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SPECIAL ISSUE

Assessing the relevance of subsurface processes for the simulation of evapotranspiration and soil moisture dynamics with CLM3.5: comparison with field data and crop model simulations

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Abstract Plant water uptake is a crucial process linking water fluxes in the soil–plant–atmosphere continuum. Soil water extraction by roots affects the dynamics and distribution of soil moisture. Water supply of plants controls transpiration, which makes up for an important fraction of the energy balance at the land surface, and influences soil–vegetation–atmosphere feedback processes. Therefore, efficient algorithms for an accurate estimation of root water uptake are essential in land-surface models that are coupled with climate models, in agricultural crop models that predict water budget and plant growth at the field and plot scale, and in hydrological models. Due to different purposes and demands on computational time, the degree of detail in representing belowground processes varies considerably between these model types. This study investigates the impact of the degree of detail in process descriptions of root growth and water uptake and of information about soil hydraulic properties on simulated seasonal patterns of evapotranspiration and soil moisture in a field study with winter wheat (*Triticum aestivum L. cv. Cubus*). Evapotranspiration was well simulated by CLM3.5 until the beginning of crop senescence, but it overestimates the water flux through plants in the last three weeks of the vegetation period and showed a lower performance in simulating soil moisture compared to crop models. The best simultaneous fit of soil moisture and latent heat flux was achieved by the crop model XN-SPASS, which consists of the most detailed representation of root growth dynamics. The results indicate the importance of implementing improved belowground process descriptions for advanced simulations with coupled hydrological and atmospheric models.

Keywords Land-surface model · Crop model · Latent heat · Soil parameterization · Root water uptake · Crop senescence

Introduction

The interface between the two subsystems of the terrestrial water cycle, the atmosphere and the subsurface hydrogeo system, is the land surface. The transfer of water and energy across this interface is predominantly governed by the processes in the soil–vegetation continuum. Soil moisture, latent heat flux, which is the flux of heat from the land surface to the atmosphere associated with evaporation and transpiration, and the state of the lower atmosphere are therefore closely linked by several feedback processes. While climate directly influences vegetation and water fluxes in hydrogeo systems, the land surface feeds back through heat and water fluxes to the atmospheric boundary layer influencing its dynamic and thermodynamic structure and development (Santanello et al. 2009). For predicting

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the effect of land-use and climate change on hydrological systems, a detailed understanding of the interaction between climate, hydrology, and ecology is therefore required (Overgaard et al. 2006). Ideally, this understanding should result in a fully coupled model system, in which the relevant atmospheric and subsurface hydrological processes are consistently linked by a land-surface scheme with advanced biogeophysics.

Land-surface schemes for modeling the hydrological processes in the soil–vegetation continuum were developed at different temporal and spatial scales in atmospheric science, catchment hydrology, and agriculture, according to the requirements of the different disciplines (e.g., Bonan et al. 2002; Ittersum et al. 2003; Jones et al. 2003; Maxwell and Miller 2005; Priesack 2006; Niu et al. 2011; Wolf 2011). These models differ considerably in the degree of detail at which vegetation and soil processes are represented. While most land-surface schemes, which are linked to atmospheric models for global or regional climate studies, consist of a detailed description of aboveground vegetation processes such as canopy microclimate and stomata regulation, belowground hydrological and vegetation processes such as soil moisture dynamics, root growth, and root water uptake are typically poorly represented. Conversely, most agricultural models, which are designed for simulating water budget, nitrogen turnover, and crop growth at field scale, have a higher awareness of seasonal dynamics of root and leaf development, soil hydraulic properties, and root water uptake.

To test the adequacy of land-surface models, simulation results are frequently evaluated at the plot scale, where data can be gathered with relatively high accuracy and in high temporal resolution (Dirmeyer et al. 2006; Schädler 2007; Mahecha et al. 2010; Ingwersen et al. 2011; Li et al. 2012). The evaluation can be done by “offline” runs, that is, without coupling to an atmospheric model. In this case, the atmospheric forcing has to be provided by measured time series of the relevant variables or by a synthetically generated weather, which meets the statistical moments of climate at the investigated site. In studies that compared simulated fluxes of water and energy from the land surface to the atmosphere against measured fluxes at the plot scale, land-surface models have proven to perform well (Overgaard et al. 2006; Stöckli et al. 2008; Niu et al. 2011). However, for the simulation of the entire hydrogeo system, models should additionally be able to match the dynamics of the vertical soil moisture distribution (Grathwohl et al. 2013). With respect to this crucial requirement, considerable deficits of land-surface models have been identified. For example, Dirmeyer et al. (2006) compared simulation results from more than 10 land-surface models designed for global weather and climate simulations with observed soil moisture and energy flux data. The authors conclude that none of these models were simultaneously able to adequately simulate soil moisture, latent heat flux, and their interrelationship.

Further, it was shown that the predictions of regional climate models are sensitive to parameterization of land-surface processes. Van den Hurk et al. (2002) showed in a simulation study that the temporal and spatial distribution of precipitation in the Baltic Sea catchment depends on the choice of the land-surface scheme. Hauck et al. (2011) demonstrated with a coupled atmosphere/land-surface model that the simulated precipitation is significantly influenced by a bias in soil moisture and that soil moisture has a considerable impact on convective precipitation. Similarly, a study by Patton et al. (2005) demonstrated that land-surface heterogeneities have a strong influence on structure and circulation of the atmospheric boundary layer. It can therefore be expected that a better representation of the soil water regime in land-surface schemes will enhance the accuracy of atmospheric model predictions.

Recent efforts to improve vegetation components of land-surface models have mainly focused on the aboveground parts of plants (Bonan et al. 2011; Niu et al. 2011). However, up to now, little attention has been given to use the more detailed descriptions of subsurface processes from field scale vegetation models in the land-surface schemes of hydrological and atmospheric models. In particular, it is an open question how strongly simplifications in the parameterization and process description of soil–root interactions influence the simulated water fluxes in large-scale models of the soil–plant continuum and to which extent a higher level of information about soil hydraulic properties can improve model predictions.

CLM3.5 is a typical land-surface model which is frequently used in global and regional climate studies (Gibbard et al. 2005; Davin et al. 2011; Subin et al. 2011). We analyze the performance of a plot-scale implementation of this model in off-line mode to reproduce water fluxes in the soil–plant continuum observed at an agricultural site in South–West Germany and compare simulation results with results from two crop models. The aim of this study is to explore the level of information required for model parameterization and the degree of detail needed for describing root water uptake to accurately simulate both soil moisture dynamics and latent heat flux. To identify the most critical processes for a coherent simulation of the system, we perform our analysis in the following steps: First, we apply CLM3.5 in a “low information modus.” We initialize the model only with relatively easy to acquire data, which at best are soil texture and a reasonable estimation of the leaf area development during the season at the site. In the next step, in “high information modus,” we use field data of soil moisture and soil matric potential to improve the parameterization of the soil hydraulic processes. We complement these steps by a third procedure, in which we additionally adjust one preset crop parameter to the actual situation at the field site. This crop parameter describes the effect of nitrogen availability on photosynthesis. In a first attempt to investigate the role of the model structure on simulation results, we compare the CLM3.5 simulations described above with these of two different crop models of the model system Expert-N (Priesack 2006; Biernath et al. 2011). These models use a more complex parameterization of soil hydraulic functions than CLM3.5 as well as a more detailed description of plant root growth and root water uptake.

Materials and methods

Simulation models

In this study, we evaluate the performance of the community land model (CLM) version 3.5 (CLM3.5) to simultaneously simulate latent heat fluxes and soil moisture dynamics at the plot scale. Simulation results were compared with observed data and with simulations of two crop models that are implemented in the model system Expert-N 3.0 (Priesack 2006; Biernath et al. 2011). Compared to CLM3.5, the two Expert-N crop models apply a simpler representation of stomatal regulation but a more detailed description of soil water transport, root growth, and root water uptake. Latent heat flux is simulated as the sum of the heat flux associated with evaporation from soil, evaporation from wet leaves, and transpiration. The latter is equivalent to root water uptake, as no changes of water storage in plant tissues are considered. In the following, we briefly describe the different methods used in the CLM3.5 and in the crop models to simulate soil hydrology and root water uptake.

The community land model CLM3.5

The community land model CLM is the land-surface component of the global community climate system model (CCSM) (Oleson et al. 2004, 2008). Because of its comprehensive representation of land-surface processes, it has also been used for regional climate simulations (Steiner et al. 2005; Davin et al. 2011; Subin et al. 2011). The version 3.5 of CLM is available as a stand-alone model, which we used in off-line mode, that is, decoupled from an atmospheric model. For the atmospheric forcing, we used the data set obtained from field measurements in half-hourly resolution. CLM3.5 simulates several biogeophysical processes which control energy partitioning at the land surface and hence, among others, the turbulent fluxes of latent heat from the soil and the canopy. These processes include the radiation interactions with the vegetation canopy and the soil; the momentum and turbulent fluxes from the canopy and the soil; the heat transfer in soil and snow; the hydrology of canopy, soil, and snow, as well as stomatal physiology and photosynthesis processes (Oleson et al. 2008). Vegetation is represented in CLM3.5 by plant functional types (PFTs) which differ in their ecophysiological and hydrological properties. To represent the winter wheat considered in this study, we chose the PFT "Crop1." Leaf area development can be simulated prognostically in "CN-mode" or provided as monthly input. We decided for the latter option to reduce uncertainties resulting from inaccurate crop development simulation.

Soil water fluxes are calculated by the Richards equation using a Campbell/Clapp-Hornberger parameterization of hydraulic functions (Clapp and Hornberger 1978) that are widely applied in meteorological models:

$$\psi_i = \psi_{sat,i}\left(\frac{\theta_i}{\theta_{sat,i}}\right)^{-B_i} \tag{1a}$$

$$k_i = k_{sat,i}\left(\frac{\theta_i}{\theta_{sat,i}}\right)^{2\cdot B_i+3} \tag{1b}$$

where ψ_i [mm], θ_i [mm^3 mm^{-3}], and k_i [mm s^{-1}] denote the matric potential, the volumetric soil water content, and the hydraulic conductivity in soil layer *i*, respectively. The water content at saturation, $\theta_{sat,i}$ [mm^3 mm^{-3}], the saturated soil matric potential, $\psi_{sat,i}$ [mm], the saturated conductivity, $k_{sat,i}$ [mm s^{-1}], and the exponent B_i [-] are the parameters determining the shape of the hydraulic functions in layer *i*. The soil is divided into 10 layers in CLM3.5. The thickness of the simulation layers increases exponentially with depth. Below the lower boundary of the modeled soil column (fixed at 3.43 m in CLM3.5), an unconfined aquifer is assumed. In addition, $k_{sat,i}$ is assumed to decrease exponentially with depth.

The impact of soil moisture stress on stomatal resistance and plant transpiration is considered by a soil water availability factor which sums up the soil water deficits in the individual soil layers, depending on the soil matric potential and the fraction of the root system in the respective soil layer, and the critical potentials at which the stomata are either fully opened or closed. The root distribution is assumed to be constant during the entire vegetation period. Processes such as an increase in rooting depth or dying of roots during plant senescence are not considered in CLM3.5. To calculate root water uptake from a soil layer, the actual transpiration is distributed over the soil column as a function of the root distribution and the soil matric potential in each layer.

Expert-N crop models

Expert-N 3.0 is a model package consisting of numerous modules for simulating different processes in the soil–plant–atmosphere system that can be coupled in various combinations (Priesack 2006). The present simulation study was carried out by coupling two different crop models with the soil carbon and nitrogen turnover simulation method according to the SoilN model (Johnsson et al. 1987), with modules for soil heat and nitrogen transport of the model LEACHN (Hutson and Wagenet 1992), and with the Richards equation for soil water transport as implemented in the model Hydrus-1D (Simunek et al. 1998). The two crop models were (a) the crop modules of the model LEACHN (Hutson and Wagenet 1992) and (b) the model SPASS (Wang and Engel 2000), in the following referred to as XN-LEACHN and XN-SPASS. The variables of the crop models are updated at daily time steps, whereas the simulation time step of the soil model is governed by the solver of the Richards equation for soil water transport and varies between 0.001 and 0.1 days.

For the soil hydraulic functions, we used the van-Genuchten-Mualem approach:

$$\psi_i(\theta_i) = -\frac{1}{\alpha_i}\left(\Theta_i^{n_i/(1-n_i)} - 1\right)^{\frac{1}{n_i}} \tag{2a}$$

$$k_i(\theta_i) = k_{sat,i}\,\Theta_i^{-1/2}\left[1 - \left(1 - \Theta_i^{n_i/(1-n)}\right)\right]^{(n_i-1)/n_i} \tag{2b}$$

with

$$\Theta_i = \left(\frac{\theta_i - \theta_{r,i}}{\theta_{sat,i} - \theta_{r,i}}\right),$$

where $\theta_{sat,i}$ [mm^3 mm^{-3}], $k_{sat,i}$ [mm s^{-1}], the parameters α_i [mm^{-1}] and n_i [-], and the residual water content $\theta_{r,i}$ [mm^3 mm^{-3}] are the shape parameters for soil layer *i*. Compared to the hydraulic functions used in CLM3.5, the van-Genuchten-Mualem model has the potential to better match measured relationships between soil and water content and matric potential, because the van-Genuchten model can represent an possibly existing inflection point of the retention curve and thus is more flexible. In addition, we refined the discretization of the soil column with 27 equidistant simulation layers in XN-LEACHN and XN-SPASS. As lower boundary condition, we assumed free drainage at a depth of 108 cm.

In contrast to CLM3.5, the Expert-N crop models do not simulate the radiation balance at the land surface in detail. Instead, potential evapotranspiration is calculated from daily weather input using the Penman–Monteith equation (Monteith 1981). The actual transpiration is calculated directly from potential transpiration by a reduction factor that takes into account the soil matric potential and the spatial and temporal distribution of root length density.

XN-LEACHN Root water uptake from a certain soil layer is calculated in XN-LEACHN according to Nimah and Hanks (1973) from the time- and depth-dependent root length density, the gradient of the hydraulic potential between soil and root xylem, the soil hydraulic conductivity and the mean distance between roots, for which a value of 10 mm is assumed. The actual value of the water potential in the root at the soil surface is determined iteratively until the amount of water, which is taken up by the whole root system, equates to the value that is given by the potential transpiration. Through constraining root water potential to a lower boundary of $-3{\cdot}10^5$ mm and soil water potential to a lower boundary of $-1.5{\cdot}10^5$ mm, transpiration can be reduced to values lower than potential transpiration. Similar as in CLM3.5, vertical root length distribution is a predefined model input. However, root growth can be mimicked by variable values during the vegetation period.

XN-SPASS XN-SPASS is a prognostic model for simulating crop growth including leaf area development and root growth. The extension of the root system is calculated from the maximum root extension rate under optimum conditions and two reduction factors taking into account the impact of unfavorable temperature and soil moisture conditions in the deepest rooted soil layer. In each time step, the change of active roots in the individual soil layers results from root growth and root death caused by root turnover and senescence processes. The distribution of newly formed roots within the rooted soil zone is simulated by modulating the species-specific vertical root length distribution function in a way that root growth is favored in soil layers with high availability of nitrogen and water. Similarly, in XN-SPASS, the dieback of roots in a given time step is distributed to the individual soil layers in a way that roots die preferentially in layers with low nitrogen and water content. Root senescence depends on soil temperature, soil moisture, and the phenological stage of the plants. In XN-SPASS, the potential root water uptake from a soil layer is either limited by the presence of roots in the respective soil layer, or by maximum water uptake capacity per root length which is assumed to equal 0.03 cm^3 cm^{-1} d^{-1}, or by the resistance of water transport from soil to roots. The latter is expressed by an empirical function to describe the effect of soil water content on root water uptake (Jones and Kiniry 1986). The total potential water uptake by plants is the sum of the potential water uptake from all layers. If it exceeds potential transpiration, which is calculated from the Penman–Monteith equation and the actual LAI of the canopy, water uptake from each individual soil layer is proportionally reduced.

To facilitate the comparison of XN-SPASS with the soil water and root water uptake components of CLM3.5 and XN-LEACHN and to be consistent with the corresponding predefined LAI–input curves of these models, three parameters of XN-SPASS were adjusted to match the measured leaf area index. These parameters are the specific leaf area and two phenological parameters of XN-SPASS, the physiological development days from the emergence to anthesis and the days from anthesis to maturity. The parameters were adjusted by trial and error to avoid uncertainties in the simulation results arising from insufficient predictions of LAI. Soil moisture and latent heat flux data were not considered in this fitting procedure.

Experimental setup

Field data

Measurements of water fluxes in the soil–vegetation continuum were taken in high temporal resolution during the course of one vegetation period. A detailed description of the field site, instrumentation, and measurements is given in Ingwersen et al. (2011). We therefore outline here only the most important aspects of the experiment which are relevant for this simulation study.

Winter wheat was sown on November 6, 2008 at an open and flat field of about 15 ha in southwestern Germany (48.92°N, 8.70°E) and harvested on August 6, 2009. Leaf area index (LAI) was recorded biweekly during the vegetation period at five subplots of 4 m^2. The soil is a Stagnic Regosol, which developed from a loess layer of several meters thickness over shell limestone. The main soil properties are given in Table 1.

To measure net radiation, turbulent fluxes of sensible and latent heat, and soil heat fluxes, an eddy covariance (EC) station was installed on April 16, 2009. The station is equipped with a Licor 7500 open path infrared CO_2/H_2O gas analyzer (LI-COR Biosciences Inc., USA) and a CSAT3 3D sonic anemometer (Campbell Scientific Inc., UK). Moreover, air temperature, humidity, and rainfall are measured on site, and time domain reflectometer probes (TDR) were installed at 5, 15, 30, 45, and 75 cm depths to measure the temporal dynamics of soil moisture content. The soil moisture data have been aggregated to daily values.

A general problem of EC flux data in heterogeneous landscapes is that its energy balance is typically not closed. Therefore, in modeling studies, the flux data are usually post-processed to close the gap. At the current state of knowledge, however, it is unknown how the missing energy is partitioned. Two approaches for post-closing EC flux data are described in the literature, the Bowen ratio correction (Twine et al. 2000) and the sensible heat flux correction (H-correction, Ingwersen et al. 2011). In the first approach, it is assumed that the missing turbulent fluxes have the same ratio between sensible and latent heat (Bowen ratio) as the measured ones, and in the latter, the energy imbalance is assigned to the sensible heat flux. Indications and the theoretical foundation of the H-correction are discussed in Foken (2008). In the study of Ingwersen et al. (2011), which used exactly the same flux data from the same station as is used in this study, the application of Bowen ratio-corrected latent heat fluxes resulted in a distinctive overestimation of soil water depletion by the NOAH model. The best agreement between observed and simulated soil water dynamics was achieved with uncorrected, that is, H-corrected, latent heat fluxes. Therefore, in the present study, the H-correction was used for post-closing the EC flux data.

Aggregation of eddy covariance measurements

As usual in measuring turbulent fluxes with the eddy covariance method, some of the latent heat flux data had to be filtered out, because they do not fulfill the required quality criteria (Rebmann et al. 2005). The remaining data of latent heat flux were aggregated in different ways to provide appropriate data sets for the evaluation of model outputs at different time scales. For a direct evaluation of the high-resolution output of the CLM3.5 model, diurnal cycles of latent heat flux over several days with contrasting weather conditions were needed. The longest period during which such data were available at hourly resolution was from June 5 to 14. Since in the other periods a larger part of the measured values had to be filtered out, we restricted the direct evaluation of simulated diurnal cycles of latent heat flux to this period. However, to test the ability of CLM3.5 to simulate latent heat flux dynamics over the entire vegetation period, we averaged the available half-hourly values to weekly mean diurnal cycles of latent heat fluxes. Standard deviations of half-hourly values were calculated to estimate the variability in the measurements. Simulation results were aggregated in the same way. A third

Table 1 Soil properties at the experimental site

Horizon	Thickness	Bulk density	Texture			Organic matter
	(cm)	(g cm^{-1})	Sand (%)	Silt (%)	Clay (%)	(% by mass)
Ap	32	1.37	2.5	79.4	18.2	1.75
Sw-eCv1	16	1.51	2.0	79.2	18.8	0.61
Sw-eCv1	42	1.48	0.9	80.4	18.7	0.42

aggregation method was applied because the Expert-N models provide simulated latent heat fluxes only as daily values. From the averaged diurnal cycles of latent heat flux, weekly averages of daily rates were calculated for the 16 weeks of the vegetation period (April 17–August 6). Again, simulation results were aggregated correspondingly for testing the performance of the three models.

Simulation runs

To test the impact of the information level for the parameterization of soil hydraulic functions on simulation results, we applied CLM3.5 in a “low information modus” and in a “high information modus.” In the “low information” run, values for $\theta_{sat,i}$, $\psi_{sat,i}$, $k_{sat,i}$, and B_i are estimated from soil texture using the pedotransfer functions of Clapp and Hornberger (1978). Such a parameterization is common if CLM3.5 is applied to large domains and in the coupled mode where usually texture data are taken from soil maps. In the “high information” run, we use field data of soil moisture and soil water potential measured at five different soil depths to improve the parameterization of the soil hydraulic function by direct fitting the retention curve to the field data. In this way, we reduce the parameter uncertainty introduced by the pedotransfer functions. As no field measurements of soil hydraulic conductivity were available, we used the pedotransfer functions for k_{sat} also in this run. Uncertainties in the estimated water retention curves resulting from hysteresis in measured soil moisture–potential relations or from inaccuracies in the measurements of soil texture and soil organic content were not considered in this study. In the following sections, we refer to the “low information” run as CLM3.5#1 and to “high information” run as CLM3.5#2.

The impact of nitrogen limitation on photosynthesis (and hence stomatal conductance and transpiration) is considered in CLM3.5 by a constant reduction factor f_{Nitr} [-], which represents the proportion of potential photosynthesis that is realized in the case of nitrogen limitation (Oleson et al. 2008). By default, this factor is set to a value of 0.61 for PFT “Crop1” estimated from CLM simulations in CN-mode for a pre-industrial state. To find a more realistic value of f_{Nitr} for a managed field like in our experiment, we applied the crop model XN-SPASS (Gayler et al. 2002; Wang and Engel 2000) according to the boundary conditions of the experiment. During the growing season from April 17 to August 6, an average of 9 % reduction in photosynthesis due to nitrogen limitation was simulated. We therefore run a third model variant, CLM3.5#3, in which f_{Nitr} was set to 0.91.

Like CLM3.5, we also applied the crop models in a “low information mode” and in a “high information mode.” Again, we started with simulations providing the models only with basic soil data and, in case of the simpler model, with data of leaf area development (XN-LEACHN#1 and XN-SPASS#1). In this case, the parameters $\theta_{sat,i}$, $\theta_{r,i}$, $k_{sat,i}$, n_i, and α_i of the van-Genuchten-Mualem model were estimated using the pedotransfer functions from the Rosetta database (Shaap et al. 2001). Finally, we ran both crop models with high information using hydraulic parameters obtained from field data (XN-LEACHN#2 and XN-SPASS#2).

With the exception of simulation run CLM3.5#3, in which the parameter considering the effect of nitrogen limitation on photosynthesis was set to a more realistic value, all parameters of CLM3.5 and XN-LEACHN were left on their default values. The only model parameter fitting in this study was the adaptation of the specific leaf area and of two of the phenological parameters in the prognostic model XN-SPASS, to ensure that this model matches the observed dynamics of LAI as accurate as the other models. In no case, parameters were fitted to the target observations, latent heat fluxes, and soil water content.

Performance measures

Two widely used statistical measures were applied to assess the performance of latent heat flux and soil moisture simulations, the normalized root mean square error NRMSE as defined by Wallach and Goffinet (1989),

$$\mathrm{NMRSE} = \frac{1}{\bar{O}} \sqrt{\frac{\sum_{i=1}^{n} (P_i - O_i)^2}{n}},$$

and the Nash–Sutcliffe efficiency NSE (Nash and Sutcliffe, 1970)

$$\mathrm{NSE} = 1 - \frac{\sum_{i=1}^{n} (P_i - O_i)^2}{\sum_{i=1}^{n} (\bar{O} - O_i)^2}$$

O_i and P_i are the observed and predicted values of the considered variable, and n is the number of data pairs. $\bar{O}$ is the mean of observations. NRMSE ≥ 0 provides the average deviation between predicted and observed values, proportioned against the mean observed value. The closer the value of NRMSE is to 0, the better the fit between model and observation. NSE can range from $-\infty$ to 1. NSE $= 1$ corresponds to a perfect match between simulated and observed data. NSE > 0 indicates that the model predictions are more accurate than the mean of the observed data. Using both measures provides some complementary information about the adequateness of simulation runs. NRMSE delivers a percentage term divided by 100 of the deviations between observations and simulation, whereas NSE focuses rather on an adequate simulation of the observed variability.

Results and discussion

Simulated soil water contents were evaluated for all models at daily time intervals at depths where TDR probes were installed (Figs. 1, 2). It was assumed that each measurement represents a soil volume of 4 cm thickness. As in CLM3.5 the discretization of the upper soil layers has a higher spatial resolution than the soil volumes represented by the measurements, simulation results were aggregated to correspond with measurements.

The CLM3.5#1 "low information" simulations resulted in a NRMSE of 0.30 and a negative NSE (−0.33) for soil moisture (Table 2). This weak performance is due to a strong overestimation of soil moisture and a clear underestimation of temporal variability down to a depth of 0.45 m during most of the simulation period (Fig. 1). In the "high information" run, CLM3.5#2, the more realistic parameterization significantly enhances the fit to soil moisture (NRMSE = 0.23, NSE = 0.22) (Table 2). The level and the variability of soil moisture in the upper soil horizon are now much closer to the measurements than in the CLM3.5#1 run (Fig. 1). A further improvement of simulated soil moisture dynamics could be achieved with simulation run CLM3.5#3 where the parameter f_{Nitr} was set to 0.91. It resulted in an increase in NSE of soil moisture to a value of 0.35 (Table 2).

Applied in "low information mode," soil moisture simulations by both crop models (XN-LEACHN#1 and XN-SPASS#1) achieved better performance measures than CLM3.5#1 (Table 2). Like in CLM3.5, the higher level of information strongly improves the simulation of soil moisture by both crop models. Also in the "high information" runs (XN-LEACHN#2 and XN-SPASS#2), the crop models, which use the van-Genuchten-Mualem approach instead of the Campbell/Clapp-Hornberger parameterization, perform better than CLM3.5 in simulating soil moisture dynamics (Table 2; Fig 2). The good performance of the crop models is caused by a more accurate simulation of the vertical soil moisture distribution and a better representation of the soil moisture

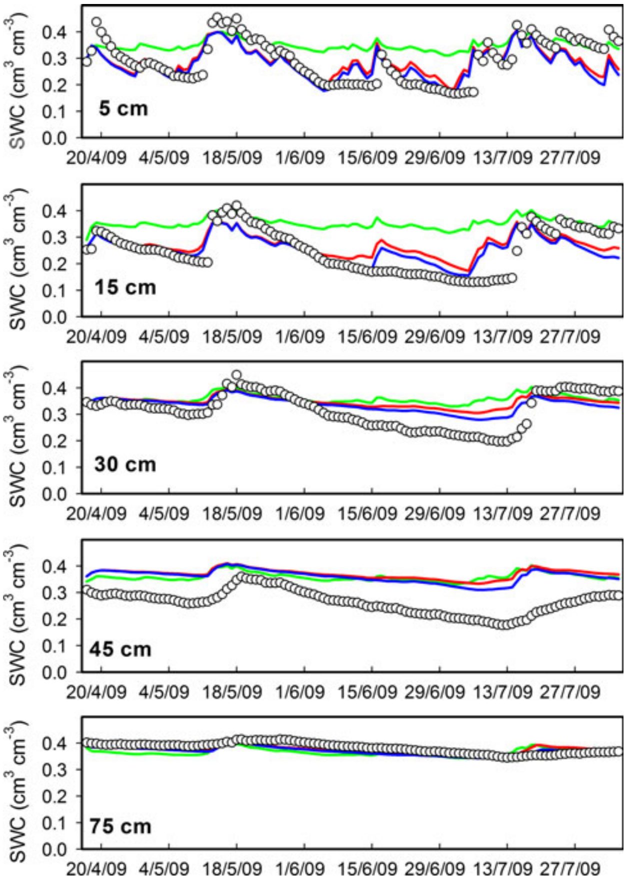

Fig. 1 Soil moisture dynamics at five different depths simulated by CLM3.5. Observed values are symbolized by *circles*. *Green lines* soil parameters calculated from pedotransfer functions (CLM3.5#1), *red lines* soil parameters fitted to field data (CLM3.5#2), *blue lines* in addition f_{Nitr} adapted to actual field conditions (CLM3.5#3)

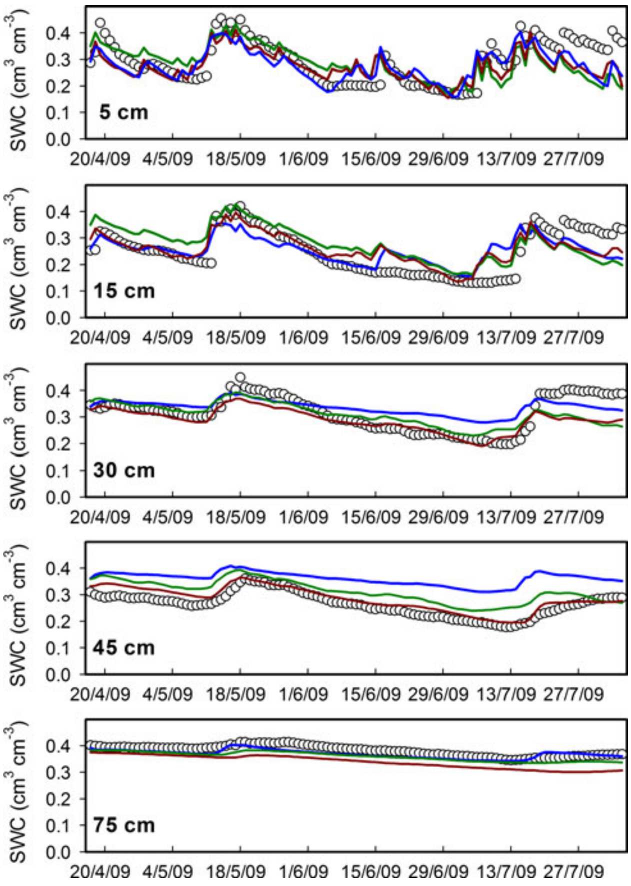

Fig. 2 Soil water content dynamics at five depths simulated by the different models (*lines*) together with observed values (*circles*). *Blue line* CLM3.5#3, *dark green line* XN-LEACHN#2, *dark red line* XN-SPASS#2

Table 2 Normalized root mean square errors and Nash–Sutcliffe efficiencies of CLM3.5 and Expert-N simulation runs compared to measured weekly averaged daily latent heat fluxes (left) and daily values of soil moisture over one vegetation period (right)

	Soil moisture	
	NRMSE	NSE
CLM3.5#1	0.301	−0.332
CLM3.5#2	0.231	0.220
CLM3.5#3	0.210	0.352
XN-LEACHN#1	0.239	0.171
XN-LEACHN#2	0.172	0.571
XN-SPASS#1	0.247	0.118
XN-SPASS#2	0.144	0.702

variability in the individual soil layers (Fig. 2). This seems to confirm findings of Braun and Schädler (2005), who compared the two parameterizations in mesoscale meteorological models. One reason for the more accurate soil moisture simulations by the crop models could lie in the different representations of the shape of the water retention curve between the two models. Other than Campbell/Clapp-Hornberger, which assumes a simple exponential law, the van-Genuchten-Mualem parameterization provides for an inflection point of the retention curve, which allowed a slightly better match with field data. However, besides different parameterizations of the hydraulic functions, further differences between CLM3.5 and the crop models in rooting structure, in the discretization of the soil column and in the lower boundary condition, could be responsible for the observed deviations between soil moisture simulations by CLM3.5 and Expert-N crop models. A rigorous examination of the impact of the different possible sources on these deviations would only be possible by additional simulations after substituting the different parameterizations of the hydraulic functions between the individual models. However, this is beyond the scope of this study.

In this study, CLM3.5 was the only model that simulates diurnal cycles of latent heat fluxes. Therefore, only for this model, simulations of diurnal cycles of latent heat fluxes were evaluated based on both hourly values for the 10-day period from June 5 to 14 and on weekly averaged half-hourly values in the whole vegetation period (Table 3; Figs. 3, 4). To allow for a comparison of CLM3.5 with the two crop models, which only provide daily output values, daily simulated latent heat fluxes were also averaged at weekly time intervals (Fig. 5).

In the “low information” run CLM3.5#1, simulated latent heat fluxes match with hourly measurements during the 10-day evaluation period fairly well with a NRMSE of 0.54 and a NSE of 0.66. The simulation of weekly averaged half-hourly values over the entire vegetation period achieved an NRMSE of 0.47 and an NSE of 0.79 (see Table 3). Simulated weekly averages of daily latent heat fluxes yielded a markedly better NRMSE but a lower NSE (Table 3). This is caused by a smaller number of data pairs in the evaluation and a smaller variation between single values compared to the diurnal cycles. Variability between single days was well simulated by CLM3.5. For example, low values of latent heat flux on June 6 in succession of high fluxes on June 5 and the subsequent increase until June 10 could be reproduced (Fig. 3). In most cases, the model matched morning and afternoon values of latent heat fluxes well, both during the 10-day evaluation period (Fig. 3) and during the whole vegetation period (Fig. 4). During midday hours, however, the fluxes were frequently underestimated. This is almost independent from the degree to which soil moisture is matched by the simulations. Differences between CLM3.5#1 and CLM3.5#2 simulations of more than 15 % of volumetric water content in the upper soil horizon during the 10-day evaluation period from June 5 to 14 have almost no effect on simulated latent heat flux. Obviously, latent heat flux is mainly a function of radiation and not of soil water availability in this period. This is a common and important situation over cropped surfaces between full soil coverage and crop ripening in midlatitudes.

However, a significant increase in the NSE of simulated latent heat flux can be observed when using a more realistic value of the parameter regulating the effect of soil nitrogen availability on photosynthesis and thus on stomatal opening, f_{Nitr} in the CLM3.5#3 run, both for the 10-day evaluation period and for the weekly means of daily flux rates (Table 3). This is due to higher midday fluxes (Fig. 3), which also increase the weekly means of daily fluxes (not shown). In case of weekly means of diurnal cycles over the whole vegetation period, performance measures were not improved (Table 3). The parameter adjustment enhances the agreement with observed latent heat fluxes during the first months of the vegetation period, but also increases the discrepancy between simulations and observations during the last weeks of the vegetation period, when crops became senescent (Fig. 4). This conflict to find one adequate value of f_{Nitr} that applies to the whole vegetation period hints to structural deficits of the model, which does not consider an increase in the hydraulic resistance of water flow through plants during senescence. A similar shortcoming concerning vegetation dynamics was discussed by Ingwersen et al. (2011). In their study with the land-surface model Noah (Chen and Dudhia 2001), they could improve the match between measured and simulated energy fluxes by enforcing a strong increase in the minimum stomatal resistance at the end of the vegetation period.

Regarding latent heat flux, the higher level of information has no effect on the performance of XN-LEACHN and

Table 3 Normalized root mean square errors (NRMSE) and Nash–Sutcliffe efficiencies (NSE) of CLM3.5 simulations of latent heat fluxes

	Latent heat flux					
	10-day period		Weekly averaged diurnal cycles		Weekly averaged daily rates	
	NRMSE	NSE	NRMSE	NSE	NRMSE	NSE
CLM3.5#1	0.54	0.66	0.47	0.79	0.293	0.084
CLM3.5#2	0.54	0.65	0.46	0.80	0.289	0.107
CLM3.5#3	0.45	0.76	0.51	0.76	0.282	0.149
XN-LEACHN#1					0.266	0.252
XN-LEACHN#2					0.266	0.251
XN-SPASS#1					0.145	0.777
XN-SPASS#2					0.163	0.719

Left: calculated for diurnal cycles over the 10-day evaluation period; right: calculated for weekly means of diurnal cycles over one vegetation period

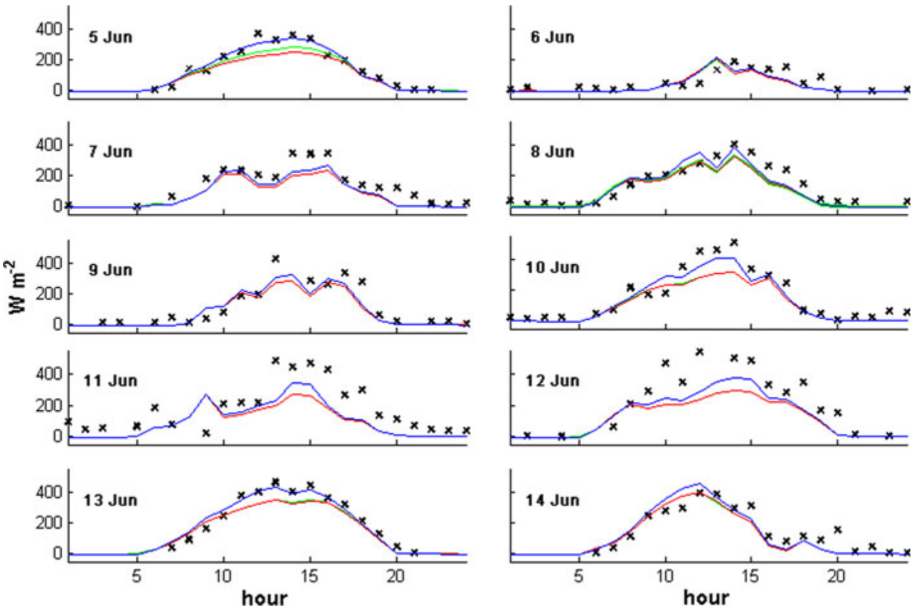

Fig. 3 CLM3.5 simulations of the diurnal cycles of latent heat flux over a period of 10 days (June 5–14, 2009) together with observed values (*black crosses*). *Green lines* (partially hidden): soil parameters calculated from pedotransfer functions (CLM3.5#1); *red lines* soil parameters fitted to field data (CLM3.5#2), *blue lines* in addition f_{Nitr} adapted to actual field conditions (CLM3.5#3)

a slightly negative effect on that of XN-SPASS (Table 3). However, compared to CLM3.5, both crop models achieved better performance criteria values for weekly averaged daily latent heat fluxes in both the “low information mode” (XN-LEACHN#1 and XN-SPASS#1) and the “high information mode” (XN-LEACHN#2 and XN-SPASS#2). Whereas the differences between XN-LEACHN and CLM3.5 are rather small, the model XN-SPASS shows a very good performance with NRMSE < 0.2 and NSE > 0.7 in both modes (Table 3). The good performance is mainly caused by the capability of XN-SPASS to simulate the strong decrease in water flux at the end of the vegetation period caused by the senescence of the root system. This physiological effect cannot be simulated by the other models (Fig. 5).

Similar to the CLM3.5 simulations, the latent heat flux simulated by the crop models is widely independent from soil water availability for most of the vegetation period. This is in accordance with the observed close relationship between weekly means of incoming radiation and measured latent heat fluxes during the first months of the vegetation period (not shown). This correlation in measured data does not hold toward the end of the vegetation period when observed latent heat fluxes decrease rapidly. However, soil moisture deficiency is not responsible for this decrease, because soil moisture contents increased after strong precipitation events in the second half of July.

Our simulation results show that better information and more detailed process descriptions increase the accuracy of simulated soil moisture dynamics and latent heat flux rates. None of the CLM3.5 simulations runs attained a simultaneous match of observed weekly means of daily latent heat flux and soil moisture data as good as the crop model simulations. The best simultaneous fit of soil moisture and

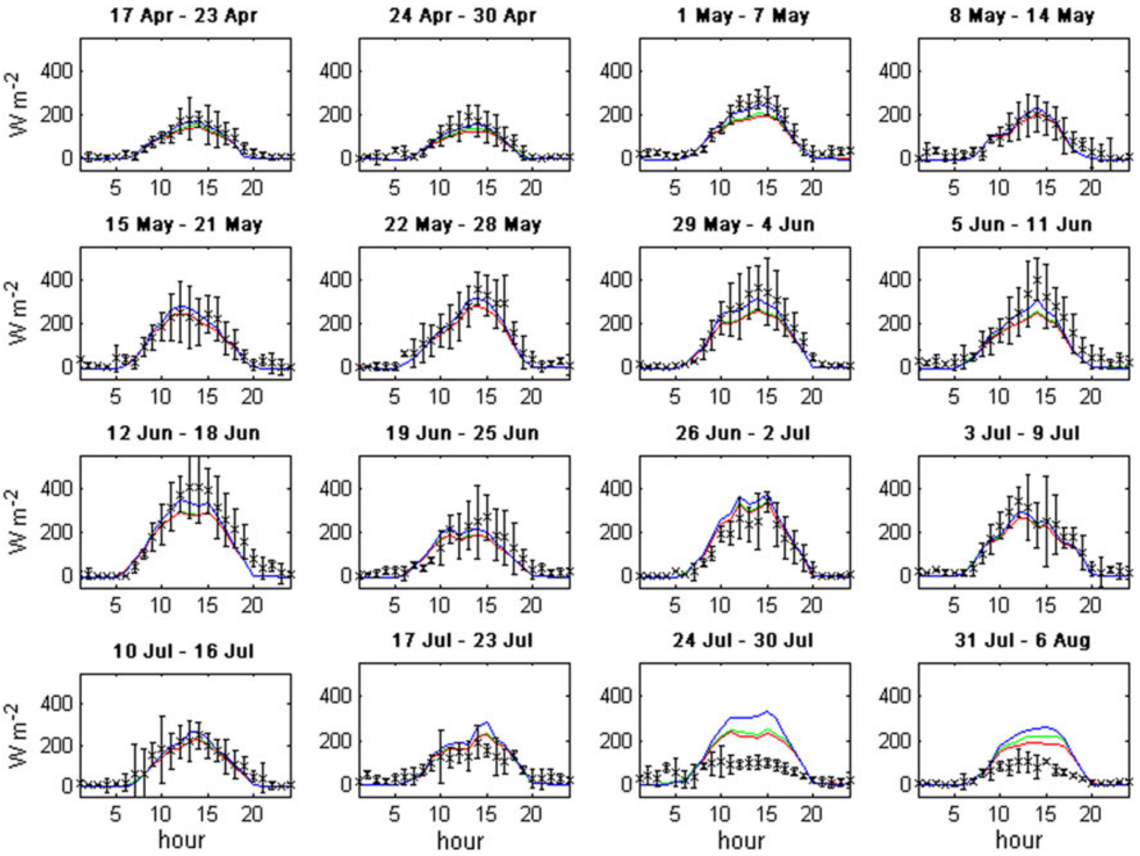

Fig. 4 Weekly averaged CLM3.5 simulations of diurnal cycles of latent heat fluxes during the growing season 2009 (April 17–August 6), together with observed values (*black crosses*). *Error bars* symbolize standard deviations resulting from the weekly averaging of observations. *Green lines* soil parameters calculated from pedotransfer functions (CLM3.5#1), *red lines* soil parameters fitted to field data (CLM3.5#2), *blue lines* in addition f_{Nitr} adapted to actual field conditions (CLM3.5#3)

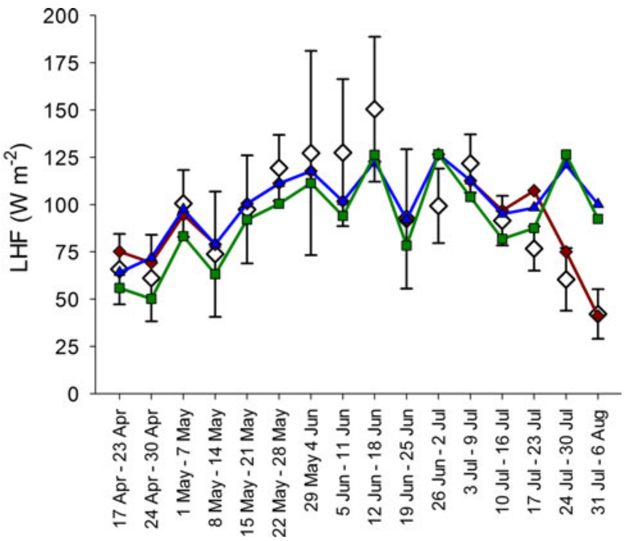

Fig. 5 Weekly means of latent heat fluxes simulated by the different models (*colored symbols with lines*) together with observed values (*white symbols with error bars*). *Blue line and triangles* CLM3.5#3, *dark green line and squares* XN-LEACHN#2, *dark red line and diamonds* XN-SPASS#2

latent heat flux was achieved by XN-SPASS. As this was not achieved by parameter fitting, the good performance is not due to the higher degree of freedom of the more complex model. Instead, it indicates the extent to which simplifications in the other models can reduce the accuracy of model predictions. XN-SPASS is the only model in this study which reproduces the decrease in latent heat flux at the end of the vegetation period, because it simulates root senescence and consequently a strong degeneration of the hydraulic system at the end of the vegetation period, which is associated with an increasing resistance of water flux through plants. Empirical evidence for a strong decrease in living root biomass, which comes along with leaf senescence at the end of the vegetation period, was recently presented by Huang et al. (2012) in field experiments with winter wheat and maize. Variability in living fine root biomass with its implications on plant hydraulic conductivity is an important factor at crop sites, where annual plants are cultivated and harvested. It plays a minor role in other vegetation types like forests and grassland communities. Thus, our results suggest the implementation of the relevant root growth and senescence routines from the SPASS model in CLM3.5 for the PTFs "crop1" and "crop2," in particular if CLM3.5 is applied in regional or catchment scale studies in agriculture-dominated regions.

Summary and conclusions

A consistent simulation of water fluxes in the soil–plant–atmosphere system must reproduce both the latent heat flux from the land surface to the atmosphere and the soil water dynamics with high accuracy. Our study has shown that this requires an enhanced level of detail in the representations of soil hydraulic functions and plant processes, in particular root growth dynamics. Parameterizations of soil hydraulic properties from basic soil data (e.g., texture, bulk density, or organic matter content) using pedotransfer functions can result in clearly insufficient simulations of the vertical distribution of soil moisture and its dynamics. The use of hydraulic parameters derived from locally measured time series of soil moisture and soil matric potential markedly improved both CLM3.5 and Expert-N crop model simulations. The results can be seen as an estimation of uncertainty caused by an inevitably poor model parameterization in larger-scale applications of CLM3.5, for which this model is rather adapted than for matching plot-scale measurements. Moreover, it makes clear that more sophisticated concepts for the estimation of soil parameters are urgently needed, if a model such as CLM3.5 is to be applied in catchment scale studies (e.g., Pause et al. 2013).

The inaccuracies in soil water simulations of "low information" runs had almost no effect on simulated latent heat fluxes as long as the soil was fully covered by crops and evapotranspiration was widely independent of soil moisture. In contrast, using models with a more detailed description of plant processes such as root growth and root senescence showed a positive impact on simulated seasonal dynamics of latent heat flux as well as on the vertical distribution of soil moisture. An excellent simultaneous agreement of both weekly averaged daily latent heat fluxes and soil moisture was only possible with the most detailed model, XN-SPASS. Consequently, we conclude that coupling of hydrological and atmospheric models necessitates more detailed process descriptions of soil water transport and root water uptake than currently implemented in land-surface models. Moreover, we expect that corresponding improvements in land-surface schemes in atmospheric models will lead to more accurate weather and climate forecasts.

The comparison with crop models, which simulate root water uptake at a much higher degree of detail, can only be seen as a first attempt to investigate the role of structural model uncertainty in CLM3.5. In a next step, the relevant processes will be implemented in the source code of CLM3.5 to directly investigate the impact of better process descriptions on the simulations of diurnal and seasonal evolution of latent heat flux and on the temporal and spatial dynamics of soil moisture. However, we are aware that improving single components of a complex model does not necessarily result in a better performance of the complete model system. As shown by Winter et al. (2009), for example, the performance of the regional climate model RegCM3 to match FLUXNET observations of latent heat flux could be improved by coupling it with the Integrated Biosphere Simulator IBIS, but the performance of other output variables decreased at the same time. We will therefore extend our study to other output variables of CLM3.5, for which observations are available (sensible heat flux, ground heat flux). In addition, we will include existing data sets from different years and from a contrasting field site on Swabian Alb in Southern Germany to identify situations in which the variability of soil moisture feeds back to processes in the atmosphere.

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