ	$6.621 \cdot 10^{-3}$	$7.402 \cdot 10^{-3}$	$1.042 \cdot 10^{-2}$		810
	SS_Δψ_Δt	$7.511 \cdot 10^{-3}$	$8.780 \cdot 10^{-3}$	$1.378 \cdot 10^{-2}$	5838	7535

Table 7: Relative errors and number of iterations obtained for the iterative algorithm depending on different convergence criteria for TC3 (n.c.: non convergence in less than 10^7 iterations, * convergence failed for 10^{-3} , $\tau_r=0.90 \cdot 10^{-3}$).



Tol.	Algorithm	L₁	L₂	L_∞	N_{param}	N_{sol}
10 ⁻⁵	TA_T	9.814 10 ⁻³	9.949 10 ⁻³	1.286 10 ⁻²	8369	8703
	TA_S	7.980 10 ⁻⁵	8.797 10 ⁻⁵	1.472 10 ⁻⁴	1357075	1357160
10 ⁻⁴	TA_T	1.731 10 ⁻²	1.760 10 ⁻²	2.748 10 ⁻²	2653	2934
	TA_S	1.067 10 ⁻⁴	1.247 10 ⁻⁴	1.997 10 ⁻⁴	135386	135498
10 ⁻³	TA_T	2.922 10 ⁻²	3.105 10 ⁻²	4.545 10 ⁻²	889	1153
	TA_S	1.433 10 ⁻⁴	1.788 10 ⁻⁴	3.367 10 ⁻⁴	13314	13397
10 ⁻²	TA_T	1.996 10 ⁻²	2.449 10 ⁻²	5.536 10 ⁻²	347	515
	TA_S	1.851 10 ⁻³	2.051 10 ⁻³	3.925 10 ⁻³	1232	1283

Table 8: Relative errors and number of iterations obtained for the time-adaptive algorithm depending on different convergence criteria for TC3.



List of Figures

Figure 1: Relative hydraulic conductivity as a function of the pressure for the three test cases (L1, L2 and L3 are the three layers for test case 3).

Figure 2: Water saturation as a function of the pressure for the three test cases (L1, L2 and L3 are the three layers for test case 3).

Figure 3: Specific moisture capacity as a function of the pressure for the three test cases (L1, L2 and L3 are the three layers for test case 3).

Figure 4: Evolution of the L_2 relative error with computational costs for TC1.

Figure 5: Pressure profiles in the domain for the TA_T algorithm.

Figure 6: Evolution of the L_2 relative error with computational costs for TC2.

Figure 7: Time step magnitudes during the simulation for TC2.

Figure 8: Evolution of the L_2 relative error with computational costs for TC3.

Figure 9: Time step magnitudes during the simulation for TC3 for the time stepping strategy based on truncation error (TA_S in blue, TA_T in black, time varying boundary conditions at the top).

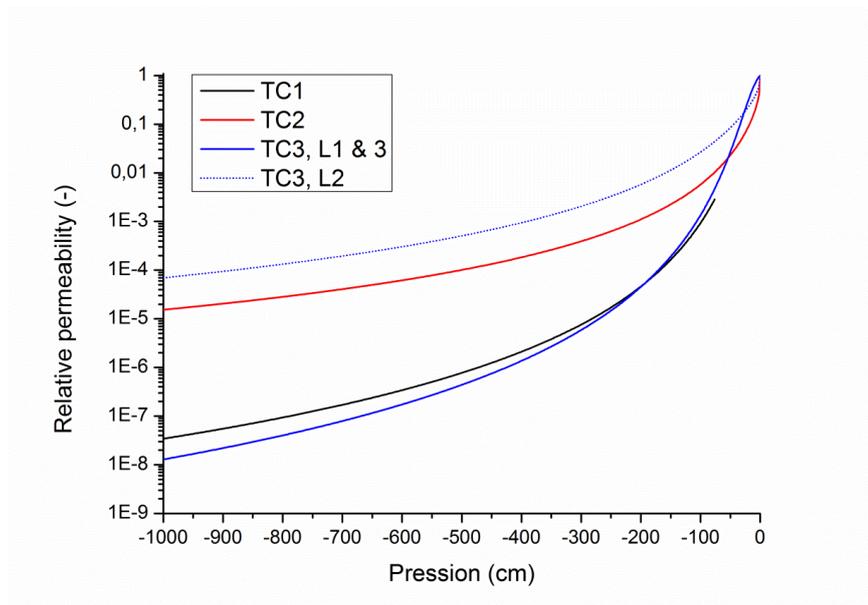


Figure 1: Relative permeability as a function of the pressure for the three test cases (L1, L2 and L3 are the three layers for test case 3).

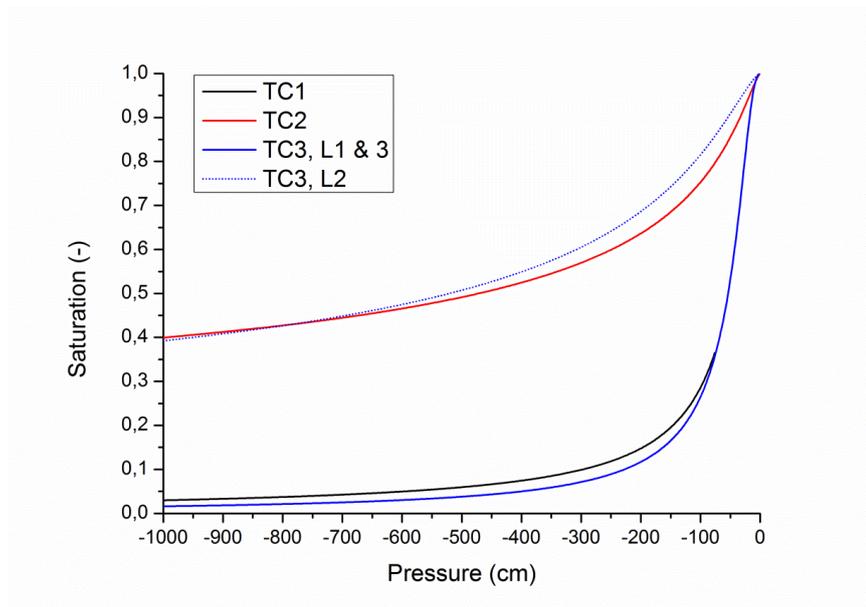


Figure 2: Water saturation as a function of the pressure for the three test cases (L1, L2 and L3 are the three layers for test case 3).

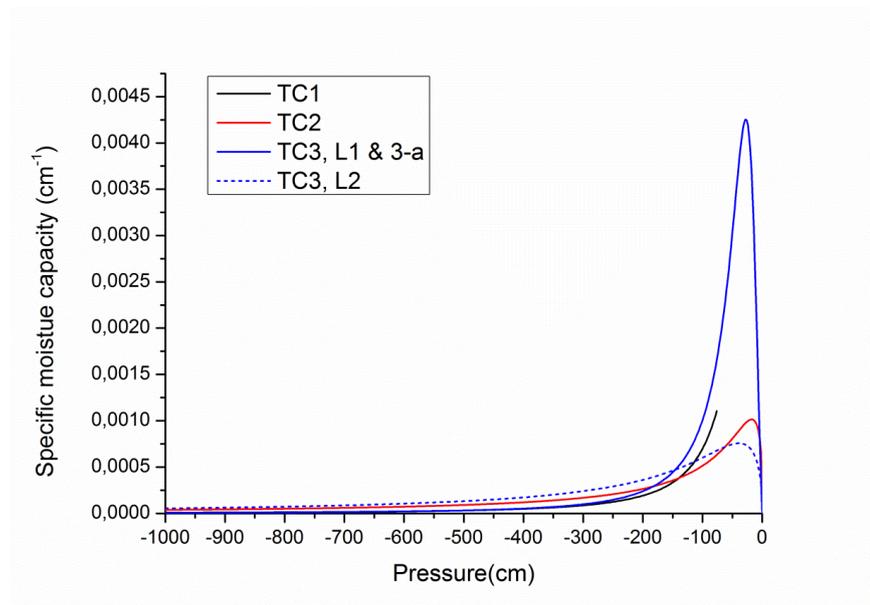


Figure 3: Specific moisture capacity as a function of the pressure for the three test cases (L1, L2 and L3 are the three layers for test case 3).

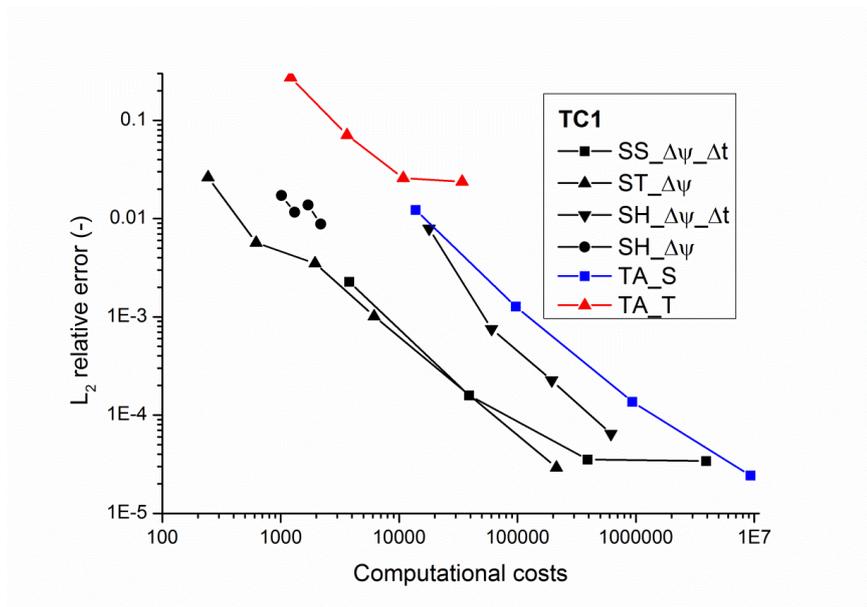


Figure 4: Evolution of the L_2 relative error with computational costs for TC1.

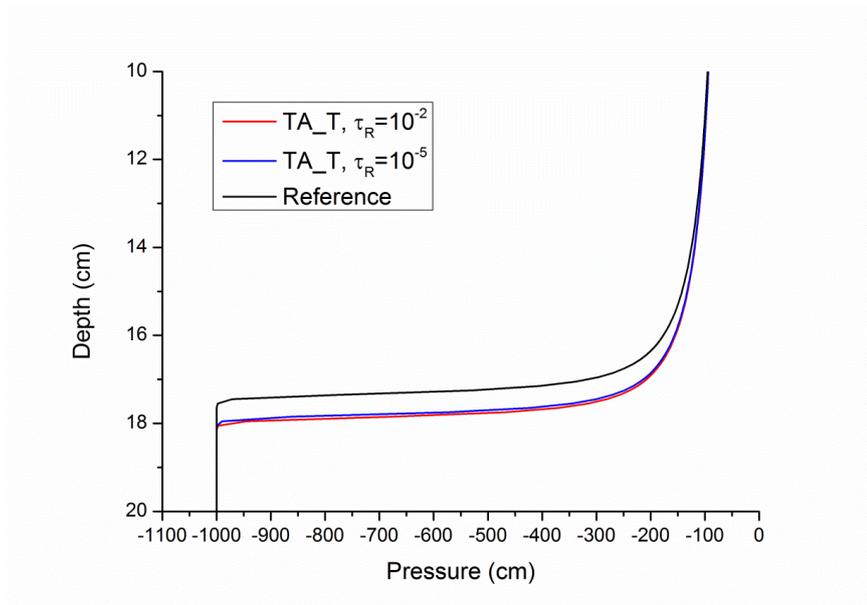


Figure 5: Pressure profiles in the domain for the TA_T algorithm.

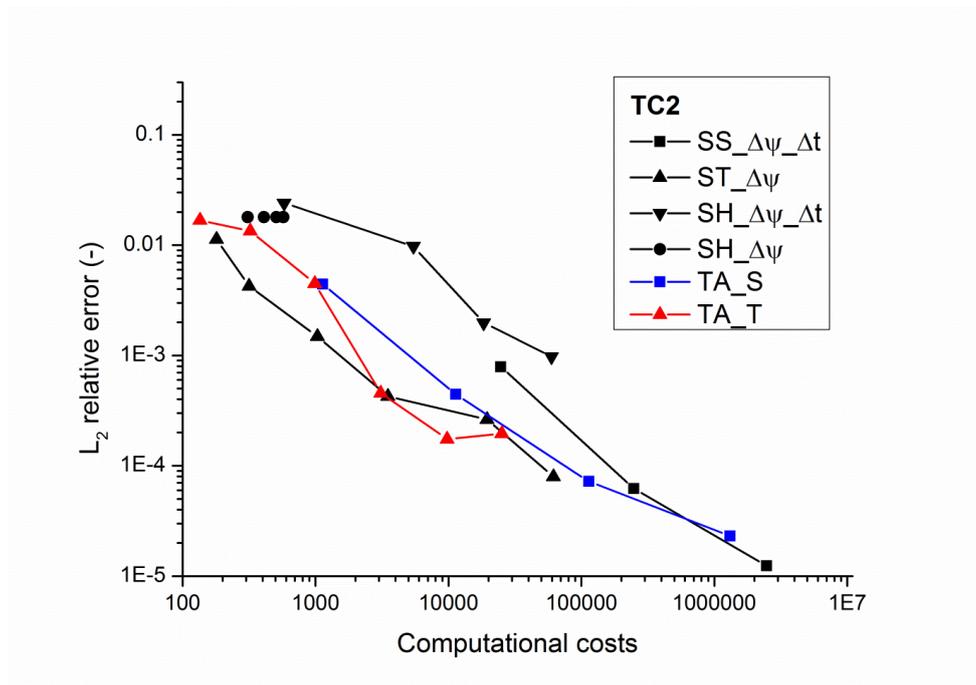


Figure 6: Evolution of the L_2 relative error with computational costs for TC2.

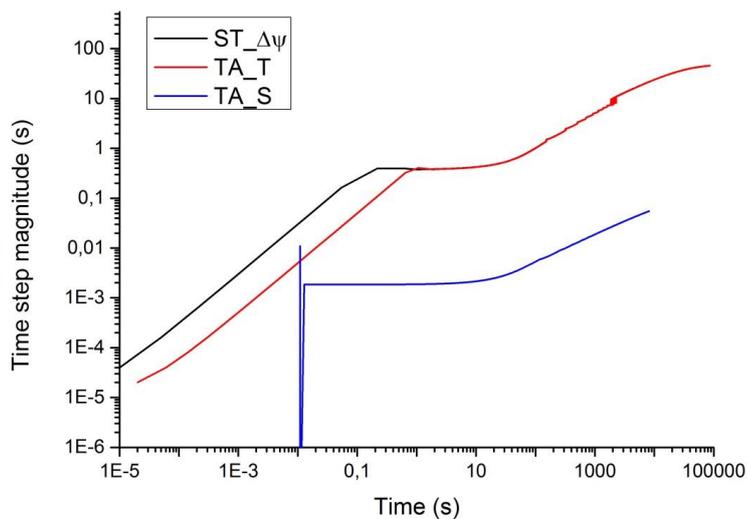


Figure 7: Time step magnitudes during the simulation for TC2.

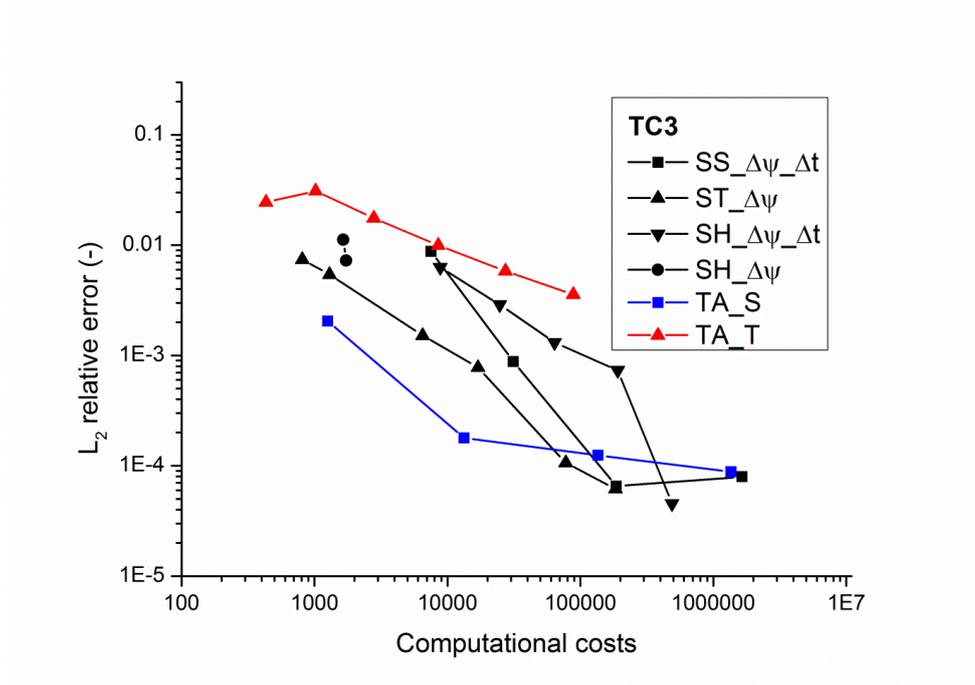


Figure 8: Evolution of the L_2 relative error with computational costs for TC3.

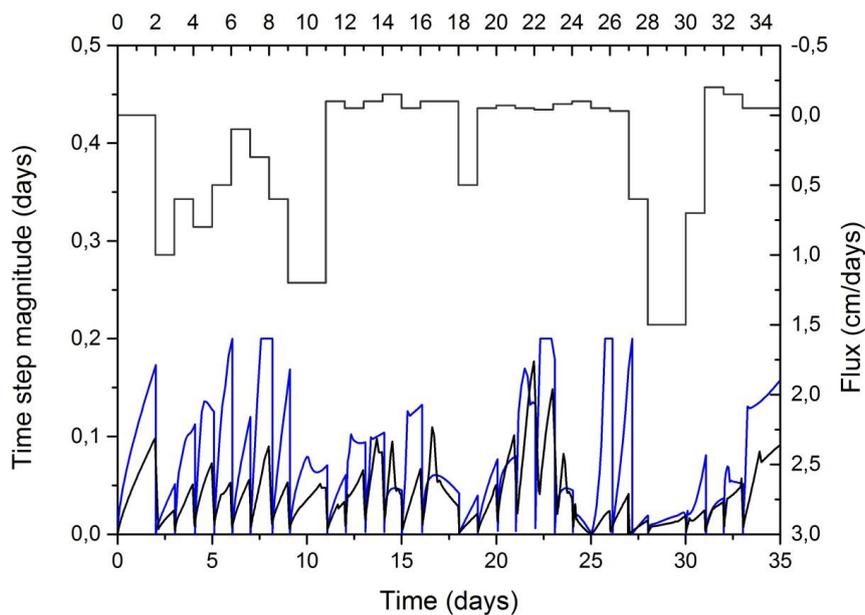


Figure 9: Time step magnitudes during the simulation for TC3 for the time stepping strategy based on truncation error (TA_S in blue, TA_T in black, time varying boundary conditions at the top).