ASSESSING THE IMPACT ON GROUNDWATER OF SOLUTE TRANSPORT IN CONTAMINATED SOILS USING NUMERICAL AND ANALYTICAL MODELS

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ABSTRACT

Expansion of human activities causes dispersion of pollutants in the subsurface environment. The fate and movement of dissolved substances in soils and groundwater has generated considerable interest out of concern for the quality of the subsurface environment. Many analytical solutions for partial differential equations exist in soil science. Numerical solutions are more general, and often more difficult to verify. Because of the difficulty in obtaining analytical solutions, numerical solutions are used; the mathematical model error has to be kept as small as possible. In order to determine the model error, the examination of numerical methods through an analysis of their ability compared with analytical methods is strongly recommended. The objective of the study is to compare between numerical and analytical solution models for solute transport equation. In this study, the numerical solution calculated with the WAVE-model was compared with the analytical solution calculated with CXTFTT-model. The study scenarios were built up with the combinations of compartment depth, applied flux at the top and soil dispersivity under steady-state conditions. The simulations depend on 27 solute infiltration scenarios. The solute concentrations were calculated with the WAVE-model and the CXTFIT-model for each scenario. The WAVE-model error was evaluated with three methods: absolute average maximum error, relative average maximum error and relative average area error. The study implied that, the WAVE-model error was increasing with the increasing of the compartment depth; the WAVE-model error was decreasing with the increasing of the soil dispersivity; and the WAVE-model error was decreasing with the increasing of the flux. The study recommended using compartment depth as thin as possible to minimise the WAVE-model error. Furthermore, it will be more useful to use several numerical solution models, such as HYDRUS-2D model, to evaluate and examine the WAVE-model.

Keywords: numerical solutions; analytical solutions; simulations; steady-state conditions; solute infiltration scenarios

INTRODUCTION

Expansion of human activities causes dispersion of pollutants in the subsurface environment. Today, acid rain, hazardous chemical wastes, fertilisers, pesticides, heavy metals, nuclear deposits, solvents and sewage sludge are amongst other things, a serious threat to soil and groundwater quality. Therefore, existing groundwater and soil conservation policies and strategies are reconsidered; while new are developed (Jury et al., 1991). The fate and movement of dissolved substances in soils and groundwater have generated considerable interest out of concern for the quality of the subsurface environment. The behaviour of solutes over relatively long spatial and temporal scales has to be assessed with the help of theoretical models since it is usually not feasible to carry out experimental studies over sufficiently long distances and/or time periods (Vanderborght et al., 1996). The fate of the chemicals in the subsurface environment is characterised by a set of complex processes, subject to varying boundary conditions in space and time.

Mathematical models are developed to unravel and integrate knowledge of the processes controlling the transport and transformation of contaminants in soils, and to predict the fate of chemicals as they disperse into the vadose environment (Toride et al., 1995). Many analytical solutions for partial differential equations exist in soil science (Beitman et al., 1995). Most of them are for special cases or as approximations due to simplifying theoretical assumptions. These “closed” solutions are much desired because they are easily and quickly adapted for those special cases for which the simplifying assumptions are approximately fulfilled. Numerical solutions are more general, and often more difficult to verify. Therefore, analytical solutions are important as a measure of the quality of the numerical solutions. Whenever it is possible to compare a numerical with an analytical solution, such a comparison is strongly recommended. In order to predict the transport of pollutants and in order to assess the risk of pollutants towards soil and groundwater, mathematical models are frequently used nowadays. These models are an approximation of the real transport of water and pollutants (pesticides, nitrates ...etc.) in the soil.

With solution of a numerical model, a model error is generated which has to be kept as small as possible (Snadgrass et al., 1997). In order to determine the model error, model output is compared with analytical solutions. In this study the numerical solution is calculated with the WAVE-model (Water and Agrochemicals in soil, crop and Vadose Environment (Vanclooster et al., 1994)) and the analytical solution is calculated with the CXTFIT-model (Code for Estimating Transport Parameters from Laboratory or Field Tracer Experiments (Toride et al. 1995)). In the vertical direction, the WAVE model considers the existence of heterogeneity in the form of soil layers within a soil profile. The soil layers are subdivided in space intervals called the soil compartments. Halfway each soil compartment a node is identified, for which state variable values are calculated. All soil compartments have the same thickness and the user can specify the thickness depending on the desired accuracy. Increasing the compartment thickness will decrease the calculation time but also the numerical accuracy. The objective of this research is to examine the numerical methods used in WAVE model through an analysis of their ability compared with analytical methods to measure the quality of the numerical solutions of WAVE model. Numerical solutions of the transport equation often exhibit oscillatory behaviour and/or excessive numerical dispersion near relatively sharp concentration fronts. In this study, the numerical solutions calculated with the WAVE-model, was compared with the analytical solutions calculated with the CXTFIT-model. The three basic variables cause oscillatory behaviour and/or excessive numerical dispersion are flux, soil dispersivity and compartment depth so that, the different solute infiltration scenarios were built up with combinations of those basic variables for steady-state conditions to evaluate the WAVE model mathematical error.

SOLUTION METHODS

Because of the difficulty in obtaining analytical solutions to groundwater flow problems, many investigators are using numerical solutions. The mathematical model error has to be kept as small as possible. In order to determine the model error, numerical solutions are compared with analytical solutions.

Numerical solution using WAVE-model

In the vertical direction, the model considers the existence of heterogeneity in the form of soil layers within a soil profile. The soil layers are subdivided in space intervals called the soil compartments. Halfway each soil compartment a node is identified, for which state variable values are calculated using finite difference techniques. All soil compartments have the same thickness and the user can specify the thickness depending on the desired accuracy. Increasing the compartment thickness will decrease the calculation time but also the numerical accuracy. The WAVE-model uses a time step smaller than a day to calculate the different system state variables, for processes which are strongly dynamic (water transport, heat transport, solute transport, solute transformation). The time step is variable, and is chosen to limit mass balance errors induced by solving the water flow equation. However, the time size criterion can be input to change the model's robustness. The model input is specified on a daily basis and flux type boundary conditions are assumed constant within the time span of a day. State variables are integrated after each day to yield daily output. The simulation period should not exceed one single year. The simulation starts at midnight of the specified starting date and ends at midnight of the specified ending date. The WAVE-model was run two times, the first time to reach the steady state flow conditions. After catching the steady state, the second run started to simulate solute transport.

WAVE-model Input

In order to solve the numerical equations, the following parameters and state variables are initialised for each soil compartment: the soil moisture content (θ); the soil pore water velocity (Vm); the soil bulk density (ρ); the chemical diffusion parameters (Dif, a, b); the hydrodynamic dispersivity (λ); the ratio mobile versus total moisture content (θ_m/θ); the mass distribution coefficient (k_d); and the fraction of the sorption sites in the mobile soil region (f). To ensure convergence and to minimise numerical dispersion, a Crank Nicolson numerical scheme is used to solve the transport equation in the mobile soil region. A flux type boundary condition is used to define the top boundary in the WAVE-model:

$$J_s = C_f \,.\, q_w \quad \text{for qw} < 0.0 \text{ (infiltration)} \tag{1}$$

Where: C_f is the solute flux concentration ($M\,L^{-3}$)
J_s is the solute mass flux ($M\,L^{-2}\,T^{-1}$)
q_w is the Darcian water flux ($L\,L^{-1}\,T^{-1}$)

To define C_f, an artificial solute mass reservoir is assumed to exist outside the soil profile. When solute is applied (with a fertilisation or irrigation event), it dissolves in the mass of water entering the profile during the day of solute application (or the first day when infiltration occurs). Hence, the solute mass flux Js is determined by the water flow across the soil surface, filling or depleting the hypothetical reservoir. During infiltration, solute mass enters only the mobile soil region. Assuming zero dispersion in the hypothetical reservoir, the solute concentration at the soil surface is set equal to $C_f = J_s/q_w = C_s$. In the WAVE-model, a zero concentration gradient at the bottom of the flow domain is considered:

$$\left.\frac{\partial C_m}{\partial x}\right|_{x=L} = 0 \tag{2}$$

In discretised form, the bottom boundary condition definition is defined as:

$$C_{m\,n+1}^{\;j+1} = C_{m\,n}^{\;j+1} \tag{3}$$

Where: C_m is the mobile solute concentration (M L-1);
j is the time position in finite difference scheme;
n is the depth position in finite difference scheme.

Analytical solution using CXTFIT-model

The CXTFIT-model is used to estimate parameters in several models for transport during steady state one-dimensional flow by fitting the parameters to observed laboratory or field data obtained from solute displacement experiments. The CXTFIT-model is used for direct problem to predict solute distributions versus time and/or space for specified model parameters. Traditional deterministic approaches based upon the convection-dispersion equation (CDE) for chemical transport and the Richards equation for water flow work relatively well for homogenous, soils and packed laboratory soil columns.

CXTFIT-model Input

The analytical solutions of the equilibrium model will be used to model local-scale transport. The variables are the pore water velocity, v, in combination with the dispersion coefficient, D, and the distribution coefficient for linear adsorption, K.

MATERIALS

The numerical solution calculated with the WAVE-model is compared with the analytical solution, calculated with the CXTFIT-model. The scenarios are built up with combinations of compartment depth, applied flux at the top, and soil dispersivity for steady-state conditions. The soil profile is divided into different soil compartments of equal size. The different compartments are grouped into one soil layer. In the study, it is assumed that:

- one solute is applied in the first compartment;
- The applied amount of solute (in mg/m^2 is equal in the three cases (compartment depths 20 mm, 50 mm and 100 mm, respectively), but smeared out in a different way depending on the compartment depth. The solute amount was applied in the first compartment depth for different scenarios, so the total amount was always 1000 mg/ m^2 per compartment depth;
- the soil profile consists of one layer;
- the simulations are done to 2 m depth (the soil profile has a total depth of 2 m);
- non-reactive solute.

The simulations depend on 27 solute infiltration scenarios which resulted from combination of three basic variables: flux; soil dispersivity; and compartment depth. The variables are shown in Table 1 and the different solute infiltration scenarios are shown in Table 2.

Table 1: The three basic variables

Flux (mm/day)	2	5	10
Soil dispersivity (mm)	20	50	100
Compartment depth (mm)	20	50	100

Table 2: The different solute infiltration scenarios

Scenario	Flux (L/T)	Soil Dispersivity (L)	Compartment Depth (L)	Water Content (L^3/L^3)	Pore-Water Velocity[+] (L/T)	Dispersion Coefficient[++] (L^2/T)
1	2	20	20	0.3405	5.8737	117.474
2	2	50	20	0.3405	5.8737	293.685
3	2	100	20	0.3405	5.8737	587.370
4	2	20	50	0.3405	5.8737	117.474
5	2	50	50	0.3405	5.8737	293.685
6	2	100	50	0.3405	5.8737	587.370
7	2	20	100	0.3405	5.8737	117.474
8	2	50	100	0.3405	5.8737	293.685
9	2	100	100	0.3405	5.8737	587.370
10	10	20	20	0.3756	26.6240	532.480
11	10	50	20	0.3756	26.6240	1331.200
12	10	100	20	0.3756	26.6240	2662.400
13	10	20	50	0.3756	26.6240	532.480
14	10	50	50	0.3756	26.6240	1331.200
15	10	100	50	0.3756	26.6240	2662.400
16	10	20	100	0.3756	26.6240	532.480
17	10	50	100	0.3756	26.6240	1331.200
18	10	100	100	0.3756	26.6240	2662.400
19	5	20	20	0.3612	13.8430	276.860
20	5	50	20	0.3612	13.8430	692.150
21	5	100	20	0.3612	13.8430	1384.300
22	5	20	50	0.3612	13.8430	276.860
23	5	50	50	0.3612	13.8430	692.150
24	5	100	50	0.3612	13.8430	1384.300
25	5	20	100	0.3612	13.8430	276.860
26	5	50	100	0.3612	13.8430	692.150
27	5	100	100	0.3612	13.8430	1384.300

\+ Pore-water velocity = flux / water content

++ Dispersion coefficient = Pore-water velocity * soil dispersivity

RESULTS AND DISCUSSION

Numerical solutions of the transport equation often exhibit oscillatory behaviour and/or excessive numerical dispersion near relatively sharp concentration fronts. These problems can be especially serious for convection-dominated transport characterised by small dispersivities. Oscillations can often be prevented by selecting an appropriate combination of space and time discretizations. To achieve acceptable numerical results, the spatial discretization must be kept relatively fine and the relative extent of numerical oscillation which is associated with the time discretization small.

The solute concentrations were calculated with the WAVE-model and the CXTFIT-model for each scenario. For flux is 2 mm/day, the solute concentration profiles were retained chosen at 21-Jan., 10-Feb. and 2-Mar., for flux is 5 mm/day at 9, 17 and 25

Jan. and for flux is 10 mm/day at 5, 9 and 13 Jan. The solute infiltration scenarios were compared, the results are shown in Fig. 1. The results of different solute infiltration scenarios using WAVE-model as numerical solution and, CXTFIT-model as analytical solution are analyzed to find:

- the relation between the WAVE-model error and the compartment depth;
- the relation between the WAVE-model error and the soil dispersivity;
- the relation between WAVE-model error and the flux.

1. Solution difference between WAVE-model and CXTFIT-model

Fig. 2 shows the solution difference between the solute concentration calculated with WAVE-model and CXTEIT-model at each compartment node. The shape of error is the same for different infiltration scenarios, whatever the value of flux, soil dispersivity or compartment depth. For example, the error curve of 21-Jan. for scenarios 1, 4 and 7 has the same shape although the compartment depths are 20 mm, 50 mm and, 100 mm respectively. The error curve of the same day for scenarios 1, 2 and, 3 has also the same shape although the soil dispersivities are 20 mm, 50 mm and, 100 mm respectively.

The same results were produced for scenarios 1, 10 and, 19 with fluxes of 2 mm/day, 10 mm/day and, 5 mm/day respectively. This means that the WAVE-model error (the difference between WAVE-model and CXTFIT-model) is symmetrical whatever the value of flux, soil dispersivity or, compartment depth. The error gets smaller if the soil dispersivity equals or greater than 5 multiplying by compartment depth and smeared out in depth when soil dispersivity is big because the spatial discretization is kept relatively fine.

2. Evaluation of the error

The WAVE-model error was evaluated with three methods:
- absolute maximum error;
- relative maximum error (Loague and Green, 1991);
- relative area (Tseng and Jury, 1994).

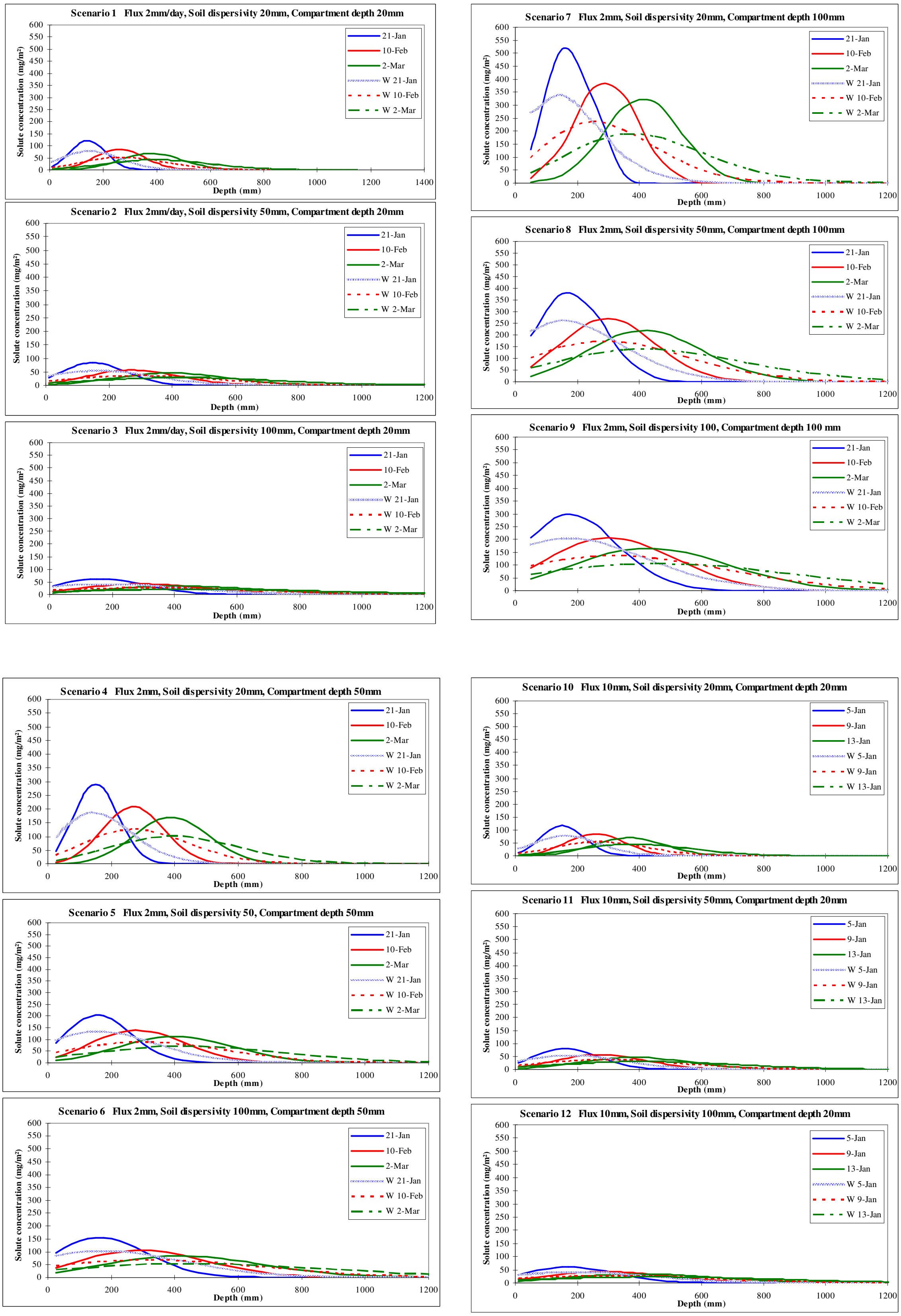

Fig. 1: Comparison between the solute concentrations for scenarios 1 to 12 calculated with CXTFIT-model (5-Jan., 9 Jan. and 13 Jan.) and WAVE-model (W 5-Jan., W 9 Jan. and W 13 Jan.)

2.1. Absolute maximum error method

In this method, the WAVE-model error is evaluated with calculating the average absolute maximum solute concentration difference between the WAVE-model and CXTFIT-model.

2.2. Relative maximum error method

The relative maximum error is given by:

$$RME = MAX_i^n = [ABS(O_i - S_i)]100/\overline{O} \quad (4)$$

Where:

RME	is the relative maximum difference between concentrations calculated with CXTFIT-model and WAVE-model, respectively;
O_i	is the solute concentrations calculated with CXTFIT-model;
S_i	is the solute concentration calculated with WAVE-model;
$\overline{O}$	is the peak solute concentration calculated with CXTFIT-model.

2.3. Relative area method

The relative area error is given by:

$$RA = \sum_{i=1}^{n} [ABS(O_i - S_i)].d / \sum_{i=1}^{n} S_i.d \quad (5)$$

Where:

RA	is the relative area;
d	is the compartment depth.

3. Relation between the WAVE-model error and compartment depth

For the same flux and soil dispersivity the WAVE-model error calculated with absolute average maximum error is increasing with the increasing of the compartment depth. For the same flux and soil dispersivity of 20 mm, the WAVE-model error calculated with relative average area method is increasing with the increasing of the Compartment depth. Meanwhile, for the soil dispersivities of 50 mm and, 100 mm, it was found that the model error is decreasing with the increasing of the compartment depth.

Calculating the WAVE-model error with the relative average maximum error method implied that the error is increasing with the increasing of the compartment depth for the same flux and soil dispersivity. Increasing of error depends on the fact that, with numerical solution, increasing of compartment thickness will decrease the numerical accuracy (numerical dispersion increases when the compartment depth increases). The amount of solute which applied in first compartment might affect the error magnitude. The total amount of solute (in mg/m^2) is the same for the three cases (compartment depths of 20 mm, 50 mm and 100 mm, respectively), but smeared out in a different way depending on the compartment depth. The solute amount was applied in the first compartment depth for different scenarios, so the total amount was always 1000 mg/m^2 per compartment depth.

4. Relation between the WAVE-model error and soil dispersivity

For the same flux and compartment depth, the WAVE-model error is decreasing with the increasing of the soil dispersivity. These results were produced by calculating the WAVE-model error with absolute average maximum error method, relative average area method and relative average maximum error method. With higher soil dispersivity better results were obtained and the error was decreasing because higher soil dispersivity causes some early arrival of solute in the soil and reduces the problems of numerical solutions which result from oscillatory behaviour and/or excessive numerical dispersion.

5. Relation between WAVE-model error and flux

For the same compartment depth and soil dispersivity, the WAVE-model error is decreasing with increasing of the flux. This result was produced by calculating the error with the three different methods to evaluate the WA VE-model error. The WAVE-model error is smaller for flux = 10 mm/day than for flux = 5 mm/day and smaller for flux = 5 mm/day than for flux = 2 mm/day. Increasing the flux increases the pore- water velocity (the pore-water velocity = flux/water content) and causes early arrival of solute in the soil decreasing also the problem of numerical solutions, so the error decreases.

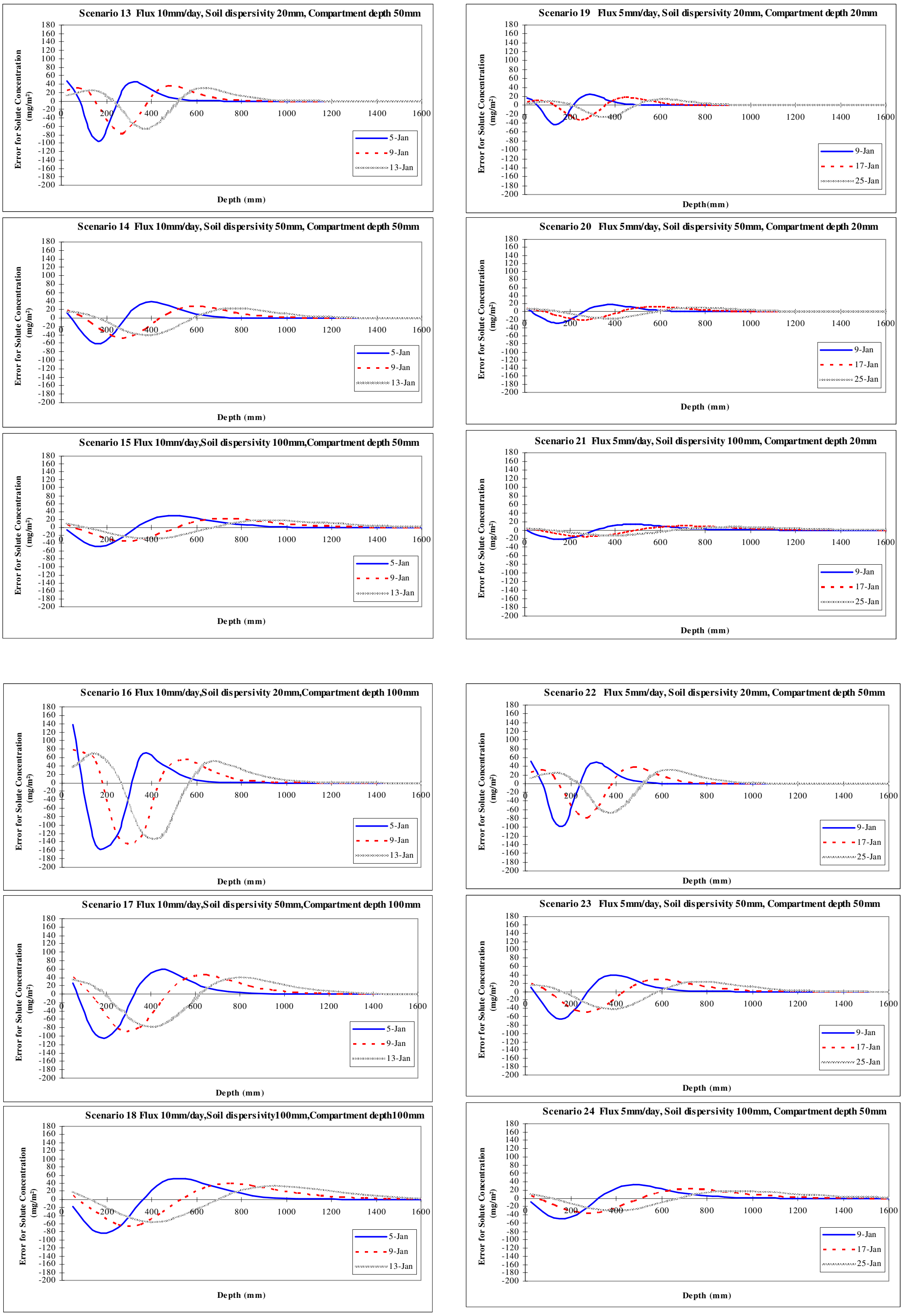

Fig. 2: WAVE-model error for scenarios 13 to 24

CONCLUSIONS

The examination of numerical methods through an analysis of their ability comparing with analytical methods is strongly recommended to measure the quality of the numerical solutions. Numerical solutions of the transport equation often exhibit oscillatory behaviour and/or excessive numerical dispersion near relatively sharp concentration fronts. In this study, the numerical solutions calculated with the WAVE-model, was compared with the analytical solutions calculated with the CXTFIT-model. The different solute infiltration scenarios were built up with combinations of three basic variables: flux, soil dispersivity and compartment depth for steady-state conditions. The simulations depend on 27 solute infiltration scenarios.

The numerical solution was calculated with the WAVE-model and the analytical solution was calculated with the CXTFIT-model for solute concentration for each scenario, for each compartment (at the node) every day. The solute infiltration scenarios were compared and the WAVE-model error was evaluated with three methods: absolute average maximum error, relative average maximum error and relative average area error. The study implied that:

- The WAVE-model error was increasing with the increasing of the compartment depth. Increasing the compartment thickness decreased the calculation time but also the numerical accuracy (numerical dispersion increases when the compartment depth increases). Generally, one can select a numerical scheme which decreases the magnitude of one problem at the expense of increasing the effect of the other.
- The WAVE-model error was decreasing with the increasing of soil dispersivity. With higher soil dispersivity better results were obtained and the error was decreasing because higher soil dispersivity causes some early arrival of solute in the soil and reduces the problems of numerical solutions which result from oscillatory behaviour and/or excessive numerical dispersion.
- The WAVE-model error was decreasing with the increasing of flux. Increasing the flux increases the pore-water velocity (the pore-water velocity = flux / water content) and causes early arrival of solute in the soil decreasing also the problem of numerical solutions, so the error decreases. Finally the study recommended using compartment depth as thin as possible where, the WAVE-model error will be smaller.

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