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# A one dimensional solute transport model for hydrological response units

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***Abstract***: The transport of solutes in soils is often modelled using the advection diffusion equation. Analytical solutions are only available for overly simplistic scenarios, so numerical formulations are applied in most models (Vanderborght *et al.* 2005). However, modelling of advection problems is not a trivial task with problems ranging from numerical instability to mass conservation, specially when modelling of discontinuities and steep fronts are required (Leonard 1979; Leonard 1991).

One of several methods that can be used to overcome problems associated with solving the advection diffusion equation was proposed by Leonard (1979), using quadratic upstream interpolation to solve the advection diffusion equation. This method is known as Quadratic Upstream Interpolation for Convective Kinematics with Estimated Upstream Terms (QUICKEST). The model presented here is the solute transport component of WASOM1, the Water and Solute Movement in 1 dimension. WASOM1 uses a cascading bucket model coupled with the QUICKEST scheme with a monotonic resolution scheme (ULTIMATE) to simulate the transport of solutes in soils.

Comparison of the results obtained using the ULTIMATE code from WASOM1, the analytical solution and HYDRUS (Simunek *et al.* 2005) different finite element implementations are shown in Figure 1. The solution due to WASOM1 predicts the position of the solute front accurately and is free of oscillations. The other methods based on finite elements (FE) either did not predict the position of the front correctly, due to numerical dispersion or suffered from oscillations.

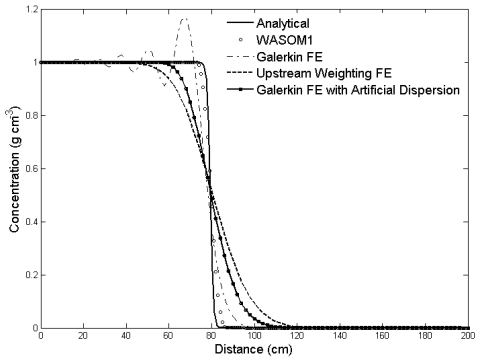


**Figure 1.** Analytical and numerical solutions for the transport of a tracer. Finite Element (FE) solutions obtaiuned from HYDRUS (Simunek *et al.* 2005).

The solute transport scheme is independent of the water balance, so it can be adapted for use with other water balance models. WASOM1 is capable of simulating the transport of non-adsorbed solutes, solutes that follow linear, Langmuir and Freundlich isotherms and undergo zero or first order decay. The scheme is mass conservative avoiding mass loss common in models such as MT3DMS (Zheng and Wang 1999). It also produces minimal numerical dispersion. The basic numerical scheme of WASOM1 is described and its advantages over other methods are presented by comparison with an analytical solution and other methods. Finally, and example of its application the transport of bromide in soils is given.

***Keywords:*** *water quality, numerical methods, numerical dispersion, advection diffusion*

## 1. INTRODUCTION

The increase in interest on catchment management has seen an increase in the number of models available to simulate water and solute transport, with varying degrees of complexity and accuracy (Borah and Bera 2003). In models that simulate transport of solutes in the soil profile, the movement is usually described using the advection-diffusion equation, with extra terms to account for adsorption and reaction (Zheng and Bennett 2002). The form of these terms varies according to the problem in hand, such as linear or non-linear adsorption or first and second order reactions. The equations associated with these models are usually non-linear and each problem has its own set of boundary conditions. In real situations, soil properties and initial conditions are non-uniform, so numerical methods are required for the solution of the governing equations as analytical solutions are only available for simple cases (Vanderborght *et al.* 2005). In particular, numerical modelling of advection dominated problems on the presence of discontinuities and steep fronts are not trivial (Leonard 1979; Leonard 1991).

Finite difference methods can be used to solve the advection dispersion equation, either using backward, forward or central differencing. This methods however can result in artificial oscillation (under or over shooting) or numerical dispersion due to truncation errors of the discretization. Application of backwards finite difference results in an implicit scheme which is always convergent but is computationally expensive and introduces considerate numerical dispersion (Zheng and Bennett 2002). The use of central differencing (such as Crank Nicholson schemes) in the discretization can cause numerical oscillation in the form of "wiggles" when implicit schemes are used. If an explicit formulation is used instead the solution often is non-convergent (Leonard 1979). Numerical oscillation can be minimized by the use of upstream weighting, but this leads to considerable numerical dispersion owing to truncation errors (Zheng and Bennett 2002). Another solution for artificial oscillation is the use of finer grids, with a choice based on the Peclet number:

$$Pe = u * \Delta x / D \tag{1}$$

where $u$ is the flow velocity [L $T^{-1}$] , $\Delta x$ is the grid spacing [L] and $D$ is the diffusivity [$L^2$ $T^{-1}$]. A $Pe$ number < 2 can greatly reduce or eliminate numerical oscillation, but usually the associated computational cost due to excessively fine grids is impractical (Zheng and Bennett 2002).

The alternative of upstream differencing introduces artificial numerical diffusion terms and becomes inaccurate due to large truncation errors. Again, these problems can in theory be solved with grid refinement, but in most practical applications the degree of refinement required is computationally prohibitive (Leonard 1979). Another possible solution is the introduction of an apparent numerical diffusion coefficient, to "counteract" the numerical dispersion introduced by the discretization, but this can only be use 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).

One of several methods that can be used to overcome these oscillation and truncation problems was proposed by Leonard (Leonard 1979), using quadratic upstream interpolation is used to solve the advection diffusion equation. This method is known as Quadratic Upstream Interpolation for Convective Kinematics with Estimated Upstream Terms (QUICKEST). The model presented here is WASOM1, the Water and Solute Movement in 1 dimension, and it uses the QUICKEST scheme with a monotonic resolution scheme (ULTIMATE) to solve the advection diffusion equation. The water balance is solved using a cascading bucket model which provides the water fluxes for the solute transport solved with the QUICKEST scheme. The solute scheme is independent of the water balance, so it can be used with other water balance models.

WASOM1 is capable of simulating the transport of non-adsorbed solutes, solutes that follow linear, Langmuir and Freundlich isotherms and undergo zero or first order decay. The basic numerical scheme to solve the advection diffusion equation in WASOM1 is described and its advantages over other methods are presented by comparison with an analytical solution and other methods. Finally, and example of the application of WASOM1 is given by the simulating the transport of bromide in soils.

## 2. MODEL DESCRIPTION

Using the water fluxes from the water balance, WASOM1 solves the advection-dispersion equation with terms accounting for reaction and adsorption:

$$\theta \frac{\partial C}{\partial t} + \rho_b \frac{\partial \bar{C}}{\partial t} + \frac{\partial C\theta u}{\partial x} = \frac{\partial}{\partial x}\left( \theta D \frac{\partial C}{\partial x} \right) - \lambda_1 C\theta - \lambda_2 \rho_b \bar{C} \tag{2}$$

Where $C$ is the dissolved concentration of a solute [M $L^{-3}$], $\theta$ is the porosity [$L^3$ $L^{-3}$], $t$ is the time [T], $\overline{C}$ is the solute concentration adsorbed on the subsurface solids [M $L^{-3}$] [M $L^{-3}$], $\lambda_1$ is the first-order reaction rate for the dissolved phase [$T^{-1}$], $\lambda_2$ is reaction rate for the sorbed (solid) phase [$T^{-1}$] and $\rho$ $\rho_b$ is the bulk density [M $L^{-3}$].

### 2.1. QUICKEST Scheme

The QUICKEST method uses a three-point upstream weighted interpolation to obtain a numerical scheme which is stable in highly advective flows, without a substantive increase in computational load in comparison to the upstream or central differencing schemes.

However, as demonstrated by Leonard (Leonard 1991), several numerical schemes such as second order schemes (central and upwind), third order schemes such as QUICKEST and even higher order methods are prone to small oscillations and/or overshooting, specially near sharp gradients. Thus, the method used in WASOM1 is modified to use the ULTIMATE (Universal Limiter for Transient Interpolative Modelling of Advective Transport Equation) QUICKEST method to achieve monotonic resolution. The adoption of the ULTIMATE strategy involves minimal extra computational cost while avoiding oscillations that could lead to appearance of negative concentrations near steep fronts.

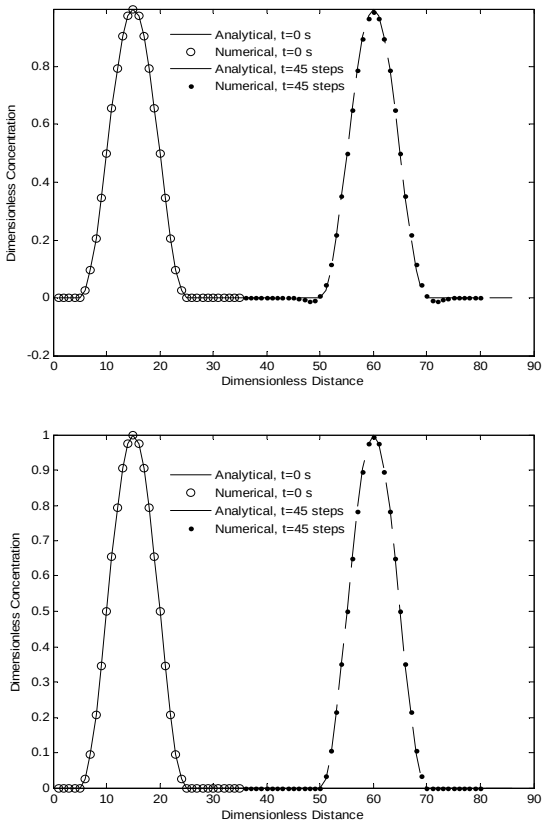


**Figure 2.** Numerical and analytical solutions for the translation of a sine-squared wave using QUICKEST (top) and ULTIMATE QUICKEST (bottom).

The benefit of the ULTIMATE scheme can be seen by comparing the top and bottom sections of Figure 2, which shows the solutions after a translating of 45 $\Delta$x to the right of a sine-squared wave. For more detail, please referred to Leonard (1991)

As can be seen from Figure 2, the QUICKEST solution is in excellent agreement to the analytical solution, but for the overshooting which lead to negative concentrations. In the ULTIMATE scheme, introduction of the universal limiter increases accuracy near steep fronts without causing spurious oscillations.

### 2.2. Coupling the water balance and the solute transport

In WASOM1, the water balance and the solute transport are solved independently, using different spatial and temporal discretizations. The water balance operates on a daily time step and its spatial discretization is chosen according to the soil information available and usually it will be much coarser than the spatial discretization of the solute code. The solute code further divides the soil layers of the water balance using a finer discretization to minimize numerical dispersion. Hence, one of the soil layers from the water balance can contain several solute layers. The only requirement is that the boundary between layers in the water balance model layers matches one of the solute model boundaries. The flow between the different solute layers (embedded in a single water content layer) is calculated using a linear interpolation while maintaining the overall water content within the water layer.

The QUICKEST method has two stability criteria to avoid oscillation, based on the Courant number Co and the diffusion parameter $\chi$, defined as (Leonard 1979):

$$Co_r = u\Delta t / \Delta x \leq 1 \tag{3}$$

$$\chi_r = D\Delta t / \Delta x^2 \leq 0.5 \tag{4}$$

The stability region of the QUICKEST method can be extended to Co < 2, but is subject to further restrictions on the diffusivity parameter value. As the spatial discretization of the solute transport is fixed at the model setup, the only parameter available to guarantee the stability of the QUICKEST scheme is through variable time stepping. The time step chosen is the minimum between daily (water balance time step) or one of the values required by constraints given by eqns 3 and 4. Note that the eqns 3 and 4 allow for stability in cases where advective flow is dominant (i.e., large PE numbers).

The water balance model used here is a cascading bucket model with modifications to allow for improved soil evaporation, see (Cook *et al.* 2006) for details.

### 2.3. Adsorbed solute

WASOM1 is also capable of modelling adsorbed solutes, as a mass transfer process between the dissolved phase and the porous medium (solid phase). WASOM1 follows the assumption of local instantaneous equilibrium, where the adsorption/desorption are much faster than the flow velocity. The relationship between the adsorbed and dissolved concentrations can be described using three possible isotherms: linear, Langmuir and Freundlich. The isotherms can be incorporated into the transport model using a retardation factor, $R$ [M $L^{-3}$] defined as (Kutílek and Nielsen 1994; Zheng and Bennett 2002):

$$R = 1 + \frac{\rho_b}{\theta}\frac{\partial \overline{C}}{\partial C} \tag{5}$$

So the transport equation can now be written as:

$$R\theta\frac{\partial C}{\partial t} + \frac{\partial C\theta u_x}{\partial x} = \frac{\partial}{\partial x}\left(\theta D\frac{\partial C}{\partial x}\right) - \lambda_1 C\theta - \lambda_2 \rho_b \overline{C} \tag{6}$$

Hence for the Freundlich isotherm for example:

$$\overline{C} = K_f C^a \tag{7}$$

$$R = 1 + \frac{\rho_b}{\theta} K_f a C^{a-1} \tag{8}$$

where $K_f$ is the Freundlich constant [$M^{1-a}$ $L^{-3(1-a)}$] and $a$ is the Freundlich exponent.

A common occurrence with solute transport models is lack of mass conservation such as in MT3DMS (Zheng and Wang 1999). In the simulation for adsorbed solutes (as well as non-adsorbed), WASOM conserved mass in all instances. There are two features in WASOM that ensure mass conservation, the correct use of the retardation factor and the treatment of the adsorbed mass/dissolved mass in absence of water flow but in presence of evaporation.

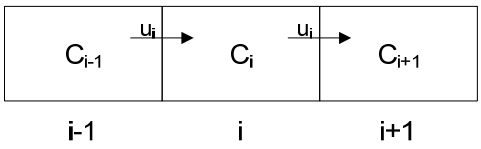


**Figure 3:** Advection only schematic

In the MT3DMS (Zheng and Wang 1999) and WASOM codes, the retardation factor R is calculated for every cell in the model at the beginning or every time step (or sub-step if needed to avoid oscillation). The difference in approach is that MT3DMS uses that factor based on the "local" cell concentration for every flow of material entering or leaving the cell whereas WASOM on the other hand uses the retardation of the upstream and downstream cells were appropriate For pure advection, constant spacing $\Delta x$ and time step $\Delta t$ the fluxes entering and leaving the cells in Figure 3 are given by:

| *WASOM* | *Local Conservation* |
|---|---|
| $for\ i-1 \Rightarrow -\Delta t u_i C_{i-1} / \Delta x R_{i-1}$ | $for\ i-1 \Rightarrow -\Delta t u_i C_{i-1} / \Delta x R_{i-1}$ |
| $for\ i \Rightarrow \Delta t u_i C_{i-1} / \Delta x R_{i-1} - \Delta t u_i C_i / \Delta x R_i$ | $for\ i \Rightarrow \Delta t u_i C_{i-1} / \Delta x R_i - \Delta t u_i C_i / \Delta x R_i$ |

(3)

As R is dependent on $C$, it is obvious that if $C_{i-1}$ and $C_i$ are different, so will $R_{i-1}$ and $R_i$ be. If one uses only the local concentration, $C_i$ and $R_i$ are used to calculate the fluxes in and out of cell "i", but $R_{i-1}$ is used to calculate the flux leaving cell "i-1". In the local conservation scheme, the fluxes out of "i-1" and the flux into

"i" are calculated using a different retardation factor and this may cause a mass conservation problem. The flux leaving cell "i-1" is divided by $R_{i-1}$ and hence it can be different from the flux entering cell "i" as it is divided by $R_i$

## 3. RESULTS

The performance of the model was tested by comparisons with analytical solutions and also the simulation of bromide transport in field plots. Here, we consider the transport of a non-adsorptive conservative solute in a semi-infinite column with a uniform initial concentration and a constant boundary condition. The analytical solution is given by Wexler (1992). The test conditions are identical of the test problem by Huang *et al* (1997), with a constant flow velocity of 4 cm/d and dispersivity of 0.16 cm. At the inflow boundary, the solute concentration was fixed at 1 $g.cm^{-3}$ for a period of 20 days. The Peclet number was equal to 25, the time step was 0.1 d and the grid spacing was 1 cm.

Comparison of the results obtained using the ULTIMATE code from WASOM1, the analytical solution and HYDRUS (Simunek *et al.* 2005) with different finite elements implementations is shown in Figure 1. It is clear that all the other finite element (FE) methods either did not predict the position of the front correctly due to numerical dispersion (Upstream Weighting FE and Galerkin FE with Artificial dispersion) or suffered from oscillations (Galerkin FE). WASOM1 predicts the position of the front accurately and is free of oscillations.

A second test of WASOM was to simulate the transport of bromide in soil plots (Verburg *et al.* (1996), comparing its performance against both measured data and simulations using SoilWat (Probert *et al.* 1998) and SWIM (Ross *et al.* 1992). In this field experiment, 12 plots were used to measure the leaching of bromide from May to November. Bromide was injected at four occasions a week apart at a depth of 2 cm and concentration of 0.16 $mol/m^2$ and concentration profiles were subsequently measured at 3 occasions. For more details, please refer to Verburg *et al* (1996).

The parameters used in the simulation to simulate the soil in WASOM1 are shown in Table 1. Other parameters used in the simulation are:

- Diffusivity of bromide in water = $2x10^{-9}$ $m^2/s$
- Dispersivity = 0.15 m (Beven *et al.* 1993);

Table 1. Soil properties for the WASOM1 simulation of the Wagga dataset

| Layer | Hydraulic Conductivity (m/d) | Water Diffusivity ($m^2/s$) | Porosity | Field Capacity | Wilting Point | Z (m) |
|---|---|---|---|---|---|---|
| 1 | 1.2 | 0.088 | 0.29 | 0.2 | 0.15 | 0.1 |
| 2-5 | 0.87 | 0.088 | 0.29 | 0.2 | 0.13 | 0.2-0.5 |
| 6-10 | 0.1308 | 0.088 | 0.3 | 0.23 | 0.18 | 0.6-1.0 |
| 11-13 | 0.877 | 0.088 | 0.3 | 0.173 | 0.15 | 1.1-1.3 |
| 14-15 | 1.68 | 0.088 | 0.32 | 0.191 | 0.2 | 1.4-1.5 |
| 16-18 | 1.68 | 0.088 | 0.32 | 0.23 | 0.2 | 1.6-1.8 |
| 19-20 | 1.68 | 0.088 | 0.32 | 0.256 | 0.2 | 1.9-2.0 |

Rainfall was identical as used by Verburg *et al* (1996), while potential evaporation was calculated by APSIM-SoilWat, on basis of weather information. However, while in the experiments the bromide was injected at 2cm, in the modelling it was added at 2.5 cm (5 cm layers) or 5 cm (10 cm layers), as the model assumes that the mass is concentrated at a node at the centre of the layer.

The results for the simulated concentrations in SoilWat, SWIM and WASOM as well as the 95 % confidence interval of the measured concentration are shown in Figure 4. WASOM 1 and SWIM reproduce the shape measured bromide concentration curves very well, with some small disagreements in the magnitude of the peaks. In general, the results from WASOM1 are very satisfactory, with quality of results and order or errors of a similar magnitude as reported for SWIM and SoilWat. The use of 5 or 10 cm layers for the solute model did result in small differences in the modelled concentrations, however the differences are not significant in this context.

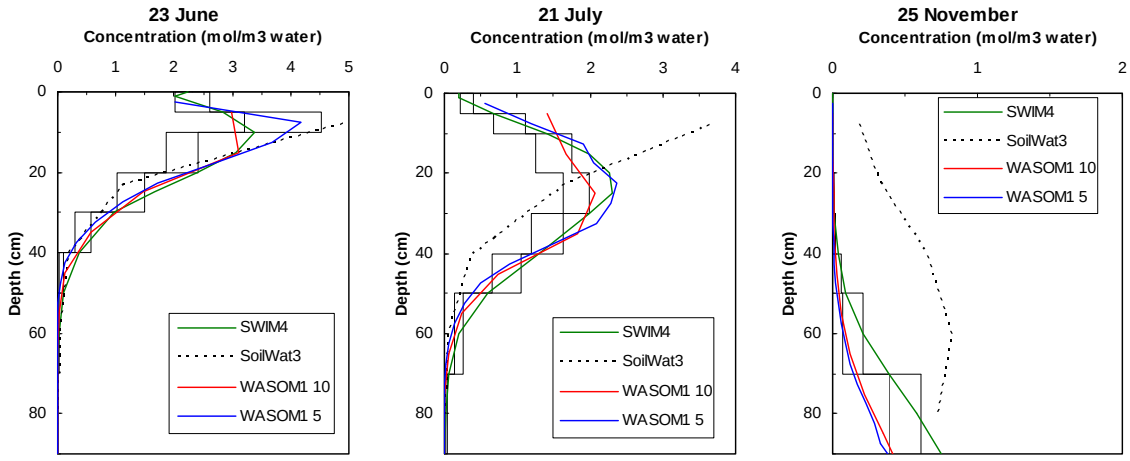


**Figure 4:** Comparison between WASOM1 and experimental (shown as histograms of 95% intervals around the mean for each depth interval) and modelling results from Verburg (Verburg 1996).

Table 2. Total solutes at different depths and dates as modelled by WASOM1 and measured Verburg *et al* (1996).

| | | Total solutes (mol/m^2) | | |
|---|---|---|---|---|
| Date | Depth (cm) | Measured | Modelled (5 cm layers) | Modelled (10 cm layers) |
| 23-Jun | 0-50 | 0.159 | 0.160 | 0.160 |
| | 0-90 | 0.16 | 0.160 | 0.160 |
| 21-Jul | 0-50 | 0.146 | 0.154 | 0.159 |
| | 0-90 | 0.16 | 0.160 | 0.160 |
| 25-Nov | 0-50 | 0.002 | 0.003 | 0.009 |
| | 0-90 | 0.029 | 0.046 | 0.049 |

## 4. DISCUSSION

An analysis of Table 2 and Table 3 show that the model's predictions compare well with either the measured or the model's results from Verburg *et al*(1996) study, with good agreement in the total water and solute present at different depths. The predicted drainage rates are slightly higher than the rates that were predicted by Verburg *et al*(1996), however this over prediction is attributed only to the water balance model here, with no relation to the solution scheme of the advection diffusion equation.

Table 3. Total water at different depths and dates as modelled by WASOM1 and measured Verburg *et al* (1996).

| | | Total water (mm) | |
|---|---|---|---|
| Date | Depth (cm) | Measured | Modelled |
| 23-Jun | 0-50 | 99 | 99.1 |
| | 0-90 | 181 | 191.1 |
| 21-Jul | 0-50 | 113 | 100 |
| | 0-90 | 215 | 192.0 |
| 25-Nov | 0-50 | 109 | 98.6 |
| | 0-90 | 197 | 190.6 |

Verburg *et al* (1996) remarked that SWIM predicts the transport of bromide fairly well, whilst the results for SoilWat are somewhat poorer in the initial stages failing to reproduce the peak around 20-30 on July 21$^{st}$ and under predicting the subsequent transport. The results for SWIM and WASOM1 are in good agreement, with WASOM1 showing a larger flushing of the profile by the end of November, but this is due to the over prediction of the water fluxes by the water balance model. For both models the prediction of the solutes is closely linked with the correct prediction of water content and fluxes. The same is certainly true for

WASOM1, where different parameterizations (not shown) which overestimate the modelled fluxes by more than 20% resulted in a complete flushing of the Bromide from the 0-90 cm profile by November 25th.

## 5. CONCLUSIONS

This study introduced WASOM1, a water balance model coupled with a numerical solution of the advection diffusion equation. The advantages of the quadratic interpolation scheme QUICKEST with the universal limiter for monotonicity used to solve the advection solution equation is shown for two analytical solutions. The numerical scheme avoids numerical oscillations and has minimal numerical dispersion, with clear advantages over other finite element methods that use upwinding or artificial dispersion for stability.

WASOM1 was also applied to simulate the one dimensional transport of bromide in field plots. The model was capable of accurately predicting the water fluxes and the transport of bromide in the soil profile, with its performance on a similar level as SWIM but with fewer limitations on maximum Peclet number for the simulations.

## ACKNOWLEDGMENTS

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