Multiobjective calibration of coupled soil-vegetation-atmosphere models

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Abstract The modular system Expert-N is adopted to analyse the effect of the complexity of soil-vegetation-atmosphere models on their calibration results. Four different models with increasing complexity are calibrated using time series of observed soil moisture, evapotranspiration, and LAI field data from a winter wheat field plot in Kraichgau, southwest Germany. The calibration of each model is posed in a multiobjective framework and three different objective functions are used to summarize the distance between measurements and simulations of different data types. The AMALGAM evolutionary search algorithm is utilized to simultaneously estimate the most important soil hydraulic and plant module parameters. Results show for most models a considerable trade-off appears in the fitting of different data types. If a mechanistic description of plant growth is considered the trade-off reduces considerably. The simplest plant model in our study performs relatively well but requires the availability of key development data of the plant. If such data are not available to the user, such models are rather useless for predictive purposes.

Key words soil-vegetation-atmosphere modelling; evapotranspiration; soil moisture; leaf area index; multiobjective parameter optimization; AMALGAM; Pareto analysis; model calibration

INTRODUCTION

The ability to describe fluxes of water, energy, and carbon in the soil–plant–atmosphere continuum is essential in soil, plant and climate research. To understand the complex interplay of the processes involved, various physically-based soil-plant-atmosphere system models have been developed during the past decades (Priesack & Gayler, 2009). Many of the parameters in these models require calibration before the model can be used for predictive purposes. However, as such models simulate different processes simultaneously, the problem arises which data to use for model calibration, and in what manner. Different data types may contain contrasting information about the system states and fluxes. As a consequence, the fitting of a model to one data type may result in poor agreement to another data set. This trade-off in the fitting of different data types is caused by structural inadequacies in the model and other potential sources of error, including calibration and forcing data errors.

To analyse the impact of plant model structural complexity on the simultaneous fit to different data types, we selected four different plant models and coupled them to a common soil water flow model. The plant models utilized herein are LEACHN (Hutson & Wagenet, 1992), CERES (Ritchie, 1988), SPASS (Wang, 1997; Gayler *et al*., 2002), and GECROS (Yin & Laar, 2005). These four disparate models are all incorporated in the modular Expert-N system and simultaneously describe evapotranspiration, root water and solute uptake, soil heat fluxes, and plant growth processes at different levels of detail and abstraction.

Priesack *et al*. (2006) used CERES, SPASS and the SUCROS model by van Laar *et al*. (1992) to investigate the impact of the choice of the crop growth model on simulated water and nitrogen balances. They found only subtle differences among the different models in their simulation of the water balance, but comparatively large differences in their performance to predict C and N turnover. It was concluded that the simulation of root growth and plant residue mineralisation needs improvement. More recently, Biernath *et al*. (2011) used the CERES, SPASS, SUCROS, and GECROS models to evaluate their ability to predict different environmental impacts on spring wheat grown in open-top chambers. The most adequate simulation results were obtained with SUCROS, followed by the SPASS, GECROS and CERES models. It was concluded that the more mechanistic plant growth models, GECROS and SPASS, do not necessarily exhibit better predictive performance.

Despite this progress made, these previous studies have failed to recognize the influence of the calibration data and parameter estimation method on the final conclusions. Coupled models of the soil–plant–atmosphere continuum typically contain many distinctly different parameters whose values can only be accurately determined by calibration against different data types. In this paper we simultaneously use measurements of leaf area index, transient soil water content, and actual evapotranspiration from a winter wheat field plot in the Kraichgau region to calibrate by multiobjective optimization four different soil–plant–atmosphere models with different levels of complexity. We are especially concerned with the ability of the different models to adequately describe the different components of the ecohydrologic system.

FIELD EXPERIMENTS

Winter wheat was sown on 6 November 2008 at an open and flat field of about 15 ha in the so-called "Kraichgau" region in southwestern Germany (48.92°N, 8.70°E). The subsurface consists of a loess soil of several metres thickness with the groundwater table more than 25 m below the surface in the underlying limestone. Five subplots of 4 m^2 were selected to measure leaf area index (LAI) and phenological development. Harvest at grain maturity took place on 6 August 2009. An eddy-covariance (EC) station was installed on 16 April 2009 to measure sensible and latent heat fluxes. Moreover, air temperature, humidity, and rainfall were measured on site, and TDR probes were installed at 5, 15, 30, 45 and 75 cm depths to measure temporal dynamics of soil moisture content. The EC data were corrected by the Foken method (2008), and aggregated to weekly values. All other sensor data were aggregated to daily values for use in our simulations. A detailed description of the field site, instrumentation and measurements appears in Ingwersen *et al*. (2011) and is therefore not repeated here. The duration of the cropping season was 268 days. For model calibration we used the data records from day 174 (EC installation) until harvest.

COUPLED SOIL–VEGETATION–ATMOSPHERE MODELLING

In this study, we use the model system Expert-N which comprises several modular sub-models to simulate vertical transport of water, solute and heat in the unsaturated zone, organic matter turnover, and crop growth (Stenger *et al*., 1999; Priesack, 2006). The sub-models currently available in Expert-N have either been taken from published models such as LEACHN 3.0 (Hutson & Wagenet, 1992), SOILN (Johnsson *et al*., 1987), HYDRUS (Šimůnek *et al*., 2005), CERES-Wheat 2.0 (Ritchie, 1988), and GECROS (Yin & Laar, 2005), or have been developed by the Expert-N team such as the crop growth model SPASS (Wang, 1997; Gayler *et al*., 2002).

The four soil–plant–atmosphere models considered here differ in their underlying representation of crop processes, but use identical modules to simulate water, heat and nitrogen transport through the loess soil. Soil water flow is modelled with the Richards equation (as implemented by Šimůnek *et al*., 2005) and the van-Genuchten Mualem model (van-Genuchten, 1980) is used to parameterize the soil hydraulic functions. In all our simulations we assume three horizontal soil layers with depths ranges from 0 to 0.32 m, 0.32 to 0.48 m, and 0.48 to 0.90 m. Heat transfer and soil nitrogen transport are calculated using LEACHN, whereas soil carbon and nitrogen turnover are simulated with the SOILN model. In all cases, potential evapotranspiration is calculated following the Penman-Monteith equation using crop factors for winter wheat (Allen, 2000). Plant water uptake and transpiration are simulated by CERES, SPASS and GECROS. In contrast, LEACHN crop growth is estimated directly from LAI and root distribution that are required inputs for the model.

Photosynthesis, biomass accumulation, leaf area development, root distribution and senescence are calculated depending on several environmental impacts such as temperature, irradiance, water and nitrogen availability. However, distinct differences exist between the four models used here. In CERES, a curvilinear relation between carbon assimilation and daily absorbed solar radiation (simulated by a simple "big-leaf" approach) is assumed. Biomass accumulation and assimilate distribution is based on the concept of radiation use efficiency and an empirical sink-source concept. In contrast, intercepted photoactive radiation (PAR) is calculated in SPASS and GECROS by considering direct and diffusive radiation components, shaded and sunlit leaves, and different spatial layers within the canopy. In addition, the diurnal variation of incident radiation is explicitly considered. In each of five canopy layers, photosynthesis rates of shaded and sunlit leaves are calculated and subsequently integrated numerically from the top of the canopy to the soil surface. In SPASS, photosynthesis follows a hyperbolic dependency on PAR, as proposed by Goudriaan & vanLaar (1994). The SPASS and CERES models use identical routines for root growth and root water uptake. Of all the different models, GECROS is most detailed in that it explicitly considers photosynthesis as well as plant internal distribution of assimilates and nitrogen to different plant organs. In this model, photosynthesis is calculated according to the biochemical approach of Farquhar (1981) which depends on leaf internal CO_2 concentration. Consequently, this approach includes a detailed model of stomatal conductivity that considers the close interdependency between CO_2 assimilation and water losses due to transpiration. GECROS also assumes an optimum criterion for carbohydrate and nitrogen distribution between roots and shoot.

The four different soil–plant–atmosphere models used herein differ substantially in their degree of process representation of plant water relations and plant growth processes, as shown in Fig. 1.

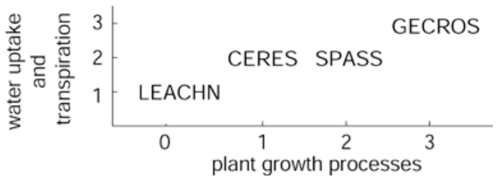

Fig. 1 Complexity of the utilized soil–vegetation–atmosphere models.

MULTIOBJECTIVE MODEL CALIBRATION

To estimate the parameters of the four soil–vegetation–atmosphere models, we pose the calibration problem in a multiobjective framework and use three different sum-of-square-error (SSE) objective functions, F_1, F_2, and F_3, to separately measure the ability of the different models to fit the measured soil water content, LAI, and actual evapotranspiration (ETA) data, respectively. The AMALGAM method (Vrugt & Robinson, 2007) was used to analyse the trade-off between the fitting of the three different objective functions. AMALGAM combines simultaneous multimethod search and self-adaptive offspring creation, to ensure a reliable and computationally efficient solution to multiobjective optimization problems. For further details on the method, please refer to Vrugt & Robinson (2007) and Wöhling *et al*. (2008).

Five different van-Genuchten model parameters are estimated for each of the three soil layers. This involves the saturated water content, θ_s ($m^3\ m^{-3}$), the shape parameters of the water retention function, α and n, the saturated hydraulic conductivity, K_s ($cm\ d^{-1}$), and the pore-connectivity parameter l (-). In addition, we included four plant model parameters that appeared most sensitive to the model predictions. The maximum root extension rate, δ_r ($cm\ d^{-1}$), the specific root length density λ_R ($m\ Kg^{-1}$), the maximum water uptake rate, ζ_W ($cm^3\ cm^{-1}\ d^{-1}$), and the specific leaf weight, λ_L ($Kg\ ha^{-1}$ leaf area) were estimated for both the CERES and SPASS models. Specific leaf area, s_{la} ($m^2\ g^{-1}$ leaf), critical root weight density, w_{Rb} ($g\ m^{-2}\ cm^{-1}$ depth), minimal leaf-N, $n_b = 0.01\ \varepsilon / s_{la}$ ($g\ N\ m^{-2}$), and the slope of the maximum carboxylation rate *versus* leaf-N, $\Delta V_{c,max}$

(μmol s^{-1} g^{-1} N) were calibrated in the GECROS model. LEACHN does not feature explicit plant model parameters (see above). The total number of estimated parameters is 19 for the CERES, SPASS, and GECROS models and 15 for LEACHN.

The sole algorithmic AMALGAM parameter to be defined by the user is the population size which is set to s = 100. The initial sample in AMALGAM was generated using Latin hypercube sampling with parameter ranges reported in Table 1. After calibration, model performance was also evaluated with the Nash-Sutcliffe efficiency (NSE).

Table 1 Upper and lower parameter bounds.

Sub-model	HYDRUS – MVG					CERES, SPASS				GECROS			
Parameter	θ_s	α	n	K_s	l	δ_r	λ_R	ζ_W	λ_L	s_{la}	w_{Rb}	ε	$\Delta V_{c,max}$
Lower bound	0.4	0.001	1	10	–10	1	5E3	0.01	300	0.0167	0.1	0.7	40
Upper bound	0.6	1.0	5	3000	10	3	2E4	0.1	600	0.0333	0.5	1.3	70

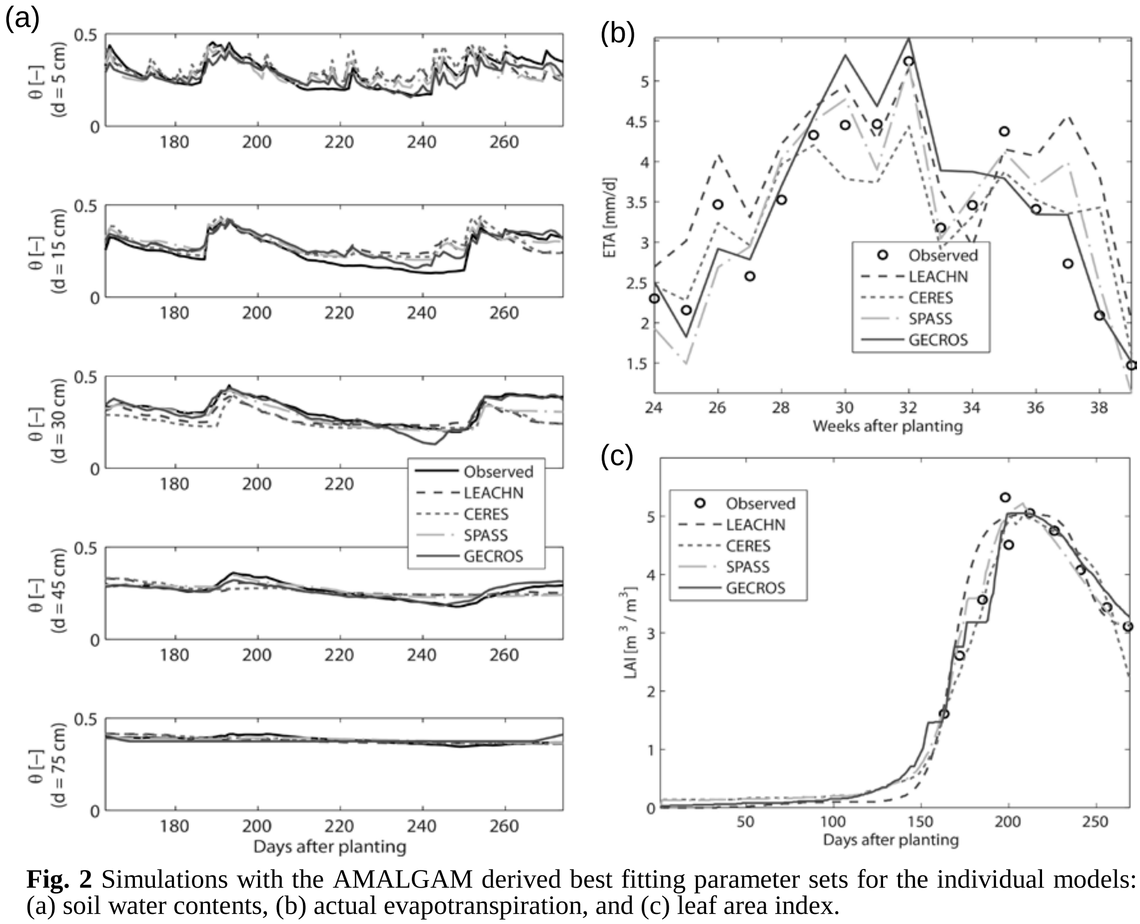

Fig. 2 Simulations with the AMALGAM derived best fitting parameter sets for the individual models: (a) soil water contents, (b) actual evapotranspiration, and (c) leaf area index.

RESULTS

The AMALGAM calibration runs for the four soil–plant–atmosphere models considered herein were terminated after 100 000 model evaluations when convergence to a stable Pareto surface was observed. To streamline the discussion we first report the best attainable fits of the four different models to each of the three objective functions. The GECROS model achieves the closest fit to the soil moisture data, followed by SPASS, LEACHN, and CERES (Table 1 and Fig. 2(a)). Surprisingly, the CERES model does not perform better than LEACHN, which excludes plant processes. The

CERES big leaf approach is probably not complex enough to accurately simulate root water uptake processes. In addition, LEACHN had a "head start" by providing accurate phenomenological data as model input. The SPASS model exhibits the closest fit to the LAI measurements, followed by GECROS and CERES (Table 1 & Fig. 2(b)). GECROS ranks again first for the fit to ETA data and is followed by SPASS, CERES, and LEACHN (Table 1 and Fig. 2(c)). Our results demonstrate that the mechanistic models with the largest level of complexity, GECROS and SPASS, yield a better agreement to single data types as compared to LEACHN.

Table 2 Performance criteria for the best fitting parameter sets.

	LEACHN		CERES		SPASS		GECROS	
	SSE	NSE	SSE	NSE	SSE	NSE	SSE	NSE
best fit water content	1.438	0.58	1.581	0.54	0.888	0.74	0.596	0.83
best fit LAI	1.526	0.88	1.27	0.90	0.43	0.96	0.86	0.93
best fit ETA	1.03	0.38	0.46	0.72	0.41	0.76	0.29	0.83

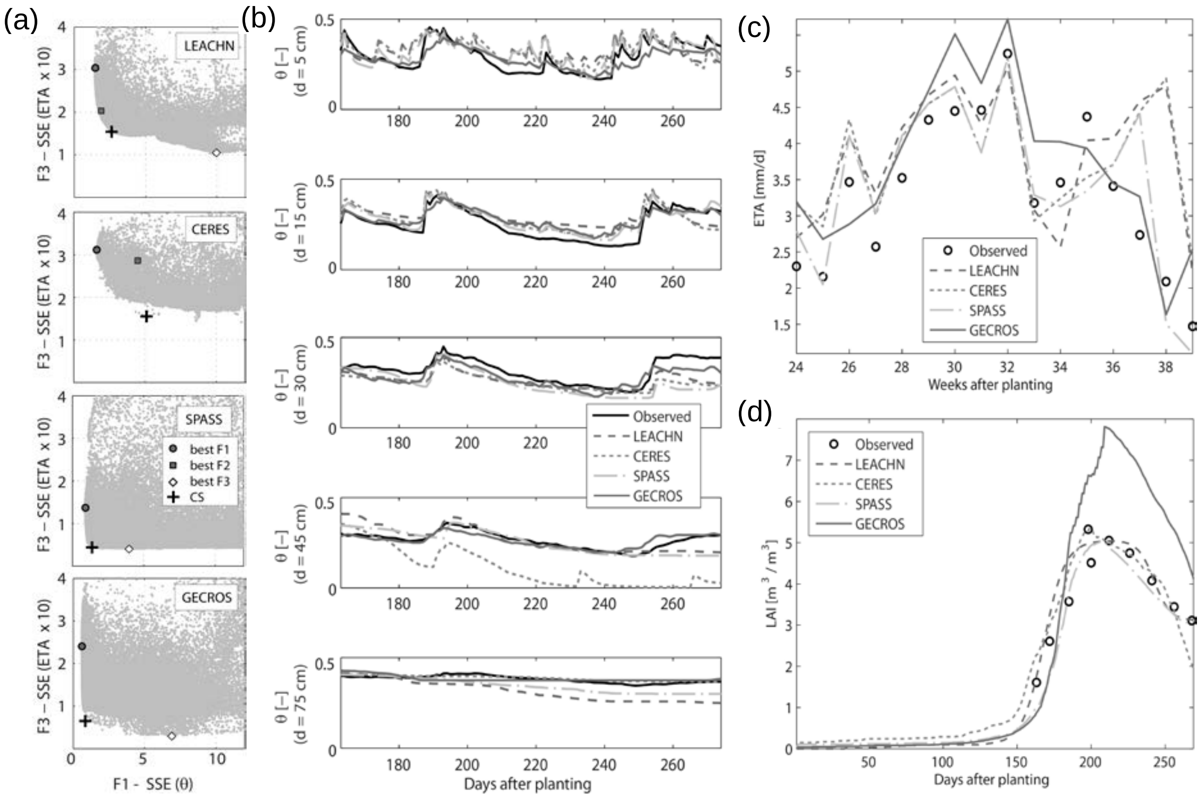

Fig. 3 (a) Trade-off between objective functions F_1 and F_3 and simulations with the AMALGAM derived compromise solution parameter sets: (b) soil water contents, (c) ETA, (d) LAI.

A good model performance for individual objective functions does not guarantee a *simultaneous* fit to all data types. This is analysed for each model by the AMALGAM derived set of non-dominated, or Pareto solutions that define the trade-off between the three different objective functions. We focus here on the trade-off between the fit to soil moisture data (F_1) and ETA (F_3), which is depicted for the different models in Fig. 3(a). The curved shape of the F_1–F_3 Pareto fronts for the LEACHN and CERES models indicate that no parameter set exists that satisfies both objective functions equally well. In contrast, the trade-off between F_1 and F_3 is small for SPASS, as indicated by the angular shape of the Pareto front. We now select from the Pareto set a minimum error parameter set, or compromise solution, for the objectives F_1–F_3 and their corresponding predictions are indicated with the "+" symbol in Fig. 3(a). The model performance with these parameter sets shows that the mechanistic models GECROS and SPASS exhibit the best overall fit to the soil moisture and evapotranspiration data (Table 3). However, some structural discrepancies are also visible for these models. Although GECROS performs well for θ and ETA (Fig. 3(c)–(d)), the LAI peak is largely overestimated (Fig. 3(d) and Table 3). The best simultaneous fit to all data types is achieved by the compromise solution of the SPASS model, which is confirmed by the lowest aggregated SSE and corresponding large NSE values (Table 3). CERES ranks last for the overall fit, mainly due to its inability to adequately simulate the observed soil moisture dynamics.

Table 3 Performance criteria for the compromise solution parameter sets.

Model	Pareto solution	Water contents SSE	NSE	LAI SSE	NSE	ETA SSE	NSE
LEACHN	Compromise F_1, F_3	2.62	0.24	–	–	1.54	0.08
	Compromise F_1, F_2, F_3	2.62	0.24	1.53	0.88	1.54	0.08
CERES	Compromise F_1, F_3	5.10	–0.49	–	–	1.55	0.07
	Compromise F_1, F_2, F_3	5.10	–0.49	2.01	0.84	1.55	0.07
SPASS	Compromise F_1, F_3	1.38	0.60	–	–	0.44	0.74
	Compromise F_1, F_2, F_3	1.80	0.47	2.23	0.82	0.63	0.62
GECROS	Compromise F_1, F_3	0.84	0.75	–	–	0.65	0.61
	Compromise F_1, F_2, F_3	0.84	0.75	33.02	–1.70	0.65	0.61

SUMMARY AND CONCLUSIONS

With our proposed multiobjective parameter calibration method, parameter sets could be found for most models that yield a satisfactory match to observations of single data types. However, the trade-off in the fitting of soil moisture and evapotranspiration data can be quite large, particularly for the LEACHN and CERES models. The mechanistic models SPASS and GECROS are superior in this respect and exhibit the smallest possible trade-off between the different objective functions. Our results confirm that a better simultaneous representation of the fluxes of water, heat and nutrients through the coupled soil–plant–atmosphere system can be gained by using mechanistic models, but only if the level of complexity of the individual plant-sub modules and the soil water transport model is sufficient and consistent with the other sub-modules.

Our Pareto analysis demonstrates the presence of significant model structural inadequacies. The GECROS model, for example, provides an adequate fit to the soil moisture and evapotranspiration data but at the expense of a significant overestimation of biomass production. The simplest model LEACHN performance is acceptable only if plant development data are readily available to the user and provided as input to the model. This limits the predictive ability of the model as this type of data is often not easily available.

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