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Implementation of quadratic upstream interpolation schemes for solute transport into HYDRUS-1D

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ABSTRACT

Numerical solution of the advection–dispersion equation, used to evaluate transport of solutes in porous media, requires discretization schemes for space and time stepping. We examine use of quadratic upstream interpolation schemes QUICK, QUICKEST, and the total variation diminution scheme ULTIMATE, and compare these with UPSTREAM and CENTRAL schemes in the HYDRUS-1D model. Results for purely convective transport show that quadratic schemes can reduce the oscillations compared to the CENTRAL scheme and numerical dispersion compared to the UPSTREAM scheme. When dispersion is introduced all schemes give similar results for Peclet number $Pe < 2$. All schemes show similar behavior for non-uniform grids that become finer in the direction of flow. When grids become coarser in the direction of flow, some schemes produce considerable oscillations, with all schemes showing significant clipping of the peak, but quadratic schemes extending the range of stability tenfold to $Pe < 20$. Similar results were also obtained for transport of a non-linear retarded solute transport (except the QUICK scheme) and for reactive transport (except the UPSTREAM scheme). Analysis of transient solute transport show that all schemes produce similar results for the position of the infiltration front for $Pe = 2$. When $Pe = 10$, the CENTRAL scheme produced significant oscillations near the infiltration front, compared to only minor oscillations for QUICKEST and no oscillations for the ULTIMATE scheme. These comparisons show that quadratic schemes have promise for extending the range of stability in numerical solutions of solute transport in porous media and allowing coarser grids.

1. Introduction

The transport of solutes in soils is usually described using the advection–dispersion equation, with extra terms to account for adsorption and reactions (Šimůnek and van Genuchten, 2006; Zheng and Bennett, 2002). The form of these extra terms varies according to the constituents and soil types and can take forms such as linear or non-linear adsorption, or first- and second-order reactions. The one-dimensional convection–dispersion equation of a solute is described by:

$$\frac{\partial C}{\partial t} = -\frac{\partial (uC)}{\partial x} + \frac{\partial}{\partial x}\left(D\frac{\partial C}{\partial x}\right) + S \qquad (1)$$

where t is time [T], C is a solute concentration [M L^{-3}], u is the velocity of the fluid [L T^{-1}], D is the dispersion coefficient [L^2 T^{-1}], x is the space dimension [L], and $S(C, x, t)$ is a source/sink term, accounting for reactions [M L^{-3} T^{-1}]. Although in the examples described below more complex forms of the convection–dispersion equation are used (e.g. with variable water contents and/or linear/non-linear retardation factors), the simpler form shown in Eq. (1) is used here to simplify the description of the numerical methods.

For most problems of interest, when water flow is transient, and soil properties and initial conditions are non-uniform, analytical solutions are generally not available and/or cannot be derived, so numerical methods must be employed for the solution of the governing equations (Vanderborght et al., 2005). Numerical methods are in general more suitable for solving practical problems involving complicated geometries that reflect complex natural geologic and hydrologic conditions, spatially and temporarily

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variable flow and transport parameters, more realistic initial and boundary conditions, and/or non-linear constitutive relationships (Šimůnek and van Genuchten, 2006). However, numerical modeling of advection dominated problems in the presence of discontinuities and steep concentration fronts is not trivial (Leonard, 1979, 1991) and robust numerical methods are still being sought.

A large number of methods are available to solve Eq. (1) numerically, but they can be broadly grouped as Eulerian, Lagrangian, and mixed Lagrangian–Eulerian methods. In the Eulerian methods, the transport equation is discretized by means of a finite difference or finite element method on a fixed grid system, while for the Lagrangian approach the mesh moves along with the flow or remains fixed in a deforming coordinate system. In the Lagrangian-Eulerian approach, a two-step method is used. The first step is to estimate convective transport using particle trajectories in a Lagrangian approach, with all other processes modeled with an Eulerian approach in the following step (Šimůnek, 2005). While Lagrangian methods are widely used when simulating transport in groundwater, the most common methods used to solve Eq. (1) for transport in unsaturated zone are Eulerian, including methods of finite differences, finite elements, and/or finite volumes, and these are the methods solely discussed here. Many groundwater flow problems are either steady-state problems or problems with gradually changing flow fields in time, and use relatively coarse spatial discretization. The Lagrangian methods are either well suited for such conditions (former) or even required (latter), because of the stability constraints on Eulerian methods. On the other hand, the flow problems in the vadose zone are inherently transient with quickly changing water contents and velocities in time and space. Eulerian methods are often considered suitable for such conditions, since the numerical solution of the highly non-linear Richards equation often requires stricter constrains on temporal and spatial discretization than groundwater flow problems.

The finite difference method can be used to solve the advection–dispersion equation either using backward, forward, or central temporal differencing. However, for certain problems such as convection-dominated transport or the transport of steep fronts this method can lead to artificial oscillations (under or over shooting) or numerical dispersion due to truncation errors of the discretization. The use of forward differencing in the temporal discretization (explicit method) can often lead to non-convergent schemes. If a backward scheme (implicit formulation) is chosen, the method is always convergent but can result in numerical oscillations in the form of "wiggles" with under and over shooting of the solution (Leonard, 1979). The use of central differencing (such as Crank–Nicholson schemes) improves accuracy but is more computational expensive than explicit methods and is still prone to numerical oscillation. Numerical oscillation can be minimized by the use of upstream weighting, but this can lead to considerable numerical dispersion owing to truncation errors (e.g. Zheng and Bennett, 2002).

One alternative is the introduction of an apparent numerical diffusion coefficient, to artificially damp the numerical dispersion introduced by the discretization (Huang et al., 1997; Moldrup et al., 1994; van Genuchten and Gray, 1978), but this can only be used for simple problems where the numerical dispersion coefficient can be estimated (Zheng and Bennett, 2002). The introduction of artificial damping also affects the accuracy of the method (Leonard, 1979). Another solution to problems with artificial oscillations is the use of finer grids, with a choice based on the dimensionless Peclet number:

$$Pe = u \cdot \Delta x / D \tag{2}$$

where Δx is the grid spacing. Spatial discretization resulting in a *Pe* number smaller than 2 can eliminate numerical oscillations, while a *Pe* number smaller than 10 can greatly reduce such oscillations. However, the associated computational cost due to excessively fine grids may become impractical in some applications (Huyakorn and Pinder, 1986) usually associated with groundwater flow, multi-dimensional calculations, or multi-component solute transport.

Two methods that potentially can be used to overcome these oscillation and truncation problems were proposed by Leonard (1979), using quadratic upstream interpolation to solve the advection diffusion equation. These explicit methods are known as QUICK (**Q**uadratic **U**pstream **I**nterpolation for **C**onvective **K**inematics) and QUICKEST method (QUICK with **E**stimated **U**pstream **T**erms). Both schemes have little numerical dispersion, and the later scheme has a large (in comparison to other methods) stability region and shows minimal oscillations.

In many applications the presence of even minimal oscillations (such as negative concentrations) can corrupt the solution. As noted by Leonard (1991), there exists a large family of schemes that aim to suppress such oscillations, commonly referred to as Total Variation Diminution (TVD) schemes (e.g. MUSCL (Van Leer, 1979); Superbee (Roe, 1985)). Leonard (1991) derived a scheme to improve the solution near steep gradients and remove under and over shoot problems by preserving local monotonicity. This scheme is known as ULTIMATE (the **U**niversal **L**imiter for **T**ransient **I**nterpolative **M**odeling of **A**dvective **T**ransport **E**quation). While these three methods by Leonard (1979, 1991) have been used widely in a broad range of convection–dispersion problems in hydrodynamics and computational fluid mechanics (e.g. Cole and Wells, 2006; Lin and Falconer, 1997; Romero et al., 2004), the use of TVD schemes in the subsurface hydrology has been limited to only few studies. In porous media the non-monotonic QUICK and QUICKEST schemes have been used in groundwater (Carter et al., 1984; Lin and Medina, 2003) and QUICK in soil (Chu and Marino, 2007), with the ULTIMATE scheme used for groundwater (Zheng and Wang, 1999) and soils (Neumann et al., 2009).

The objective of this study is to demonstrate the implementation of the explicit QUICK, QUICKEST, and ULTIMATE schemes into HYDRUS-1D (Šimůnek et al., 2008a), one of the most widely used flow and transport programs in vadose zone hydrology. The implementation of the quadratic schemes is verified for a series of problems of increasing complexity, against analytical solutions for purely convective transport problems and against standard implicit schemes in HYDRUS-1D for non-linear transport or transient flow problems. Performance of the numerical schemes for uniform and non-uniform grids, uniform and non-uniform velocities, reactive transport and other conditions will be discussed. The results will demonstrate the improvements provided by some of the quadratic schemes for situations of larger Peclet numbers or steep fronts, where non-oscillatory behavior is attained.

2. Methods

In this section the QUICK, QUICKEST, and ULTIMATE schemes, and the main ideas behind them, are briefly introduced. Complete descriptions are presented by Leonard (1979, 1991), while the other methods implemented in HYDRUS-1D are also discussed in detail elsewhere (Šimůnek et al., 2008a). The QUICK and QUICKEST schemes, both explicit methods, for the solution of Eq. (1) are derived using a control-volume approach for spatial discretization and finite differences approach for temporal discretization of Eq. (1). This results in the requirement to calculate the discrete fluxes entering and leaving the control-volume, or the so-called face values, associated with a node within the grid. The control-volume for node *i*, and upstream and downstream nodes are defined as shown in Fig. 1.

Using definitions from Fig. 1, the concentration at a nodal point *i* for a new time level $(j + 1)$ can be calculated as:

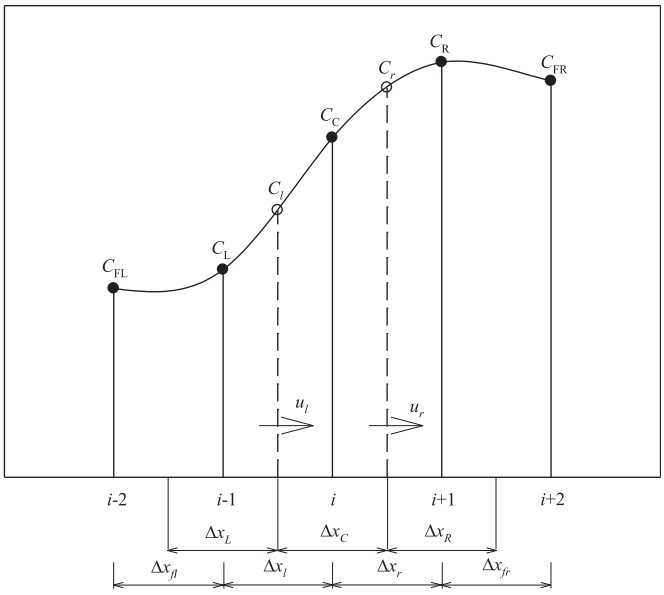

Fig. 1. Schematic showing a control-volume for node *i* (indicated by the dashed lines), concentrations C at upstream and downstream nodes, grid spacing and face velocities (u_l, u_r). Subscripts *FL*, *L*, *C*, *R*, and *FR* refer to the far left, left, central, right, and far right nodes. Subscripts *l* and *r* refer to the left and right faces.

$$C_i^{j+1} = C_i^j + \frac{\Delta t}{\Delta x_C}\left(u_l C_l^* - u_r C_r^* - D_l\left(\frac{\partial C}{\partial x}\right)_l^* + D_r\left(\frac{\partial C}{\partial x}\right)_r^*\right) + \Delta t\bar{S} \tag{3}$$

where superscripts *j* and $j+1$ refer to previous and new time levels, Δt is the time step, C_l^* and C_r^* are concentrations at the left (l) and right (r) faces of the finite volume *i*, $\bar{S}$ is the average sink term for the control-volume during the time step, D_l and D_r are corresponding dispersion coefficients, and $(\partial C/\partial x)_l^*$ and $(\partial C/\partial x)_r^*$ are associated concentration gradients. The estimation of the face and gradient values is discussed below.

2.1. The QUICK method

The QUICK method uses a quadratic upstream interpolation to obtain face values of concentrations as shown in Fig. 2. The method can be interpreted as a linear interpolation, given by the first term on the right hand side of Eq. (4), corrected by a term proportional to the upstream-weighted curvature, given by the second term on the right hand side.

For flow to the right and for uniform grids the face values are estimated as:

$$\begin{aligned} C_l^* &= \frac{1}{2}(C_L + C_C) - \frac{1}{8}(C_{FL} + C_C - 2C_L) \\ C_r^* &= \frac{1}{2}(C_C + C_R) - \frac{1}{8}(C_L + C_R - 2C_C) \end{aligned} \tag{4}$$

and for non-uniform grids we obtain:

$$\begin{aligned} C_l^* &= \frac{1}{2}(C_L + C_C) - \frac{\Delta x_l^2}{8}\frac{1}{\Delta x_L}\left(\frac{C_C - C_L}{\Delta x_l} - \frac{C_L - C_{FL}}{\Delta x_{fl}}\right) \\ C_r^* &= \frac{1}{2}(C_C + C_R) - \frac{\Delta x_r^2}{8}\frac{1}{\Delta x_C}\left[\frac{C_R - C_C}{\Delta x_r} - \frac{C_C - C_L}{\Delta x_l}\right] \end{aligned} \tag{5}$$

The general formula for the QUICK scheme is shown in Eq. (6). Note that the QUICK scheme uses the concentrations at the beginning of the time step to calculate the face values.

$$\begin{aligned} C_l^* &= \frac{1}{2}(C_L + C_C) - \frac{\Delta x_l^2}{8}Curv_l = \frac{1}{2}(C_L + C_C) - \frac{\Delta x_l^2}{8}\left[\frac{1}{\Delta x_L}\left(Grad_l - Grad_{fl}\right)\right] \\ C_r^* &= \frac{1}{2}(C_C + C_R) - \frac{\Delta x_r^2}{8}Curv_r = \frac{1}{2}(C_C + C_R) - \frac{\Delta x_r^2}{8}\left[\frac{1}{\Delta x_C}(Grad_r - Grad_l)\right] \end{aligned} \tag{6}$$

where *Curv* represents (upstream-weighted) concentration curvatures and *Grad* concentration gradients (compare Eq. (5) and (6) for their definitions). Similar equations can be derived for flow in the opposite direction (to the left). For the QUICK scheme, the concentration gradients in Eq. (3) are identical to the ones used in Eq. (6). As discussed by Leonard (1979), the stability criteria for QUICK are more restrictive than in the case of central differencing, but in theory QUICK can be used for cases when $Pe > 2$. However, as will be shown in the next section, the QUICK method is still prone to oscillations.

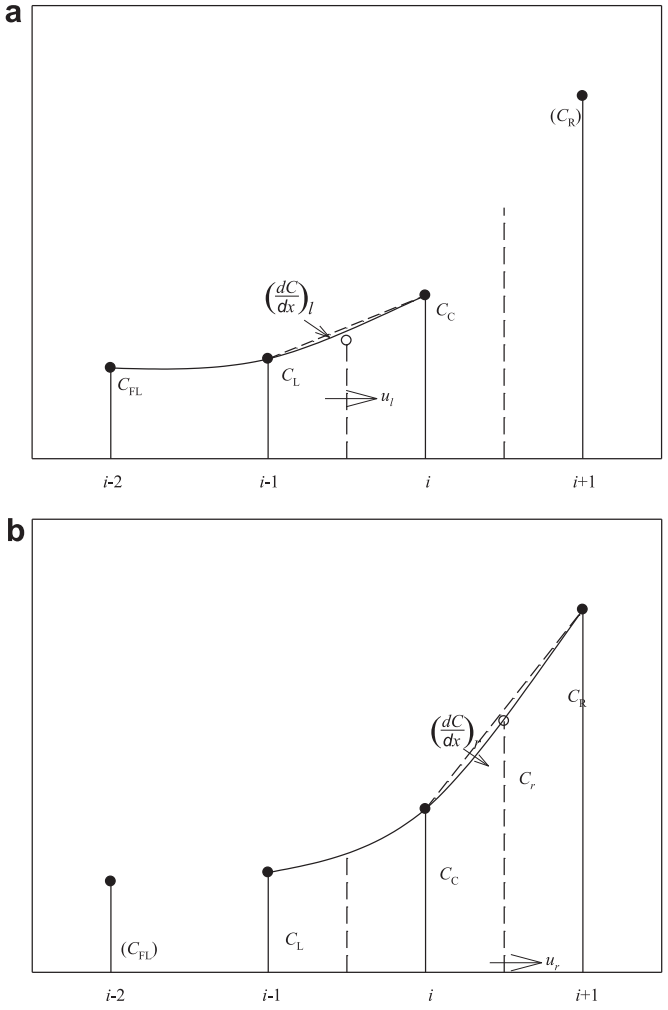

Fig. 2. Quadratic upstream interpolation for face values of concentrations C_l (a) and C_r (b), and definition of face concentration gradients $(\partial C/\partial x)_l$ and $(\partial C/\partial x)_r$ used by the QUICK method (Leonard, 1979).

2.2. The QUICKEST method

Rather than using the quadratic upstream interpolation only at the old-time level to obtain face concentration values as in the QUICK scheme, the QUICKEST method attempts to obtain these values as an average over a time increment Δt between the old and new time levels. The average face concentrations are estimated assuming that the concentration profile approximated using the quadratic upstream interpolation at the old-time level is "swept" downstream unchanged, as shown in Fig. 3. The QUICKEST formulation uses the same approach of averaging over a time step for the physical diffusion terms and the effect of diffusion on wall values.

This leads to the following definition of the right face concentration and concentration gradient values, respectively:

$$C_r^* = \frac{1}{2}(C_C + C_R) - \frac{\Delta x_r}{2}Co_r Grad_r + \frac{\Delta x_r^2}{2}\left[\chi_r - \frac{1}{3}\left(1 - Co_r^2\right)\right]Curv_r \tag{7}$$

$$\left(\frac{\partial C}{\partial x}\right)_r^* = Grad_r - \frac{\Delta x_r}{2}Co_r Curv_r \tag{8}$$

where *Grad* and *Curv* are defined as above. Similar equations can be derived for the left face values and for flow in the opposite direction (to the left).

Eq. (7) and (8) contain two dimensionless terms, the Courant number and the diffusion parameter χ, defined respectively as:

$$Co_r = \frac{u_r \Delta t}{\Delta x} \tag{9}$$

$$\chi_r = \frac{D_r \Delta t}{\Delta x_r^2} \tag{10}$$

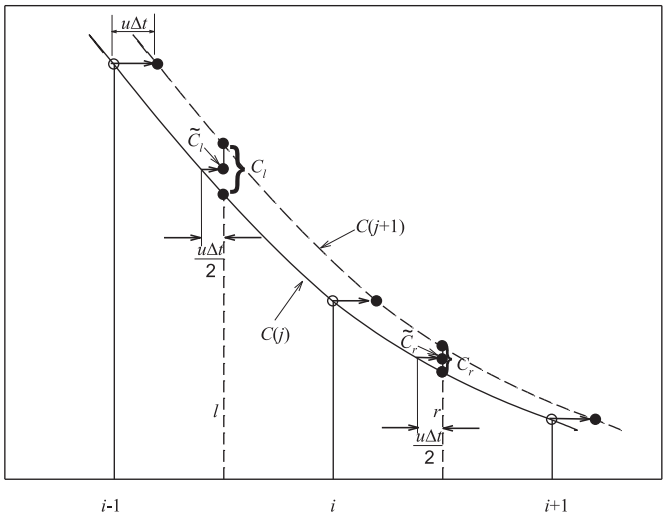

Fig. 3. Control-volume face values C_l and C_r are estimated in the QUICKEST method as an average of $C(j)$ and $C(j+1)$. $C(t+\Delta t)$ is obtained by simply translating $C(t)$ to the right by a distance $u\Delta t$, assuming pure (retarded, when adsorption is considered) convection.

Leonard (1979) demonstrated that the QUICKEST method is stable in the (Co,χ) plane if $0 \le Co \le 1$ and $0 < \chi \le 0.5$. The stability region is extended to parts of the (Co,χ) plane if $Co > 1$ and $\chi < 0.5$, and to $\chi > 0.5$ if $Co < 1$. The method is also stable for the region where pure convective flow dominates ($\chi = 0$) if the Courant number does not exceed unity.

The adoption of the estimated upstream terms using the new time level in the QUICKEST scheme greatly reduces the amount of over and under shooting and numerical dispersion. However, as demonstrated in the next sections and also by Leonard (1991) the QUICKEST method is still prone to small oscillations and/or overshooting, especially near sharp gradients. The presence of such oscillations can lead to negative concentration values. The presence of these oscillations can be eliminated by using a scheme that preserves local monotonic resolution.

2.3. The ULTIMATE method

The ULTIMATE method adopted here aims to suppress oscillation by using a TVD scheme to preserve local monotonicity of the solution. The ULTIMATE scheme is derived using the Normalized Variation Diagram (NVD) concept, based on normalized variables defined as:

$$C_C^{\text{norm}} = \frac{C_C^j - C_U^j}{C_D^j - C_U^j} \tag{11}$$

$$C_f^{\text{norm}} = \frac{C_r^* - C_U^j}{C_D^j - C_U^j} \tag{12}$$

where C_U^j and C_D^j are the concentration upstream and downstream of the central node "C" at time step "j". The ULTIMATE scheme uses the normalized variables from the NVD concept to set the boundaries, between which each nodal value must remain to suppress oscillations. Fig. 4 shows the necessary conditions imposed on C_c^{norm} used in the ULTIMATE scheme to preserve monotonicity, based on the fact that $C_D^{\text{norm}} = 1$ and $C_U^{\text{norm}} = 0$.

In order to preserve monotonicity, the following limits for the maximum normalized face values are:

$$C_C^{\text{norm}} \le C_f^{\text{norm}} \le 1 \quad \text{for} \quad 0 \le C_C^{\text{norm}} \le 1 \tag{13}$$

$$C_f^{\text{norm}} \le \frac{C_C^{\text{norm}}}{Co} \quad \text{for} \quad 0 < C_C^{\text{norm}} \le 1 \tag{14}$$

If $C_c^{\text{norm}} < 0$ or $C_c^{\text{norm}} > 1$, it is simple to just set $C_f^{\text{norm}} = C_C^{\text{norm}}$, which is the equivalent of setting the wall face value to the node value. The adoption of the ULTIMATE strategy involves minimal extra computational load and as will be shown in the following section, it avoids oscillations that could lead to appearance of negative concentrations near steep fronts.

2.4. Implicit schemes used in HYDRUS-1D

The governing flow and transport equations are solved in HYDRUS-1D numerically using Galerkin-type linear finite element schemes. Mass lumping is invoked by redefining the nodal values of the time derivative as weighted averages over the entire flow region. The Galerkin method is used only for approximating the spatial derivatives while the time derivatives are discretized by means of finite differences. Different finite difference schemes can be selected by users depending upon the value of the time-weighting coefficient ϵ (=0: explicit scheme, = 0.5: Crank–Nicholson scheme, = 1: fully implicit scheme). Higher-order approximations for the time derivative in the transport equation as derived by van Genuchten and Gray (1978) are implemented.

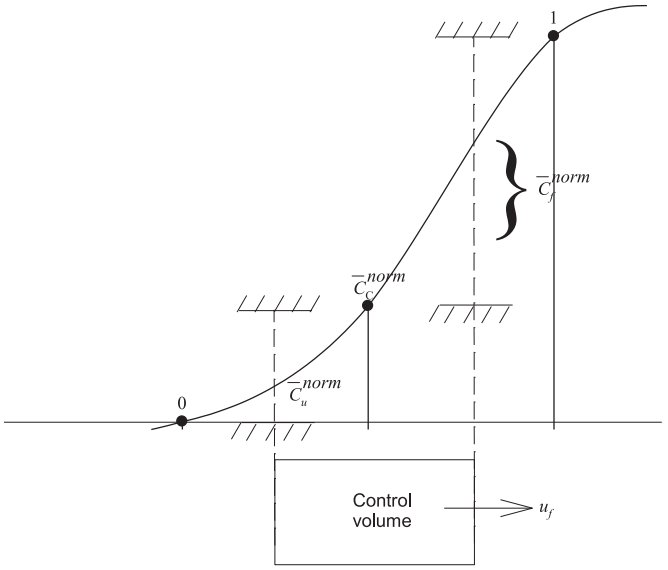

Fig. 4. Normalized node values in the case of locally monotonic behavior. Hatching shows necessary conditions on the face value of interest C_f^{norm}, and on the corresponding upstream control-volume face value C_u^{norm} (Leonard, 1991).

Upstream weighing is provided as an option in HYDRUS-1D to minimize some of the problems with numerical oscillations when relatively steep concentration fronts are being simulated. For this purpose the flux term of Eq. (1) is not weighted using regular linear basis functions, but instead with the special non-linear functions that ensure that relatively more weight is placed on the flow velocities of nodes located at the upstream side of an element. The extent of increased weight on upstream nodes is evaluated using the equation of Christie et al. (2005); a larger weight is placed on upstream nodes for larger Peclet numbers and a standard weight is placed on them for small Peclet numbers.

The acronym CENTRAL is used below in the Results Section for the Crank–Nicholson implicit scheme with central spatial differencing. The acronym UPSTREAM is used below for the Crank–Nicholson implicit scheme with upstream spatial weighting. The results obtained using the quadratic explicit schemes (i.e., QUICK, QUICKEST, and ULTIMATE) are compared only with the results obtained using the Crank–Nicholson implicit schemes, since these schemes are considered either less prone to numerical instabilities or superior in view of solution precision than explicit and fully explicit schemes, respectively (Šimůnek et al., 2008a). Note that the explicit scheme, although in general available in HYDRUS-1D, is disabled in its graphical user interface, in order to discourage HYDRUS-1D users from its use.

3. Results

Implementation into HYDRUS-1D of various quadratic upstream interpolation schemes, i.e., QUICK, QUICKEST, and ULTIMATE, and their performance is verified in this section on multiple problems of increasing complexity. The first set of problems involves challenging purely convective transport with uniform grids and velocities, with the results compared against analytical solutions.

The second set of problems introduces dispersion and non-uniformity of grids, with results compared against the results obtained using the standard implicit finite element numerical schemes of HYDRUS-1D that have been verified many times before (e.g. Scanlon et al., 2002; Šimůnek et al., 2008a; Vanderborght et al., 2005). In particular, the central spatial weighting and the Crank–Nicholson temporal differencing are used for this purpose.

The final set of more complex problems involves cases with transient water flow, non-uniform velocities and reactions. All results discussed below, other than those in which negative concentrations were set to zero, were mass conservative and produced mass balance errors significantly less than 1% for the overall simulations over the entire domain.

Boundary conditions for the quadratic schemes are prescribed by either assigning a node concentration value (Dirichlet) or a cell face concentration value as described in Tkalich (2006, 2007). From the point of view of numerical stability, both Dirichlet and Cauchy boundary conditions behaved similarly and did not present any problems. All problems presented here used a Dirichlet boundary condition, with the exception of the last problem where we have used a Cauchy boundary condition by prescribing the flux at the boundary and used a zero concentration gradient at the bottom.

3.1. Purely convective transport

As outlined in previous sections, standard numerical schemes, such as Crank–Nicholson Finite Element (or Finite Difference) schemes with central spatial differencing are not suited to deal with purely convective flow, producing spurious oscillations. The quadratic upstream interpolation schemes presented here were designed to overcome partly or fully this oscillatory behavior. We compare below these new numerical schemes using two test examples involving (a) a unit step change at the boundary (Leonard, 1991), and (b) the transport of an isolated sine-squared wave (Sweby, 1984). Results obtained using standard implicit schemes are shown for comparison.

3.1.1. A unit step change at the boundary

A unit step change in concentration at the boundary at time zero represents a basic test for most numerical schemes. The following physical parameters are used in this example. The transport domain is 1 m long and is discretized using 101 nodes ($\Delta x = 0.01$). Since dispersion, D, is assumed to be zero, the Peclet number ($Pe = v\Delta x/\mathrm{D}$) is equal to infinity. Mean pore water velocity, v, is assumed to be equal to 1 m/d. A constant time step (Δt) of 0.001 d is used and the final time ($t_{\max}$) is 0.5 d. The corresponding Courant number ($Co = v\Delta t/\Delta x$) is equal to 0.1.

Fig. 5 compares results obtained using the implicit schemes (i.e., CENTRAL and UPSTREAM) with the explicit schemes (QUICK, QUICKEST and ULTIMATE) and the analytical solution. The CENTRAL scheme shows, as expected, clear oscillations behind the concentration step, with a maximum oscillation wave on the order of 0.2. Oscillations, propagating all the way toward the inflow boundary, would keep increasing for longer simulation times, eventually corrupting the entire solution. On the other hand, the UPSTREAM scheme shows, again as expected, a very gradual change of concentrations around the front, rather than the abrupt change as predicted by the analytical solution. While this scheme is monotonic, i.e., it does not display any oscillations, it clearly introduces large artificial numerical dispersion, which is an inherent property of this numerical scheme.

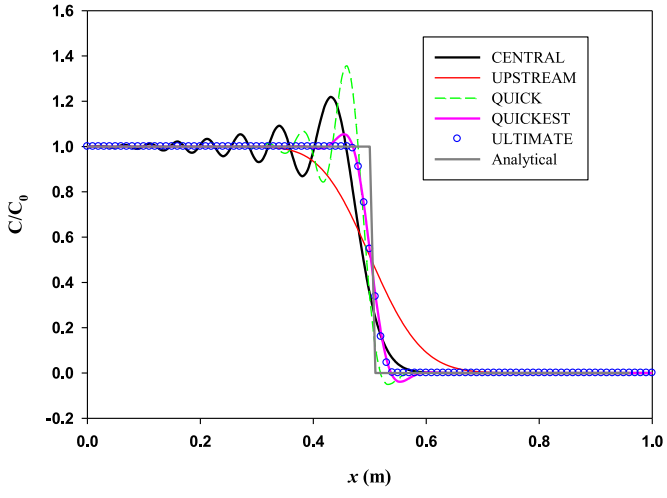

Fig. 5. Comparison of various numerical schemes (CENTRAL, UPSTREAM, QUICK, QUICKEST, and ULTIMATE) against the analytical solution for a unit step change example.

The QUICK scheme shows the largest oscillations both in front of and behind the traveling concentration step (the largest oscillation is about 0.4). Compared to the CENTRAL scheme, oscillations quickly dissipate toward the inflow boundary. The sharp change in concentrations is better approximated than by the CENTRAL scheme. Leonard (1979) suggests that oscillations in the QUICK method are less likely to corrupt the solution.

The QUICKEST scheme significantly reduces oscillations toward the inflow (there is actually only a single overshoot wave of about 0.05) compared to the QUICK scheme, while preserving a good approximation of the step increase due to small numerical dispersion. Finally, the ULTIMATE scheme entirely removes the oscillations both in front of and behind the concentration step, while still preserving a good description of the concentration step. Since all these results correspond closely with results of Leonard (1991), we can conclude that all three new explicit numerical schemes were likely implemented into HYDRUS-1D correctly.

3.1.2. An isolated sine-squared wave

While in the previous test example, the concentration change was imposed using the boundary condition, in this example concentrations are specified using the initial condition. This test follows Sweby (1984) by specifying an isolated sine-squared wave of width $20\Delta x$ as an initial condition:

$$\begin{aligned} C(x, t = 0) &= \sin^2\left(\frac{\pi x}{20\Delta x}\right) \quad \text{for} \quad 0 \le x \le 20\Delta x \\ &= 0 \qquad\qquad\qquad\quad \text{otherwise} \end{aligned} \tag{15}$$

This function represents a relatively smooth profile with a continuously changing gradient on both sides of a single local maximum (Leonard, 1991). All other physical conditions, i.e., spatial and temporal discretizations and velocity, are the same as for the unit step change example.

Fig. 6 compares results obtained using the implicit schemes with the explicit schemes and the analytical solution. Two solutions are shown with the CENTRAL scheme, one where negative concentrations are not allowed (by resetting them to zero; denoted CENTRAL1), and a second denoted CENTRAL2 without any resetting. Apart from minor oscillations behind the traveling wave, the standard CENTRAL scheme shows a very good approximation of the traveling sine-squared wave. When negative concentrations are not allowed (by resetting them to zero), the CENTRAL1 scheme shows an almost perfect description of the traveling wave. The UPSTREAM scheme shows, again as expected, an unacceptably large clipping (underestimation of maximum concentrations) of the concentration peak due to numerical dispersion, even though the scheme is monotonic and free of any oscillations.

The worst results were obtained using the QUICK scheme that quite dramatically overestimated the concentration peak, as well as displayed significant oscillations behind the traveling wave. Once again, the QUICKEST scheme improves on the QUICK results, with an almost perfect description of the traveling wave. It shows a small amount of clipping as it slightly underestimated the concentration

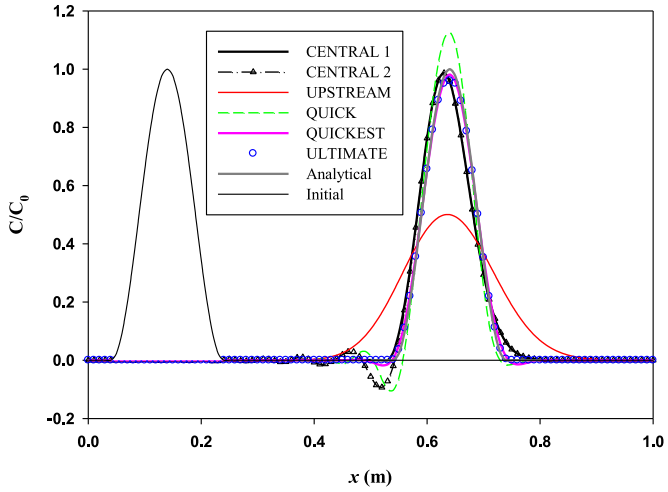

Fig. 6. Comparison of various numerical schemes (CENTRAL, UPSTREAM, QUICK, QUICKEST, and ULTIMATE) against the analytical solution for an isolated sine-squared wave and purely convective transport.

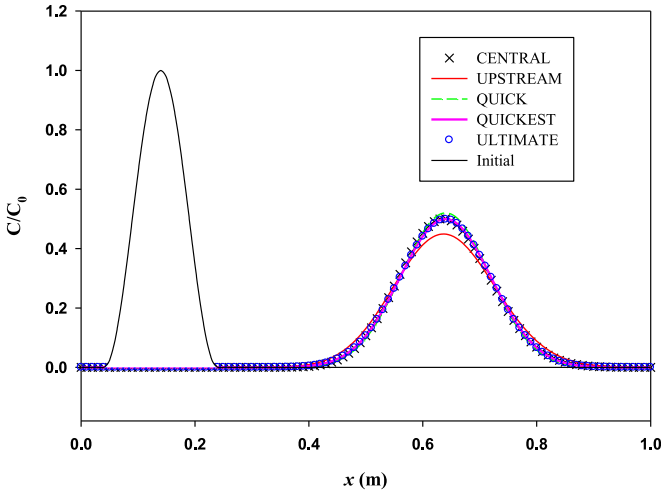

Fig. 7. Comparison of various numerical schemes (CENTRAL, UPSTREAM, QUICK, QUICKEST, and ULTIMATE) for an isolated sine-squared wave and a convective-dispersive transport with Pe = 2.

peak ($C_{max} = 0.982$). The scheme also shows small undershoot both in front of and behind the traveling wave (<0.018). Minor oscillations produced by the QUICKEST scheme were completely removed by the ULTIMATE scheme, although at the expense of a small increase in clipping ($C_{max} = 0.96$).

All schemes, other than the UPSTREAM scheme, described well a continuously changing gradient on both sides of a single local maximum of the sine-squared traveling wave.

3.2. Convective-dispersive transport

3.2.1. Uniform grids

As described earlier, numerical oscillations in implicit numerical schemes (e.g. CENTRAL) can be virtually eliminated when local Peclet numbers do not exceed about 2. Although acceptably small oscillations may be obtained with local Peclet numbers as high as 10 (Huyakorn and Pinder, 1986) unacceptably large oscillations are obtained when local Peclet numbers are larger than 10 (as shown above in Fig. 5). As such, for cases where *Pe* equals 2 all numerical schemes should converge to the true solution.

The previous example with a traveling isolated sine-squared wave was modified by introducing a diffusion coefficient D equal to 0.005 m^2/d and keeping all other parameters the same, so the local Peclet number is equal to 2 ($P = v\Delta x/D = 1 \times 0.01/0.005 = 2$). The result is shown in Fig. 7 and, in this particular example, results of all numerical schemes, other than QUICK and UPSTREAM, converged to the same solution. While the QUICK scheme slightly overestimated the concentration peak (by about 0.02), the UPSTREAM scheme underestimated the concentration peak more significantly (by about 0.05). Even for the local Peclet number of 2, the UPSTREAM scheme introduced some, although limited, numerical dispersion.

3.2.2. Non-uniform grids

All numerical schemes were further tested using spatially non-uniform grids, with the grid spacing either gradually increasing or decreasing. All other physical parameters other than the initial condition and spatial discretization are identical to the example for a purely convective transport shown in Fig. 6. In both cases the transport domain was discretized using 101 nodes; in the first case, the largest element was on the left side of the grid, and the grid was made gradually finer from left to right using a multiplication factor of 1/1.01. In the second case, the smallest element was on the left side of the grid, which was made gradually coarser from left to right using a multiplication factor of 1.01. In both cases the smallest element was 0.00181818 m and the largest 0.0181818 m. In both cases an isolated sine-squared wave was specified as an initial condition over the same number (i.e., 20) of grid nodes. Consequently, different solute mass was initially in the transport domain in these two cases since the initial sine-squared wave was spread over different parts of the domain (grids have different sizes).

As shown in Fig. 8, all numerical schemes, except for UPSTREAM which again produced significant numerical dispersion, performed reasonably well when the grid becomes finer in the direction of flow. However, none of the numerical schemes performed well when the grid becomes increasingly coarser in the direction of flow, as shown in Fig. 9. In this case both oscillatory schemes, i.e., CENTRAL and QUICK, suffered from large (larger than for the uniform grid) oscillations behind the traveling wave, and as in the uniform grid case, oscillations of the CENTRAL scheme propagated

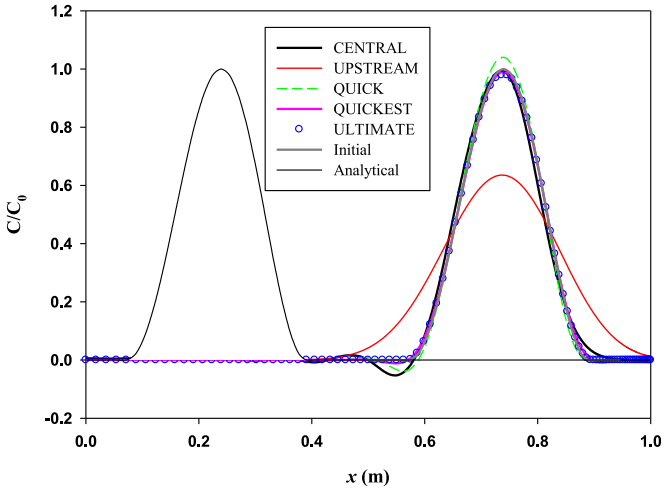

Fig. 8. Comparison of various numerical schemes (CENTRAL, UPSTREAM, QUICK, QUICKEST, and ULTIMATE) against the analytical solution for an isolated sine-square wave, a purely convective transport, and a gradually finer grid.

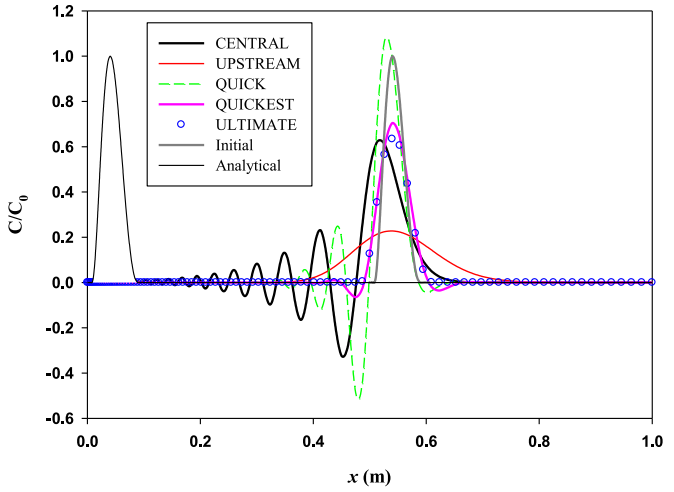

Fig. 9. Comparison of various numerical schemes (CENTRAL, UPSTREAM, QUICK, QUICKEST, and ULTIMATE) against the analytical solution for an isolated sine-squared wave, a purely convective transport, and a gradually coarser grid.

much further upstream than for the QUICK scheme. All non-oscillatory schemes produce significant clipping of the peak concentration and the QUICKEST scheme again produced only a single undershoot at both sides of the traveling wave, with no undershoot in the ULTIMATE case. Once more, the UPSTREAM scheme produced much higher levels of numerical dispersion, although in this case, all non-oscillatory regimes are affected by numerical dispersion.

Although this is clearly a disturbing finding, it is important to emphasize that these results are for purely convective transport, for which the standard numerical schemes, such as CENTRAL and UPSTREAM, are not expected to be either stable or accurate. In most soil applications (if not all), such conditions are not encountered as the transport is likely to also always contain dispersion.

It is thus necessary to investigate, for what conditions with gradually coarser grids these quadratic upstream weighting schemes (mainly QUICKEST and ULTIMATE) provide reasonable solutions. Fig. 10 presents the same problem with additional dispersion so that the three scenarios shown have Peclet numbers 2, 20 and 200. To provide a benchmark, these three additional runs are compared to the CENTRAL scheme (denoted below as CENTRAL#) applied on a much finer uniform grid, for which the stability conditions were satisfied, i.e., $Pe < 2$.

As expected all numerical schemes studied, i.e., CENTRAL, QUICKEST and ULTIMATE converged to a true solution provided by CENTRAL# when the Peclet number was equal to 2. Relatively good results were still obtained for a Peclet number equal to 20 by the QUICKEST and ULTIMATE schemes, which only slightly underestimated the concentration peak. The CENTRAL scheme already shows relatively minor oscillations beyond the sine-squared wave. Finally, for a Peclet number of 200, all three schemes produced significant clipping, similarly as for purely convective transport, while the CENTRAL scheme additionally suffered from significant oscillations and the QUICKEST scheme shows undershooting before and after the sine wave. Significant oscillations encountered with the CENTRAL scheme caused slight lagging of the sine wave front behind the analytical solutions.

Although for increasingly coarser non-uniform grids the QUICKEST and ULTIMATE schemes cannot be used for infinite Peclet numbers (i.e., purely convective flow), they nevertheless quite dramatically expand the interval of stability ($Pe = 20$, i.e., at least ten times) compared to standard implicit schemes.

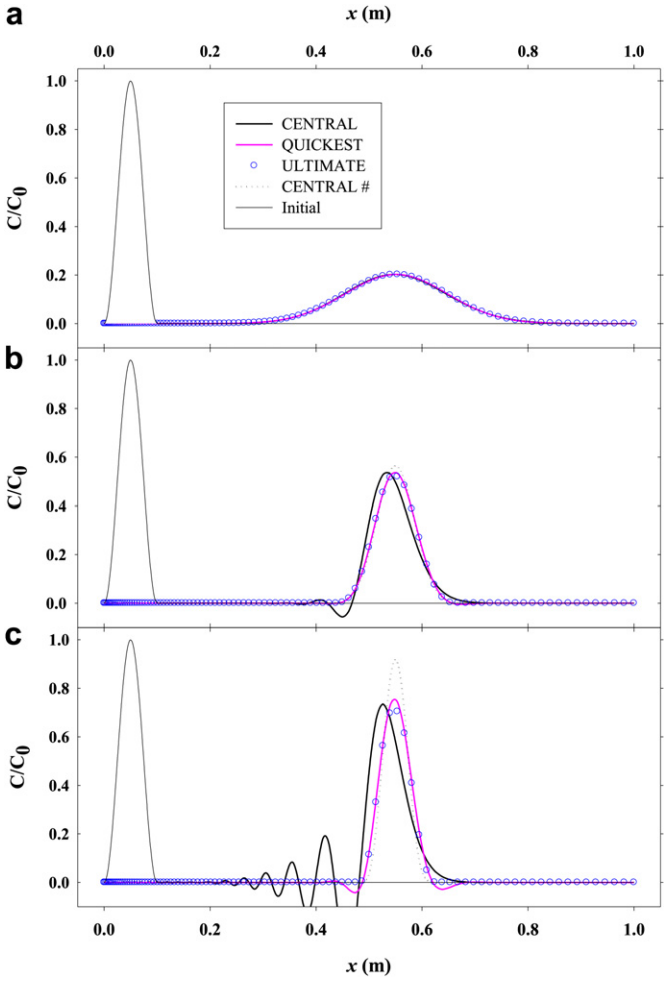

Fig. 10. Comparison of various numerical schemes (CENTRAL, QUICKEST, and ULTIMATE) for a convective-dispersive transport characterized by a Peclet number of 2 (a), 20 (b), and 200 (c) on a gradually coarser grid. CENTRAL# represents the CENTRAL scheme on a very fine grid, representing the true solution.

3.3. Non-uniform velocities and adsorption

Non-uniform velocities cannot be generated for a one-dimensional problem without compensating at the same time for changes in velocities by changes in water contents, which would lead to a transient water flow problem (addressed below). However, non-uniform "retarded" velocities can be generated by considering transport of a solute undergoing non-linear sorption while keeping water contents constant (unity so far). In this case the convection–dispersion equation

$$R\frac{\partial C}{\partial t} = -u\frac{\partial C}{\partial x} + D\frac{\partial^2 C}{\partial x^2} \tag{16}$$

can be reformulated using the so-called retarded velocities (v_R) and retarded dispersion coefficients (D_R) (Jury and Horton, 2004) as follow:

$$\begin{aligned}\frac{\partial C}{\partial t} &= -\frac{u}{R}\frac{\partial C}{\partial x} + \frac{D}{R}\frac{\partial^2 C}{\partial x^2}\\ \frac{\partial C}{\partial t} &= -u_R\frac{\partial C}{\partial x} + D_R\frac{\partial^2 C}{\partial x^2}\end{aligned} \tag{17}$$

where for non-linear sorption the retardation factor R is defined as:

$$R = 1 + \frac{\rho ds}{\theta dC} \tag{18}$$

and for the Freundlich adsorption isotherm:

$$s = K_d C^n$$
$$R = 1 + \frac{\rho n K_d C^{n-1}}{\theta} \tag{19}$$

where s is the sorbed concentration [MM^{-1}], ρ is the soil bulk density [ML^{-3}], θ is the water content [-], and K_d [$M^{1-n}L^{3n}M^{-1}$] and n [-] are empirical Freundlich coefficients. Note that Eq. (17) with retarded velocity and dispersion has the same form as Eq. (1), for which the quadratic numerical schemes discussed in this paper were developed, and they can thus be used for problems involving retardation, without any major modifications.

However, for the QUICKEST (and consequently ULTIMATE) scheme, the method estimates the wall values as an average over the time interval, so we solve a modified form of Eq. (16) with R inside of the temporal derivative, and a different definition of R as given below (Huang et al., 1997):

$$\frac{\partial RC}{\partial t} = -u\frac{\partial C}{\partial x} + D\frac{\partial^2 C}{\partial x^2} \tag{20}$$

$$R = 1 + \frac{\rho K_d C^{n-1}}{\theta} \tag{21}$$

Note that the Freundlich exponent n appears as multiplicator in the definition of the retardation factor in Eq. (19) and not in Eq. (21). This is because the retardation factor defined by Eq. (19) is outside of the temporal partial derivative in Eq. (17) and thus the sorbed concentration was subject to the ordinary derivative given in Eq. (18), while the retardation factor defined in Eq. (21) is inside of the temporal partial derivative in Eq. (20). Since the explicit approach was used for evaluating the retardation factor, i.e., the retardation factor was evaluated using concentrations at the old-time level, no iterative procedure was required for non-linear problems.

Thus, when there is a traveling concentration wave in the transport domain, although actual water velocities may be uniform, retarded velocities will be non-uniform, because of spatially changing concentrations and consequently changing retardation factors.

The problem presented here, involving steady-state water flow and non-linear solute transport in a homogeneous soil profile, follows a benchmark traveling wave problem suggested by Vanderborght et al. (2005) and an analytical solution by van der Zee (1990). The physical parameters for this problem were as follows. The soil column was 200 cm deep and was discretized using 101 nodes. The water content and velocities were uniform and equal to 0.004 and 0.05 m/d, respectively. The soil profile was initially solute free and the inflow concentration was 10 mg mL^{-1}. The soil bulk density was 1000 mg mL^{-1}, the Freundlich exponent n was 2/3, and the Freundlich sorption coefficient K_d was 0.001 $mL^n\ mg^{-1}\ mg^{(1-n)}$. The dispersivity λ was equal to 0.01 m, leading to a local Peclet number ($Pe = v\Delta x/D = v\Delta x/\lambda v = \Delta x/\lambda$) of 2. A constant time step (Δt) of 0.04 d was used and the final time (t_{max}) was 60 d. The corresponding maximum local Courant number (variable in space because of non-uniform v_R, $Co = v_R\Delta t/\Delta x$) was about 0.05.

Notice that due to the relatively low Pe number all numerical schemes, except for the QUICK scheme, provided as expected almost identical solutions similar to the one obtained by the analytical solution (Fig. 11). The UPSTREAM schemes shows again limited numerical dispersion because of a relatively low local Peclet number.

Similar verification for transport with the Freundlich exponent larger than 1 ($n = 4/3$) shows similar agreement between the models. However, since concentration fronts for $n < 1$ are steeper, and thus more difficult to solve numerically, only results for this case (i.e., $n = 2/3$) are presented here.

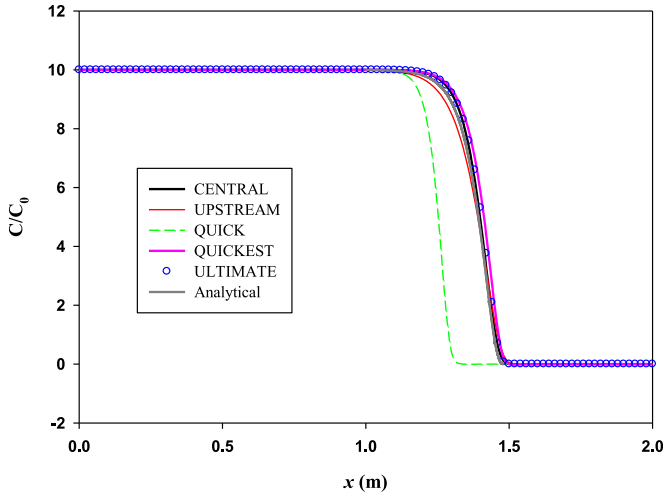

Fig. 11. Comparison of various numerical schemes (CENTRAL, UPSTREAM, QUICK, QUICKEST, and ULTIMATE) for a traveling wave problem.

3.4. Convective-dispersive-reactive transport

The next problem involves, in addition to physical processes of dispersion and retardation, also reactive chemical processes of degradation and production. The problem involves first-order decay and zero-order production. HYDRUS-1D has been shown in multiple studies (e.g. Šimůnek et al., 2008a; Vanderborght et al., 2005) to correctly solve such problems, and thus in the following example it is considered to provide a true solution that other schemes will be compared against.

The following physical parameters are used in this example. The transport domain is again 1 m long and is discretized using 101 nodes ($\Delta x = 0.01$ m). Mean pore water velocity, v, is assumed to be equal to 1 m/d. Since dispersion, D, is assumed to be 0.001 $m^2\ d^{-1}$, the Peclet number ($Pe = v\Delta x/D$) is equal to 10. The linear distribution coefficient K_d is equal to 1 $g^{-1}\ cm^3$. A constant time step (Δt) of 0.005 d is used and the final time (t_{max}) is 1.0 d. The corresponding Courant number ($Co = v_R\Delta t/\Delta x$) is equal to 0.25. The solute is additionally subject to the first-order decay with a rate constant μ equal to 1 d^{-1} and the zero-order production with a rate constant γ equal to 0.0001 g $m^{-3}\ d^{-1}$. The reaction term of Eq. (1) is thus defined as:

$$S = -\mu c + \gamma \tag{22}$$

Comparison of various numerical schemes for this reactive transport problem is shown in Fig. 12. Notice that the CENTRAL, QUICKEST and ULTIMATE schemes produce almost identical results, similarly as in the two previous examples. The QUICK and UPSTREAM schemes, similarly as above in Figs. 6 and 7, overestimate and underestimate the concentration peak, respectively. When the dispersion D was increased to 0.005 $m^2\ d^{-1}$, i.e., the Peclet number was reduced to 2, the correspondence between results obtained by individual numerical schemes (not shown) was similar as in Fig. 7.

3.5. Transient water flow

An ultimate test for each numerical scheme for solute transport is how it performs under transient water flow conditions. So in the

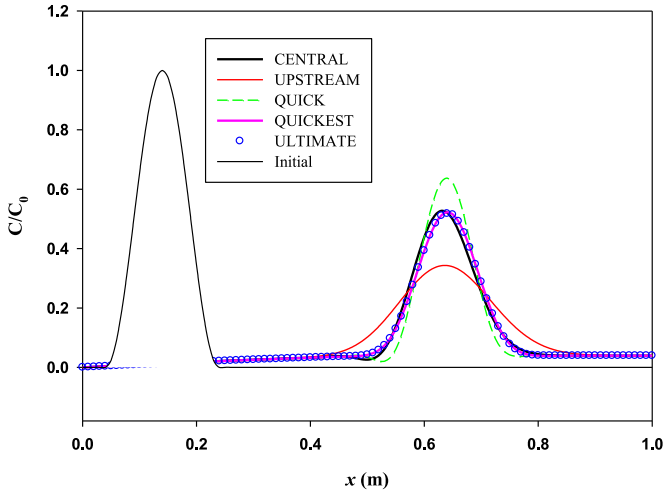

Fig. 12. Comparison of various numerical schemes (CENTRAL, UPSTREAM, QUICK, QUICKEST, and ULTIMATE) for a transport of an isolated sine-squared wave subject to retardation, production, convection, and dispersion.

last example transient water flow conditions are generated by imposing ponding (a pressure head of zero) at the surface of a 1-m deep loamy soil profile.

The following physical parameters are used in this example. The transport domain is discretized using 101 nodes ($\Delta x = 0.01$ m). Diffusion is not considered, but the dispersivity λ is considered using two values, either 0.005 or 0.0005 m. Even though the local velocities are not constant, the local Peclet numbers are constant throughout the profile when a uniform grid is used (since $Pe = v\Delta x/v\lambda = \Delta x/\lambda$) and equal to 2 ($\lambda = 0.005$ m) and 20 ($\lambda = 0.0005$ m). The former case is used to demonstrate that various numerical schemes converge to the same solutions when Pe is about 2, while the latter case shows the improvement of the ULTIMATE scheme for problems with high Peclet numbers.

To obtain transient values of water contents and pore water velocities required by the convection–dispersion equation for transient water flow, the Richards equation for variably-saturated water flow in porous media was solved using standard numerical techniques of HYDRUS-1D. Soil hydraulic parameters for loam from the Carsel and Parrish (1988) database were used. For this soil, the saturated hydraulic conductivity K_s is equal to 0.249 m d^{-1}, the residual and saturated water contents are 0.078 and 0.43, respectively, and the van Genuchten shape parameters α and n (van Genuchten, 1980) are 3.6 m^{-1} and 1.56, respectively. Initial pressure head was equal to −100 cm and the free drainage boundary condition was used at the bottom of the soil column.

The time step (Δt) was determined by requirements of the numerical solution of the Richards equation and varied from the initial value of 0.0001 d to a maximum value of 0.008 d. The final time (t_{max}) was 1.0 d. The corresponding Courant numbers ($Co = v\Delta t/\Delta x$) varied between 0.1 and 0.5. The solute was assumed not to be subject to any chemical reactions. The governing convection–dispersion equation for transient flow equation solved in this case is:

$$\frac{\partial \theta c}{\partial t} = -\frac{\partial u\theta c}{\partial x} + \frac{\partial}{\partial x}\left(\theta D \frac{\partial c}{\partial x}\right) \tag{23}$$

Similarly as above for the non-linear problem, the partially implicit approach in the QUICKEST and ULTIMATE methods was applied only to concentrations, and water contents, fluxes, and dispersion coefficients were evaluated at the old-time level.

Fig. 13 shows generated water content profiles after 0.2, 0.4, 0.6, and 1.0 d. The water content front reaches the depth of about 0.40 m after 0.2 d and the bottom of the soil profile after about 0.65 d. Fig. 13 also shows concentration profiles after 0.2, 0.4, 0.6, 0.8, and 1.0 d obtained using the CENTRAL, QUICKEST, and ULTIMATE schemes. All three numerical schemes converged to the same solution since the local Peclet numbers were equal to 2, i.e., no oscillations were expected to develop.

Fig. 14 shows concentration profiles for the same transient flow conditions, however for transport conditions with the Peclet number equal to 20. As discussed above, this is significantly above the range of Peclet numbers for which the solution is expected to be oscillation free for the CENTRAL scheme. And indeed, significant oscillations developed behind the concentration front. In this case the concentrations were constrained to positive values, similarly as in the example shown in Fig. 6 above. If this constraint was not used, small negative oscillations in front of the concentration front and significantly larger oscillations behind the front would have developed (data not shown). The QUICKEST scheme showed only a minor undershoot and overshoot in front of and immediately behind the concentration front, respectively. The ULTIMATE scheme completely eliminated negative values ahead of the concentration front and dramatically reduced the overshoot behind the front.

4. Discussion

Test examples shown in the previous section demonstrate that the quadratic interpolation schemes QUICKEST and ULTIMATE,

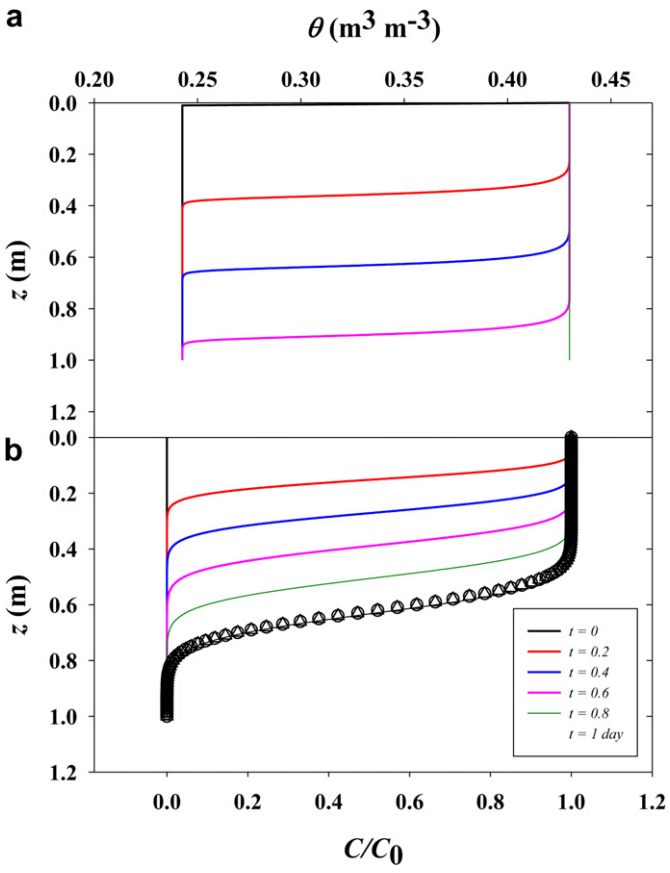

Fig. 13. Water contents (top) and concentrations (bottom) for the transient flow example and dispersivity of 0.5 cm ($Pe = 2$). Results obtained for $t = 1$ day using CENTRAL (solid lines), QUICKEST (○), and ULTIMATE (Δ) schemes at are also shown.

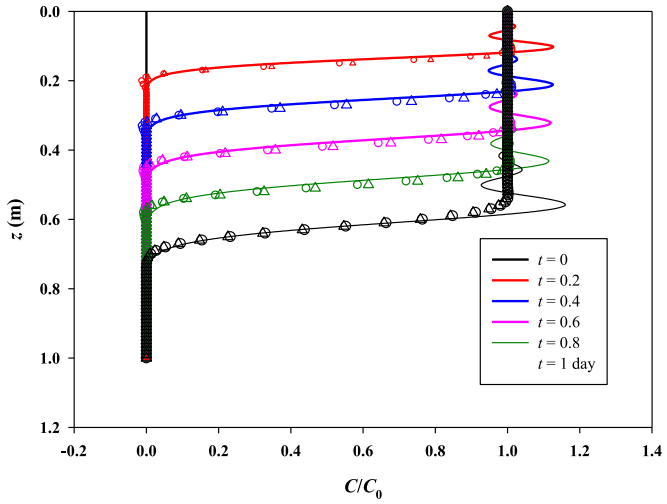

Fig. 14. Concentrations for the transient flow example and dispersivity of 0.05 cm ($Pe = 20$). Results obtained using CENTRAL (solid lines), QUICKEST (○), and ULTIMATE (Δ) schemes.

implemented in HYDRUS-1D, were able to adequately solve various presented transport problems. It is also important to emphasize that the examples, in which the standard implicit schemes, i.e., CENTRAL and UPSTREAM, failed or did not produce reasonable results, were for purely convective transport or very large local Peclet numbers. Such transport is only encountered in few applications and is very unlikely to occur in vadose zone hydrology. As shown above, numerical oscillations in implicit numerical schemes (e.g. CENTRAL) can be virtually eliminated when local Peclet numbers do not exceed about 2. Furthermore with local Peclet numbers as high as 10 (Huyakorn and Pinder, 1986) acceptably small oscillations can still be obtained. Even for problems with larger Peclet numbers, the oscillations can be minimized or virtually eliminated when the time step is adjusted appropriately. Perrochet and Bérod (1993) proposed a stability criterion:

$$Pe \cdot Cr \leq \omega_s (= 2) \tag{24}$$

where ω_s is the performance index [-]. This criterion indicates that convection-dominated transport problems having large Peclet numbers can be safely simulated provided Co (by, in fact, reducing the time step) is reduced according to the equation above (Perrochet and Bérod, 1993). Imposing these constraints, i.e., either $Pe<2$ or $\omega_s < 2$, numerical oscillations can be virtually eliminated and the CENTRAL scheme is expected to provide precise solutions (Šimůnek et al., 2008b). When small oscillations in the solution can be tolerated, ω_s can be increased to about 5 or 10.

For real-life one-dimensional problems encountered in vadose zone hydrology, it is usually not a problem to adjust the spatial discretization grid so that these criteria are fulfilled, and usually the numerical solution of the Richards equation requires finer temporal discretization than that required by solute transport. If needed, having hundreds or even several hundreds of nodes, is usually not a problem either in terms of memory or solution time for most one-dimensional applications. It is worthwhile noting that, as shown in Figs. 6, 10 and 14, the QUICKEST and ULTIMATE schemes quite dramatically expand the stability range, compared to standard implicit schemes, to $Pe \sim 20$ for non-uniform grids and up to infinity for uniform grids.

There are, however, several other areas where these non-oscillatory techniques can be used with a great advantage. One such area is in multi-dimensional applications. Larger two-dimensional, and certainly three-dimensional, applications in the vadose hydrology can easily have several hundreds of thousands, or even millions, of elements (volumes), as required by various stability criteria. Reducing the number of elements for these applications by relaxing the constraints on maximum grid spacing can still produce significant computational savings. Both QUICKEST and ULTIMATE schemes have been used in many multi-dimensional codes of hydrodynamics (e.g. Cole and Wells, 2006; Lin and Falconer, 1997; Romero et al., 2004) and it is our goal, after this initial testing presented in this manuscript, to also implement them in the multi-dimensional versions of HYDRUS (Šimůnek et al., 2008b).

The second area where these numerical schemes can be used with a great advantage is in codes simulating multicomponent reactive chemistry (e.g. Jacques et al., 2008; Wissmeier and Barry, 2010, 2011). Such codes are usually developed by coupling the flow and transport codes with the reactive chemistry codes, such as PHREEQC (Parkhurst and Appelo, 1999), and simulations with these codes often fail when they are provided with negative element concentrations by the transport codes. As shown in Figs. 13 and 14, the ULTIMATE scheme does not produce oscillations and suppresses negative concentrations. The ULTIMATE scheme preserves sharp concentration fronts while maintaining monotonicity of the solution, which is especially relevant in flow situations with high grid Peclet numbers.

As shown above, the accuracy of the ULTIMATE scheme greatly exceeds the accuracy of commonly applied first- and second-order schemes currently used in HYDRUS for problems, in which convective transport dominates over the dispersive transport, and other problems with sharp concentration fronts. Note that sharp concentration fronts may not necessarily be a result of a dominant convective transport, but can also be result of involved chemical reactions, such a sorption (Borkovec et al., 1996; Frey, 1987), cation exchange (Voegelin et al., 2000), or precipitation/dissolution (Lake et al., 2002). All these reactions can under certain conditions (e.g. for $n < 1$ in the Freundlich adsorption isotherm) lead to self-sharpening concentration fronts, which are difficult to handle by traditional implicit schemes.

5. Conclusions

Two quadratic interpolations schemes (QUICK and QUICKEST) and one TVD scheme (ULTIMATE) have been successfully implemented in HYDRUS-1D and tested against a series of analytical and numerical solutions. Both quadratic schemes showed small numerical dispersion. The QUICKEST scheme showed reduced oscillatory behavior when compared to the QUICK scheme or unbound central differencing. The incorporation of the TVD scheme removed the oscillatory behavior near sharp fronts for large Peclet numbers.

The QUICKEST and ULTIMATE schemes presented here have a larger stability region in terms of the Peclet number, compared to standard implicit schemes. Even if this advantage is of limited application in 1D cases, it shows a large potential to be employed in multi-dimensional applications to relax Peclet number constraints on grid spacing.

Finally, the ULTIMATE scheme shows improved stability near steep fronts due to non-oscillatory behavior and reduced numerical dispersion. This suggests an improvement in stability in reactive transport applications, as the absence of negative values is likely to improve the convergence of such models.

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