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Sensitivity and predictive uncertainty of the ACASA model at a spruce forest site

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Abstract

The sensitivity and predictive uncertainty of the Advanced Canopy-Atmosphere-Soil Algorithm (ACASA) was assessed by employing the Generalized Likelihood Uncertainty Estimation (GLUE) method. ACASA is a stand-scale, multi-layer soil-vegetation-atmosphere transfer model that incorporates a third order closure method to simulate the turbulent exchange of energy and matter within and above the canopy. Fluxes simulated by the model were compared to sensible and latent heat fluxes as well as the net ecosystem exchange measured by an eddy-covariance system above the spruce canopy at the FLUXNET-station Waldstein-Weidenbrunnen in the Fichtelgebirge Mountains in Germany. From each of the intensive observation periods carried out within the EGER project (ExchanGE processes in mountainous Regions) in autumn 2007 and summer 2008, five days of flux measurements were selected. A large number (20 000) of model runs using randomly generated parameter sets were performed and goodness of fit measures for all fluxes for each of these runs calculated. The 10% best model runs for each flux were used for further investigation of the sensitivity of the fluxes to parameter values and to calculate uncertainty bounds.

A strong sensitivity of the individual fluxes to a few parameters was observed, such as the leaf area index. However, the sensitivity analysis also revealed the equifinality of many parameters in the ACASA model for the investigated periods. The analysis of two time periods, each representing different meteorological conditions, provided an insight into the seasonal variation of parameter sensitivity. The calculated uncertainty bounds demonstrated that all fluxes were well reproduced by the ACASA model. In general, uncertainty bounds encompass measured values better when these are conditioned on the respective individual flux only and not on all three fluxes concurrently. Structural weaknesses of the ACASA model concerning the soil respiration calculations were detected and improvements suggested.

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1 Introduction

The exchange of energy and matter between the ground and the atmosphere is an important process within an ecosystem and influences its meteorological, hydrological and ecological properties. To model this exchange process and the corresponding sensible and latent heat fluxes as well as the CO₂ flux, soil-vegetation-atmosphere transfer (SVAT) models have been developed. Due to the large variety of model scopes, SVAT models differ greatly in their complexity (Falge et al., 2005). Simpler model representations, so called “big leaf” models (e.g., Sellers et al., 1996), are applied when aiming for larger temporal and spatial scales, such as in land surface schemes of climate models. Within these models, the vegetation is depicted as one “big leaf” which represents the properties of the whole canopy and therefore is described with “effective” parameters. In multilayer SVAT models (e.g., Wohlfahrt et al., 2001; Baldocchi and Meyers, 1998), the emphasis is placed on a more detailed description of canopy processes and thus the vegetation is represented with more than one layer. Such SVAT models incorporate a large number of process descriptions varying in complexity, such as radiative transfer or photosynthesis schemes.

SVAT models can also be classified based on their implementation of turbulent transfer within and above the canopy. The most common turbulence closure is the first-order flux-gradient closure or *K*-theory. Here, fluxes of a meteorological variable are calculated from the gradients of the mean of this variable and an exchange coefficient *K*. This simple closure scheme works well in representing the turbulent exchange above short canopies, but is limited in the correct reproduction of the turbulence structure inside tall canopies such as forests (e.g., Shaw, 1977; Denmead and Bradley, 1985). Higher-order closure schemes have been developed to adequately simulate the turbulent structure and permit the simulation of second moments inside tall canopies. Second-order closure was proposed by Wilson and Shaw (1977) and Wilson (1988) and a third-order closure was developed by Meyers and Paw U (1986), which was successfully coupled to leaf energy balance equations and a radiative transfer model

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(Meyers and Paw U, 1987). Comparisons of these closure schemes found a similar performance of second- and third-order closure for wind speed and scalar concentration profiles as well as fluxes (Katul and Albertson, 1998; Juang et al., 2008). However, both closure schemes failed in reproducing the third moments close to the canopy-atmosphere interface.

All SVAT models, even the ones with less complexity, require a large number of model parameters to be specified by the user, such as morphological and optical properties of the vegetation or physical properties of the soil. The more processes that are explicitly described in a SVAT model, the more parameters are needed. These parameters are often not easily determined, as the scale at which they are measured in the field varies, such as the leaf scale for photosynthesis parameters and the stand scale for plant morphological parameters.

When calibrating SVAT schemes against (eddy) flux measurements at high temporal resolution, the problem of model equifinality has been reported (Franks et al., 1997; Mo and Beven, 2004; Prihodko et al., 2008; Schulz et al., 2001). In all these studies, there was not a single optimum parameter set but rather many different sets of parameters that gave equally good fits to the observed data and were from physically feasible ranges. The Generalized Likelihood Uncertainty Estimation (GLUE) methodology (Beven and Binley, 1992) addresses the problem of parameter equifinality and assesses the predictive uncertainty of a model from the runs that are classified as “behavioral”. This method has been frequently applied in hydrological modeling, especially in run-off modeling (e.g., Beven and Freer, 2001; Freer et al., 1996; Choi and Beven, 2007), but was also employed in other model applications such as the estimation of critical loads (Zak and Beven, 1999) and the simulation of the nitrogen budget (Schulz et al., 1999), as well as the analysis of ground heat flux calculation approaches (Liebethal et al., 2005). The GLUE methodology is also well suited to the analysis of SVAT-models (Franks et al., 1997; Franks et al., 1999; Mitchell et al., 2009; Mo and Beven, 2004; Prihodko et al., 2008; Schulz and Beven, 2003; Schulz et al., 2001; Poyatos et al., 2007). In a study comparing uncertainty analysis techniques for a

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Within this sensitivity study, five days from each IOP that were chosen due to the good weather conditions and the good performance of the measuring devices were considered (IOP-1: 20–24 September 2007, day of year 263–267; IOP-2: 28 June–2 July 2008, day of year 180–184). IOP-1 was carried out during a relatively wet and cool autumn, whereas during IOP-2 hot and dry summer weather prevailed, which allows us to investigate different meteorological periods. The meteorological conditions during the two five-day periods are shown in Fig. 2. During IOP-1, global radiation, temperature and vapor pressure deficit were lower than during IOP-2. The wind speed reached comparable magnitudes during both IOPs. Soil conditions differed greatly during both IOPs, with a colder and wetter soil during IOP-1.

2.3 The ACASA model

The Advanced Canopy-Atmosphere-Soil Algorithm (ACASA, Pyles, 2000; Pyles et al., 2000), which was developed at the University of California, Davis, was used to model the turbulent fluxes of heat, water vapor and CO₂ within and above the canopy. This multi-layer canopy-surface-layer model incorporates a diabatic, third-order closure method to calculate turbulent transfer within and above the canopy on the theoretical basis of the work of Meyers and Paw U (1986, 1987). The multi-layer structure of ACASA is reflected in 20 atmospheric layers evenly distributed between the canopy and the air above extending to twice the canopy height, and in 15 soil layers. Leaf, stem and soil surface temperatures are calculated using the fourth-order polynomial of Paw U and Gao (1988), allowing the calculation of temperatures of these components where these may deviate significantly from ambient air temperatures. Energy flux estimates consider multiple leaf-angle classes and direct as well as diffuse radiation absorption, reflection, transmission and emission. Plant physiological response to micro-environmental conditions is calculated by a combination of the Ball-Berry stomatal conductance (Leuning, 1990; Collatz et al., 1991) and the Farquhar and von Caemmerer (1982) photosynthesis equation following Su et al. (1996). The soil module used to calculate soil surface evaporation, soil moisture, and soil temperature is adapted

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from MAPS (Mesoscale Analysis and Prediction System; Smirnova et al., 1997, 2000). Additionally, canopy heat storage and canopy interception of precipitation are included in ACASA.

The model was adapted from a version from October 2009. The model source code was modified in two parts. The first change concerns the soil respiration calculations. A soil moisture attenuation factor that is meant to reduce microbial soil respiration when soil moisture falls below the wilting point soil moisture was disabled in this study, as it not only reduced soil microbial respiration during dry periods but also enhanced respiration rates to unreasonably high values during wet periods, a finding that is consistent with Isaac et al. (2007). As in the original ACASA version, respiration R_T at temperature T_s is calculated with an Arrhenius type equation with basal respiration rate R_0 at 0 °C and the Q_{10} as input parameters (e.g., Hamilton et al., 2001):

$$R_T = R_0 \cdot \exp(0.1 \cdot T_s \cdot \ln(Q_{10})) \quad (1)$$

Here, R_0 is given in ($\mu\text{mol m}^{-2} \text{s}^{-1}$), based on the surface area of the roots or microbes. Soil respiration is simulated for microbes and roots separately, using Eq. (1), and summed up to form the total soil respiration. Each of the two components is the sum of the respective respiration contributions from the 15 soil layers, weighted by the root fractions of these layers. To obtain the total soil respiration per ground surface area, it is assumed that the sum of the total root and microbe surface area resemble the leaf area index.

The second change in the source code was made within the plant physiology sub models in the calculation of photosynthesis. The temperature dependence of the maximum catalytic activity of Rubisco at saturated ribulose biphosphate (RuBP) and saturated CO₂, $V_{c\text{max}}$ ($\mu\text{mol m}^{-2} \text{s}^{-1}$) follows a third-order polynomial given by Kirschbaum and Farquhar (1984), which was derived from measurements made in a temperature range of 15 to 32 °C. For temperatures below 10 °C this third-order polynomial results in an unrealistic increase of $V_{c\text{max}}$, as was already noticed by Leuning (1997). As temperatures of less than 10 °C are very common at our site, the third-order polynomial was

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heat fluxes. Whereas for the NEE for both IOPs the behavioral parameter sets contain more values from the upper half of the parameter range, the cumulative frequency curves for the other two fluxes suggest optimal parameter values from the lower half of the parameter ranges, with a much stronger response for IOP-2, where values are completely confined to the lower half of the parameter range.

To quantify whether the distribution of parameter values for the 10% best model runs follows the uniform distribution or not, and thus to identify the parameters the model is sensitive to and to list these parameters in order of importance, the Kolmogorov-Smirnov test was performed. Table 4 gives an overview of the sensitive model parameters for the respective fluxes according to the Kolmogorov-Smirnov test for IOP-1 and IOP-2.

There was a difference in the number of sensitive parameters between the two IOPs with a larger number of sensitive parameters for NEE for IOP-1 than for IOP-2 and a larger number of sensitive parameters for the combined fluxes for IOP-2 than for IOP-1.

As the *lai* appears as the first or one of the first parameters in the parameter rankings for all fluxes, the importance of this parameter as one of the most influential parameters is illustrated once more. The other two plant morphological parameters, the canopy height, *hc*, and the mean leaf diameter, *xldiam*, are not listed among the influential parameters. The leaf drag coefficient, *drx*, used in the third order closure turbulence subroutines only appears in the parameter rankings for the sensible heat flux.

Also among the most influential parameters for all fluxes are the parameters determining leaf respiration, with the leaf basal respiration rate, *r0l*, and the Q_{10} of leaf respiration, *q10l*. The parameters for stem respiration (*r0s*, *q10s*) do not appear in the parameter rankings, whereas the parameters for root and microbial respiration (*r0r*, *q10r*, *r0m*, *q10m*) are listed amongst the most influential parameters for the NEE and also appear for the combined fluxes. Radiation parameters (*pr0*, *pv0*, *tr0*, *tv0*) only appear for IOP-1, with the sensible heat flux being sensitive to *pr0* and *pv0*.

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The parameters of the photosynthesis and stomatal conductance subroutines contribute to the ranked parameters in roughly the same proportion as they do to the overall number of investigated parameters for the sensible heat flux and the NEE, but in a larger proportion for the latent heat flux and in a smaller proportion for the combined fluxes. Of the parameters that determine the temperature dependence of the maximum catalytic activity of Rubisco V_{cmax} , only the maximum rate of carboxylation, *vcmax25*, appears to be influential for the NEE for IOP-1. The corresponding activation energy, *eavc*, does not appear in the parameter rankings. The picture for the maximum rate of whole-chain electron transport at saturated light J_{max} is different, with the potential rate of electron transport at 25 °C, *jmax25*, appearing as an influential parameter for the NEE for both IOPs and the latent heat flux for IOP-1, and the activation energy, *ejmax*, appearing also for NEE for IOP-1.

The radiation dependence of the potential rate of whole-chain electron transport is affected by the curvature factor, *theta0*, and the quantum efficiency, *iqe*, with the latter being influential for all fluxes except the combined fluxes, and the former not being influential for any flux. The slope of the Ball-Berry formula, *cm*, to calculate stomatal conductance appears for all fluxes and the combined fluxes as the first or one of the first parameters, thus as one of the most influential parameters. In contrast, the second parameter in the Ball-Berry formula, its intercept *cb*, only appears for the sensible and latent heat fluxes in IOP-2 in combination with *cm*.

3.3 Model uncertainty

Predictive uncertainty bounds were calculated for each flux for the individual best 10% model runs and the model runs resulting from the combination of all three likelihood measures for both IOPs (Figs. 7 and 8). Table 5 lists the percentage of observations that are enclosed by the uncertainty bounds and those that lie without. In general, the calculated uncertainty bounds capture the measured values for all three fluxes reasonably well. The narrowest uncertainty bounds were observed for the sensible heat flux. Maximum daytime values as well as night-time values were simulated by the model

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number and ranking of influential parameters (Table 4) consequently varies for the two time periods, indicating the need to seasonally adjust several parameter values. But as only two short periods are considered here, such recommendations are of limited justifiability. In order to draw general conclusions about the seasonality of parameters and to cover all relevant processes, it is necessary to include much longer time periods with a larger meteorological variability, as was done by Prihodko et al. (2008). An extension of the time period studied was also suggested as a possible solution to the parameter equifinality problem by Schulz et al. (2001).

Our findings of parameters that appeared to be influential in our sensitivity analysis revealed similarities with results from other sensitivity studies or studies that used inversion methods for parameter estimation. Even though other models – including different process descriptions and thus different parameters investigated – were analysed, stomatal parameters were also among the most sensitive or best constrained parameters (Mitchell et al., 2009; Prihodko et al., 2008; Knorr and Kattge, 2005). Wang et al. (2001) included the slope of the Ball-Berry formula in their parameter estimation, whereas all fluxes proved to be insensitive to the intercept of the Ball-Berry formula. Our observations revealed a similar result, with the slope of the Ball-Berry formula being among the most influential parameters and its intercept being not influential for any flux. Furthermore, the parameter inversion performed by Knorr and Kattge (2005) found that amongst the photosynthesis parameters most information was gained for quantum efficiency and maximum carboxylation rate. We found quantum efficiency to be an influential parameter; however, maximum carboxylation rate was less influential. As in our study, strong sensitivity to the leaf area index was found by Mitchell et al. (2009).

The sensitivity to parameter values for the three studied fluxes was not the same for all parameters. There was a very similar response for all three fluxes to some parameters (e.g. lai for IOP-2, Fig. 3), whereas other parameters were only influential for one flux (e.g. r0m for the NEE, Fig. 5). But the sensitivity of the latent heat flux and the NEE to some plant physiology parameters (cm, iqe, jmax25) was even opposite,

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with cumulative frequency plots indicating optimal parameter values from the lower part of the parameter range for one flux and from the upper part of the parameter range for the other flux (e.g. iqe in Fig. 5). Thus, difficulties arise when trying to deduce optimal parameter values from the results of this study, and the model user has to decide in favor of either the latent heat flux or the NEE. The sensible heat flux either showed a response similar to that of the latent heat flux or was not sensitive to the respective parameter.

A complex process-based model like ACASA requires a large number of input parameters. In this study, 24 parameters were of interest and concurrently varied to create 20 000 random parameter sets, which is very few with regard to the number of parameters. A much larger number of parameter sets would be required to sample the whole range of variation in combinations of parameters, which would hardly be realizable due to the large computational power required. However, as with Prihodko et al. (2008), who had an even larger number of parameters, we expect that an important range of the parameter space is already covered by 20 000 model runs.

In order to not only cover a larger range of variation in combinations of parameters but also to reduce the problem of parameter equifinality, the results of the present GLUE analysis could be used to fix relatively insensitive parameter values, to constrain parameter ranges and to improve the model structure for a subsequent GLUE analysis (Prihodko et al., 2008). Alternatively, Schulz et al. (2001) not only suggest prescribing as many parameter values as possible using measurements to reduce the degrees of freedom, but also mention the gap between scales of measured parameters and parameters needed to run models. For the photosynthesis parameters, this is especially evident, where parameters of the gas exchange response of a few sample leaves is used as average leaf parameterization of the entire stand.

4.2 Identification of structural weaknesses of the model

As noted before, results of an analysis following the GLUE methodology are always conditional on the model input data, the parameter sets, the observations and the

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choice of likelihood measure (Beven and Freer, 2001). Therefore, it is difficult to determine whether the observed errors are the result of structural weaknesses of the model or errors in the input data or the observations. Nevertheless, Mitchell et al. (2009) demonstrated how to use a GLUE study to detect problems in model structure. Our analysis also revealed indications to structural weaknesses, such as in the soil respiration calculations of the model, which will be discussed in the following.

For the NEE, the basal respiration rates for the soil and the leaves as well as the lai are the most influential parameters for both IOPs. On the one hand, this could suggest respiration as the most important process for the CO₂ exchange within the ACASA model, but on the other hand could also be caused by an inappropriate choice of parameter ranges, as the results are conditional on all the subjective choices concerning likelihood measures, rejection criteria and parameter ranges. The equations governing the soil respiration calculations were introduced in Chap. 2.3, with the basal soil respiration rates r_{0r} and r_{0m} being defined per root area and per microbial surface area, respectively. The sum of the root and microbial surface areas are, in turn, assumed to be equal to the lai value. Thus, the effective basal respiration rate for the soil strongly depends on the lai, and an interaction of these two parameters is expected. The scatter plot of the parameters basal respiration rate of the roots, r_{0r} , versus the leaf area index, lai, for coefficients of efficiency for the NEE larger than 0.6 confirms this assumption (Fig. 9). The effective basal respiration rate for the roots ($r_{0r} \cdot lai$) for most model runs was between 0.2 and $2 \mu\text{mol m}^{-2} \text{s}^{-1}$, which encompasses values measured for spruce sites (0.65 to $1.16 \mu\text{mol m}^{-2} \text{s}^{-1}$, references see Table 2). Figure 9 also illustrates that the parameter ranges as chosen result in a very large possible range for the effective basal respiration rate, which leads to very large and inappropriate root respiration for combinations of large r_{0r} and large lai, dominating the NEE and leading to low model performances.

Measurements of the ratio of root area to leaf area are scarce, and do not necessarily find values close to 0.5. Even though a value close to unity was found for some sites, such as old-growth beech stands in Germany reported by Leuschner et al. (2004),

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there were variations of this ratio observed, for example variations with age for young eucalyptus trees (O'Grady et al., 2006) and with elevation within a tropical mountain forest in Ecuador (Röderstein, 2006). We therefore suggest using the basal root respiration rate based on the soil surface as it is measured at many sites, rather than assuming a root respiration rate based on root surface and assuming the root surface as being equal to the lai. Such a reduction of complexity, even though it only concerns one sub model, could help to reduce the problem of parameter equifinality, as suggested by Schulz et al. (2001) and Franks et al. (1997).

4.3 Predictive uncertainty of the modeled fluxes

The ACASA model was capable of reproducing all fluxes reasonably well as reflected by the uncertainty bounds in Figs. 7 and 8. For the latent heat flux, maximum daily values were not captured by the model for IOP-1. For the first days, this underestimation can probably be attributed to evaporation from interception due to a rainy period before day 263, which was not included in the simulation period and therefore cannot be adequately represented by the model. During each of the IOPs there was one night where measured fluxes behaved differently than during all other nights, with all fluxes being close to zero (night 265/266 for IOP-1 and night 181/182 for IOP-2). This divergent behavior was not simulated by ACASA. Instead, the modeled fluxes during these nights were comparable in magnitude to the fluxes of the other nights. During these two nights measured wind speeds were much lower (Fig. 2), stabilities higher and friction velocities smaller than during the other nights, indicating decoupling of the canopy and the air above. Close to the soil surface, decoupling was also observed during these periods (Riederer, 2009). The ACASA model is probably not capable of representing this process and therefore overestimates the fluxes above the canopy during periods of strong decoupling.

It is suspected, or at least hoped, that a parameter set that achieves good results for one flux would also achieve good results for the other fluxes, as the aim of SVAT models is usually to represent all fluxes well. The comparison of the single-objective and

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Table 1. Meteorological input parameters of the ACASA model and the corresponding measurements at the Waldstein-Weidenbrunnen site.

Parameter	Unit	Sampling location	Sampling height (m)	Instrument, Manufacturer
Precipitation rate	mm	Clearing	1	OMC 212, Adolf Thies GmbH & Co. KG
Specific humidity	g kg ⁻¹	Main tower	31	Vent. psychrometer (Frankenberger, 1951), Theodor Friedrichs & Co
Mean wind speed	m s ⁻¹	Main tower	31	Cup anemometer, Theodor Friedrichs & Co
Downwelling short-wave radiation	W m ⁻²	Main tower	30	CM14, Kipp & Zonen
Downwelling long-wave radiation	W m ⁻²	Main tower	30	CG2, Kipp & Zonen
Temperature	K	Main tower	31	Vent. psychrometer (Frankenberger, 1951), Theodor Friedrichs & Co
Pressure	hPa	Clearing	2	Barometric pressure sensor, Ammonit Gesellschaft für Messtechnik mbH
CO ₂ concentration	ppm	Main tower	32	LI-7000, LI.COR Biosciences GmbH

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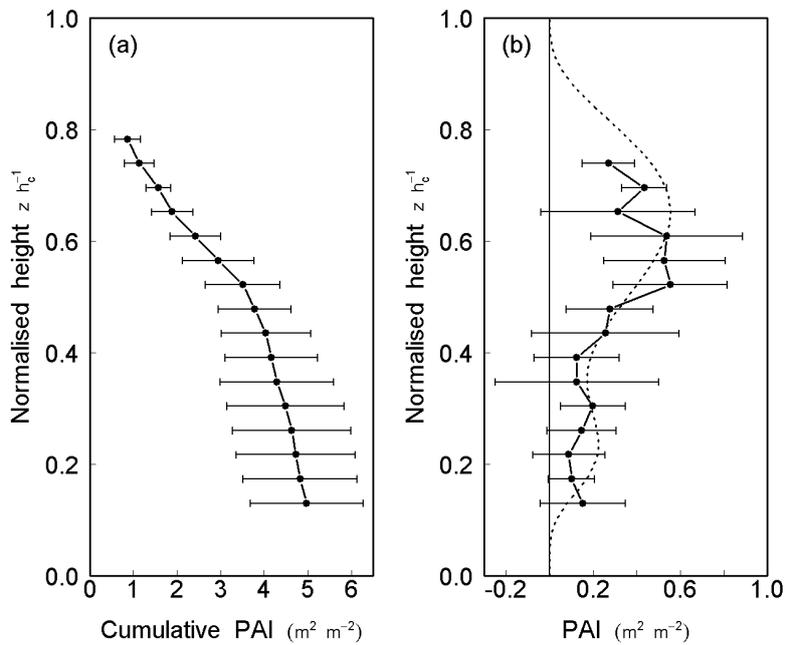


Fig. 1. Vertical profiles of the cumulative **(a)** and absolute **(b)** plant area index (PAI) at the Waldstein-Weidenbrunnen site (May 2008, Foken et al., 2010). Profiles are mean values of five measured PAI profiles with the corresponding standard deviations indicated. The dashed line in **(b)** represents the fitted PAI profile for the ACASA model (weighted sum of two beta distributions fitted to the measured data following Simon et al., 2005, 101 data points).

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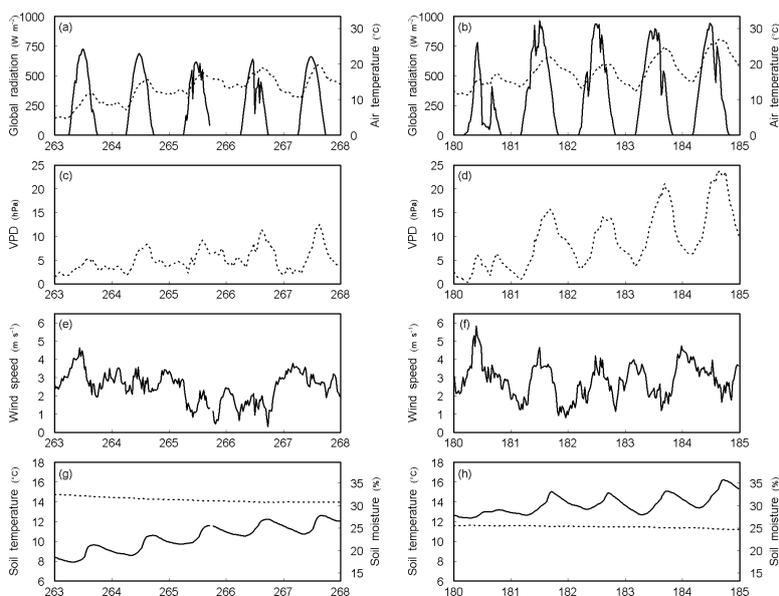


Fig. 2. Meteorological conditions during the two five day periods (left: IOP-1, right: IOP-2). **(a and b)**: Global radiation (solid line) and air temperature (dotted line) above the canopy (30 m and 31 m). **(c and d)**: Vapor pressure deficit above the canopy (31 m). **(e and f)**: Wind speed above the canopy (31 m). **(g and h)**: Soil temperature (solid line) and soil moisture (dotted line) at 10 cm depth.

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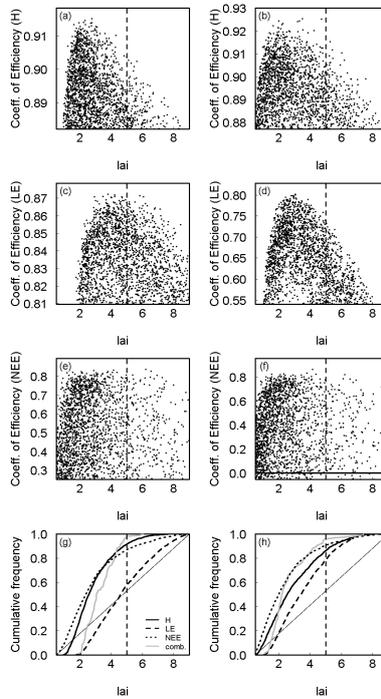


Fig. 3. Sensitivity graphs showing the range of the single-objective coefficients of efficiency for the best 10 percent parameter sets (left: IOP-1, right: IOP-2) for the sensible (H, **a** and **b**) and latent (LE, **c** and **d**) heat flux and the NEE (**e** and **f**) across the range of the leaf area index, lai [$\text{m}^2 \text{m}^{-2}$]. The vertical dashed line denotes the reference parameter value. Cumulative frequencies are plotted in (**g** and **h**) for the three fluxes as well as for the combined likelihood measure with the diagonal solid line showing a uniform parameter distribution for comparison.

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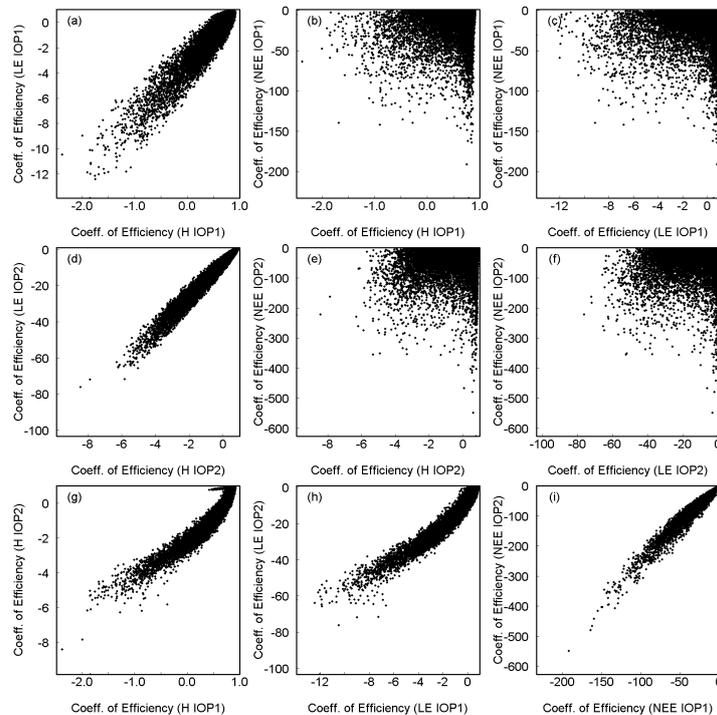


Fig. 4. Scatter plots of the coefficients of efficiency for the three fluxes. Each dot represents one parameter set. (**a–c**): Individual coefficients of efficiency for IOP-1 compared to each other. (**d–f**): Same as (**a–c**) but for IOP-2. (**g–i**): For each flux, coefficients of efficiency compared for the two IOPs. Note the differences in the axis ranges.

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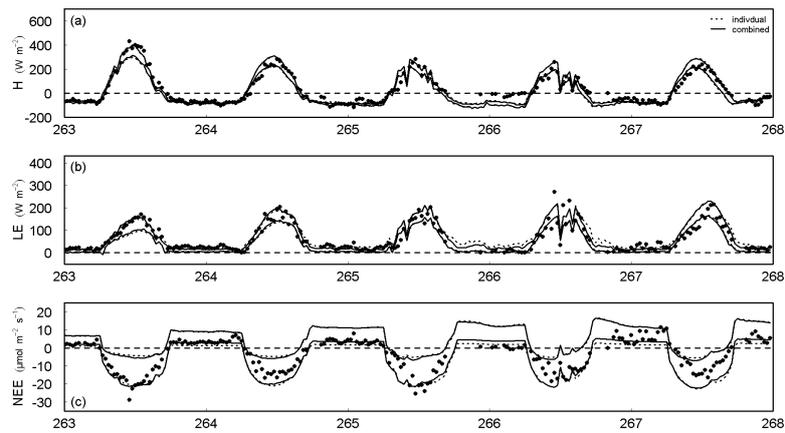


Fig. 7. Predictive uncertainty bounds (5th and 95th quantile) and observed values (black dots) for the sensible heat flux (H , **a**), the latent heat flux (LE , **b**) and the net ecosystem exchange (NEE , **c**) for the coefficient of efficiency (IOP-1, dotted lines: individual best 10%, solid lines: combined).

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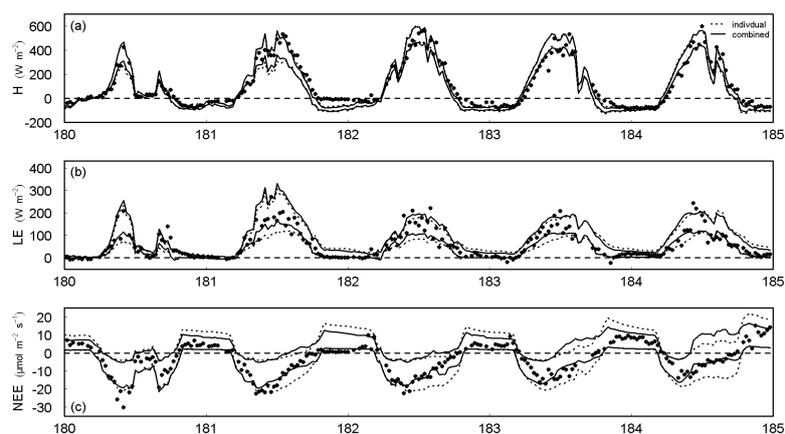


Fig. 8. Predictive uncertainty bounds (5th and 95th quantile) and observed values (black dots) for the sensible heat flux (H , **a**), the latent heat flux (LE , **b**) and the net ecosystem exchange (NEE , **c**) for the coefficient of efficiency (IOP-2, dotted lines: individual best 10%, solid lines: combined).

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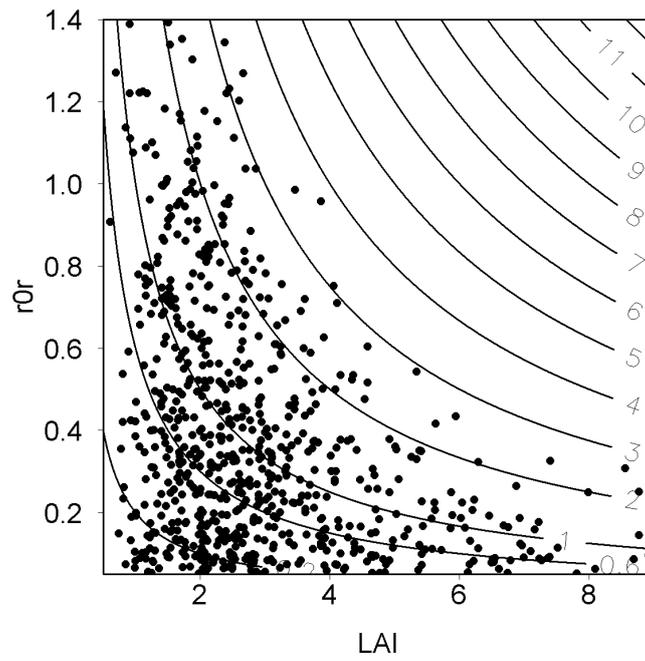


Fig. 9. Scatter plot of root basal respiration rate at 0°C, r_{0r} [$\mu\text{mol m}^{-2} \text{s}^{-1}$], vs. leaf area index, lai [$\text{m}^2 \text{m}^{-2}$], for model runs that achieved a coefficient of efficiency of better than 0.6 for the NEE. Contours indicate the effective root basal respiration rate at 0°C [$\mu\text{mol m}^{-2} \text{s}^{-1}$] ($r_{0r} \cdot \text{lai}$).