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EFFECTS OF HYSTERESIS AND TEMPORAL VARIABILITY IN METEOROLOGICAL INPUT DATA IN MODELING OF SOLUTE TRANSPORT IN UNSATURATED SOIL USING HYDRUS-1D

Effekten av hysteresis och tidsupplösning av meteorologiska indata på modellering av föroreningstransport i den omättade zonen med HYDRUS-1D

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Abstract

A one-dimensional, unsaturated transport model was used to simulate non-reactive transport of solutes. The effects of soil water hysteresis, and temporal variability in precipitation and evapotranspiration input data were evaluated. Simulations were conducted in HYDRUS-1D code for the period 1996–2008 for three different geographic locations in Sweden and for three different soil textures. Simulations were run for the period from March to September for both hysteretic and non-hysteretic cases with different temporal variability of precipitation and evapotranspiration input data (half-hourly, hourly, 2-hours, 4-hours, and daily). The results show that under non-hysteretic water flow solute migration is faster. Analysis of the downward migration of the solutes indicates that the effect of hysteresis is more pronounced in the coarse textured soils. The simulations show that a lower temporal resolution of the meteorological input data increases both underestimation of the downward movement of the solutes for non-hysteretic simulations and overestimation for hysteretic ones. Meanwhile, in most cases, this over and underestimation rises with increasing hydraulic conductivity of the soil. Finally, analysis of the results displays that the differences between hysteretic and non-hysteretic simulations are negligible when using daily input data.

Key words – HYDRUS-1D; Unsaturated zone; Hysteresis; Solute transport; Temporal variability of precipitation

Sammanfattning

Föroreningstransport genom den omättade markvattenzonen modellerades med en endimensionell numerisk modell kallad HYDRUS-1D. Effekten av hysteresis och tidsupplösning av regn undersöktes. Simuleringar med HYDRUS-1D gjordes för tre olika platser och tre olika jordtyper i Sverige under perioden 1996–2008. För varje år gjordes simuleringar under perioden mars till september. Simuleringarna gjordes både med och utan hysteresis samt med olika tidssteg för indata; 0,5, 1, 2, 4 och 24 h. Resultaten visar att transporthastigheten överskattades när hysteresis inte beaktades. Denna effekt är mer påtaglig i grövre jordar. Simuleringarna visade också att tidsupplösningen var viktig. När hysteresis beaktades överskattades transporten vid en lägre tidsupplösning medan för fallen utan hysteresis var det tvärtom. Dessa effekter var större ju högre hydraulisk konduktivitet jorden hade. En slutsats man kan dra från resultaten in denna studie är att för 24 h tidsupplösning spelar hysteresis ingen större roll, därför rekommenderas att hysteresis inte beaktas för denna tidsupplösning för att minska simuleringstiden.

1 Introduction

The zone between ground surface and groundwater table is defined as the unsaturated zone or the vadose zone which contains in addition to solid soil particles, air and water. The unsaturated zone acts as a filter for the aquifers by removing unwanted substances that might come from the ground surface such as hazardous wastes, fertilizers and pesticides. This filtering is attributed to the high contents of organic matters and clay, which motivates biological degradation, transformation of contaminants and sorption. Therefore, the vadose zone can be considered as a buffer zone protecting the groundwater. Thus, the hydrogeological properties of this zone are of great concern for the groundwater pollution (Selker et al., 1999, Stephens, 1996).

Many chemical and physical processes occur in the soil horizon. These processes are attributed to different soil phases, due to the existence of solid particles, water and air. In order to be able to model water and solute transport in the unsaturated zone and provide acceptable outputs concerning water and solute solution profiles, it is required to make some simplifications and assumptions due to the heterogeneous and complex nature of soil (Selker et al., 1999).

From hydrologic point of view, the transmission of water to aquifers, to water on the surface, and to the atmosphere is greatly controlled by the processes in unsaturated zone. For these reasons, the study and modeling of water flow and solutes transport in the unsaturated zone is becoming an issue of major concern, generally, in terms of water resources planning and management, and especially in terms of water quality management and groundwater contamination (Rumynin, 2011).

A large number of models have been developed during the past several decades to evaluate the computations of water flow and solute transfer in the vadose zone. In general, they are either analytical or numerical models for predicting water and solute movement between the soil surface and the groundwater table. Amongst the most commonly used ones are the Richards equation for variably saturated flow, and the Fickian-based convection-dispersion equation (CDE) for solute transport (Šimůnek et al., 2009). These two equations are solved numerically using finite difference or finite element methods (Arampatzis et al., 2001, Šimůnek et al., 2009), which requires an iterative implicit technique (Damodhara Rao et al., 2006). HYDRUS is one of the computer codes which simulates water, heat, and solutes transport in one, two, and three dimensional variably saturated porous media on the basis of the finite element method. The Richards equation for variably-saturated water flow and advection-dispersion type equations (CDE) for heat and solute transport are solved deterministically (Šimůnek et al., 2009).

In this study, HYDRUS-1D version 4.14 is used as a tool to analyze water and solute movement in the vadose zone in Sweden through investigating downward movement of the centre of mass of solutes and general patterns of concentration profiles. Among the specific objectives are identifying the effect of hysteresis on the movement of solutes for different kinds of soils in different geographic locations throughout Sweden. In addition, the effect of temporal variability in precipitation and implications of precipitation patterns on the downward movement of solutes in different types of soils in different geographic locations throughout Sweden was examined.

2 Theory

2.1 Water Flow in Unsaturated Zone

Water flow in the unsaturated zone is usually described by Richards equation (1). In this study water flow and solute transport was numerically simulated by the numerical model HYDRUS-1D. The software uses a modified Richards equation and describes infiltration into vadose zone by modeling it as one dimensional vertical flow.

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left[K(\theta)\left(\frac{\partial H}{\partial z} - 1\right)\right] - S \qquad (1)$$

Where θ is the volumetric water content, $[L^3L^{-3}]$, t is time [T], q is the volumetric flux density $[LT^{-1}]$, z is the spatial coordinate [L], and S is a general sink or source term $[L^3L^{-3}T^{-1}]$, for example, root water uptake, K is an unsaturated hydraulic conductivity, $[LT^{-1}]$, H is a soil water pressure head, [L], relative to atmospheric pressure ($H \leq 0$). Richards equation is partially differential and highly non-linear as θ–H–K has a non-linear relationship in nature, which also indicates its strongly physically based origin.

Essential hydraulic soil property that describes soil water movement is volumetric water content which differs with soil water suction, H. Suction usually expressed by the soil water matric head, (strictly negative) or soil suction (strictly positive). If suction is very low (higher moisture contents) water retention depends on capillary surface tension effects, and the last depends on pore size and soil structure. If suctions are higher (lower moisture contents) water retention influenced mainly by adsorption which depends on soil texture and specific surface (i.e. surface area per unit of volume) of material (Ward and Robinson, 2000b).

Another important hydraulic soil property that describes soil water movement is the relation between the soil's unsaturated hydraulic conductivity, K, and volumetric water content, θ. Hydraulic conductivity reflects the ability of porous medium to transfer the water. Hydraulic conductivity depends on size, shape of filled with water pores (Wang, 2009) and how they are connected between each other, the flowing fluid and θ of the soil (Simunek and Genuchten, 2006).

The unsaturated hydraulic soil properties, $\theta(h)$ and $K(h)$ for this study was defined by a simple single-porosity hydraulic model which describes uniform flow in porous media and disregards the preferential flow. The model is based on van Genuchten equation which expresses unsaturated hydraulic conductivity as function of soil water retention parameters (van Genuchten, 1980).

2.2 Hysteresis in soil hydraulic properties

Water content at a given suction depends not only on the value of that suction but also on hysteresis or moisture 'history' of the soil (Ward and Robinson, 2000b). The retention curves will be different for drying and wetting soils: at a given matric pressure the water content for wetting soils will be less than for drying ones. The main drying curve describes the drying from the highest reproducible saturation degree to the residual water saturation. But the main wetting curve describes the wetting from the residual θ to the highest degree of saturation.

Several studies were conducted recently to investigate the effect of hysteresis and many of them showed that hysteresis has an effect on unsaturated soil water movement and solute transport (Russo et al., 1989, Yang et al., 2012, Lehmann et al., 1998, Kool and Parker, 1987) as well as disregarding hysteresis might lead to significant errors in prediction of solute movement and contaminant concentrations (Kool and Parker, 1987). The main factors which affect hysteresis are the complexity of the pore space geometry, the presence of entrapped air, shrinking and swelling and thermal gradients. There are many mechanisms by which hysteresis is propagated but the main ones are considered to be 'ink bottle' and 'contact angle' effects (Ward and Robinson, 2000a).

- 'ink bottle effect' implies that water drains the pore at a larger suction as larger suction is needed to enable the air to enter the narrow pore neck, than for filling the pore with water, as it is controlled by the lower curvature of the air-water interface in the wider pore itself.
- The 'contact angle' affect implies that the contact angle of the solute interfaces is likely to be larger when the interface is advancing (wetting) than when it is receding (drying), so at a given θ the suction will be greater for drying than for wetting (Ward and Robinson, 2000a). However, it might be assumed that the contact angle is something that is not fully understood as it is very difficult to measure (Nimmo, 2006).

3 Materials and methods

3.1 Input data

Meteorological data

Precipitation and evapotranspiration during study period 1996–2008 were given as input for time variable boundary conditions in HYDRUS-1D. The meteorological data for all the three sites under investigations (Löddeköpinge, Norrköping, and Petisträsk) were obtained from Swedish Metrological and Hydrological Institute (SMHI). Initially precipitation data were given in half-hourly time resolution. In order to investigate the effect of time resolution of the input on the model, half-hourly input was converted into 1, 2, 4, and 24 h input.

Potential evapotranspiration was given as monthly data. Monthly data can give only hourly average values during a day which cannot give a good picture of reality, as evapotranspiration varies during the day and the season. For this study a model was built to calculate hourly ET according to diurnal variations. The model was completed in a simplified manner and it was assumed that:

- There is no ET during the night, 18:00 until 6:00;
- ½ of the diurnal ET is during 8 hours, between 6:00 and 10:00, and between 14:00 and 18:00;
- ½ of diurnal ET occurs during 4 hours between 10:00 and 14:00.

Soil hydraulic properties

Investigation of coupled water and solute transport was done for different climatic conditions and for the soils with different physical properties. For this soil 1 (Persson and Berndtsson, 2002), soil 2 (Zhang, 1991) and soil 3 have been chosen which are considered to be representative for typical Swedish agricultural soils. Three 250 cm deep multi layered soil profiles were used as input data for HYDRUS-1D for 3 sites of interest (Table 1).

Contaminant sources

The top 5 cm of soil with area 1 m^2 was assumed to be contaminated with 100 g of non-volatile and non-reactive solute. For the simulation of the solute transport the initial concentration in liquid phase (mass solute per volume of water) has been used as input to the model. The volume of water in the top 5 cm soil was calculated.

Table 1. *Soil profiles for study sites.*

	Depth (cm)	Sand (%)	Silt (%)	Clay (%)	Bulk density (g/cm^3)
Soil 1					
	0–20	80	16.5	3.5	1.53
	20–45	78.8	18.3	2.9	1.55
	45–70	84.3	11.8	3.9	1.55
	>70	93.4	4.8	1.8	1.56
Soil 2					
	0–20	68.0	27.2	4.8	1.48
	20–150	58.15	32.99	8.86	1.48
	>150	40.5	44.6	14.9	1.65
Soil 3					
	0–120	59.0	25.6	15.4	1.45
	120–150	36.9	32.8	30.3	1.50
	>150	35.3	36.5	28.2	1.60

Volumetric water content for the soil was calculated according to van Genuchten (1980). van Genuchten hydrodynamic parameters θ_r and θ_s were predicted by Hydrus-1D from the particle size distribution and bulk density of the soils (Table 2) The following initial liquid phase concentrations were obtained for different soil types: $C_{soil\ 1}$=23.2 mg/cm^3, $C_{soil\ 2}$ =13.5 mg/cm^3 and $C_{soil\ 3}$=9.31 mg/cm^3.

3.2 Modeling with HYDRUS-1D

In this study, three different kinds of soil profiles were used; Soil 1, Soil 2, and Soil 3. The total depth of each soil profile is 250 cm, representing the average depth of the unsaturated zone in Sweden. The finite element model was constructed by dividing the entire profile into 100 layers of a thickness of 2.5 cm.

The period 1st of March to 25th of September was used for simulation purposes (5000 h). This period was selected due to the fact that a large amount of annual precipitation occurs in this period in Sweden. In addition, problems associated with soil freezing could be neglected.

For modeling purposes, the van Genuchten-Mualem single porosity model was used, both with and without hysteresis. The parameters needed for the van Genuchten-Mualem single porosity model are residual and saturated water contents, saturated hydraulic conductivity, pore connectivity parameter, and the empirical coefficients α and *n*. To predict the values of these parameters, HYDRUS-1D uses Rosetta DLL (Dynamically Linked Library) (Schaap et al., 2001).

Modeling with HYDRUS-1D was performed for the cases with and without hysteresis for all the three sites with different temporal variability of precipitation and evapotranspiration input data. First, half-hourly precipitation and evapotranspiration data were applied to simulate in the model, then 1, 2, 4, and finally 24 h.

Three objective functions were used to achieve the aims of this research, depth of the centre of mass of solutes (COM), depth to a limit concentration (LC), and the mass of solutes leached into the groundwater (M_{gw}).

3.3 Limitations

The study of the unsaturated zone is a complex work due to the heterogeneous nature of soil; therefore, to be able to model movement of water and solutes, and in an attempt to achieve the aim and specific objectives of the study, some simplifications and limitations were made:

- Because of time limitations, only 13 years were simulated. In addition, the selected period for simulations

Table 2. *Soil hydraulic parameters obtained from Hydrus-1D, using the single porosity flow model.*

	Depth, cm	θ_r (V/V)	θ_s (V/V)	α (1/m)	*n*	K_s (m/d)	l
Soil 1	0–20	0.039	0.372	0.0437	1.818	5.01	0.5
Soil 2	0–20	0.034	0.371	0.0383	1.476	2.70	0.5
Soil 3	0–120	0.052	0.397	0.021	1.438	1.27	0.5

(1st of March–25th of September) might not be the worst condition for downward migration of solutes in all the locations.

- It was assumed that the water-table is constant (250 cm below the ground surface) throughout the simulation period.
- The effect of root-water uptake was neglected.
- A one-dimensional vertical movement was assumed and simulated in the model, though three-dimensional flow representing more correctly the reality. However, the one-dimensional vertical movement is the dominant direction of flow in the unsaturated zone, but in a large-scale field condition it could be seen as a simplification of the reality.
- A single porosity model was used to describe the uniform flow in the unsaturated porous media which neglects both the variability in the soil properties, and non-equilibrium flow.
- Simulations were conducted for the non-reactive solute transport. This might be an overestimation of the real downward migration of solutes.
- The input precipitation and evaporation data could be another factor of uncertainty, especially the downscaling of the evapotranspiration input data.

4 Results and discussion

4.1 Effect of hysteresis

First, the effect of hysteresis on the downward movement of solutes is evaluated. During the study period (1996–2008) precipitation varies between 243 to 577 mm, 288 to 409 mm, and 270 to 500 mm in Malmö, Norrköping, and Petisträsk, respectively. The depths to COM against measured precipitations for soil 1 in all sites are displayed in Figure 1. It is obvious that the depth of COM is deeper when hysteresis is neglected. This is generally in agreement with a previous study conducted by Russo et al. (1989), in which overestimated values of solute velocities have been noticed in transient flow models when neglecting hysteresis. Pickens and Gillham (1980) also reported that for "a hypothetical case involving one-dimensional transport of slug of water containing a nonreactive tracer during an infiltration-redistribution sequence in a vertical sand column", there is a lag in hysteretic concentration profiles compared to that of non-hysteretic case. This behavior could be due to the fact that under hysteretic conditions, only small changes in moisture content can be resulted from large changes in pressure head. In such a case, hysteretic simulations show slower changes than the non-hysteretic simulations (Bashir et al., 2009).

On the other hand, the trend line is steeper when ignoring hysteresis with higher R^2 values, which refers to more rapid response to the precipitation increase and stronger linear relationship between solute movement and precipitation.

The depth of COM versus measured precipitation plots in Norrköping shows a different pattern compared to the same soil profiles in Malmö and Petisträsk (Figure 1). The relationship between precipitation and depth of COM is unclear (non-linear). This could be attributed, at least partially, to the precipitation pattern. For better understanding the implications of precipitation pattern in all the sites on the downward movement of water and solutes more investigation is required. The relationship between depth of COM and precipitation in a specific soil type does not depend only on the amount of pre-

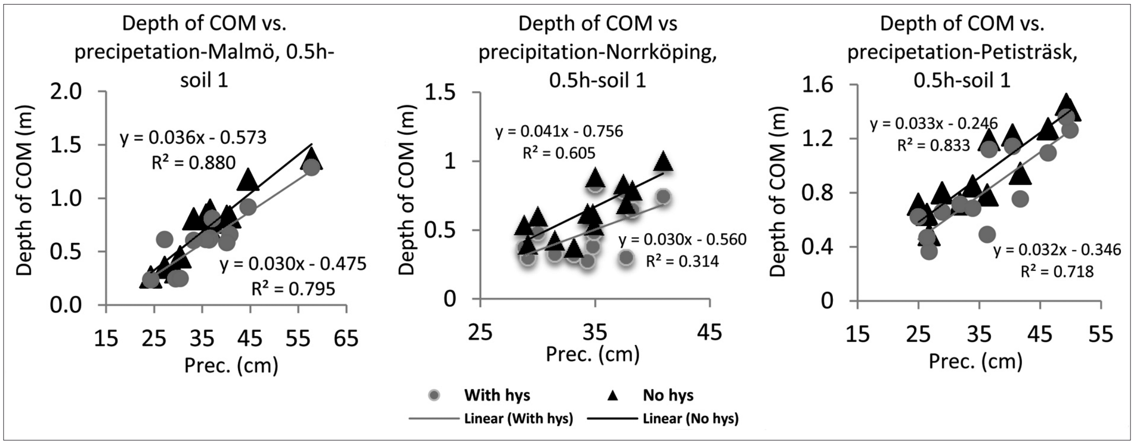

Figure 1. *Depth of COM of solutes versus measured precipitations in soil 1, soil 2, and soil 3 in all the three sites for the period 1996–2008, for both non-hysteretic (triangular dots) and hysteretic (circular dots) models.*

Table 3. *The average depths of COM in m for all the three soil types for the period 1996–2008.*

	Soil 1		Soil 2		Soil 3	
	Hysteresis	No hysteresis	Hysteresis	No hysteresis	Hysteresis	No hysteresis
Malmö	0.619	0.739	0.303	0.381	0.2726	0.295
Norrköping	0.482	0.640	0.260	0.308	0.214	0.241
Petisträsk	0.8285	0.9607	0.4511	0.5071	0.3813	0.4025

cipitation (non-deterministic relationship). One might expect that, for instance, precipitation pattern could be another important factor.

When evaluating the effect of hysteresis and comparing between different soil profiles, it is found that, on average, the depth of COM in Malmö is deeper in non-hysteretic water system by 19 % in soil 1, 26 % in soil 2, and 8 % in soil 3. While in Norrköping the depth of COM is deeper in non-hysteretic system by 33 % in soil 1, 18 % in soil 2, and 13 % in soil 3. Finally, in Petisträsk the depth of COM is deeper in non-hysteretic system by 16 % in soil 1, 12 % in soil 2, and 6 % in soil 3 (Table 3). In other words, the differences are most pronounced in coarse textured soils (Parlange et al., 2006, Ward and Robinson, 2000a).

The importance of time resolution of the input data on hysteresis is illustrated by investigating the depth of COM in all the three sites for the three soil profiles under investigation. In Table 4 the average depths to COM with half hourly, 4-hourly, and daily input data during study period are shown. The results display that the differences between hysteretic and non-hysteretic simulations decrease with decreasing time resolution of the input data. It seems that the differences almost disappeared when using daily input data.

It is expected to have less variation in soil moisture when using averaged daily input data. In other words, the effect of moisture history of the soil will be vanished over short time periods (hours), which play an important role when finding water content at a specific suction. This means that the effect of hysteresis will not be that important, since the mechanism of hysteresis is more pronounced over short time periods (hours).

4.2 Effect of temporal variability in rainfall and evapotranspiration

We started analyzing the effects of temporal averaging of precipitation and evapotranspiration input data on the downward movement of moisture and contaminants by examination of the two functions, COM and LC. For soil 1 in all sites solute movement was simulated with half hourly meteorological input as well as with 1, 2, 4, and 24 h. For soil 2 and soil 3 the simulations were done but only with half hourly, 4 h and 24 h inputs. To be able to analyze the effect of temporal averaging of the

Table 4. *The average depths of COM in m with half hourly, 4 h, and daily input data, for all the soils, for the period 1996–2008.*

Time-step (h)	Soil 1		Soil 2		Soil 3	
	Hysteresis	NO hysteresis	Hysteresis	NO hysteresis	Hysteresis	NO hysteresis
Malmö						
0.5	0.6192	0.739	0.3033	0.381	0.2726	0.295
4	0.6146	0.7248	0.3392	0.3940	0.2798	0.2927
24	0.6929	0.6693	0.3590	0.3628	0.2966	0.2872
Norrköping						
0.5	0.4818	0.6398	0.2601	0.3082	0.2135	0.2407
4	0.5500	0.6177	0.2763	0.3029	0.2377	0.2391
24	0.5329	0.5404	0.2752	0.2853	0.2338	0.2304
Petisträsk						
0.5	0.8285	0.9607	0.4511	0.5071	0.3813	0.4025
4	0.8559	0.9484	0.4561	0.5035	0.3804	0.3979
24	0.9111	0.9080	0.4927	0.4906	0.3917	0.3933

Table 5. *Averaged depths of COM as a percentage of half hourly COM during 1996–2008 without considering hysteresis.*

Time-step (h)	Malmö			Norrköping			Petisträsk		
	Soil 1	Soil 2	Soil 3	Soil 1	Soil 2	Soil 3	Soil 1	Soil 2	Soil 3
0.5	100	100	100	100	100	100	100	100	100
1	100	–	–	100	–	–	100	–	–
2	99	–	–	99	–	–	100	–	–
4	98	99	100	96	98	99	99	99	99
24	89	95	98	83	92	95	94	97	98

Table 6. *Averaged depths of COM as a percentage of half hourly, during 1996–2008 years, with effect of hysteresis.*

Time-step (h)	Malmö			Norrköping			Petisträsk		
	Soil 1	Soil 2	Soil 3	Soil 1	Soil 2	Soil 3	Soil 1	Soil 2	Soil 3
0.5	100	100	100	100	100	100	100	100	100
1	98	–	–	106	–	–	102	–	–
2	97	–	–	116	–	–	102	–	–
4	100	111	104	117	108	111	104	102	100
24	113	118	109	119	107	109	112	109	102

meteorological data we took 0.5 hour input as a base point, assuming that the higher time resolution, the more adequate outputs. This allowed us to calculate the percentages of different time resolutions with regard to the base point for each year. Later, the averages during the whole period for each soil type for each location were computed.

Investigating the migration of COM with different inputs, one can see that for all three locations the averaged inputs seem to lead to rising of underestimation of COM migration with increasing time step. In addition, the rate of underestimation is rising proportionally with hydraulic conductivity of soil in the non-hysteretic model. This shows that contaminant transport in the unsaturated zone is influenced to a large degree by the hydraulic properties and its heterogeneity. For instance, in soil 3 even when using half-hourly short intense precipitations, the whole amount of water may not totally infiltrate due to low infiltration capacity. This means small differences might occur when comparing half hourly results to daily ones in soil 3. Moreover, recent study by Wang (2009), seems to support this finding. It is worthwhile to notice that the underestimation of COM migration is very small for 1, 2 and 4 h time steps for all soil types in all sites, and in average does not exceed 1 %. For the 24 h time step the overestimation is also relatively small, 6.5 % in average. The exception is Norrköping soil 1 with 24 h time step, where the underestimation is 17 %, see Table 5.

Concerning COM movement in hysteretic models, one may see that in many cases lower input resolution leads, on the contrary to non-hysteretic ones, to an overestimation of COM migration. It also seems that the overestimation also rises with increasing hydraulic conductivity of the soil but the overestimation is a quite small (Table 6).

The reason why the COM is overestimated in hysteretic model when using daily input data compared to half-hourly is that the effect of the soil history disappears (variations in the soil moisture are neglected) which in turn leads to deeper percolation. In other words, the hysteretic simulation results will tend to be more similar to those of the non-hysteretic case.

Analyzing how the temporal averaging the input data effects on the depth to LC one may see that for all sites and all soil types in non-hysteretic model, the depth to LC is almost stable for hourly, 2 hours and 4 hours input. As in case with COM here we may also observe that it seems that the depth to LC is more underestimated for coarse textured soils compared to finer ones, see Table 7.

For hysteretic case the depth to LC as the depth to COM is slightly overestimated and the overestimation also rises with time step as well as with increasing hydraulic conductivity in the soil. Average overestimation of depth to LC for all sites and for hourly time-step is 2 %, for 2 h time step zero, for 4 h time step 1 %, and for 24 h is 3 % (Table 8).

Table 7. *Averaged depths to LC as a percentage of half hourly LC during 1996–2008 years, without considering hysteresis.*

Time-step (h)	Malmö			Norrköping			Petisträsk		
	Soil 1	Soil 2	Soil 3	Soil 1	Soil 2	Soil 3	Soil 1	Soil 2	Soil 3
0.5	100	100	100	100	100	100	100	100	100
1	100	–	–	100	–	–	100	–	–
2	100	–	–	99	–	–	100	–	–
4	99	99	99	98	99	99	99	100	100
24	100	96	99	90	98	99	96	99	100

Table 8. *Averaged depths to LC as a percentage of half hourly input, during 1997–2008 years, with effect of hysteresis.*

Time-step (h)	Malmö			Norrköping			Petisträsk		
	Soil 1	Soil 2	Soil 3	Soil 1	Soil 2	Soil 3	Soil 1	Soil 2	Soil 3
0.5	100	100	100	100	100	100	100	100	100
1	100	–	–	104	–	–	102	–	–
2	98	–	–	102	–	–	102	–	–
4	104	103	101	104	103	102	96	101	100
24	106	101	103	108	102	101	100	104	101

4.3 Effect of geographic location

The results clearly demonstrate that the depth of COM is deeper in Petisträsk compared to the other two sites. It can also be seen that the lowest depths of COM occurred in Norrköping.

The average precipitations are 365, 343, and 365 mm in Malmö, Norrköping, and Petisträsk respectively. The deeper migration of COM of solutes in Petisträsk could be, at least partially due to higher net precipitation compared to the other two sites (Table 3).

5 Conclusions and recommendations

Water and solutes movement in the unsaturated zone is incredibly complex process due to the heterogeneous nature of soil and variable atmospheric boundary conditions at the soil surface over short time periods. Despite all the simplifications which were made, HYDRUS-1D is a powerful tool to simulate the movement of water and solutes in partially saturated porous media, since it can deal with different water flow and solute transport boundary conditions. However, to be able to validate the model performance, more data collection and measurements are needed which in turn means more cost-effective sampling and analysis methodologies must be developed.

Results of the study show the following;

- Generally, under non-hysteretic water flow, solute migration is faster which in turn refers to an overestimation of the solute velocity, especially with high resolution input data.
- Analysis of the downward migration of the solutes indicates that the effect of hysteresis is more pronounced in the coarse textured soils
- Generally, the leaching of solutes into the groundwater (GW) starts beyond some threshold precipitation values, although even the maximum concentrations leached into the GW at the end of simulation period are small, especially in Norrköping.
- The results demonstrate that the concentration profiles of solutes in Norrköping and Malmö are lagged behind that of Petisträsk, since the results show that the average depth of COM is deeper in Petisträsk. It is also found that the lowest depths of COM occurred in Norrköping. This could be an indication that the groundwater is more susceptible to contamination in Petisträsk and Malmö in comparison to Norrköping. Though in real conditions, there are many other key factors affecting migration of contaminants from ground surface into the groundwater, for instance, land use, topography, etc.
- Lower time resolution of the input data leads to increasing both underestimation of the depth of COM

for non-hysteretic simulations and overestimation for hysteretic ones.

- In most cases overestimation and underestimation of the depth to COM is rising with increasing hydraulic conductivity of the soil.
- It is found that the differences between hysteretic and non-hysteretic simulations are very small when using daily input data. Consequently, we may recommend neglecting the effect of hysteresis when using daily input data.

Finally, from the results and preceding discussion and conclusions, we propose a number of recommendations;

- Since in this study the simulations were conducted using only 13 years of data which might not be long enough to find out and understand the tendency of the downward migration of solutes, so it could be useful to extend the study period.
- It might be also useful to try different simulation periods and compare between them to discover the worst downward migration scenarios.
- Finally, further investigation is required to evaluate the implications of precipitation pattern on the solute transport.

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