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Unsaturated flow modeling with HYDRUS and UZF: calibration and intercomparison

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ABSTRACT

A groundwater flow model of the unconfined aquifer in a small interfluve area (~20 km²) of NE Belgium is presented. Two different packages are tested for the simulation of unsaturated flow: the HYDRUS package (Seo et al., 2007) for MODFLOW-2000 (Harbaugh et al., 2000) and the UZF package (Niswonger et al., 2006) for MODFLOW-2005. Transient boundary conditions (weekly potential evapotranspiration and precipitation for 14 years) are used to calculate the recharge. The discharge of groundwater flow to the ground surface (or seepage) is also simulated. In the HYDRUS-MODFLOW model, 8 homogeneous zones (based on land cover and steady-state groundwater depth) are defined, which keeps the computation time reasonable (3 min). In contrast, UZF (kinematic wave approach) makes calculations for every model cell of the top layer and the computation time of a single run is 11 min. A sensitivity analysis and local optimization is performed with UCODE (Poeter et al., 2005). The advantages and limitations of using HYDRUS or UZF for simulating unsaturated flow are discussed.

INTRODUCTION

In zones of shallow, unconfined aquifers, it is important that groundwater models include recharge and evapotranspiration processes in an appropriate way. Different approaches have been tested to find a balance between the need of an accurate description of vadose zone processes and addressing computational resource issues. At one extreme, flow under variably saturated conditions is neglected and one recharge value is applied to the groundwater model. At the other extreme, a full representation of vadose zone flow is implemented using Richards' equation. Examples of the latter include the VSF package (Thoms et al., 2006) for MODFLOW, Hydrogeosphere (Therrien et al., 2005) or InHM (Vanderkwaak, 1999). Although their applicability to real-world problems has been demonstrated (e.g. Jones et al., 2008; Goderniaux et al., 2009), such models may rapidly become intractable for large modeling domains or when multiple runs are required (e.g. for global uncertainty analysis).

Between these extremes, an adequate compromise may lie in symplifying the conceptualisation of vadose zone processes, as illustrated by the UZF package for MODFLOW (Niswonger et al., 2006), which implements a kinematic wave equation to describe the infiltration front. Alternatively, the HYDRUS package for MODFLOW (Seo et al., 2007) solves Richards' equation for the vadose zone but, in the coupling of HYDRUS to MODFLOW, "zones" can be implemented for which a single 1-D soil profile is defined. As a consequence of this clustering, the CPU requirements substantially decrease.

The objective of the present work is to assess, in a real case study, the benefits and limitations of using HYDRUS-MODFLOW in comparison to UZF-MODFLOW. First, a local sensitivity analysis (SA) of both models is carried out using UCODE. The results are then used to select the most sensitive parameters to include in a calibration against a 10-year time series of piezometric observations.

PROBLEM DESCRIPTION

The modeling domain is a small interfluve area in the Campine region, NE Belgium. Altitude ranges between 16 and 31 m.a.s.l. (Fig.1a) and the climate is temperate oceanic (yearly average precipitation 895 mm y^{-1}, average temperature 10.4°C). In the river and brook valleys, land cover is dominated by grassland and deciduous woods, while the rest of the study area is a mix of crop land, urban or industrial areas and forests. Land cover is shown in Fig. 1b, and was simplified for the models into four classes: urban, crop, pasture and forest (heather and dune were assigned to pasture). Surface hydrological features include the canal Bocholt – Herentals and several lakes, some of which artificially created by the sand extraction industry. The study area is delimited in all directions by rivers and brooks. Vertically, the modeling domain includes four geological layers of an unconfined aquifer: Mol Sands, Kasterlee Sands, the Kasterlee-Diest Transition layer (KDTL, consisting of the clayey parts of the Kasterlee and Diest formations), and Diest Sands.

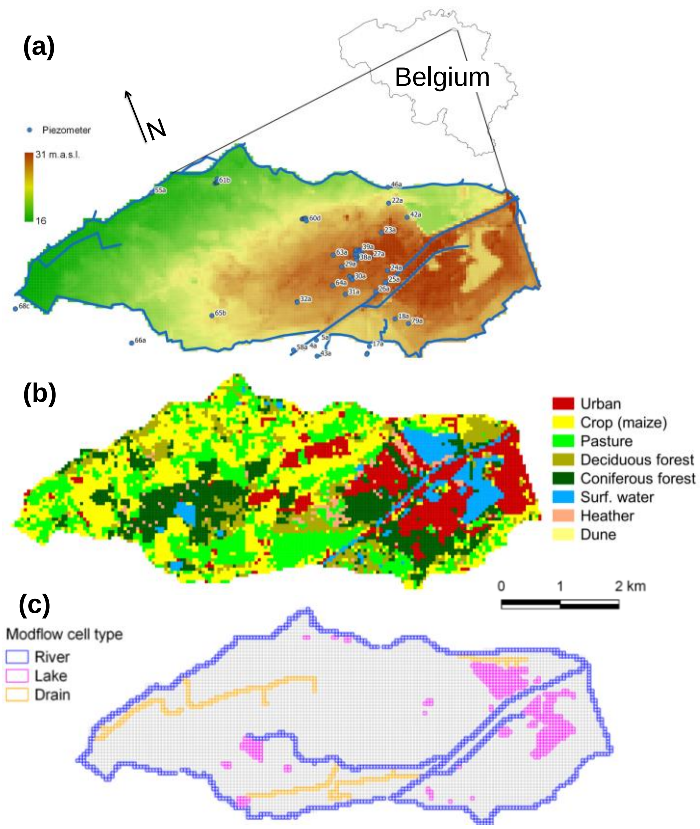

Figure 1. (a) Topography and piezometer network, (b) land cover in the study area and (c) inclusion of surface hydrological features in MODFLOW.

We compare two approaches for simulating the unsaturated zone and groundwater recharge: (i) HYDRUS-MODFLOW and (ii) UZF-MODFLOW. Piezometric observations and a time series of weather observations (precipitation and potential evapo-transpiration, ET_0, calculated using the Penman-Monteith method) are available for the period 2000-2013. Daily precipitation and ET_0 is used as the top boundary condition, with interception and ET_0 calculated specifically for each land cover. Surface water bodies are represented using the drain, river and lake packages (Fig. 1c).

Before the parameter SA, the sensitivity of groundwater recharge to the number of zones defined in the HYDRUS package was tested. Using 4 land cover and 1 soil types, the number of zones was varied by defining different expected groundwater depth intervals. Results are shown in Table 1. The simulated recharge averaged on the whole study area ("TOTAL" in Table 1) is relatively insensitive to the number of zones. However, for a given land cover, it seems that taking only one groundwater depth interval (and thus a total of four zones) neglects the spatial variability of recharge due to different water table depths. Therefore, we decided to proceed for the rest of the study with two intervals (adapted to 0-0.5 m and 0.5-9 m compared to the results presented in Table 1).

SENSITIVITY ANALYSIS AND PARAMETER ESTIMATION

The list of parameters included in the SA is presented in Table 2. The SA was performed in UCODE on a 7-year simulation (2007 to 2013) using 3194 head measurements from 25 piezometers as observation data. Results are expressed in terms of composite scaled sensitivities.

		Average GW recharge [mm y^{-1}]				
Number of HYDRUS zones	GW depth intervals [m]	Urban	Grass	Crop	Forest	TOTAL
4	0-9	157.4	347.4	254.4	181.1	234.1
8	0-1	136.9	383.6	354.3	248.8	244.3
	1-9	120.3	345.1	282.5	181.7	
12	0-1	136.5	382.6	353.8	248.3	243.2
	1-2	137.8	331.5	252.9	181.2	
	2-9	158.1	345.5	226.9	175.5	
16	0-0.5	198.8	425.6	343.4	333.9	243.8
	0.5-1	135.0	385.4	291.2	182.9	
	1-2	137.6	331.3	252.6	181.2	
	2-9	158.2	345.7	226.9	175.6	

Table 1. Sensitivity of groundwater recharge to different numbers of HYDRUS zones defined by the expected groundwater depth intervals.

	Parameter		Starting value	Lower bound	Upper bound
CHD_mlt	Head multiplier of fixed-head cells	[-]	1	0.95	1.05
DRN_mlt	Drain conductance multiplier	[-]	1	0.5	2.5
RIV_mlt	River conductance multiplier	[-]	1	0.5	2.5
SS_whole	Specific storage (all layers)	[m^{-1}]	0.00001	0.000001	0.0001
SY_1st	Specific yield (top layer)	[-]	0.47	0.25	0.95
HK_Mol	Hydraulic conductivity Mol Formation	[$m\ d^{-1}$]	1	0.01	100
HK_Kast	Hydraulic conductivity Kasterlee Formation	[$m\ d^{-1}$]	2.73	0.273	273
HK_KDTL	Hydraulic conductivity KDTL	[$m\ d^{-1}$]	0.23	0.023	23
HK_Diest	Hydraulic conductivity Diest Formation	[$m\ d^{-1}$]	1.21	0.121	121
VANI_KDTL	Ratio of horizontal to vertical hydraulic conductivity KDTL	[-]	3224	322.4	32240
VANI_MOL	Ratio of horizontal to vertical hydraulic conductivity Mol Formation	[-]	1	0.1	10
VANI_REST	Ratio of horizontal to vertical hydraulic conductivity Kasterlee and Diest Formations	[-]	1	0.1	10
FINF001	Unit infiltration rate at land surface†	[$m\ d^{-1}$]	0.0001	0.00005	0.0005
PEV001*	Unit potential evaporation rate†	[$m\ d^{-1}$]	0.0001	0.00005	0.0005
PTR001*	Unit potential transpiration rate†	[$m\ d^{-1}$]	0.0001	0.00005	0.0005
PET001**	Unit potential evapotranspiration rate†	[$m\ d^{-1}$]	0.0001	0.00005	0.0005
EXTD_UR	ET extinction depth for urban land cover‡	[m]	0.05	0.01	1
EXTDC*	Wilting point pressure head	[m]	−80	−160	−10
EXTWC**	Extinction water content	[$m^3\ m^{-3}$]	0.1	0.001	0.2
VKS	saturated vertical hydraulic conductivity of the (top horizon of the)*,# unsaturated zone	[$m\ d^{-1}$]	2.03	0.000203	203
EPS**	Brooks-Corey epsilon of the unsaturated zone	[-]	5.9	5	7
THTS	Saturated water content of the (top horizon of the)*,# unsaturated zone	[$m^3\ m^{-3}$]	0.47	0.3	0.6
THTR	Residual water content of the (top horizon of the)*,# unsaturated zone	[$m^3\ m^{-3}$]	0.06	0.01	0.1
ALP01*,#	Parameter alpha in van Genuchten model (top horizon)	[m^{-1}]	1.3	0.8	1.9
NVG01*,#	Parameter n in van Genuchten model (top horizon)	[m^{-1}]	1.68	1.4	2.3

† All infiltration and PET rates are expressed in terms of derivative parameters as multipliers of the unit rates (e.g. to specify an infiltration rate of 0.0025 m d¯1 the derivative parameter FINF025 = 25*FINF001 is used)
‡ ET extinction depth for other land covers are expressed as multipliers of the depth for urban land cover (for cropland EXTD_MA = EXTD_UR/0.05*2.0, for grassland EXTD_GR = EXTD_UR/0.05*0.3, and for deciduous forest EXTD_DC = EXTD_UR/0.05*1.7)
# in HYDRUS package, van Genuchten parameters for the soil horizons below the top horizon are expressed as mutipliers of values in the latter

Table 2. Starting value, lower and upper bound of parameters included in the sensitivity analysis. Parameters specific to HYDRUS are marked with * and those specific to UZF with **.

The composite scaled sensitivities obtained for both models are displayed in Fig. 2 (average results from two different starting points – only the first one is given in Table 2). The head multiplier of fixed-head cells (CHD_mlt) is the most sensitive parameter in both models, followed by the infiltration parameter (THR001 for HYDRUS; FINF001 for UZF). The parameter ranking is similar between both models, at the exception of saturated hydraulic conductivity of the unsaturated zone. For UZF, VKS is not identified as a sensitive parameter, while VKS01 is ranked as a sensitive parameter in the HDYRUS-MODFLOW model. Parameter selection for the calibration step was based on the threshold of 0.01 of the maximum sensitivity (Hill, 1998).

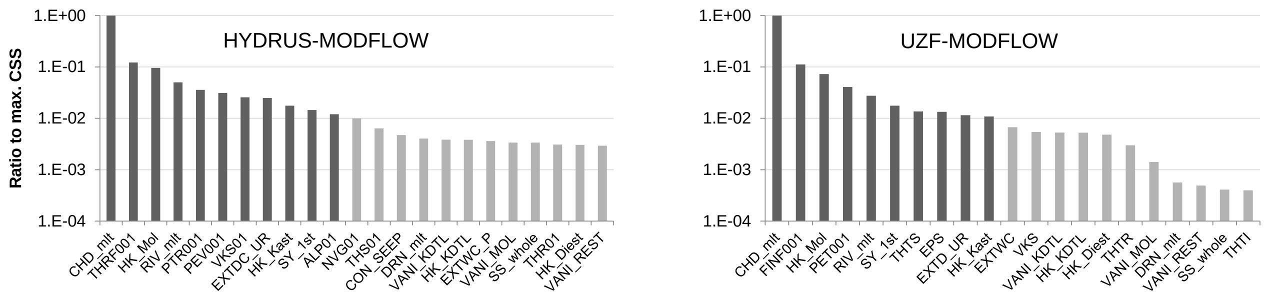

Figure 2. Parameter sensitivity plotted as the ratio to the maximum composite scaled sensitivity (CSS) for the HYDRUS-MODFLOW (left) and UZF-MODFLOW (right) models. Parameters selected for the calibration step are displayed in dark grey.

Calibration

After the local SA, calibration was performed in UCODE using the observed groundwater heads for the years 2000 to 2009. During calibration, parameters with a composite scaled sensitivity less than 0.01 of the maximum sensitivity were omitted. The maximum number of iterations (=10) was reached for both UZF-MODFLOW and HYDRUS-MODFLOW without parameter estimation convergence. For UZF-MODFLOW, the minimum sum of squared, weighted residuals was 13224 m² after the 10th iteration. For HYDRUS-MODFLOW, the minimum sum of squared, weighted residuals was 10718 m² at the 9th iteration.

Fig. 3 shows the fit obtained with the best parameter estimates of HYDRUS (in red) and UZF (in yellow) for 8 of the 25 piezometers of the calibration data set. Although seasonal variations are visible, Fig. 3 shows that their amplitude is underestimated in both models. This poor fit is probably due to the model conceptualization, in which the modeling domain is laterally not defined by no-flow boundaries. Since the boundary conditions other than climate forcings (river stage, fixed head cells…) are kept constant throughout the simulation period, the seasonality of groundwater recharge (and discharge to surface water bodies) can hardly be captured and the simulated heads too heavily depend on these bottom boundary conditions (cf. the high sensitivity of CHD_mlt).

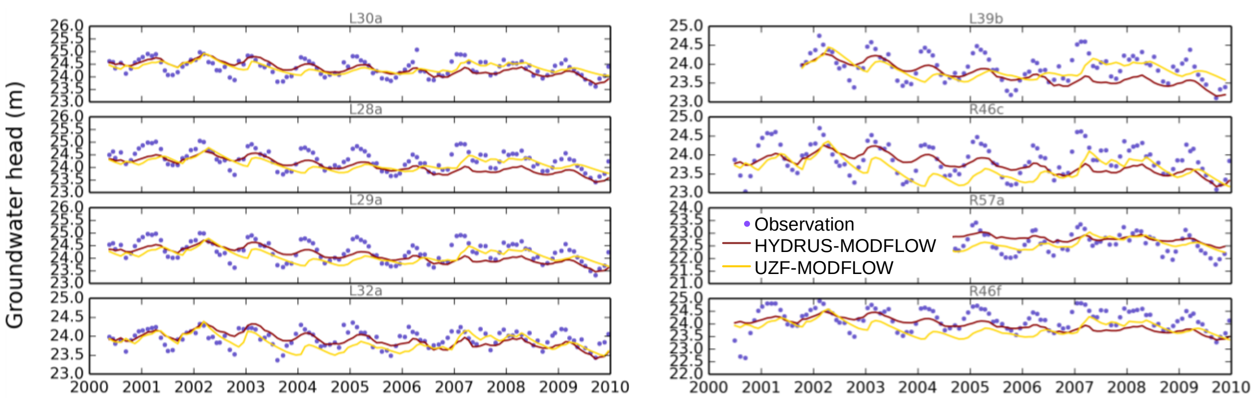

Figure 3. Simulated values of the model calibration (HYDRUS-MODFLOW in red and UZF-MODFLOW in yellow) and groundwater head observations in a subset of the piezometer network (see location in Fig.1a).

DISCUSSION AND SUMMARY

HYDRUS-MODFLOW and UZF were compared for the coupling of water flow in the unsaturated zone to a groundwater model. For this case study, the HYDRUS-MODFLOW model needed 3 min. for a forward run, while the UZF-MODFLOW model lasted 11 min. This computational advantage of HYDRUS is likely to increase when larger modeling domains are used, as the number of zones can remain relatively limited as opposed to the UZF number of cells. Moreover, in the present simulations, UZF discretization parameters NTRAIL2 and NSETS2 needed to be set at higher values than default, thus requiring more computation time than expected.

The SA highlighted the importance of a correct description of vadose zone processes for transient flow simulations. Infiltration (or throughfall) was one of the most sensitive parameters. Fixed-head cell boundary conditions had the highest sensitivity. However, since they were kept constant for the entire modeling period (like drain and river stage boundary conditions), this resulted in a relatively poor fit of both HYDRUS-MODFLOW and UZF-MODFLOW models. The parameter estimation did not converge for any of the two models tested. HYDRUS-MODFLOW performed slightly better, but the seasonal amplitude of groundwater head variations was strongly underestimated in both models.

In order to improve the model fit for transient simulations, the study area should be extended to a "true" hydrogeological catchment (i.e. no-flow boundaries), or transient boundary conditions should be implemented for the lake and river stages as well as for fixed-head cells (CHD package). Also, a global method for the sensitivity and uncertainty analysis would be profitable for the parameter estimation process.

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