TOWARDS AN IMPROVED ASSESSMENT OF THE WATER BALANCE AT THE CATCHMENT SCALE: A COUPLED MODEL APPROACH

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RESUMEN. Se presenta una metodología de acoplamiento de modelos para calcular el balance hídrico detallado a escala de cuenca. El modelo MARMITES, que simula las zonas superficial y no saturada, es acoplado con el modelo de agua subterránea MODFLOW. El objetivo es cuantificar espacio-temporalmente los flujos en las zonas saturada y no saturada y evaluar el impacto de flujos tradicionalmente subestimados, así como la transpiración y la evaporación de agua subterránea, sobre los recursos hídricos subterráneos.

ABSTRACT. We present a coupled model approach to improve the water balance at the catchment scale. The model is composed of a land surface and unsaturated zone model (MARMITES) coupled with the groundwater model MODFLOW. We aim to quantify spatio-temporally the water fluxes of the unsaturated and saturated zones and to assess the impact of typically underestimated water fluxes, such as groundwater transpiration and groundwater evaporation, on groundwater resources.

1.- Water balance at the catchment scale

The water balance of a catchment is controlled by several hydrological processes (i.e. precipitation, interception, evapotranspiration, infiltration, runoff, percolation, groundwater flow) that regulate the storage and exchange of water between the reservoirs (i.e. surface, vegetation, unsaturated zone and aquifer). The reliable closure of subsurface water balance is challenging because: (i) subsurface water fluxes, due to their inaccessibility, are by far more difficult to assess than surface water fluxes; (ii) subsurface water fluxes quantities are generally small; (iii) methods of estimation of subsurface water fluxes are still highly uncertain; (iv) subsurface water fluxes vary spatio-temporally, being affected not only by spatio-temporal variability of rainfall and evapotranspiration but also by unpredictable depth-wise heterogeneity of subsurface; (v) it is difficult to separate groundwater fluxes from unsaturated zone water fluxes.

Due to these difficulties, common modeling practices apply simplistic estimates of the hydrological fluxes (typically evapotranspiration and groundwater recharge) that are adjusted a-posteriori during model calibration. Such practices lead to bias in parameter estimation and erroneous groundwater balances (Lubczynski, 2009; Lubczynski, 2011).

We present a coupled model approach to improve the catchment water balance. We developed a transient and distributed land surface and unsaturated zone model (MARMITES) that we coupled with the groundwater model MODFLOW (Harbaugh et al., 2000). The main features and novelties of this approach are: (i) spatio-temporal quantification of sub-surface water fluxes; (ii) sourcing of the subsurface water fluxes, i.e. the allocation of these water fluxes to unsaturated or saturated zones; and (iii) partitioning of the evapotranspiration into evaporation and transpiration.

First, we define the components of the water balance at the catchment scale. Next, we describe the coupled model that we developed to compute the water balance. Finally, we present the preliminary results of the model application to a synthetic case study developed to validate the model. We also refer the field experiments we performed in the Sardón catchment (Salamanca) study case since the results will be implemented in the Sardón model to compute the catchment water budget.

2.- Water balance components

We considered the following 3 catchment reservoirs (Fig. 1): land surface, unsaturated zone and saturated zone (in the text, the index ‘s’ refers to the surface, index ‘u’ to the unsaturated zone and the index ‘g’ to the groundwater reservoir). The surface water balance equation is written as:

$$\frac{dS_s}{dt} = RFe - E_s - Ro \text{ with } RFe = RF - I \tag{1}$$

where S_s is surface water storage, RF is precipitation, RF_e is precipitation excess, I is interception by vegetation, E_s is evaporation from open water, Ro is run-off and t is time. All water fluxes are expressed in [L/T] and storage in [L]. RF_e is defined as the fraction of precipitation that reaches the surface and infiltrates. If the root zone is saturated, RF_e is stored in the surface water reservoir. When the maximum capacity of the surface storage is reached, Ro occurs.

The unsaturated zone water balance is:

$$\frac{dS_u}{dt} = RFe - E_u - T_u - Rp + DRN \tag{2}$$

where S_u is soil moisture, E_u is evaporation from bare soil, T_u is transpiration, Rp is percolation and DRN is groundwater exfiltration into the unsaturated zone. Rp is converted in groundwater recharge R using the following convolution equation (van der Lee and Gehrels, 1990):

$$R = Y_n = \frac{f}{1+f}\sum_{i=0}^{n}(1+f)^{-i}Y_{n-i}^{*} \text{ with } Y_0 = \frac{1+f}{f}Rp \tag{3}$$

where f is the unsaturated recession constant, n is the number of reservoirs, Y^* refers to the result from the previous time step and Y_0 is the upper boundary condition.

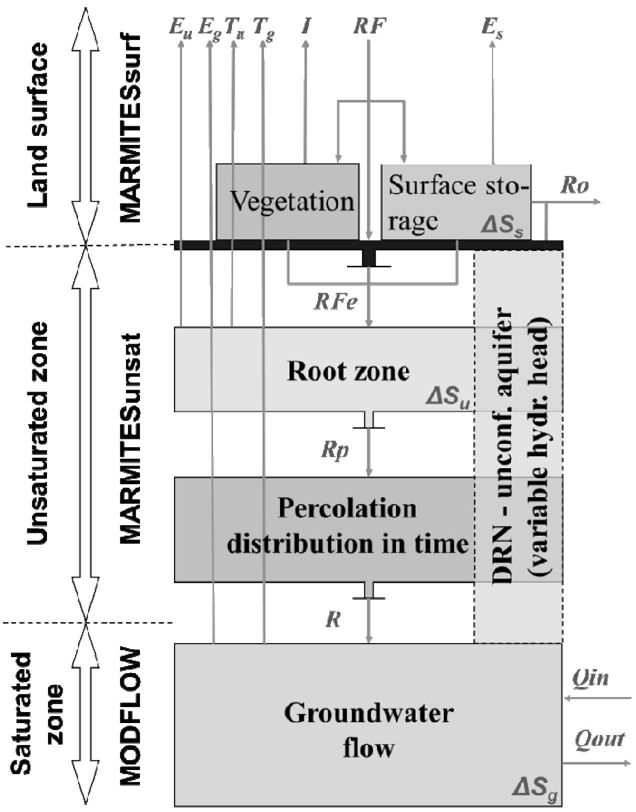

Fig. 1. Conceptual model of the coupled model, water fluxes partitioning and sourcing (fluxes in [L/T] and storage in [L]). Land surface: rainfall *RF*, rainfall excess *RFe*, interception *I*, evaporation from open water E_s, surface runoff *Ro*, storage change ΔS_s. Unsaturated zone: evaporation E_u, transpiration T_u, percolation *Rp*, recharge *R*, groundwater exfiltration *DRN*, storage change ΔS_u. Saturated zone: evaporation E_g, transpiration T_g, inflow/outflow *Qin*/*Qout*, storage change ΔS_g.

The groundwater balance is:

$$\frac{dS_g}{dt} = R + Qin - Qout - E_g - T_g - DRN \tag{4}$$

where S_g is groundwater storage, E_g is evaporation, T_g is transpiration, *Qin* and *Qout* are respectively groundwater inflow and outflow and *DRN* is groundwater drainage (exfiltration).

In the previous equations, we incorporated the water fluxes resulting from the partitioning and sourcing of the evapotranspiration (*ET*). The total evaporation and transpiration fluxes at the catchment scale, written respectively *E* and *T*, can be formulated as (Lubczynski, 2009; Lubczynski, 2011; Lubczynski and Gurwin, 2005):

$$E = I + E_s + E_u + E_g \tag{5}$$

$$T = T_u + T_g \tag{6}$$

These water balance concepts are implemented in the coupled model described in the next section.

3.- Coupled model approach

The coupled model approach incorporates 3 components (Fig 1): land surface (MARMITESsurf), unsaturated zone (MARMITESunsat) and saturated zone (MODFLOW). MARMITES is a distributed grid-based model that simulates the hydrological processes at the land surface (meteorological forcing, interception, surface storage, runoff and evaporation from open water) and in the unsaturated zone (evapotranspiration, percolation and soil moisture storage). MARMITES provides the groundwater recharge to MODFLOW that computes the groundwater flow and budget. Both models share the same spatial and temporal discretization. The catchment is divided in grid cells that are parameterized with vegetation, soil and aquifer parameters. Each grid cell supports one soil type and several vegetation types that are characterized by the fractional area that they occupy in the cell. The basic hydro-meteorological variables necessary to obtain the time series of driving forces (*RF* and potential evaporation and transpiration, respectively *PE* and *PT*) and calibration state variables (hydraulic heads and soil moisture) are typically acquired using monitoring network equipped with automatic data acquisition system.

MARMITES is developed using the Python programming language (version 2.6.6). The input and output files are read and stored in portable formats such as ASCII files (variables and driving forces time-series and non spatio-temporal parameters) and ASCII ESRI grid (spatial parameters and variables). The MODFLOW packages are implemented using the FloPy code (Post, 2008), also developed in Python.

Next, we describe the 3 components of the coupled model, the coupling and calibration methods and the model output.

- Land surface

The land surface component (MARMITESsurf) performs the rainfall analysis and computes interception (Equation 1), potential transpiration (*PT*) of the vegetation and potential evaporation (*PE*) of bare soil (used to derive E_u and T_u of Equation 2, see section 3.2).

The rainfall analysis is hourly based and computes the rainfall intensity and duration. These values are used in the computing of the interception from the several vegetation types. We applied the storm-based analytical model (Gash, 1979) reformulated by Gash et al. (1995) to account for sparse forest. This model considers unit area of canopy to perform the computing of evaporation of the intercepted rainfall. It combines the advantages of low data demand with simplicity, still maintaining a realistic approach of the interception process.

PT and *PE* are computed using the Penman-Montheith equation as formulated in Allen et al. (1998). The potential evapotranspiration is defined following Gieske (2003): "The maximum possible evapotranspiration according to prevailing atmospheric conditions and vegetative properties. The land surface in question (can be any part of the landscape that contains a certain fraction of vegetation) should be well supplied by water such that soil moisture forms no limitation in the stomatal aperture. [...] the biophysical properties of a potentially evaporating vegetation are spatially and temporally variable.” To compute *PE*, the surface resistance of bare soil was computed using van de Griend and Owe (1994).In addition to 4 meteorological variables (wind speed, air relative humidity, air temperature and solar short wave incoming radiation), the model requires vegetation and soil parameters such as leaf conductance, shelter factor, vegetation height, canopy capacity, leaf area index, albedo and soil specific yield. The definition and values for standard vegetation and soil types of these parameters can be found for instance in Dingman (2002). When temporally variable, these parameters are averaged seasonally. The model computes the open water evaporation E_o rate as defined by Penman (Gieske, 2003) that is used to compute E_s in Equation 1.

-Unsaturated zone

MARMITESunsat solves the water balance of Equation 2 on a daily basis in the root zone using linear relationships between water fluxes and soil moisture (Fig. 2). The root zone is parameterized with basic soil hydraulic properties (soil porosity, specific retention, wilting point, saturated hydraulic conductivity and thickness). The spatial prediction of these soil properties can be efficiently performed using a combination of techniques such as invasive sampling, remote sensing, geophysics and statistics (Francés and Lubczynski, 2010). S_u (Equation 2) is defined as the product of actual volumetric soil moisture content times the thickness of the layer. *Rp* is computed assuming that the pressure head in the soil reservoir is constant over depth and thus the potential gradient approximate zero. This approximation is valid if the potential flux term is negligible in relation to the gravitational term (van der Lee and Gehrels, 1990).

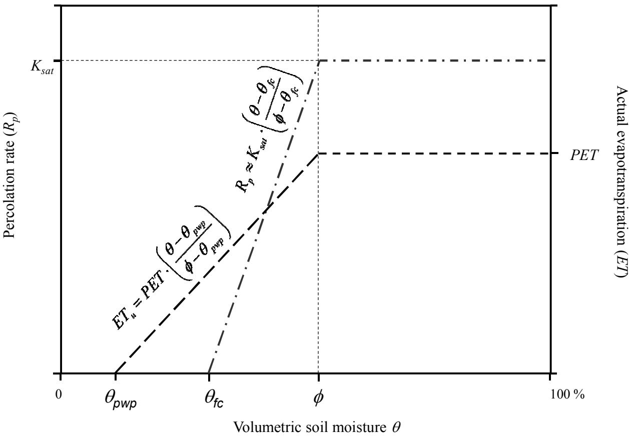

Fig.2. Linear relationship between actual volumetric soil moisture (θ) in the root zone and: (i) evapotranspiration (ET_u); and (ii) *Rp*. ϕ is porosity, θ_{fc} is soil moisture at field capacity, θ_{pwp} is permanent wilting point and K_{sat} is saturated hydraulic conductivity.

The partitioning of ET_u is performed as followed:

$$E_u = PE \cdot \left(\frac{\theta-\theta_{pwp}}{\phi-\theta_{pwp}}\right) \tag{7}$$

$$T_u = PT \cdot \left(\frac{\theta-\theta_{pwp}}{\phi-\theta_{pwp}}\right) \tag{8}$$

where θ is actual volumetric soil moisture, ϕ is porosity, θ_{fc} is soil moisture at field capacity, θ_{pwp} is permanent wilting point and K_{sat} is saturated hydraulic conductivity. Equation 7 is applied in bare soil and Equation 8 is applied for each vegetation type, taking into account the fractional grid cell area.

-Saturated zone

Groundwater flow and budget are computed in MODFLOW through the following partial-differential equation (Harbaugh et al., 2000):

$$\frac{\partial}{\partial x}\left(K_{xx}\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_{yy}\frac{\partial h}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_{zz}\frac{\partial h}{\partial z}\right)+W=S_s\frac{\partial h}{\partial t} \tag{9}$$

where K_{xx}, K_{xx} and K_{xx} are the values of hydraulic conductivity along the x, y and z coordinate axes (assumed to be parallel to the major axes of the hydraulic conductivity tensor *K*), *h* is hydraulic head, *W* is water sources or sinks (e.g. *R*, E_g, T_g), S_s is specific storage and *t* is time. This equation is numerically solved using the finite-difference method and applied to both confined and unconfined aquifers. The time domain is divided into stress periods (SP) during which the water fluxes are constant. The water fluxes are thus averaged in MARMITES for each SP. Each SP is itself divided in time steps from which the hydraulic heads and groundwater budget are computed.

Groundwater exfiltration (Fig. 1) is simulated using the drain package. Evaporation from groundwater (E_g) is simulated following Shah et al. (2007) that found an exponential relationship between E_g and the depth of groundwater (Equation 10) using numerical simulation and field data:

$$E_g = \begin{cases} PE & \text{for } d \le d'' \\ PE(y_0 + e^{-b(d-d'')}) & \text{for } d > d'' \end{cases} \tag{10}$$

where *d* is the depth to water table, d'' is the decoupling depth, y_0 is a correction and *b* is the decay coefficient (the last 3 parameters are soil type dependent and are provided by the authors of this equation).

The groundwater transpiration is computed as:

$$T_g = T_u\left(\frac{1}{k_{T_u}}-1\right) \text{ with } k_{T_u} = \frac{T_u}{T} \text{ and } 1 \ge k_{T_u} > 0 \tag{11}$$

where k_{T_u} is the transpiration sourcing factor.

- Coupling and calibration using PEST

The two models are run sequentially (Fig.3), being controlled by the Python code. The groundwater recharge computed by MARMITES is implemented in MODFLOW and the depth of the water table computed by MODFLOW constitutes the bottom boundary of MARMITES.

The simultaneous calibration of the two models is done against soil moisture in MARMITES and hydraulic heads in MODFLOW using the parameter estimation algorithm PEST (Doherty, 2005). The highly parameterized inversion techniques (singular value decomposition, Tikhonov regularization) of the PEST suite accommodate the spatial variation of the calibrated parameters, avoiding over-fitting, preserving realistic parameter values and incorporating spatial heterogeneity. It provides also a quantification of parameter sensitivity and uncertainty, as well as prediction uncertainty, which constitute valuable information to identify and analyze unreliable model solutions (Francés et al., 2011).

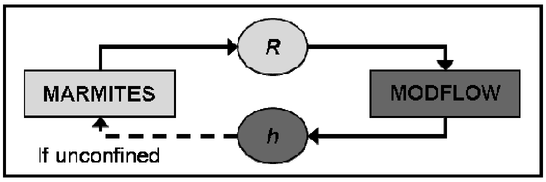

Fig. 3. Coupling of MARMITES and MODFLOW models (*R* is groundwater recharge, *h* is hydraulic heads)

- Model output

MARMITES computes a daily spatial water balance that quantifies the partitioning and sourcing of the subsurface water fluxes in each cell of the catchment. Daily water fluxes and state variables (soil moisture computed by MARMITESunsat and hydraulic heads by MODFLOW) are stored on disk in HDF5 format (Collette, 2008) and can be exported as time series or 2D sections for output visualization.

4.- Model applications

- Synthetic case study

The MARMITES-MODFLOW coupled model was validated using a synthetic case study of 130 rows, 60 columns and 2 aquifer layers (upper layer unconfined, 20 m thick, lower one confined, 50 thick, initial water table is ~90 m elevation) and 2 meteorological zones with 3 vegetation and 2 soil types (Table 1 and Fig. 4). In each grid cell (10x10m), the 3 vegetation types can coexist, each one covering a percentage of the grid cell area. The remaining area is considered as bare soil. 2 hydrological years, between October 2005 and September 2007, were simulated using a coherent compilation of meteorological data from several stations from south Portugal (www.snirh.pt). The water fluxes time series extracted at the piezometer Pz5 (see location in Fig. 4) are shown in Fig. 5. The spatial variation of water fluxes, averaged for the whole simulated period, are presented in Fig. 6.

Table 1. Hydraulic soil properties

Soil zones	ϕ	θ_{fc}	θ_{pwp}	K_{sat}	n	f
Alluvium	0.45	0.25	0.10	50.0	1	1.0
Regolith	0.35	0.20	0.10	75.0	1	5.0

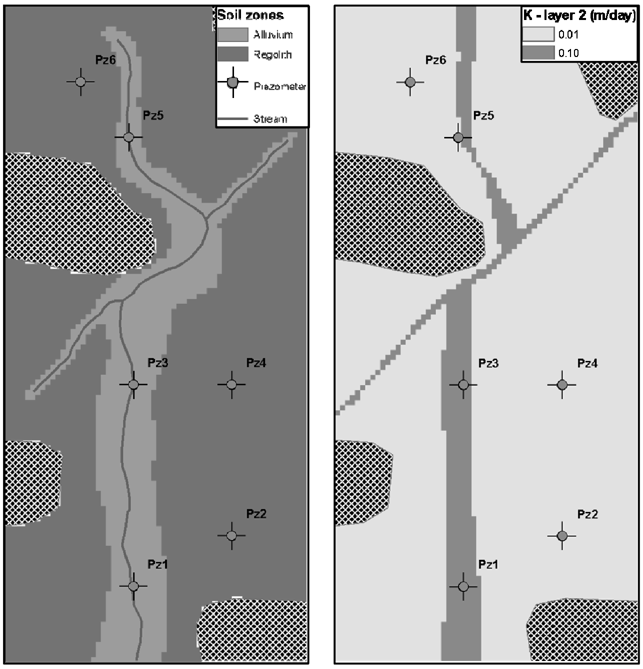

Fig. 4. Example of input grid of the MARMITES model (dashed polygons indicate inactive cells): soil zones (left) and hydraulic conductivity of the lower aquifer layer (right).

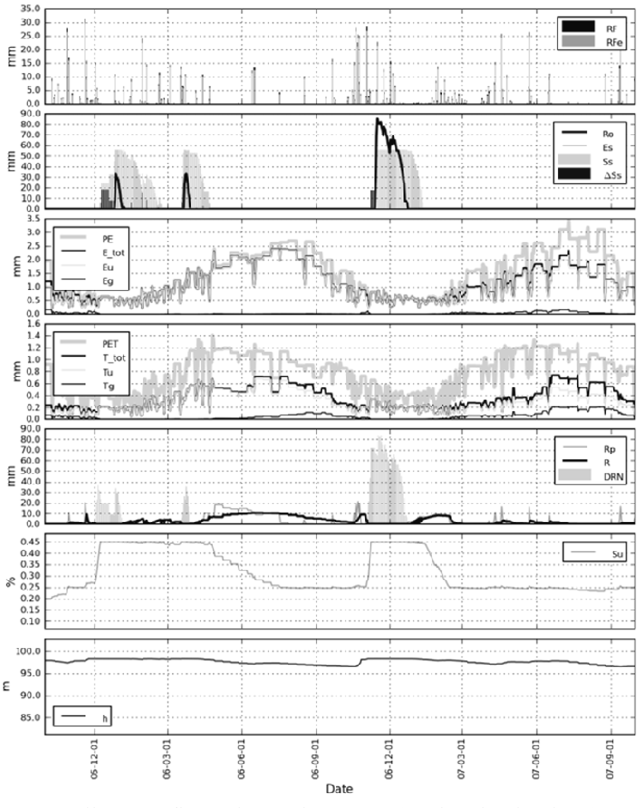

Fig.5. Daily water fluxes time series at Pz5 (see location in Fig. 4). See abbreviation in Fig. 1

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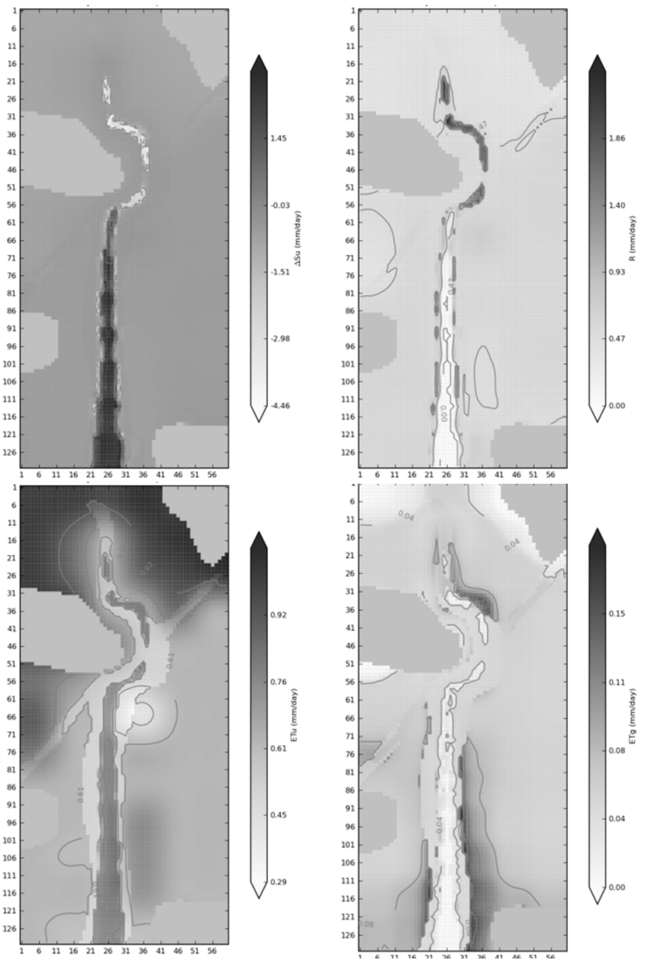

Fig.6. Example of MARMITES output: water fluxes averaged for the whole simulated period. Top left (ΔS_u): change in soil moisture; top right (R): groundwater recharge; bottom left (ET_u): unsaturated zone evapotranspiration; bottom right (ET_g): saturated zone evapotranspiration.

- Sardón case study

We aim to apply the MARMITES-MODFLOW coupled model to the Sardón catchment (~80 km^2, west of Salamanca, Spain), characterized by a semi-arid climate, granitic bedrock and shallow groundwater (~2 m depth). We performed several studies such as tree transpiration partitioning using isotopes (Reyes-Acosta and Lubczynski, 2011), *ET* assessment using eddy covariance technique and bare soil evaporation assessment using field soil-column and lysimeter (Balugani et al., 2011). We will subsequently integrate these results into the MARMITES-MODFLOW coupled models to compute a detailed catchment water balance and to assess the impact of the groundwater discharge by *Quercus ilex* and *Quercus pyrenaica* trees (the two main species present in the catchment) transpiration (T_g) and by bare soil evaporation (E_g) on groundwater resources.

5.- Discussion and Conclusion

We presented in this communication: (i) the concepts of a detailed water balance at the catchment scale that integrates the spatio-temporal quantification, the partitioning and the sourcing of the hydrological fluxes; (ii) the implementation of these concepts in a coupled model approach; and (iii) the preliminary results obtained using a validation, synthetic study case. Several authors (e.g. Miller et al., 2010; Newman et al., 2010) focused recently on fluxes partitioning and/or sourcing at the local scale. The present study complements these works, presenting the water dynamic at the catchment scale.

We will discuss in this section the concepts and methods that we selected to simulate the hydrological processes. Complex and data-demanding models based on the Richard's equation constitute the most appropriate tools to compute the surface and subsurface water fluxes at the local, site-specific scale. However, at larger scales these models perform generally not better than lumped-parameters models such as MARMITES or other (Finch, 2001; Rushton et al., 2006). This is because the bias introduced by the averaging or the upscaling of the soil hydraulic parameters at the grid cell makes the two solutions comparable. The linear relationships between water fluxes and soil moisture used in the MARMITES model were previously successfully applied in watershed models (Gehrels and Gieske, 2003; Savenije, 1999). Recently, Soylu et al. (2010) tested the impact of groundwater depth on evapotranspiration and confirmed that the HYDRUS-1D model and a single-bucket soil moisture model performed equivalently when using standard soil hydraulic parameter datasets. These authors also showed that the two models performed much better when the groundwater depth was introduced as bottom boundary. This feature is also considered in the MARMITES model through the coupling with MODFLOW.

The most challenging in the computing of the catchment water balance is the sourcing of the transpiration. A MODFLOW package was recently developed to compute T_g (Baird and Maddock Iii, 2005) but it requires vegetation specific transpiration functions that are difficult to obtain. Our approach is to integrate the results of local experiments on transpiration sourcing and upscale them at the catchment scale using the MARMITES model. Reyes-Acosta and Lubczynski (2011) performed site-specific experiments based on sap flow measurements combined with environmental isotope tracing. The experiments were conducted at several date during the dry season and on several vegetation types. We obtained the k_{T_u} sourcing factor (Equation 11) for each vegetation type that allowed us to carry out the transpiration sourcing at the catchment scale.

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