

Examples of numerical simulations of two-dimensional unsaturated flow with VS2DI code using different interblock conductivity averaging schemes

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Abstract

Flow in unsaturated porous media is commonly described by the Richards equation. This equation is strongly nonlinear due to interrelationships between water pressure head (negative in unsaturated conditions), water content and hydraulic conductivity. The accuracy of numerical solution of the Richards equation often depends on the method used to estimate average hydraulic conductivity between neighbouring nodes or cells of the numerical grid. The present paper discusses application of the computer simulation code VS2DI to three test problems concerning infiltration into an initially dry medium, using various methods for inter-cell conductivity calculation (arithmetic mean, geometric mean and upstream weighting). It is shown that the influence of the averaging method can be very large for coarse grid, but that it diminishes as cell size decreases. Overall, the arithmetic average produced the most reliable results for coarse grids. Moreover, the difference between results obtained with various methods is a convenient indicator of the adequacy of grid refinement.

Keywords: numerical modelling, Richards equation, hydraulic conductivity

1. Introduction

Numerical modelling tools often are used to simulate flow and transport processes occurring in the vadose zone. Typical applications of such models in the field of hydrogeology and engineering geology include estimation of groundwater recharge, response of unconfined aquifers to pumping, infiltration from surface water bodies, as well as estimation of seepage rates and pore pressures in natural and artificial slopes and embankments, which influence their stability. Moreover, unsaturated flow simulations often provide data for contaminant or heat transport modelling. Flow modelling tools are typically based on the Richards equation (Richards 1931), which describes water movement in partially saturated porous media and in extended form is

suitable for both unsaturated and saturated conditions. The Richards equation is strongly nonlinear due to nonlinear relationships between water content, relative permeability and water pressure (in unsaturated conditions water pressure is negative and represents the effects of capillary and adsorption forces binding water to the soil or rock matrix). The hydraulic characteristics of unsaturated porous medium are given in the form of water retention curve (also called water characteristic curve), which represents the relationship between water content (or saturation) and water pressure, and the relative permeability function, which describes the dependence of the relative hydraulic conductivity on pressure or saturation.

A number of well-documented computer programs can be used by researchers or practitioners

interested in simulations of vadose zone flow. Examples of one-dimensional flow simulators include HYDRUS 1D (Šimůnek et al. 2008), UNSAT-H (Fayer 2000), SWAP (Kroes et al. 2008). Multidimensional flow problems can be solved for example with FEMWATER (Lin et al. 1997), TOUGH2 (Pruess et al. 1999) VS2DI (Healy 2008), HYDRUS 2D/3D (Šimůnek et al. 2008), SUTRA (Voss and Provost 2002), VADOSE/W (Geo-Slope International 2008) or DUMUX (Flemisch et al. 2007). The choice of particular modelling tools depends on the considered problem settings, robustness, ease of use and availability of the simulator and on the modeller's experience. Among the codes listed above, the VS2DI package has a combination of features which makes it an attractive option for many potential applications. The package has been developed over a period of nearly 30 years by the US Geological Survey. It started as a code for variably saturated flow modelling (Lappala et al. 1987), with later extensions covering transport of dissolved substance (Healy 1990) and heat (Healy and Ronan 1996), as well as a graphical user interface (Hsieh et al. 1999). The solution domain can be one-dimensional or two-dimensional (cartesian or axi-symmetric). Different types of boundary conditions specific to subsurface hydrology problems have been implemented (infiltration, evaporation, seepage face). The code can be downloaded and used free of charge, with no limitation on the number of nodes. It is simple to use due to graphical user interface working in a Windows environment. The computational modules are available as separate programs, together with its source code, so advanced users may modify it according to their needs. Applications of VS2DI codes to various hydrogeological problems have previously been summarised by Healy (2008) and Healy and Essaid (2012).

Numerical solution of the Richards equation involves several stages: spatial discretization, time discretization, linearization and solution of systems of linearized equations. For each stage a number of techniques are available, which usually involve a variety of user-specified parameters. The efficiency and accuracy of the solution may strongly depend on the choice of numerical methods and parameters for each stage of solution. One of such issues, which is the subject of this work, concerns approximation of the average hydraulic conductivity between two adjacent nodes or gridblocks in a finite-difference type discretization. This problem is not trivial, since the nodal values of conductivity can vary by several orders of magnitude. For example, during infiltration from ponded surface into a dry sand layer the initial conductivity is close

to zero, while the conductivity at the ponded surface is equal to its maximum (fully saturated) value. Various averaging approaches have been developed in the literature, including previous work by ourselves (Haverkamp and Vauclin 1979; Belfort and Lehmann 2005; Szymkiewicz 2009; Szymkiewicz and Helmig 2011; Szymkiewicz and Burzyński 2011; Szymkiewicz 2013, and others). However, more sophisticated averaging methods are used mostly in in-house research codes. VS2D is one of few publicly available simulation programs which enable the user to choose the method of hydraulic conductivity averaging (arithmetic, geometric and upstream). To the best of our knowledge, no systematic studies have been reported which deal with this aspect of the numerical solution procedure for VS2DI code. In this paper we show results of our numerical computations for three problems involving infiltration in sand or loamy sand soils using different grid density and different averaging procedures.

2. Variably saturated flow equation and its numerical solution

Two-dimensional flow in variably saturated porous medium can be described by an extended form of the Richards equation (Richards 1931; Lappala et al. 1987), derived from the mass conservation principle:

$$\frac{\partial \theta}{\partial t} + S S_s \frac{\partial H}{\partial t} - \frac{\partial}{\partial x} \left(K_{sx} K_R \frac{\partial H}{\partial x} \right) - \frac{\partial}{\partial z} \left(K_{sz} K_R \frac{\partial H}{\partial z} \right) = 0 \quad (1)$$

where: θ – volumetric water content, t – time, $S = \theta/\phi$ – water saturation, ϕ – porosity, S_s – specific storage coefficient, K_{sx} , K_{sz} – hydraulic conductivity (permeability) at saturation in x and z directions, K_R – relative hydraulic conductivity (permeability), H – total hydraulic head, x – horizontal co-ordinate, z – vertical co-ordinate (oriented positively upwards).

Neglecting water compressibility, the total hydraulic head can be written as a sum of two components:

$$H = h + z \quad (2)$$

where: h – pressure potential head, hz – elevation above datum. The pressure head is positive below the water table (where it represents physical pressure) and negative above the water table (where it represents combined effects of capillary and adsorption forces binding water to the soil or rock matrix).

In order to solve Eq. (1) one has to know the soil hydraulic characteristics, i.e. the retention function and the relative permeability function. These functions are often specified using the Van Genuchten (1980) formulas:

$$\theta(h) = \theta_R + (\theta_s - \theta_R) \left[1 + (\alpha |h|)^n \right]^{-m} \quad (3)$$

$$K_R(h) = \frac{\left\{ 1 - (\alpha |h|)^{n-1} \left[1 + (\alpha |h|)^n \right]^{-m} \right\}^2}{\left[1 + (\alpha |h|)^n \right]^{m/2}} \quad (4)$$

where: θ_R – residual water content, θ_s – water content at saturation, α – pressure scaling parameter, n and m – shape parameters with $m = 1 - 1/n$.

Other types of hydraulic functions are also implemented in VS2DI, together with a small data base containing typical parameters for different soil textural classes.

VS2DI package solves Eq. (1) using cell-centred finite-difference / finite volume spatial discretization and implicit time discretization scheme. Details of the numerical solution are described in the code documentation (Lappala et al. 1987). Here we focus only on the intercell flux discretization. The solution domain is divided into a number of rectangular cells, with unknown values of hydraulic head located at their centres (Fig. 1). The flux terms appearing in Eq. (1) are approximated with finite difference formulas. For example, the Darcy velocity in the direction normal to the boundary between cells (i, j) and $(i+1, j)$ is computed as follows:

$$v^{(i+1/2, j)} = K_{SX}^{(i+1.2, j)} K_R^{(i+1/2, j)} \frac{H^{(i+1, j)} - H^{(i, j)}}{\Delta x^{(i+1/2)}} \quad (5)$$

where: $K_{SX}^{(i+1.2, j)}$ – average intercell saturated conductivity, $K_R^{(i+1.2, j)}$ – average intercell relative conductivity, $\Delta x^{(i+1/2)} = 0.5(\Delta x^{(i)} + \Delta x^{(i+1)})$.

The saturated conductivity between cells is calculated as a harmonic mean weighted by the grid cell sizes:

$$K_{SX}^{(i+1/2, j)} = \frac{2K_{SX}^{(i)} K_{SX}^{(i+1)} \Delta x^{(i+1/2)}}{K_{SX}^{(i)} \Delta x^{(i+1)} + K_{SX}^{(i+1)} \Delta x^{(i)}} \quad (6)$$

Such an approach is consistent with the condition of flux continuity at cell interface and provides accurate results for saturated flow when $K_R = 1$ and K_S changes abruptly at cell boundaries (Lappala et al. 1987; Szymkiewicz and Helmig 2011). In unsaturated flow simulation an additional difficulty arises

due to the need to calculate the average relative conductivity, which may vary by several orders of magnitude even for homogeneous media. VS2DI allows the user to choose among the three most commonly used averaging schemes:

arithmetic mean:

$$K_R^{(i+1/2, j)} = 0.5(K_R^{(i, j)} + K_R^{(i+1, j)})$$

geometric mean:

$$K_R^{(i+1/2, j)} = \sqrt{K_R^{(i, j)} K_R^{(i+1, j)}}$$

upstream weighting:

$$K_R^{(i+1/2, j)} = K_R^{(i, j)} \text{ if } H^{(i, j)} \geq H^{(i+1, j)}$$

$$K_R^{(i+1/2, j)} = K_R^{(i+1, j)} \text{ if } H^{(i, j)} < H^{(i+1, j)}$$

These and other formulations were compared in a number of previous studies using other numerical codes (e.g. Haverkamp and Vauclin 1979, Belfort and Lehmann 2005; Szymkiewicz 2009). In general, accuracy of each of the above methods depends on the shape of the relative conductivity function (i.e. soil type), cell size, and the initial and boundary conditions of the problem. For example, the geometric mean is more accurate than the arithmetic or upstream weighting in moderately wet, fine-textured soils, but can be very inaccurate for infiltration in dry sand. Arithmetic mean, which seems to be the most common choice, performs well for a wide range of problems, but may produce unphysical oscillations on very coarse grids. Upstream weighting ensures non-oscillatory solutions, but often significantly overpredicts the flow rate, especially for flow in an upward direction. More accurate methods to estimate the intercell relative permeability make use of information on the shape of the relative conductivity function, grid spacing and flow direction (e.g. Gasto et al. 2002; Baker 2000; Szymkiewicz 2009), but at the cost of additional algorithmic complexity.

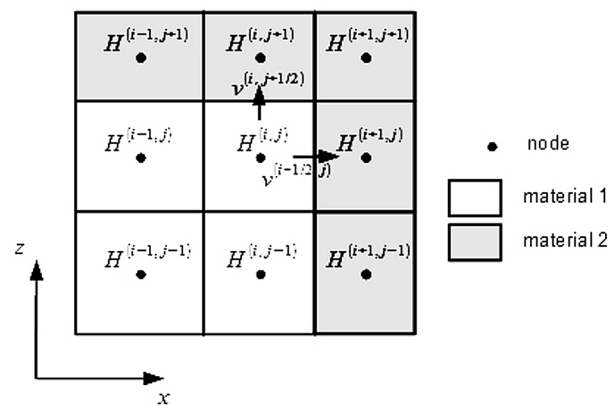


Fig. 1. Cell-centred spatial discretization used in VS2D code.

In this study we compare the performance of the three simple averaging schemes implemented in VS2DI in function of grid refinement.

3. Examples

3.1. Axisymmetric infiltration from ponded area

We considered infiltration into a dry medium sand from a circular area with a 20-cm radius. The geometry and boundary conditions are shown in Fig. 2, while the Van Genuchten parameters of the porous medium are listed in Table 1. In the source area we assume ponding conditions with a negligible ponding depth, so the water pressure head is set to 0 and kept constant during the simulation. At the bottom a free drainage condition is applied, which means a unit gradient of total head in vertical direction. This condition simulates outflow to a distant groundwater table. The time of simulation is 200 seconds. Two grids were used. The coarse one consisted of 10 by 10 uniform squares. The fine grid was also uniform, but consisted of 100 by 100 square cells.

Figure 3 shows the distribution of water saturation obtained for the coarse grid with three con-

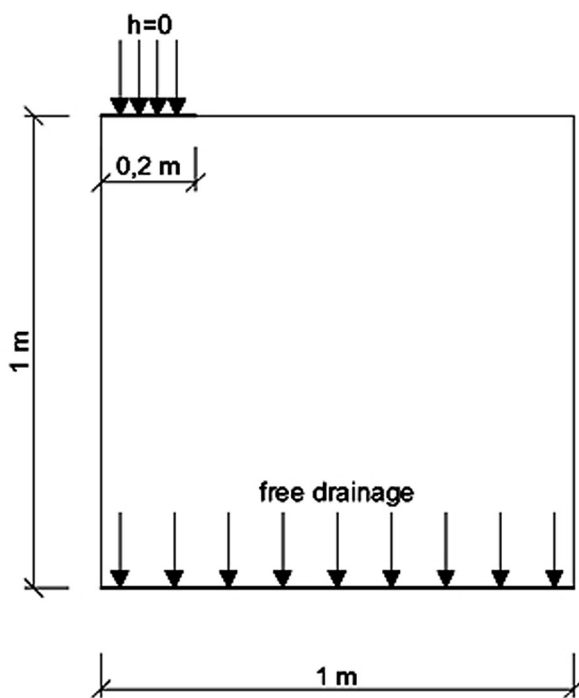


Fig. 2. Test case 1: Geometry and boundary conditions.

Table 1. Parameters of Van Genuchten (1980) hydraulic functions used in test simulations (parameters taken from VS2DI data base).

Parameter	Material		
	Medium sand	Loamy sand	Sandy loam
S_s [1/m]	10^{-4}	10^{-4}	10^{-4}
K_s [m/s]	4.63×10^{-3}	4.05×10^{-5}	1.23×10^{-5}
$n = \theta_s$ [-]	0.375	0.41	0.41
θ_R [-]	0.02	0.057	0.065
α [1/m]	4.31	12.4	7.5
β [-]	3.1	2.28	1.89

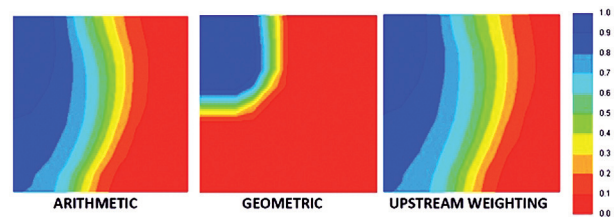


Fig. 3. Test case 1: Water saturation distribution at $t = 170$ s obtained for the coarse mesh with various averaging schemes.

ductivity averaging schemes. Large differences between averaging methods were observed. The upstream weighting method predicts the fastest movement of the wetting front, while the geometric mean predicts the slowest. The solutions obtained with various conductivity averaging schemes can also be compared in terms of cumulative infiltration, i.e. the total amount of water which infiltrated from the source in a specific time. The cumulative infiltration curves are shown in Fig. 4. It can be seen that the differences between various averaging schemes are much larger on the coarse grid than on the fine one. Assuming that all averaging schemes converge to an accurate solution as the grid is refined, the arithmetic average yields the best coarse grid approximation.

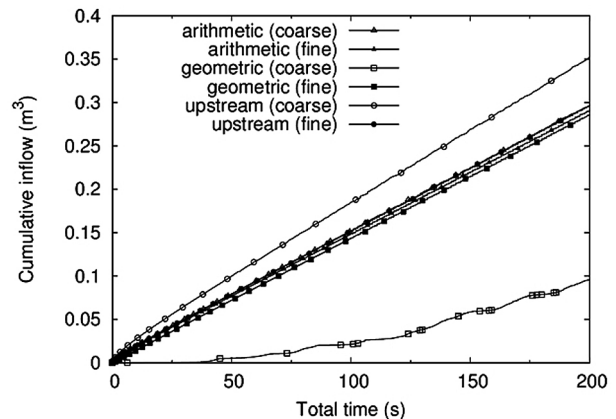


Fig. 4. Test case 1: Cumulative infiltration as a function of time for different conductivity averaging schemes.

3.2. Infiltration from a disconnected stream

In this example we considered an infiltrating stream flowing above a phreatic aquifer (Fig. 5). The stream is separated from the aquifer by an unsaturated zone. The stream bed has hydraulic characteristics that are different from those of the aquifer, due to the presence of sediment. The parameters of aquifer and the overlying vadose zone correspond to medium sand, while the sediment layer along the bottom of the stream is given sandy loam parameters (Table 2). Numerical solution to such kind of problems was presented by Jackson (2005) and Brunner et al. (2009). In the former case the simulations were also done with VS2DI. Computations presented in this paper are performed for three grid levels. The coarse grid consisted of uniform rectangles, each having a horizontal dimension of 1 m and a vertical dimension of 0.5 m. In the medium grid the horizontal spacing was reduced to 0.5 m for a 3-m zone on the right-hand side of the domain, including the streambed, while the vertical spacing was reduced to 0.2 m for the whole grid. On the finest level the vertical spacing was reduced to 0.1 m in the zone between the stream bottom and the initial position of the water table. The simulated time period was 2×10^5 s, which was enough to

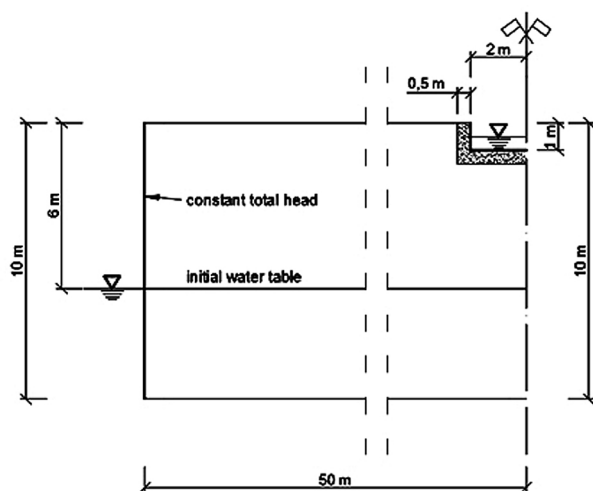


Fig. 5. Test case 2: Geometry and boundary conditions.

Table 2. Test case 2: Steady state infiltration rate [m^3/s] from disconnected stream to the aquifer for different grids and conductivity averaging schemes.

Grid	Method		
	Arithmetic	Geometric	Upstream
Coarse	1.82×10^{-4}	1.71×10^{-5}	3.43×10^{-4}
Medium	1.02×10^{-4}	4.50×10^{-5}	1.43×10^{-4}
Fine	9.12×10^{-5}	8.18×10^{-5}	1.02×10^{-4}

reach steady state conditions, with the inflow from a stream balanced by horizontal outflow on the left-hand side boundary. Note that due to the presence of a semi-permeable sediment layer, the region between the stream bed and water table did not become saturated even at steady state (contrary to the case without sediment layer).

Figure 6 shows the spatial distribution of the water saturation at transient stage of the process ($t = 6.6 \times 10^4$ s) obtained for the coarsest and finest grids using different averaging formulas. Differences in saturation patterns are clearly visible for the coarse grid, where the use of geometric mean leads to an unphysical saturation profile below the sediment, with two minimum values. Fine grid simulations produced results more closely similar to each other. In particular, the solution using arithmetic mean is close to the one obtained with upstream weighting. Additional information can be found in Table 2, where the final (steady-state) values of infiltration rate from the stream are listed. As the grid was refined the infiltration rate decreased for the arithmetic mean and upstream weighting (by a factor of about 2 and 3.5, respectively), while for the geometric mean it increased by a factor of about 5. At the finest grid level considered the maximum discrepancy between averaging method was about 20%, which is still significant, but much less than in the coarse grid, where differences exceeded 100%. It can also be seen that at the coarsest grid level the arithmetic mean yields an estimation of

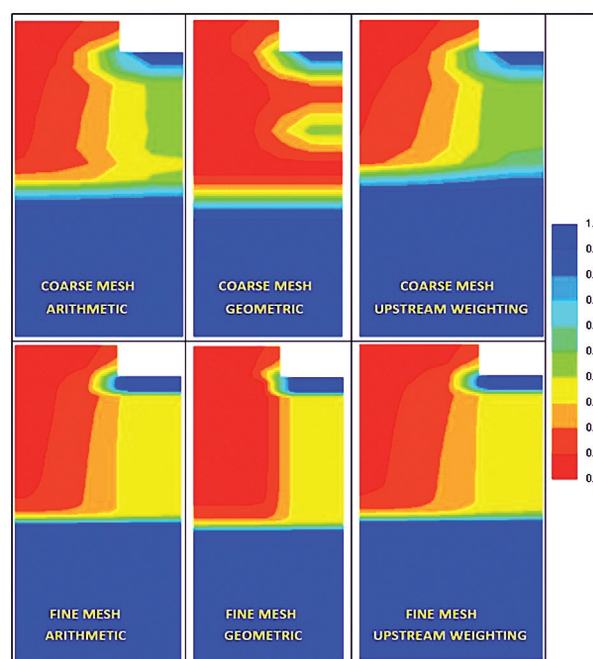


Fig. 6. Test case 2: Distribution of water saturation in the vicinity of stream bed for $t = 66000$ s.

the infiltration rate which is closest to the fine-grid estimations.

3.3. Seepage through a dyke

The last example concerned seepage in the vertical cross-section of a dyke, as shown in Fig. 7. As the initial condition we assumed equilibrium pressure distribution, with $h = 0$ at the bottom of the dike. At the outer slope the water level was instantly increased to 2.5 m above the base of the dyke. The underlying soil is assumed impermeable, so all seepage comes through the dyke, leading to the development of a seepage face at the inner (right-hand) slope. The dyke is homogeneous and the hydraulic functions of the fill material correspond to loamy sand (Table 2). Numerical solutions were obtained using two uniform grids – a coarse one with 50 cells in x direction and 25 in z direction, and a fine one with 100 by 50 cells. The total simulation time was set at 50 days, which allowed to reach steady state (inflow balanced by outflow).

Examples of saturation distribution obtained for the coarse mesh during the transient phase are shown in Fig. 8. Note that in this case the differences between various conductivity averaging methods are smaller than in the previous examples. In Fig. 9 we show the influence of various conductivity averaging schemes on the seepage flux (total discharge rate along the seepage face boundary). Initially, the seepage flux was zero and occurred only after the

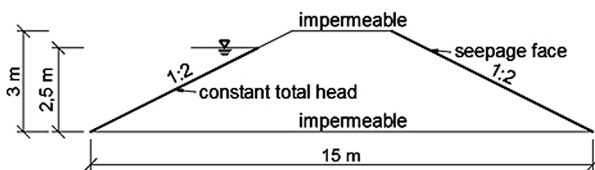


Fig. 7. Test case 3: Geometry and boundary conditions.

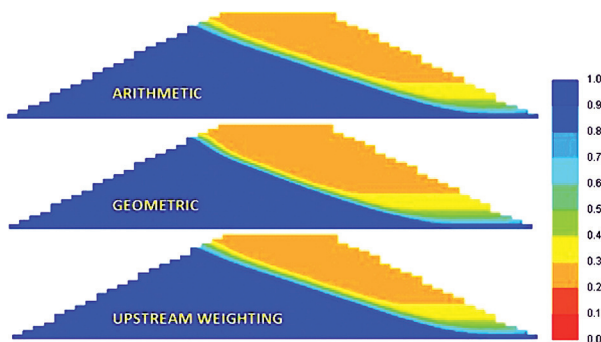


Fig. 8. Test case 3: Water saturation distribution at $t = 2.6$ day obtained for the coarse mesh with various averaging schemes.

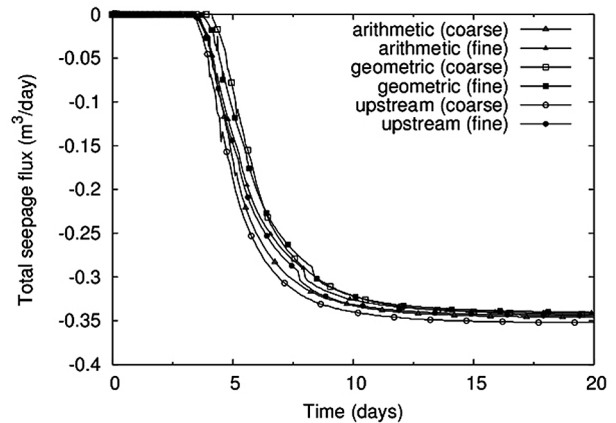


Fig. 9. Test case 3: Evolution of the seepage flux at the inner slope of dyke.

wetting front reaches the inner slope. The flux increased with increasing length of the seepage face and later stabilised when steady state water table position inside the dyke was approached. In general, the differences between various conductivity averaging methods are smaller than in the previous examples. It can be noted that the time of appearance of outflow at the seepage face is essentially the same for arithmetic and upstream averaging, irrespective of the spatial discretization. On the other hand, if the geometric mean is used, the outflow starts about 0.5 day later according to the coarse grid solution and about 0.25 day later according to the fine scale solution. Again, the arithmetic mean produces coarse grid results that are relatively close to the fine grid solutions.

4. Conclusions

A preliminary evaluation of various methods for computing intercell conductivity implemented in a VS2DI package was presented. It was shown that the choice of the averaging method may have a significant impact on the results when the grid is coarse. On more refined grids all three methods led to similar results; however, it is difficult to estimate the appropriate level of refinement in advance. In this regard, performing coarse-grid simulations with different means yields an indication of the quality of spatial discretization. For the range of problems considered here the arithmetic mean provided coarse-grid solutions that were closest to the fine-grid solutions. Further research is needed to evaluate averaging schemes for other types of problems (e.g., capillary rise or evaporation).

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