

Dear Christoph Müller,

Thank you for handling the review process. We received a good set of comments from the reviewers and we have addressed almost all in the text. Below we detail all the changes we made to the manuscript in response to each of the reviewer's comments. We also made a number of minor corrections to the manuscript to improve readability. We won't detail all those but you can see them in the marked up version of the manuscript. We are confident these changes have improved the manuscript substantially.

Sincerely,
Matthew Smith (on behalf of the authors)

Response to Reviewer 1 comments

Comment from reviewer 1: "A first criticism is that there seems to be some ambiguity about the exact objective of the predictions. In the introduction the authors speak of application to a "generic farm location", whereas evaluation is based on comparison with regional yields. Prediction for a farm, with uniform management, is quite different than prediction for a region. The paper seems more oriented toward regional prediction, since county yields are one of the data sets used as input and are also used for evaluation. On the other hand, the landcover input data was aggregated to 3km by 3 km pixels, which is generally intermediate between farm and county scale. In any case, it is essential to clarify the spatial scale of interest."

Response from Authors 1: The model is intended, in an ideal situation, to be used at the local scale. However, given the lack of availability of the data, particularly the yield information, this is difficult. The model as applied here is indeed at an intermediate scale, as the eddy flux data is always field scale, while the crop yield is regional. We agree that this discrepancy between the different spatial scales in the data has not been discussed sufficiently and we have now added this to the discussion.

Change to Manuscript 1: We have added to the end of the introduction a clarifying statement about the scale of application, such as

"While our study is part of a broader scientific objective to enable more accurate field scale predictions, the lack of availability of field scale datasets to train and validate our model means that the scale of model evaluation for our study here is a mix of field (flux tower) and regional scales (county and country level for yield estimates and 3 by 3 km scale for photosynthetic activity)."

And added a dedicated paragraph to the discussion about this issue

"One additional complication is the different spatial scales of the three datasets - while the eddy covariance data is at the scale of the flux tower footprint, which can be seen as equivalent to the individual field scale, the fAPAR and yield data correspond to larger scales (county and country level for the yield data and a 3 by 3 km scale for the fAPAR data). The assumption behind our analysis is that the conditions at field scale are representative of the regional scale, so that there would be no discrepancy between model predictions at these different scales. This is obviously a source of error, especially at the wheat sites in Europe,

which will be located over a much more heterogeneous landscape. Further sources of data at the field scale would be required to identify the model error caused by the discrepancy in spatial scales.”

Comment from Reviewer 2: “Much of the evaluation is based on comparing the model using data constrained parameters to the model with prior parameters. This is not a very interesting comparison. The prior parameters were chosen quite arbitrarily by the authors to represent essentially a total lack of information about the parameter values. The fact that adding some information improves the situation is hardly surprising.”

Response from Authors 2: This is indeed a not very surprising result. However, we have chosen the model with prior parameters as a benchmark as this offers a worst case scenario of parameter values and can be used to show relative improvement in model error and uncertainty when using the different datasets.

Change to Manuscript 2: We have included a statement in the introduction to reflect on the fact that we fully expect data constraining the model to improve predictive accuracy but that we’re more interested in how much the predictions are improved. We insert just after we state the paper aims:

“We expect the qualitative answer to the first question to be that utilising empirical data does enable the model to make better predictions because that’s a typical outcome of our parameter estimation approach. However we are more interested in the quantitative answer; i.e. how much? For example, the generation of a model that could make extremely precise and accurate predictions would suggest that data-constraining general models with the datasets we identify could provide an extremely useful tools for agricultural predictions and forecasts. Alternatively, the generation of a model that makes very imprecise predictions would suggest that more data collection and model improvement is needed for the model to have practical applications.”

Comment from Reviewer 3: “A much more relevant comparison would be between the data constrained model and long term average county yields. Does the model do better than simply assuming that the future is like the average of the past? This is analogous to comparing climate forecasts with climatology.

Response from Authors 3: This is a very good idea, however, we consider that such a comparison with long terms yields is premature. We have not performed this analysis two reasons: inadequate data and the mix of spatial scales. As mentioned our ultimate objective is to enable better field scale predictions, however the only field scale data we have, the flux datasets, typically only cover one year and different sites cover different years. This makes comparing model predictions to a data average for one site almost meaningless. Our other datasets do have longer, more complete time series. The fAPAR time series reflects vegetation dynamics over a wider spatial area of vegetation than an individual field, including non-agricultural vegetation and so itself is only a coarse indicator of field level dynamics - we are therefore not interested in how well the model captures the complete seasonal dynamics of that dataset. It would be interesting to understand whether a model such as that developed here can outperform historical data at predicting large scale yield variations. This should be dealt with in a dedicated future piece of work because a number of other analyses

should be conducted alongside such a comparison to make it insightful. For example we currently do not account for variations in environmental drivers and agricultural practices at smaller spatial scales across a region that would also help to explain yield variations observed at the larger spatial scales. These could be accounted for by simulating our model for every relevant field within the region and aggregating the predictions. A dedicated comparison of the predictions of our model with those of statistical averages over historical data is a natural avenue for future research.

Change to Manuscript 3: We thought hard about how to implement this request but, as explained above, evaluation for each dataset raises further issues. We therefore decided to defer this comparison to another study, ideally one in which our model can be trained and evaluated against a richer dataset of location specific data. We include a brief statement in the discussion (under future data needs) stating

“If this model, or any other similar process-based data constrained crop model, is to be used for scientific purposes to understand the response of crops to climate across the globe, the ideal data would be a global data set, such as space-based vegetation observations, combined with high quality field level data that would ideally include growth timeseries, final grain yield and information about agricultural practices. However, if the model is to be used for agricultural purposes, to aid decision making at the local level, high quality field level data would be sufficient. An valuable evaluation in such studies, not conducted here for brevity and due to a lack of location-specific data, would be to compare the predictive accuracy of the model against the predictive accuracy of a statistical average over the data. Such an analysis would reveal whether and how much benefit is gained by using a data constrained model for predictions”

Comment from Reviewer 4: “Another aspect of the evaluation is that uncertainty intervals are given for each prediction. This is extremely informative and pertinent, and is a very valuable addition to the comparison between the mean prediction and observed values. However, the uncertainty results need to be discussed more thoroughly. For example, it seems that the 95% intervals for yield cover all historic yields at most sites (Fig. 3a). Surely this uncertainty is so large as to render the results useless. More discussion is required here.”

Response from Authors 4: We agree that the uncertainty in yield predictions is very large, making it largely unsuitable for predicting interannual variation in crop yields. However, as the reviewer also points out, the model parametrisation method presented in our paper has the advantage that it does provide an uncertainty estimate. Hence, any future improvements in model performance, especially through added sources of data are easily quantifiable.

Change to Manuscript 4: We have expanded an existing paragraph in the discussion to read

“Model uncertainty is difficult to compare with previous crop modelling studies, as models with fixed parameter values do not often provide uncertainty estimates. In fact, providing uncertainty values for all model variables and parameters is one of the advantages of a data constrained model. In the current model, uncertainty is highest at the start of the season for all variables but decreases rapidly and final yield uncertainty is much lower. This is due to thresholds: abrupt changes from one growing stage to another when small differences in parameters can lead to large differences in resulting variables. It is, however, important to note that the uncertainty in our yield predictions remains high and the model in its current

form is unlikely to provide accurate predictions for practical applications without the addition of new data (Section 7.4). We have however shown that the use of three different data types does reduce prediction uncertainty - pointing to an avenue for future model improvement.”

Comment from Reviewer 5: “The uncertainty calculations are based on propagating uncertainty in the parameter values through the model. It is not clear if residual error is included when calculating uncertainty intervals or not. It should be.”

Response from Authors 5: The model uncertainty is calculated by sampling parameters from the posterior distributions and then computing model predictions with the sampled parameters, which results in a distribution of model predictions from which we can calculate a predicted mean and confidence intervals. We realise that this was insufficiently well explained clearly in the paper.

Change to Manuscript 5: We have included a fuller explanation of how we propagate uncertainty in the parameter values of the model:

“To calculate uncertainty for the model predictions we sample parameter values from their respective posterior distribution and compute predictions with each parameter combination, which results in a corresponding distribution of model predictions. We report this prediction distribution uncertainty using 95th percent confidence intervals. This predicted distribution does not include the prescribed or inferred uncertainty about observations, $\sigma_{x,D}$, our predicted distributions correspond to the state being predicted and not the observations of that state.”

Comment from Reviewer 6: “Also, there are other sources of uncertainty than the parameters which might be quite important, in particular uncertainty about management practices. This should at least be discussed.”

Response from Authors 6: We agree and have changed the manuscript to reflect this.

Change to Manuscript 6: We have included include a discussion of model uncertainty related to management practices, in particular sowing and harvest dates as well as fertilizer input, such as

“In addition to the three datasets used for parametrisation, the model also requires input data in the form of sowing and harvest dates and fertiliser inputs. Additional uncertainty is associated with these datasets which is not available nor accounted for in our analyses. For example, the crop calendar (Sacks et al., 2010) and Nitrogen Fertilizer Application (Potter et al., 2010) datasets are global data collections that will imperfectly represent the value for any given location. Alternatives to these global datasets would be to use location-specific data, or to infer the values. Location specific data has the advantage of more accurately reflecting the situation at a given site and would therefore be useful when the model is applied at the field scale, but such data is unlikely to be available for all sites. Successful inference of the values would depend on if there is enough information in the datasets used to infer the model parameters. If there is inadequate data then there would be excessive degrees of freedom for inference, leading to the wrong parameter values begin inferred and the model performing poorly in novel situations. Therefore, the decision whether to obtain more data or infer

unknown quantities in future applications of our model and inference framework depends on the data availability and the intended scales of application.”

Comment from Reviewer 7: “It seems that the likelihood used here for the Bayesian estimation assumes that all data are independent. This is of course almost certainly false for time series data. Taking non independence into account by dividing by the number of measurements is only a very crude approximation.”

Response from Authors 7: The division by the number of measurements is not meant to account for non independence, rather it accounts for the different number of data points in each time series so that each dataset is given equal importance for fitting purposes. We agree that the timeseries data is most likely not independent but the independence assumption is often used when fitting models to eddy covariance flux data in order to simplify the formulation of the likelihood function.

Change to Manuscript 7: We have included the point made by the reviewer after we describe our Likelihood function.

“Note that with this definition of the likelihood we are treating every data point as independent, that is the likelihood of a value at time t , is treated independently from the likelihoods at preceding times. This is only an approximation but is commonly used in parameter estimation studies because the additional mathematical and computational complexity of accounting for non-independent data.”

Comment from Reviewer 8: “More detail about the model would be helpful. How exactly is the date of flowering calculated? According to the text, the switch from vegetative to reproductive growth occurs when increased vegetative fractions would not result in an overall increase in growth rate. Is this calculated day by day or is there some averaging over environmental conditions to ensure that the plant doesn't respond to conditions on one specific day?”

Response from Authors 8: The start of the reproductive growth is calculated using an average of environmental conditions for the peak carbon criteria. Due to the continuous decrease in soil N driven only by plant uptake and the relative simplicity of the model which does not take temperature and moisture into account for nutrient uptake, this averaging is not necessary for the peak N criteria.

Change to Manuscript 8: We now include a statement in the methods about this:

“The peak nitrogen condition is achieved when an increase in root mass does not result in an increase in nitrogen uptake. This condition is achieved in nitrogen limited environments where the nitrogen available in the soil is depleted through the period of vegetative growth. This assumption can be considered valid in agricultural systems where the major nitrogen input into the system during the growing period comes solely from agricultural fertilisers. Soil nitrogen decays monotonically through the season in our model due to the simplicity with which we model nitrogen uptake and so detecting the peak nitrogen condition is straightforward. Similarly, the peak carbon flowering condition is triggered when the addition

of aboveground biomass would not lead to an increase in net carbon gain, due to self-shading in the canopy. To calculate the peak carbon trigger we use the environmental variables averaged over p days, to avoid flowering being triggered by short-term environmental fluctuations. We infer p alongside the other parameters in our model.”

Comment from Reviewer 9: “What exactly are the management inputs required for the model? The authors mention sowing and harvest date, but aren't sowing density and fertilizer inputs also required? The required management information should be made clear, as well as the sources of this information.”

Response from Authors 9: This is correct, in addition to sowing and harvest dates, fertilizer input and planting density are also required, as well as irrigation regimes for future versions of the model which would take into account water limitation.

Change to Manuscript 9: We have included these details in the methods

“Fertilizer input data were obtained from the published site descriptions (see Table 1 for references) or from the Nitrogen Fertilizer Application database (Potter et al. 2010). The model implemented in this study does not require any additional information on irrigation or soil properties.”

Comment from Reviewer 10: “There is also no information on soils. Apparently this information is not needed here thanks to the assumptions that there is no water limitation, and that initial soil N is negligible compared to fertilizer N. In general, however, it will be necessary to have soil information.”

Response from Authors 10: Additional soil information would be essential for versions of the model that include water limitation and very important if the N uptake model was made more complex, for example if we included information about rooting depth or different forms of available nitrogen.

Change to Manuscript 10: We have included in the discussion:

“The model in the version presented in this paper does not include any water limitation to growth due mainly to a lack of data constraint on any water related parameters, as we found that latent heat data from EC towers is not sufficient. Below-ground measurements of not only root growth but also soil water properties would again provide some of the necessary information. Such belowground data, especially if supplemented by nutrient concentrations can also help constrain a more complex version of the nitrogen uptake scheme, which could be improved to include more explicit soil-plant interactions and additional processes such as biological nitrogen fixation for legumes.”

Comment from Reviewer 11: “The authors suggest that the model could be tested by comparing different model structures. Perhaps more useful would be to test the model proposed here with much more detailed input data, in order to reduce the data as a source of error and thereby isolate the amount of error due to the model.”

Response from Authors 11: Comparing different model structures and including better quality data are two different, but valid ways of identifying sources of error in our analysis and the two combined would give the most accurate analysis.

Change to Manuscript 11: We believe this point is already covered by one of the final statements in our Discussion

“If this model, or any other similar process-based data constrained crop model, is to be used for scientific purposes to understand the response of crops to climate across the globe, the ideal data would be a global data set, such as space-based vegetation observations, combined with high quality field level data that would ideally include growth timeseries, final grain yield and information about agricultural practices. However, if the model is to be used for agricultural purposes, to aid decision making at the local level, high quality field level data would be sufficient.”

Comment from Reviewer 12: “P7 L23-24. ``given the model" needs to be omitted”

Change to Manuscript 12: This has been corrected.

Response to Reviewer 2

Comment from Reviewer 1: “The extensive linkage to 'food security' is not necessary and the meaning of the own contribution overstated.”

Response from Authors 1: Since GMD is not a subject specific journal we find it is helpful to include the link to the bigger picture and clarify why improving agricultural models is important. The link to food security was the main reason why we undertook the research described in the manuscript.

Change to Manuscript 1: We have not removed our original framing of the study. However, in response to comments from the other reviewer, we have included more discussion on the lack of accuracy of our current model at predicting crop yields and the need for more research with more location-specific data

“Model uncertainty is difficult to compare with previous crop modelling studies, as models with fixed parameter values do not often provide uncertainty estimates. In fact, providing uncertainty values for all model variables and parameters is one of the advantages of a data constrained model. In the current model, uncertainty is highest at the start of the season for all variables but decreases rapidly and final yield uncertainty is much lower. This is due to thresholds: abrupt changes from one growing stage to another when small differences in parameters can lead to large differences in resulting variables. It is, however, important to note that the uncertainty in our yield predictions remains high and the model in its current form is unlikely to provide accurate predictions for practical applications without the addition of new data (Section 7.4). We have however shown that the use of three different data types does reduce prediction uncertainty - pointing to an avenue for future model improvement.”

and

“If this model, or any other similar process-based data constrained crop model, is to be used for scientific purposes to understand the response of crops to climate across the globe, the ideal data would be a global data set, such as space-based vegetation observations, combined with high quality field level data that would ideally include growth timeseries, final grain yield and information about agricultural practices. However, if the model is to be used for agricultural purposes, to aid decision making at the local level, high quality field level data would be sufficient. An valuable evaluation in such studies, not conducted here for brevity and due to a lack of location-specific data, would be to compare the predictive accuracy of the model against the predictive accuracy of a statistical average over the data. Such an analysis would reveal whether and how much benefit is gained by using a data constrained model for predictions”

Comment from Reviewer 2: “The use of categories is not convincing. How can statistical models be considered non-mathematical and process based models mathematical? (line 16-17).”

Response from Authors 2: The phrasing on lines 16-17 is indeed wrong. The process-based and statistical model separation is one that is commonly used not only for crop models but also in the field of earth system models and one that we find useful in explaining how process knowledge and data are used to obtain agricultural predictions.

Change to Manuscript 2: We have edited the confusing sentence to read

“Predicting and understanding how crops respond to changes in their environment through the use of mathematical models is needed to help address such threats, enabling advanced warning of potential threats and predictions of what alterations to agricultural practices might help prevent or mitigate problems.”

We then go on to explain in detail the difference between process-based and statistical models (both are mathematical!)

Comment from Reviewer 3: “The influence of the different data sources on parametrization is not considered. For example, the inclusion of farm yield data would necessarily imply that management effects influence the parametrization. This is similar to the parametrization of statistical models and should have been addressed in a different way on page 2 lines 30-35.

Response from Authors 3: The influence of different data sources on model parametrization is the main topic of our paper. management and field level information is required in process based models but not included explicitly in statistical models, as we discuss in the paragraph mentioned by the reviewer. Unfortunately the meaning of this comment is not entirely clear.

Change to Manuscript 3: we now include more details of where we got our data for fertilizer, sowing and harvest dates – an issue also raised by the other Reviewer.

“In addition to the three datasets used for parametrisation, the model also requires input data in the form of sowing and harvest dates and fertiliser inputs. Additional uncertainty is associated with these datasets which is not available nor accounted for in our analyses. For example, the crop calendar (Sacks et al., 2010) and Nitrogen Fertilizer Application (Potter et

al., 2010) datasets are global data collections that will imperfectly represent the value for any given location. Alternatives to these global datasets would be to use location-specific data, or to infer the values. Location specific data has the advantage of more accurately reflecting the situation at a given site and would therefore be useful when the model is applied at the field scale, but such data is unlikely to be available for all sites. Successful inference of the values would depend on if there is enough information in the datasets used to infer the model parameters. If there is inadequate data then there would be excessive degrees of freedom for inference, leading to the wrong parameter values being inferred and the model performing poorly in novel situations. Therefore, the decision whether to obtain more data or infer unknown quantities in future applications of our model and inference framework depends on the data availability and the intended scales of application.”

Comment from Reviewer 4: “The introduction ends with three valid research questions, however, the concrete model that will be used to address these questions remains open.”

Response from Authors 4: We have indicated in the introduction that we intend to introduce and use a new model.

Change to Manuscript 4: We have clarified in the introduction that we use a new model

“In this paper we present a newly developed general, non-crop specific process based model and use parameter inference to infer the most likely parameters for 15 locations for winter wheat and maize using a combination of space-based vegetation indices, eddy covariance flux data and reported agricultural yields.”

Comment from Reviewer 5: “The claim for a new model (page 5 line 15) adds surprising additional dimensions to the paper.”

Response from Authors 5: As we discussed in section 7.3, we chose to use a new model as it is more general and allows us to perform our analysis for multiple sites and species. We acknowledge that the use of this new model also has certain disadvantages and we mention this in the discussion.

Change to Manuscript 5: We have partially addressed this by mentioning that the model is new in the introduction. We also already cover the need to compare our model to others in the discussion

“Here we have chosen a given model structure and extensively tested the way in which constraining the parameters with different datasets in different configurations. The question that arises is to what extent the chosen model itself affects the present results. We have chosen a novel, physiology based model which includes plant optimality concepts, which on one hand has the advantage that it is more general than some of the older models and lacks artificially set thresholds between growth stages, but does have the disadvantage of being less thoroughly tested against field observations. An ideal companion paper to this study would be a comparison of different model structures with a constant data constraining framework, providing greater insights into which parts of the model lead to high errors or uncertainty. However, given the limitations of the current study, we acknowledge this limitation and

report most error metrics as relative to prior model runs in an attempt to isolate errors created by the data and model fitting from those caused by the model itself.”

Comment from Reviewer 6: “How was the soil variability parametrized?”

Response from Authors 6: As this is a very simple model at this stage the only soil information needed was nitrogen fertilizer application.

Change to Manuscript 6: At the suggestion of both reviewers we have added a discussion of any additional soil information needed for a more detailed model.

“The model in the version presented in this paper does not include any water limitation to growth due mainly to a lack of data constraint on any water related parameters, as we found that latent heat data from EC towers is not sufficient. Below-ground measurements of not only root growth but also soil water properties would again provide some of the necessary information. Such belowground data, especially if supplemented by nutrient concentrations can also help constrain a more complex version of the nitrogen uptake scheme, which could be improved to include more explicit soil-plant interactions and additional processes such as biological nitrogen fixation for legumes.”

Comment from Reviewer 7: “The original parameter values are not given and any validation results are missing.”

Response from Authors 7: As we explain in section 4 (Parameter estimation technique) we use a Bayesian fitting method which requires prior intervals for the parameter but not prior parameter values. As explained in section 5, the prior parameter values are randomly sampled from the prior parameter distribution in a manner similar to parameters being sampled from the posterior. The paper contains extensive model validation, in fact it contains little else. Figure 1 shows a comparison of prior and posterior model performance and figures in the appendix contain site level model-data comparison as the results of cross-site validation. Model validation is discussed extensively in both the results and discussion section.

Change to Manuscript 7: We have adjusted the aim statement in the paper to make clear that we are inferring our parameters

“In this paper we present a newly developed general, non-crop specific process based model and use parameter inference to infer the most likely parameters for 15 locations for winter wheat and maize using a combination of space-based vegetation indices, eddy covariance flux data and reported agricultural yields.”

Comment from Reviewer 8: “The assigned uncertainties for the given data sources are difficult to follow. A systematic reasoning for the chosen uncertainty values is missing.”

Response from Authors 8: A description of how we include data uncertainty in model fitting can be found in section 4. We acknowledge that this can be difficult to follow for those new to, or unfamiliar with, with Bayesian fitting methods and we will extend this description

Change to Manuscript 8: We have adjusted the paragraph on data uncertainty to read.

“We adopt different techniques to estimate the standard deviation $\sigma_{(x,D)}$ above, depending on the dataset D at each location. Generally, we assume that the variation in the model predictions about the data is solely due to uncertainty in the data. The GPP data do not have an estimate of uncertainty and so we infer the uncertainty associated with those data as the parameter $\sigma_{(x,D)}$. In the case of MODIS fAPAR data we explicitly incorporate a measure of variation in the data within the geographical area used to compute the mean fAPAR as well as inferring a parameter representing additional unexplained variation. We include this parameter to account for known issue in space based remotely sensed data, such as background soil reflectance. The crop yield data already have estimates of observational uncertainty associated with them and so we use those data to define $\sigma_{(x,D)}$.”

Comment from Reviewer 9: “The presentation of the results continues the deficits of the M&M section. It does not fulfill the existing standards.”

Response from Authors 9: We have presented our results in a manner common to model-data fusion studies.

Change to Manuscript 9: Without further explanation of the reviewer’s existing standards we cannot improve this section to their satisfaction.

Comment from Reviewer 10: “What was the quantitative propagation of the initial parameter setting?”

Response from Authors 10: As explained above, the fitting method does not require initial parameter settings and in any case it is not clear to us what propagation of parameter settings refers to. We have striven to offer a clear explanation of the Bayesian fitting method used in our study but given the length limitations of a scientific paper we found that a detailed explanation of the basics of model fitting methods was not feasible.

Change to Manuscript 10: As in our reply to the other reviewer, we have expanded on our methods paragraph describing how we propagate parameter uncertainty

“To calculate uncertainty for the model predictions we sample parameter values from their respective posterior distribution and compute predictions with each parameter combination, which results in a corresponding distribution of model predictions. We report this prediction distribution uncertainty using 95th percent confidence intervals. This predicted distribution does not include the prescribed or inferred uncertainty about observations, $\sigma_{x,D}$, our predicted distributions correspond to the state being predicted and not the observations of that state.”

Comment from Reviewer 11: “This leads to my main criticism of the paper: the results given are not reproducible.”

Response from Authors 11: In accordance to the GMD publication requirements, the model code and settings are available upon request from the authors. The model fitting algorithm,

developed by our group, has been freely available for several years. All the data used is freely available and fully referenced in the text.

Change to Manuscript 11: We do not propose any changes because we already include statements about the code and data availability in the manuscript.

The impacts of data constraints on the predictive performance of a general process-based crop model (PeakN-crop v1.0)

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Abstract. Improving international food security under a changing climate and increasing human population will be greatly aided by improving our ability to modify, understand and predict crop growth. What we ~~currently~~ predominantly have at our disposal are either process based models of crop physiology or statistical analyses of yield datasets, both of which suffer from various sources of error. In the current paper we present a generic process based crop model which we parametrise using a Bayesian model fitting algorithm to three different sources of data - space based vegetation indices, eddy covariance productivity measurements and regional crop yields. We show that the model parametrised without data, based on prior knowledge of the parameters, can largely capture the observed behaviour but the data constrained model greatly improves both the model fit and reduces prediction uncertainty. We investigate the extent to which each dataset contributes to the model performance and show that while all data improves on the prior model fit, the satellite based data and crop yield estimates are particularly important for both reducing model error and uncertainty. Despite ~~the improvements in model performance we show by incorporating data into a process-based mode~~ these improvements, we conclude that there are still significant knowledge gaps, in terms of available data for model parametrisation, but our study can help indicate the necessary data collection ~~steps for improvement in~~ to improve our predictions of crop yields and crop responses to environmental changes.

1 Introduction

Improving food security is one of the greatest challenges currently facing humanity (Schmidhuber and Tubiello, 2007; Rosegrant and Cline, 2003). The increasing and developing human population is driving up food demand and changing demand patterns. This is occurring alongside increasing anthropogenic threats to supply such as climate change. Predicting and understanding how crops respond to changes in their environment through the use of mathematical ~~and statistical~~ models is needed to help address such threats, enabling advanced warning of potential threats and predictions of what alterations to agricultural practices might help prevent or mitigate problems. A continual challenge when developing models is knowing the generality of their predictions, either applied to multiple crops or ~~or~~ across different space and time scales (Rosenzweig et al., 2014): Having one model to cover all circumstances is obviously unrealistic, as is tailor-making models to every conceivable circumstance. Thus, a challenge in developing models to help address the current food security crisis is identifying ~~some~~ those that can be said to be

generally useful over particular scales of application. In the current study we present a proof of concept that such an aim can be reached through using a process-based ~~model-crop model~~, parametrised to available data using a model fitting algorithm.

Most crop models to date can be put into one of two broad categories: process-based or statistical. Process-based ~~crop~~ models have some representation of the mechanisms that determine how plants grow in their formulation (e.g. Jamieson et al., 1998; Jones et al., 2003; Stackle et al., 2003). Processes included ~~in these models can~~ cover crop phenology, carbon assimilation and biomass allocation responses to the internal plant state and the external environment ~~in order to predict crop growth responses to environmental variables~~. Such models have traditionally been specific to a particular crop, partly because of the nature of studies that employ process-based crop models, which have tended to focus on individual crops and often describe growth phases specific to a particular crop type within their formulation. However it is also partly because ~~of~~ the difficulty in developing generally applicable process based crop models; it can be unclear which aspects of the model formulation can be said to be general versus crop specific and obtaining data to assess model generality continues to be a challenge. Some studies have avoided making crop-specific models by using broad crop categories such as C3 and C4 crops, based on the functional plant type concept (Bondeau et al., 2007; Osborne et al., 2015). Other models group a family of crop-specific parametrisations into one single framework ~~which does not achieve full model~~, ~~which limits~~ generality but does ~~offer ease of~~ ~~facilitate~~ use across different scales and crops (Brisson et al., 2003; Stackle et al., 2003).

Statistical crop models aim to capture relationships between various predictor variables and crop properties without using any information of how such factors should be related from biology or ecology. For example, studies have predicted crop yields based on observed simple relationships between yield data and climate inputs (Lobell et al., 2011; Lobell and Field, 2007; Schlenker and Roberts, 2009); these have then been used to help understand past long-term trends in yields at large spatial scales and to make forward projections under climate change scenarios. Often statistical models are developed to be generally applicable to multiple crops and apply over multiple space and timescales, as these do not need to include any plant specific concepts.

Both the process-based and statistical approaches have their disadvantages when it comes to obtaining general insights. Process-based models have often only been shown to be applicable at the individual field scale, making it unclear if their predictions might provide information about crop responses at larger spatial scales. Process-based models can also be sensitive to chosen parameter values and formulation, which has rarely been identified as applicable over multiple crop types or locations (Challinor et al., 2009). Statistical models are limited by the extent to which the relationships they capture are useful in predicting crop properties outwith the circumstances that they have been verified for. This becomes a particularly important limitation given that one of the leading questions being addressed in food security is how different crops might grow in environments and under circumstances that we have not yet observed. For example, correlative models based on mean annual values of environmental variables are unlikely to capture the impacts of changes in extreme weather events or increases in atmospheric CO₂, which have been shown to be essential to understanding changes in crop yield under climate change (Porter and Semenov, 2005; Deryng et al., 2014). Furthermore, simple statistical analyses rarely incorporate information on management agricultural practices such as planting and harvest dates, irrigation and fertiliser application, which account for a large proportion of variations in yield across the globe (Calvino et al., 2003; Zwart and Bastiaanssen, 2004).

An alternative to the extremes of either purely process-based or purely statistical crop models is to apply statistical methods to process-based models to data-constrain their parameters. This technique, which is increasingly used in earth system and vegetation modelling studies (Fox et al., 2009; Raupach et al., 2005), involves allowing some parameters to have undefined values and inferring those values by comparing the model predictions to data (hence the technique is called parameter inference, or inverse modelling). The specific methods used vary but the ~~ultimate aim is~~ aim is often commonly to deduce parameters that ~~give yield~~ the best model predictive performance (another common aim is to deduce insight about the underlying processes from the inferred parameter values). The result is typically a model with improved model predictive ability (Knorr et al., 2010; Ziehn et al., 2012) when assessed using empirical data. Importantly, formally data-constraining model parameters is a technique that can be used to increase the general applicability of a given model formulation, and for that general applicability to be assessed.

The main problem with data-constraining process based models is data availability. Datasets of annual yield such as those used in statistical modelling studies are unlikely to be sufficient when data-constraining the parameters of physiologically explicit model. ~~However, because, to put it simply, they are unlikely to carry enough information to enable identification of what the different model parameters should be. However~~ two other sources of data ~~that have been widely used~~, widely used in the global vegetation modelling ~~community~~ but to a ~~much~~ lesser extent in agricultural modelling, could be of use in data constraining crop model parameters. Space based remote sensing data can provide spatially and temporally continuous information on vegetation greenness at a variety of spatial and temporal scales (Glenn et al., 2008; Tucker et al., 2005). Such data has previously been used for crop classification purposes (Wardlow et al., 2007; Howard et al., 2012) and for simple yield estimation (Doraiswamy et al., 2003; Lobell et al., 2003). The second data source is flux tower eddy covariance (EC) data which provides high resolution CO₂ fluxes at point locations (Baldocchi and Wilson, 2001). Previously, data assimilation methods have been used for an ecosystem model in croplands with earth observation data (Reville et al., 2013; Sus et al., 2013), but both studies focused on ecosystem carbon fluxes and leaf area index and included no estimates of yield.

Sites where intensive data collection has taken place do exist and can be very useful in exploring certain aspects of crop physiology, for example in the context of the agricultural model intercomparison and improvement project, AgMIP (Rosenzweig et al., 2013). However, here we aim to explore a general model-data integration system that could be applied to generic farm locations with generally available data. This makes the problem more difficult but the conclusions can be more useful to a ~~a~~ general application of the concepts.

In this paper we present a newly developed general, non-crop specific process based model ~~parametrised at~~ and use parameter inference to infer the most likely parameters for 15 locations for winter wheat and maize using a combination of space-based vegetation indices, eddy covariance flux data and reported agricultural yields. We aim to answer the following questions:

1. Does ~~a~~ our model with data constrained parameters predict empirical data better than a model with prior parameters?
2. Are the data constrained parameters similar among different sites and what are the impacts on model predictive accuracy of having site-specific versus site-shared parameters?

3. To what extent does the inclusion of the different types of data in the model fitting process influence the uncertainty in the inferred parameters and model predictions?

~~In addition, we aim to build~~ We expect the qualitative answer to the first question to be that utilising empirical data does enable the model to make better predictions because that's a typical outcome of our parameter estimation approach. However we are more interested in the quantitative answer; i.e. how much? For example, the generation of a model that could make extremely precise and accurate predictions would suggest that data-constraining general models with the datasets we identify could provide an extremely useful tools for agricultural predictions and forecasts. Alternatively, the generation of a model that makes very imprecise predictions would suggest that more data collection and model improvement is needed for the model to have practical applications.

- 10 In addition to our aims above, our goal with this paper is to provide a proof of concept ~~that a data-constrained~~ process-based ~~model constrained with widely available data crop model that~~ could be of use in practical agricultural systems ~~and to~~. To this end we include a more ~~didactic~~ ~~description~~ discussion of the methods than otherwise necessary as well as a more broad discussion of the paper's applicability.

- 15 While our study is part of a boarder scientific objective to enable more accurate field scale predictions, the lack of availability of field scale datasets to train and validate our model means that the scale of model evaluation for our study here is a mix of field (flux tower) and regional scales (county and country level for yield estimates and 3 by 3 km scale for photosynthetic activity).

2 Datasets used

2.1 Study sites

- 20 Our analysis focusses on 15 sites for which we can obtain the combination of eddy-covariance data, satellite data and crop yield data for specific crops (summarised in Table 1), of which 7 sites were growing maize (*Zea mays*) and 8 sites were growing winter wheat (*Triticum aestivum*; we refer to this simply as wheat). Most of these sites grow maize or wheat on a rotation with other crops and we identify the time period over which the species of interest is growing from the metadata associated with the eddy-covariance data. All of the maize sites are based in the United States. All but one of the wheat sites are based in western
- 25 Europe, with one ~~of the sites~~ site in the United States. For the site where information was available, the crops were not irrigated with the exception of the US-Me1 site (Suyker et al., 2004). All sites have been tilled to a certain degree, generally in accord with agricultural practices in the area. European sites have received a moderate amount of fertiliser (Moors et al., 2010).

2.2 Space-based vegetation indices

- 30 We use data on vegetation greenness from the MODIS (Moderate Resolution Imaging Spectroradiometer) Terra instrument. MODIS fraction of absorbed photosynthetically active radiation (fAPAR data) from the MOD15A product was downloaded (<https://lpdaac.usgs.gov/>) for geographic regions corresponding to each of the study sites (Table 1) for the period 2000-2010.

This data was subsequently filtered using the quality assurance (QA) indices provided so that only data points calculated using the main algorithm were retained and pixels classified as cultivated land were identified using the MODIS landcover product (MOD12A) IGBP classification.

Using the pixel closest to the flux tower site was infeasible because of data noise and gaps resulting in an uneven timeseries. Instead, we aggregated all pixels within a 3 km by 3 km square centred on the tower site in a single timeseries. The untested assumption behind this aggregation is that farming practices are constant across this scale. To separate between different crops we use a crop phenology approach (Wardlow et al., 2007). Pixels that reach maximum fAPAR before day 150 are classed as winter crops (specifically, winter wheat), while crops that peak after that date are classified as summer crops. This procedure is applied for individual years to account for crop rotations.

10 2.3 Eddy-covariance data

We use eddy covariance data for 15 sites across Europe and the United States (Table 1), consisting of 19 data years. The data was obtained from the Ameriflux (<http://ameriflux.lbl.gov/>) and the European Fluxes Database Cluster (<http://www.europe-fluxdata.eu/>). We use level 4 data of CO₂ fluxes partitioned into gross primary productivity (GPP) and gap filled using the mDS method (Reichstein et al., 2005). Sites that have a crop rotation were filtered to obtain single species timeseries. These include the maize-soybean rotation sites and European mix rotation sites that include winter wheat.

2.4 Crop yield data and agricultural dates

To obtain information on crop yield we use data provided by the US Department for Agriculture (USDA) yearly, at the county level, available for the entire study period (<https://www.nass.usda.gov/>). For the European sites we used country level data provided by the EC Eurostat database, available from 2004 onwards (<http://ec.europa.eu/eurostat>).

20 Sowing and harvest dates are required as model inputs and were extracted from the crop calendar global dataset (Sacks et al., 2010). We chose this rather than local level dates for greater model generality.

Fertilizer input data were obtained from the published site descriptions (see Table 1 for references) or from the Nitrogen Fertilizer Application database ((Potter et al., 2010). The model implemented in this study does not require any additional information on irrigation or soil properties.

25 2.5 Environmental input data

We use NASA's Modern-Era Retrospective Analysis for Research and Application (MERRA) dataset (Rienecker et al., 2011) at a spatial resolution of 0.5 degrees latitude by 0.66 degrees longitude and a temporal resolution of 3 hours which we average to a day. Temperature and direct and diffuse photosynthetically active radiation (PAR) data ~~is~~were extracted for each site. Comparison with tower based meteorological data has shown this to be an accurate estimation of conditions at the tower site for all variables and we use MERRA data for the greater generality of the model as this would allow the model to be applied at any location on the globe.

3 Model description

We propose a ~~Our~~ new general model of crop growth ~~is~~ based on the ~~hypothesis that~~ single plant model of Guilbaud et al. (2014) and like that model, assumes that annual plants show optimal biomass allocation during vegetative growth and optimal flowering in order to achieve maximum reproductive mass given available resources. ~~This model is based on the single plant model of~~

5 ~~Guilbaud et al. (2014).~~ Plant growth is divided into three stages, starting at sowing date and ending at harvest: germination, vegetative growth and reproductive growth.

3.1 Germination

The germination process is described as a degree day function with a fixed base temperature of 0°C up to a parameter germination limit $germ_{lim}$. The initial seed mass is prescribed and is expressed as grams per metre squared, incorporating information
10 about both seed size and planting density. When the germination limit is reached, all seed mass is allocated to above- and below-ground pools according to the optimality criteria described below. Initial model runs have shown that for values of the germination base temperature T_b and seed mass within realistic ranges, the model is largely insensitive to the values of these parameters, which is why they have been fixed.

3.2 Vegetative growth

15 During vegetative growth, biomass is allocated to either above or below-ground fractions to achieve an optimal carbon to nitrogen (C:N) ratio at the plant level (ρ). The net daily growth is calculated as the minimum of a nitrogen limited growth, G_{root} and a carbon limited growth G_{leaf} .

Nitrogen limited growth is considered to be a function of root mass M_{root} and available soil nitrogen N :

$$G_{root}(t) = \theta N(t) M_{root}(t-1) \rho, \quad (1)$$

20 where θ is the nitrogen uptake capacity of the roots expressed as $\text{gN g}^{-1} \text{soil N g}^{-1} \text{root C day}^{-1}$, $N(t)$ is soil nitrogen at time t (g) and $M_{root}(t-1)$ is the root mass (g) at the previous timestep. Carbon limited growth is considered to be equal to potential net carbon uptake, calculated as the difference between whole canopy photosynthesis and respiration. Photosynthesis is calculated using the model for C3 plants developed by Farquhar et al. (1980) as described in dePury and Farquhar (1997) and the alternative model for C4 species (Collatz et al., 1992; Von Caemmerer, 2000):

$$25 \quad G_{leaf}(t) = f(V_{cmax}, J_m, T(t), I(t), pCO_2, LAI(t-1)) - R_{plant} \quad (2)$$

Here V_{cmax} is a parameter representing photosynthetic Rubisco capacity ($\mu\text{mol m}^{-2} \text{s}^{-1}$), J_m is potential electron transport rate and T , I and pCO_2 are environmental inputs (temperature, solar radiation and atmospheric CO_2 partial pressure respectively). Total absorbed solar radiation I is calculated for direct and diffuse photosynthetically active radiation (PAR) using a sun-shade model (dePury and Farquhar, 1997). Partial pressure of CO_2 inside the leaf is calculated assuming a constant optimal
30 ratio λ between internal and atmospheric CO_2 in the absence of water stress (Haxeltine and Prentice, 1996). Leaf area index

(LAI) is calculated from leaf mass M_{leaf} using the leaf mass per area (LMA) parameter. Whole plant respiration is calculated as a linear function of total plant mass:

$$R_{plant} = r_{tot}(M_{leaf} + M_{root}) \quad (3)$$

Here r_{tot} represents average respiration per unit plant mass ($\text{g g}^{-1} \text{ day}^{-1}$). This total respiration component accounts for growth costs and maintenance including active nutrient uptake by the roots and is a function of temperature. Given the optimal whole plant C:N ratio that drives the vegetative biomass allocation, this formulation is ultimately equivalent to the nitrogen dependent function commonly used in vegetation models without the need to introduce further parameters for root and leaf specific C:N ratios.

Actual biomass growth is then the minimum between nitrogen and carbon limited growth:

$$G_{net} = \min(G_{root}, G_{leaf}) \quad (4)$$

This biomass is allocated to the limiting fraction, either aboveground or belowground in order to adjust the C:N supply. Crops are considered to be not water limited, as all sites are in areas with a high annual precipitation. We lacked any information on soil water availability and initial trials to data-constrain a model that included the effects of varying soil water availability led to poorly constrained parameters related to soil water constraints (see section 7).

15 3.3 Optimal flowering and reproductive growth

Reproductive growth starts at a point where the supply of any of the resources, carbon or nitrogen, reaches a maximum, which we term 'peak resource'. This is the point in time which will result in the maximum final reproductive mass as further increase in vegetative fractions would not result in an overall increase in growth rate and lead to suboptimal growth (see Guilbaud et al. (2014) for an in depth discussion of this).

20 The peak nitrogen condition is achieved when an increase in root mass does not result in an increase in nitrogen uptake. This condition is achieved in nitrogen limited environments where the nitrogen available in the soil is depleted through the period of vegetative growth. This assumption can be considered valid in agricultural systems where the major nitrogen input into the system during the growing period comes solely from agricultural fertilisers. [Soil nitrogen decays monotonically through the season in our model due to the simplicity with which we model nitrogen uptake and so detecting the peak nitrogen condition is straightforward.](#) Similarly, the peak carbon flowering condition is triggered when the addition of aboveground biomass would not lead to an increase in net carbon gain, due to self-shading in the canopy. [To calculate the peak carbon trigger we use the environmental variables averaged over \$p\$ days, to avoid flowering being triggered by short-term environmental fluctuations. We infer \$p\$ alongside the other parameters in our model.](#)

30 During the reproductive phase all new biomass produced is assigned to reproductive tissues. Nitrogen and carbon are translocated to reproductive organs at a constant rate, m_{trans} . As all biomass within the model is calculated as mass of carbon and agricultural yield data is reported as total dry mass we use a conversion parameter to account for the carbon fraction, C_{frac} . This parameter also accounts for the differences in total reproductive mass and actual mass harvested and reported as yield.

4 Parameter estimation technique

We use Bayesian parameter inference techniques to infer the parameters for the model described above. The technique involves solving Bayes' theorem which in this context states

$$P(\theta|obs) = \frac{P(obs|\theta)P(\theta)}{\int P(obs|\theta)P(\theta)d\theta}, \quad (5)$$

5 where P denotes a probability, obs is the empirical data, and θ is the set of parameters to be inferred (Gilks, 1996.). The term in the denominator can be treated as a normalising constant in our study and so we omit it here. Thus our problem reduces to $P(\theta|obs) \approx P(obs|\theta)P(\theta)$ where $P(obs|\theta)$ is usually referred to as the likelihood of the data given the model and $P(\theta)$ is the prior probability of the parameters. Prior probabilities of parameters can be determined by previous empirical evidence, such as field measurements. In our case we do not have any prior expectations about what the prior parameter values should
 10 be and so we specify that each parameter is equally likely to fall within a wide range of values (flat priors). This means that our study reduces to inferring the joint probability distribution of the parameters based on the likelihood of the data given ~~the model given~~ all possible parameter combinations. We cannot solve this inference problem exactly. Instead we use Markov-Chain Monte Carlo techniques with the Metropolis Hastings algorithm to approximate the likelihood and its associated joint parameter probability distribution, which we implemented using the Filzbach inference library as detailed in (Caldararu et al.,
 15 2012). This algorithm works by iteratively making random mutations to an existing parameter set, computing the likelihood associated with the new set of parameters, and then replacing the existing parameter set with the new set based on the ratio of their likelihoods according to the Metropolis-Hastings algorithm (Gilks, 1996.).

Three different datasets were used in combination to infer our model parameters - MODIS fAPAR, flux tower GPP and crop yield data. Each dataset contributes to the assessment of the model likelihood but each one of these has different temporal
 20 resolutions and covers different time periods, resulting in a variable number of data points. To prevent our inferred parameters from being overly-based towards explaining the datasets with the greatest quantity of data points we down-weighted the contributions to our likelihood estimates from each data point according to the quantity of data in each data set. The likelihood ~~to be inferred by function used in~~ Filzbach is therefore:

$$l(Z_{\mathbf{x}}|\theta_{\mathbf{x}}) = \sum_D \frac{1}{N_{\mathbf{x},D}} \sum_{t(\mathbf{x},D)} \ln[n(Y_{obs}(\mathbf{x}, D, t), Y_{pred}(\mathbf{x}, D, t, \theta_{\mathbf{x}}), \sigma_{\mathbf{x},D})], \quad (6)$$

25 where $\theta_{\mathbf{x}}$ is the vector of model parameters at site \mathbf{x} , $N_{\mathbf{x}}$ is the number of data points in each dataset D at each location and $n(Y_{obs}(\mathbf{x}, D, t), Y_{pred}(\mathbf{x}, D, t, \theta_{\mathbf{x}}), \sigma_{\mathbf{x},D})$ denotes the probability density for observing $Y_{obs}(\mathbf{x}, D, t)$ given a normal distribution with mean $Y_{pred}(\mathbf{x}, D, t, \theta_{\mathbf{x}})$ and standard deviation $\sigma_{\mathbf{x},D}$ which expresses the magnitude of unexplained variation in the variable Y . Y refers to the model variables corresponding to the three datasets. Note that with this definition of the likelihood we are treating every data point as independent, that is the likelihood of a value at time t is treated independently from the likelihoods at preceding times. This is only an approximation but is commonly used in parameter estimation studies because the additional mathematical and computational complexity of accounting for non-independent data.
 30

We adopt different techniques to estimate the standard deviation $\sigma_{x,D}$ above, depending on the dataset D at each location. Generally, we assume that the variation in the model predictions about the data is solely due to uncertainty in the data. The GPP data does do not have an estimate of ~~the uncertainty about that data and so instead uncertainty and so~~ we infer the uncertainty associated with ~~that data as those data as the parameter~~ $\sigma_{x,D}$. In the case of MODIS fAPAR data we explicitly incorporate a measure of variation in the data within the geographical area used to compute the mean fAPAR as well as inferring a parameter representing additional unexplained variation. We include this parameter to account for known issue in space based remotely sensed data, such as background soil reflectance. ~~In the case of The~~ crop yield data ~~σ_x is expressed solely as variation in the data.~~ ~~already have estimates of observational uncertainty associated with them and so we use those data to define $\sigma_{x,D}$.~~

5 Experimental protocol

10 In order to assess whether the model with data constrained parameters predicts empirical data better than a model with prior parameters we infer the parameters for each site individually using all of the empirical data and compare the model predictive performance to one in which the parameter values are sampled randomly from the prior range.

We compare the inferred parameters and predictive performance of models with parameters inferred using data from individual sites (the one site model) or from multiple sites together (all sites model), always keeping maize and winter wheat sites separate, to assess the effects of allowing parameters to differ between the sites. Preliminary investigations revealed that similar model parameter distributions were inferred once data from more than 3 sites were used in combination when inferring the parameters. We therefore also take the opportunity to assess the performance of the models with parameters shared between sites in predicting data that has not been used in parameter inference (evaluation model).

20 To assess the importance of different types of data-constraints we perform a data knock out experiment and we infer the model parameters for individual sites using only one or two of the different empirical datasets and assess inferred model parameters and model performance.

In general we assess model predictive performance by quantifying the root mean squared error between the model predictions and the empirical data to assess model precision and the mean error to assess model bias. We normalise both these metrics by the mean value of the different empirical dataset types to aid in comparison. We calculate ~~model prediction and parameter~~ parameter uncertainty as the 95th percentile confidence interval from the posterior distribution (Section 4).

25 ~~To calculate uncertainty for the model predictions we sample parameter values from their respective posterior distribution and compute predictions with each parameter combination, which results in a corresponding distribution of model predictions. We report this prediction distribution uncertainty using 95th percentile percent confidence intervals. This predicted distribution does not include the prescribed or inferred uncertainty about observations, $\sigma_{x,D}$, our predicted distributions correspond to the state being predicted and not the observations of that state.~~

30

6 Results

6.1 Prior and posterior model predictions

In general and as expected, the predictive accuracy of both the wheat and maize models is improved by inferring their parameters; the root mean squared error and bias of the model predictions is reduced for predicting all empirical datasets compared to the prior model (Table 3). These improvements are about a 40% reduction in RMSE for both GPP and fAPAR and an 80% reduction in RMSE for yield. Visual inspection of the predicted time series for the models with prior and posterior parameter distributions (e.g. Figure 1 for wheat in one site) highlights that the model with prior parameters predicts the same qualitative behaviour as the model with inferred parameters but that parameter inference reduces the posterior uncertainty in the predictions of the model.

In terms of uncertainty, the posterior models show a large reduction when compared to the prior of aboveground biomass (86%) and yield (97%), but a smaller reduction for the belowground variables (67% for root biomass and 20% for soil nitrogen), as there is no data in the fitting procedure to directly constrain these. Visual inspection also emphasises the importance of model structural constraints on the model dynamics e.g. the model predicts a narrow range of dynamics in some properties at certain times of the year (e.g. biomass in leaves, roots and reproductive parts soon after sowing) irrespective of the parameter values.

6.2 One site vs. all sites fit

On average the RMSEs are very similar between the models with parameters inferred for individual sites to when parameters are inferred for all sites together (Table 3). In general, we expect that if we were to infer a single set of parameters for individual sites then the predictive performance of that model will always be at least as good as when the set of parameters has been inferred for all sites. This may not necessarily be the case when inferring parameter probability distributions: the lower quantity of data could result in greater parameter uncertainty which may on average lead to a lower predictive accuracy than that using the more constrained parameter distributions obtained by inferring parameters from all sites. This explains why some of the mean RMSE scores are higher for the model with parameters inferred from ~~all~~ individual sites. The bias scores are also very similar although the bias tends to be smaller on average for the models with parameters inferred using all sites.

As expected, the uncertainty in the predicted GPP, fAPAR and yield is lower for the models with parameters inferred using all sites because more data is used to infer the parameter values for those models, leading to lower uncertainty in the inferred parameter distributions (Figure 2). When parameters are inferred for individual sites uncertainty is around 134% for GPP, 121% for fAPAR and 33% for yield, with similar values at wheat sites (Table 3). This is reduced to around 45% for GPP, 100% for fAPAR and 12% for yield estimates when parameters are inferred using data for all sites. Visual inspection of the change in uncertainty over time highlights that prediction uncertainty due to parameter uncertainty is highest at the start and end of the season (over 100%) but decreases to 50% on average for all variables in the middle of the growing period (Fig. 4).

Inspection of the inferred parameter distributions (Fig. 2) shows, as expected, that the posterior parameter uncertainty tends to be higher when parameters are inferred using data from individual sites versus using all sites together, although these distributions overlap for almost every site and every parameter. In general, these inferred parameter distributions show greater

differences between winter wheat crops and maize crops than they do as a result of using more sites for inference. One exception is the sole winter wheat site in the United States; inferred to have lower soil nitrogen, respiration rate and translocation rate of mass from vegetative to reproductive tissue. These inferred differences are probably due to differences in winter wheat crops between the USA site and the European sites such as different crop varieties or agronomic practices.

- 5 Visual inspection of the predicted time series of GPP, fAPAR and yield for maize and winter wheat predominantly show very similar predictions between the models with parameters estimated from one site versus all sites (Figure 3 shows predictions for representative sites. Appendix A shows timeseries for all sites with associated uncertainty). There tends to be greater differences between the ~~models-model predictions~~ and the empirical data ~~than between the predictions under the different model parametrisations~~ when the model has site-specific parametrisations than when parametrisations are shared between sites.
- 10 The one notable exception is again the winter wheat site in the US, for which inferring parameters for the specific site leads to much more accurate predictions compared to the model with parameters inferred for all sites (Fig. A1). Other than that that site, the time series for GPP, fAPAR and yield for maize show larger discrepancies between the data and the model predictions than from the predictions of different models. GPP tends to be reproduced well, relative to the other time series, with an average correlation coefficient of around $r^2=0.7$. fAPAR is predicted less well (around $r^2=0.4$) which is at least partly due to a
- 15 systematic under prediction of fAPAR at the start and end of the year. We attribute this to the fact that the fAPAR data reflects the light absorption by plants in a region that includes vegetated areas out with just the fields whereas the model is predicting only light absorption by the crop (discussed further below). Annual yields are predicted least well by our models (around ~~r^2~~ $r^2=0.1$) and we attribute this at least in part to the data itself having a relatively high uncertainty (discussed further below).

We evaluate the model transferability by inferring the model parameters using a subset of the sites and assessing model

20 predictive performance against the remaining sites (Fig. 3 and Table 3). In general, the model RMSE and bias do not differ between the sites that were used for parameter estimation and those that were not. Moreover, the model predictive performance is similar to that resulting when fitting to all sites. The uncertainty for GPP, fAPAR and yield at maize sites is similar to that obtained by fitting to all sites, but for the wheat sites the uncertainty in GPP and fAPAR increases, while the yield uncertainty remains at the level obtained when fitting to all sites (Table 3).

25 6.3 Impacts of using different data types

Our data type hold out experiments show clear differences in the roles played by different data types in improving model predictive accuracy, but the effects are similar for both crop types (Figure 5, this figure only shows model RMSE and bias when parameters are inferred using data for individual sites but the results are similar when all sites are used to infer model parameters). The largest effect of adding a given data type is when yield data is included, which significantly reduces RMSE

30 and bias for predicting yield. This makes intuitive sense, although interestingly including yield data alone and as part of a combination also tends to improve model predictive performance for GPP and fAPAR. Counter intuitively, including GPP data alone or fAPAR data alone only has subtle effects on the model RMSE and bias for predicting those variables and yield, but including those datasets in combination does indeed lead to improvements in RMSE and bias. –

The greatest improvements in model predictive performance for all response variables is obtained when all data types are used for parameter inference. This is not inevitable as an overall more likely model might be achieved by sacrificing predictive accuracy for one data type in order to improve predictive accuracy for another. For example, adding fAPAR data alone slightly improves model RMSE for fAPAR data, but makes it worse for GPP and yield predictions when compared to the model with prior parameter distributions. Indeed the crops do not flower for maize or wheat when only fAPAR data is used for parameter inference. Comparing knockouts with and without fAPAR data included implies a trade-off between predicting the fAPAR data well and predicting GPP well (Figure 5). Interestingly, all models underestimate GPP, although this bias is least when all data is used to infer the model parameters.

The uncertainty in model predictions (~~Fig-~~Figure 6) follows a similar pattern to model error, with the fAPAR only model having the highest uncertainty (up to 900% for GPP) while the GPP and fAPAR model ~~perform~~performs best with uncertainty values of 123%, 128% and 32% for GPP, fAPAR and yield respectively, values which are close to those obtained through fitting to all the data. The GPP and yield model also has relatively low uncertainty values for GPP and fAPAR estimates but fails to produce any yield at the wheat sites (the plants do not proceed to the flowering stage).

7 Discussion

7.1 Model performance

We show that a process-based crop model constrained using EC data, satellite fAPAR observations and regional yield estimates can improve model performance compared to the model run with prior parameter ranges and greatly reduces the uncertainty in model output. However, the resulting uncertainty in both state variables and model parameters is still relatively high.

Model uncertainty is difficult to compare with previous crop modelling studies, as models with fixed parameter values do not often provide uncertainty estimates. In fact, providing uncertainty values for all model variables and parameters is one of the advantages of a data constrained model. In the current model, uncertainty is highest at the start of the season for all variables but decreases rapidly and final yield uncertainty is much lower. This is due to ~~thresholds-~~thresholds: abrupt changes from one growing stage to another when small differences in parameters can lead to large differences in resulting variables. It is, however, important to note that the uncertainty in our yield predictions remains high and the model in its current form is unlikely to provide accurate predictions for practical applications without the addition of new data (Section 7.4). We have however shown that the use of three different data types does reduce prediction uncertainty - pointing to an avenue for future model improvement.

In terms of the posterior parameter distributions, resulting parameters show a similar degree of constraining to that observed in previous model parametrisation studies for natural ecosystems (Keenan et al., 2012). The photosynthesis related parameters are badly constrained despite the fact that GPP estimates have a relatively low uncertainty. This can be explained by the structure of the photosynthesis component which is rigid compared to other components of the model as these processes are better understood. In contrast, belowground processes are both poorly understood and lack the data to properly constrain model parameters (Pendall et al., 2004).

In terms of model performance, the model correctly predicts seasonal trajectories of GPP and final yield data. We cannot however capture the interannual variability in yields, which is most likely due to the fact that our model does not include a response to water limitation or heat damage. The fact that we use regional yield data can also lead to discrepancies between the yield at each specific flux tower site and the yield data. The model does not capture the fAPAR seasonal cycle well, especially at the maize sites, which is due to the low spatial resolution of the data. However, the predicted model fAPAR is more realistic than the fAPAR data, which is one of the advantages of using a process-based model with a more rigid structure than a statistical one.

One additional complication is the different spatial scales of the three datasets - while the eddy covariance data is at the scale of the flux tower footprint, which can be seen as equivalent to the individual field scale, the fAPAR and yield data correspond to larger scales (county and country level for the yield data and a 3 by 3 km scale for the fAPAR data). The assumption behind our analysis is that the conditions at field scale are representative of the regional scale, so that there would be no discrepancy between model predictions at these different scales. This is obviously a source of error, especially at the wheat sites in Europe, which will be located over a much more heterogeneous landscape. Further sources of data at the field scale would be required to identify the model error caused by the discrepancy in spatial scales.

7.2 Use of the different datasets

Eddy covariance data is to date the most widely used data set for parametrisation of vegetation models (Fox et al., 2009; Xiao et al., 2011). We show that removing this data from the fitting procedure does not radically decrease model performance. If we consider what information content this data provides - primary productivity and CO₂ flux seasonality, this fact is maybe not surprising. The seasonality information is already contained in the fAPAR dataset, while the primary productivity is highly constrained by the structure of the biochemical photosynthesis model. Furthermore, the GPP only fit results in an underestimation of the final yield, indicating that the sole use of EC data in crop models is not sufficient to accurately predict yields. Unlike most studies using EC data we have used sites with only one year of data as these were the only available agricultural sites and it is possible that more GPP data at one site could increase its importance in the fitting. EC data could also be a valuable tool for independent model evaluation as it provides information about plant function not included in the other available data.

Space based vegetation data has the main advantage of a large spatial and temporal coverage, so that it can be used irrespective of the local monitoring infrastructure, providing a general data source. However, the quality of the data is relatively low, especially at the high spatial resolutions needed for crop modelling. This problem is particularly obvious in the case of the maize data, which lacks the expected seasonality and is reflected in the very high error in the fAPAR only fit. However, the model fits without fAPAR (GPP and yield only) show a high error as well, indicating that the information content in vegetation indices is needed for constraining the model but not sufficient.

Some of these limitations are not general for remote sensed data, but can be attributed to the spatial and spectral resolution of the MODIS instrument. The 1 km spatial resolution can be too ~~low~~-coarse for agricultural fields, especially in areas with heterogeneous landcover. Other existing instruments, specifically the Landsat family, have a better spatial resolution (30 m), but a much poorer temporal resolution which we have found unsuitable for fitting a plant growth model where developmental

changes can be abrupt. More recent missions, such as Sentinel-2 will have more suitable spatial and temporal resolutions for use with this type of model (Herrmann et al., 2011). Some of the error in the data can also be attributed to misclassification of pixels. We use a simple phenology based approach which is one of the only ones available for data with a relatively wide bandwidth such as MODIS. This method is useful for winter crops which have different timing compared to the natural
5 vegetation, but less useful for summer crops such as maize where there is no clear separation in phenology between cropland and the surrounding vegetation. Hyperspectral data can be used more accurately for crop identification (Thenkabail, 2001) but to date no space-based instrument is available that has the required bandwidth, the spatial and temporal coverage and the spatial and temporal resolution. However, such data can be used at local scales if the measurements were available.

Crop yield is the data that is traditionally used for evaluating agricultural models and is arguably the most important to
10 predict correctly, given that the purpose of the model is to predict crop productivity. We have used county and country level reported yields rather than field level measured yield because of both the availability of the data and the generality of the method. The model fitted with yield data only gives a good fit to yields, but higher errors for the GPP and fAPAR estimates which raises questions about the correctness of models which only use final yields to assess performance and the ability of
15 such models to predict crop yields under different conditions. Crop yield data provides the final point of plant crop growth but there is potentially a multitude of model structures and parameter combinations that can result in that yield.

In addition to the three datasets used for parametrisation, the model also requires input data in the form of sowing and harvest dates and fertiliser inputs. Additional uncertainty is associated with these datasets which is not available nor accounted for in our analyses. For example, the crop calendar (Sacks et al., 2010) and Nitrogen Fertilizer Application ((Potter et al., 2010)) datasets are global data collections that will imperfectly represent the value for any given location. Alternatives to these
20 global datasets would be to use location-specific data, or to infer the values. Location specific data has the advantage of more accurately reflecting the situation at a given site and would therefore be useful when the model is applied at the field scale, but such data is unlikely to be available for all sites. Successful inference of the values would depend on if there is enough information in the datasets used to infer the model parameters. If there is inadequate data then there would be excessive degrees of freedom for inference, leading to the wrong parameter values being inferred and the model performing poorly in
25 novel situations. Therefore the decision whether to obtain more data or infer unknown quantities in future applications of our model and inference framework depends on the data availability and the intended scales of application.

7.3 Choice of model

Here we have chosen a given model structure and extensively tested the way in which constraining the parameters with different datasets in different configurations. The question that arises is to what extent the chosen model itself affects the present
30 results. We have chosen a novel, physiology based model which includes plant optimality concepts, which on one hand has the advantage that it is more general than some of the older models and lacks artificially set thresholds between growth stages, but does ~~has~~have the disadvantage of being less thoroughly tested against field observations. An ideal companion paper to this study would be a comparison of different model structures with a constant data constraining framework, providing greater insights into which parts of the model lead to high errors or uncertainty. However, given the limitations of the current study, we

acknowledge this limitation and report most error metrics as relative to prior model runs in an attempt to isolate errors created by the data and model fitting from those caused by the model itself.

7.4 Future data needs

The fact that our model shows a relatively good fit when constrained at multiple sites indicates that it would be possible to obtain a single parameter set for one cultivar given the same agricultural practices, so that the model can be fitted at a small number of locations and then applied more widely. However, the parameters are badly constrained and part of the data we have used is not sufficiently accurate to allow the use of the model at a wider variety of locations and climate conditions. Accurate yield data is essential but not sufficient and must be accompanied by a growth timeseries. Our results indicate that additional EC data is not necessary, especially given the cost of installing and maintaining a flux tower. Instead, either biomass or LAI (or fAPAR or other VIs) data could be easier to obtain at multiple locations. The belowground part of the model, describing root nitrogen uptake, is only indirectly constrained by the existing data and any observation of root mass and function would have the capacity to add extra information, especially timeseries information (Johnson et al., 2001).

The model in the version presented in this paper does not include any water limitation to growth due mainly to a lack of data constraint on any water related parameters, as we found that latent heat data from EC towers is not sufficient. Below-ground measurements of not only root growth but also soil water properties would again provide some of the necessary information. Such belowground data, especially if supplemented by nutrient concentrations can also help constrain a more complex version of the nitrogen uptake scheme, which could be improved to include more explicit soil-plant interactions and additional processes such as biological nitrogen fixation for legumes.

If this model, or any other similar process-based data constrained crop model, is to be used for scientific purposes to understand the response of crops to climate across the globe, the ideal data would be a global data set, such as space-based vegetation observations, combined with high quality field level data that would ideally include growth timeseries, final grain yield and information about agricultural practices. However, if the model is to be used for agricultural purposes, to aid decision making at the local level, high quality field level data would be sufficient. A valuable evaluation in such studies, not conducted here for brevity and due to a lack of location-specific data, would be to compare the predictive accuracy of the model against the predictive accuracy of a statistical average over the data. Such an analysis would reveal whether and how much benefit is gained by using a data constrained model for predictions.

8 Conclusions

In this paper we present a method for data constraining a process-based agricultural model to three sources of data—eddy covariance flux measurements, space-based fAPAR and regional yield estimates. We show that the data constrained model performs better than the model with prior parameter estimates, especially in terms of uncertainty and even though the data used is in some cases not sufficient to fully constrain posterior parameters it has sufficient information value to be used for model parametrisation. We apply the model to both maize and wheat sites and show that the model performs equally well for both

species. Parameters can be shared between sites of the same species with a similar performance to local parameters and reduced uncertainty. We have also investigated the impact of the different data sets on constraining the model and we show that all three types of data contribute to the model performance, but that if in a data limited world one [of](#) the data types was not available, the model can be constrained reasonably well with fAPAR and yield data only. There are still gaps in the data available for
5 model parametrisation, which are also a limitation to the models which can be parametrised, in particular in relation to water limitation on crops and we believe that a model parametrisation framework such as that presented here can help identify those gaps and the data needed to further our capacity to model crops.

9 Code availability

All model code used in this paper is available from the authors upon request.

10 10 Data availability

All data used in this paper is freely available and has been fully referenced in the text.

Appendix A: Site level model simulations

Figures A1-A3 show site level predictions for the one site and all site model parametrisation. Figures A4=A6 show results from the site knock out evaluation.

15 *Author contributions.* All authors contributed to model development and analysis

Competing interests. There are no competing interests

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References

- 5 Baldocchi, D. D. and Wilson, K. B.: Modeling CO₂ and water vapor exchange of a temperate broadleaved forest across hourly to decadal time scales, *Ecological Modelling*, 142, 155–184, doi:10.1016/S0304-3800(01)00287-3, <http://www.sciencedirect.com/science/article/pii/S0304380001002873>, 2001.
- Bondeau, A., Smith, P. C., Zaehle, S., Schaphoff, S., Lucht, W., Cramer, W., Gerten, D., Lotze-campen, H., Muller, C., Reichstein, M., and Smith, B.: Modelling the role of agriculture for the 20th century global terrestrial carbon balance, *Global Change Biology*, 13, 679–706, <http://dx.doi.org/10.1111/j.1365-2486.2006.01305.x>, 2007.
- 10 Brisson, N., Gary, C., Justes, E., Roche, R., Mary, B., Ripoche, D., Zimmer, D., Sierra, J., Bertuzzi, P., Burger, P., et al.: An overview of the crop model STICS, *European Journal of agronomy*, 18, 309–332, 2003.
- Caldararu, S., Palmer, P. I., and Purves, D. W.: Inferring Amazon leaf demography from satellite observations of leaf area index, *Biogeosciences*, 9, 1389–1404, doi:10.5194/bg-9-1389-2012, <http://www.biogeosciences.net/9/1389/2012/>, 2012.
- 15 Calvino, P., Sadras, V., and Andrade, F.: Quantification of environmental and management effects on the yield of late-sown soybean, *Field Crops Research*, 83, 67–77, <http://www.sciencedirect.com/science/article/pii/S0378429003000625>, 2003.
- Challinor, A. J., Ewert, F., Arnold, S., Simelton, E., and Fraser, E.: Crops and climate change: progress, trends, and challenges in simulating impacts and informing adaptation, *Journal of Experimental Botany*, 60, 2775–2789, doi:10.1093/jxb/erp062, <http://jxb.oxfordjournals.org/content/60/10/2775.abstract>, 2009.
- 20 Collatz, G., Ribas-Carbo, M., and Berry, J.: Coupled Photosynthesis-Stomatal Conductance Model for Leaves of C₄ Plants, *Functional Plant Biol.*, 19, 519–538, <http://www.publish.csiro.au/paper/PP9920519>, 1992.
- dePury, D. G. G. and Farquhar, G. D.: Simple scaling of photosynthesis from leaves to canopies without the errors of big-leaf models, *Plant Cell and Environment*, 20, 537–557, 1997.
- Deryng, D., Conway, D., Ramankutty, N., Price, J., and Warren, R.: Global crop yield response to extreme heat stress under multiple climate change futures, *Environmental Research Letters*, 9, 034 011, <http://stacks.iop.org/1748-9326/9/i=3/a=034011>, 2014.
- 25 Doraiswamy, P. C., Moulin, S., Cook, P. W., and Stern, A.: Crop Yield Assessment from Remote Sensing, *Photogrammetric Engineering & Remote Sensing*, 69, 665–674, <http://dx.doi.org/10.14358/PERS.69.6.665>, 2003.
- Farquhar, G. D., Caemmerer, S., and Berry, J. A.: A biochemical model of photosynthetic CO₂ assimilation in leaves of C₃ species, *Planta*, 149, 78–90, doi:10.1007/BF00386231, 1980.
- 30 Fischer, M. L., Billesbach, D. P., Berry, J. A., Riley, W. J., and Torn, M. S.: Spatiotemporal Variations in Growing Season Exchanges of CO₂, H₂O, and Sensible Heat in Agricultural Fields of the Southern Great Plains, *Earth Interactions*, 11, 1–21, doi:10.1175/EI231.1, <http://dx.doi.org/10.1175/EI231.1>, 2007.
- Fox, A., Williams, M., Richardson, A. D., Cameron, D., Gove, J. H., Quaife, T., Ricciuto, D., Reichstein, M., Tomelleri, E., Trudinger, C. M., and Wijk, M. T. V.: The REFLEX project: Comparing different algorithms and implementations for the inversion of a terrestrial ecosystem model against eddy covariance data, *Agricultural and Forest Meteorology*, 149, 1597–1615, doi:10.1016/j.agrformet.2009.05.002, <http://www.sciencedirect.com/science/article/pii/S0168192309001014>, 2009.
- 35 Gilks, W. R.: Markov chain Monte Carlo in practice edited by W.R. Gilks, S. Richardson and D.J. Spiegelhalter., 1996.
- Glenn, E. P., Huete, A. R., Nagler, P. L., and Nelson, S. G.: Relationship between remotely-sensed vegetation indices, canopy attributes and plant physiological processes: what vegetation indices can and cannot tell us about the landscape, *Sensors*, 8, 2136–2160, 2008.

- Griffis, T. J., Zhang, J., Baker, J. M., Kljun, N., and Billmark, K.: Determining carbon isotope signatures from micrometeorological measurements: Implications for studying biosphere–atmosphere exchange processes, *Boundary-Layer Meteorology*, 123, 295–316, doi:10.1007/s10546-006-9143-8, <http://dx.doi.org/10.1007/s10546-006-9143-8>, 2007.
- Guilbaud, C. S. E., Dalchau, N., Purves, D. W., and Turnbull, L. A.: Is "peak N" key to understanding the timing of flowering in annual plants?, *New Phytologist*, pp. n/a–n/a, doi:10.1111/nph.13095, <http://dx.doi.org/10.1111/nph.13095>, 2014.
- Haxeltine, A. and Prentice, I. C.: BIOME3: An equilibrium terrestrial biosphere model based on ecophysiological constraints, resource availability, and competition among plant functional types, *Global Biogeochem. Cycles*, 10, 693–709, doi:10.1029/96GB02344, 1996.
- Herrmann, I., Pimstein, A., Karnieli, A., Cohen, Y., Alchanatis, V., and Bonfil, D.: LAI assessment of wheat and potato crops by VEN μ S and Sentinel-2 bands, *Remote Sensing of Environment*, 115, 2141–2151, 2011.
- Howard, D. M., Wylie, B. K., and Tieszen, L. L.: Crop classification modelling using remote sensing and environmental data in the Greater Platte River Basin, USA, *International Journal of Remote Sensing*, 33, 6094–6108, doi:10.1080/01431161.2012.680617, <http://dx.doi.org/10.1080/01431161.2012.680617>, 2012.
- Jamieson, P., Semenov, M., Brooking, I., and Francis, G.: Sirius: a mechanistic model of wheat response to environmental variation, *European Journal of Agronomy*, 8, 161 – 179, doi:[http://dx.doi.org/10.1016/S1161-0301\(98\)00020-3](http://dx.doi.org/10.1016/S1161-0301(98)00020-3), <http://www.sciencedirect.com/science/article/pii/S1161030198000203>, 1998.
- Johnson, M., Tingey, D., Phillips, D., and Storm, M.: Advancing fine root research with minirhizotrons, *Environmental and Experimental Botany*, 45, 263 – 289, doi:[http://dx.doi.org/10.1016/S0098-8472\(01\)00077-6](http://dx.doi.org/10.1016/S0098-8472(01)00077-6), <http://www.sciencedirect.com/science/article/pii/S0098847201000776>, 2001.
- Jones, J., Hoogenboom, G., Porter, C., Boote, K., Batchelor, W., Hunt, L., Wilkens, P., Singh, U., Gijsman, A., and Ritchie, J.: The {DSSAT} cropping system model, *European Journal of Agronomy*, 18, 235 – 265, doi:[http://dx.doi.org/10.1016/S1161-0301\(02\)00107-7](http://dx.doi.org/10.1016/S1161-0301(02)00107-7), <http://www.sciencedirect.com/science/article/pii/S1161030102001077>, <ce:title>Modelling Cropping Systems: Science, Software and Applications</ce:title>, 2003.
- Keenan, T. F., Davidson, E. A., Munger, J. W., and Richardson, A. D.: Rate my data: quantifying the value of ecological data for the development of models of the terrestrial carbon cycle, *Ecological Applications*, 23, 273–286, doi:10.1890/12-0747.1, <http://dx.doi.org/10.1890/12-0747.1>, 2012.
- Knorr, W., Kaminski, T., Scholze, M., Gobron, N., Pinty, B., Giering, R., and Mathieu, P.-P.: Carbon cycle data assimilation with a generic phenology model, *Journal of Geophysical Research*, 115, G04017–, doi:10.1029/2009JG001119, 2010.
- Lobell, D. B. and Field, C. B.: Global scale climate-crop yield relationships and the impacts of recent warming, *Environmental Research Letters*, 2, 014002, <http://stacks.iop.org/1748-9326/2/i=1/a=014002>, 2007.
- Lobell, D. B., Asner, G. P., Ortiz-Monasterio, J., and Benning, T. L.: Remote sensing of regional crop production in the Yaqui Valley, Mexico: estimates and uncertainties, *Agriculture, Ecosystems & Environment*, 94, 205 – 220, doi:10.1016/S0167-8809(02)00021-X, <http://www.sciencedirect.com/science/article/pii/S016788090200021X>, 2003.
- Lobell, D. B., Schlenker, W., and Costa-Roberts, J.: Climate Trends and Global Crop Production Since 1980, *Science*, 333, 616–620, doi:10.1126/science.1204531, <http://www.sciencemag.org/content/333/6042/616.abstract>, 2011.
- Meyers, T. P. and Hollinger, S. E.: An assessment of storage terms in the surface energy balance of maize and soybean, *Agricultural and Forest Meteorology*, 125, 105 – 115, doi:<http://dx.doi.org/10.1016/j.agrformet.2004.03.001>, <http://www.sciencedirect.com/science/article/pii/S0168192304000620>, 2004.

- Moors, E. J., Jacobs, C., Jans, W., Supit, I., Kutsch, W. L., Bernhofer, C., Beziat, P., Buchmann, N., Carrara, A., Ceschia, E., Elbers, J., Eugster, W., Kruijt, B., Loubet, B., Magliulo, E., Moureaux, C., Olioso, A., Saunders, M., and Soegaard, H.: Variability in carbon exchange of European croplands, *Agriculture, Ecosystems & Environment*, 139, 325 – 335, doi:<http://dx.doi.org/10.1016/j.agee.2010.04.013>, <http://www.sciencedirect.com/science/article/pii/S0167880910001210>, the carbon balance of European croplands, 2010.
- Osborne, T., Gornall, J., Hooker, J., Williams, K., Wiltshire, A., Betts, R., and Wheeler, T.: JULES-crop: a parametrisation of crops in the Joint UK Land Environment Simulator, *Geoscientific Model Development*, 8, 1139–1155, doi:10.5194/gmd-8-1139-2015, <http://www.geosci-model-dev.net/8/1139/2015/>, 2015.
- Pendall, E., Bridgham, S., Hanson, P. J., Hungate, B., Kicklighter, D. W., Johnson, D. W., Law, B. E., Luo, Y., Megonigal, J. P., Olsrud, M., Ryan, M. G., and Wan, S.: Below-ground process responses to elevated CO₂ and temperature: a discussion of observations, measurement methods, and models, *New Phytologist*, 162, 311–322, doi:10.1111/j.1469-8137.2004.01053.x, <http://dx.doi.org/10.1111/j.1469-8137.2004.01053.x>, 2004.
- Porter, J. R. and Semenov, M. A.: Crop Responses to Climatic Variation, *Philosophical Transactions: Biological Sciences*, 360, pp. 2021–2035, <http://www.jstor.org/stable/30041392>, 2005.
- Potter, P., Ramankutty, N., Bennett, E. M., and Donner, S. D.: Characterizing the Spatial Patterns of Global Fertilizer Application and Manure Production, *Earth Interactions*, 14, 1–22, doi:10.1175/2009EI288.1, <http://dx.doi.org/10.1175/2009EI288.1>, 2010.
- Raupach, M., Rayner, P., Barrett, D., DeFries, R., Heimann, M., Ojima, D., Quegan, S., and Schimmlus, C.: Model-data synthesis in terrestrial carbon observation: methods, data requirements and data uncertainty specifications., *Global Change Biology*, 11, 378–397, <http://search.ebscohost.com/login.aspx?direct=true&db=eih&AN=16479815&site=ehost-live>, 2005.
- Reichstein, M., Falge, E., Baldocchi, D., Papale, D., Aubinet, M., Berbigier, P., Bernhofer, C., Buchmann, N., Gilmanov, T., Granier, A., Grünwald, T., Havránková, K., Ilvesniemi, H., Janous, D., Knohl, A., Laurila, T., Lohila, A., Loustau, D., Matteucci, G., Meyers, T., Miglietta, F., Ourcival, J.-M., Pumpanen, J., Rambal, S., Rotenberg, E., Sanz, M., Tenhunen, J., Seufert, G., Vaccari, F., Vesala, T., Yakir, D., and Valentini, R.: On the separation of net ecosystem exchange into assimilation and ecosystem respiration: review and improved algorithm, *Global Change Biology*, 11, 1424–1439, <http://dx.doi.org/10.1111/j.1365-2486.2005.001002.x>, 2005.
- Revill, A., Sus, O., Barrett, B., and Williams, M.: Carbon cycling of European croplands: A framework for the assimilation of optical and microwave Earth observation data, *Remote Sensing of Environment*, 137, 84 – 93, doi:<http://dx.doi.org/10.1016/j.rse.2013.06.002>, <http://www.sciencedirect.com/science/article/pii/S0034425713001879>, 2013.
- Rienecker, M. M., Suarez, M. J., Gelaro, R., Todling, R., Bacmeister, J., Liu, E., Bosilovich, M. G., Schubert, S. D., Takacs, L., Kim, G.-K., Bloom, S., Chen, J., Collins, D., Conaty, A., da Silva, A., Gu, W., Joiner, J., Koster, R. D., Lucchesi, R., Molod, A., Owens, T., Pawson, S., Pegion, P., Redder, C. R., Reichle, R., Robertson, F. R., Ruddick, A. G., Sienkiewicz, M., and Woollen, J.: MERRA: NASA's Modern-Era Retrospective Analysis for Research and Applications, *J. Climate*, 24, 3624–3648, doi:10.1175/JCLI-D-11-00015.1, <http://dx.doi.org/10.1175/JCLI-D-11-00015.1>, 2011.
- Rosegrant, M. W. and Cline, S. A.: Global Food Security: Challenges and Policies, *Science*, 302, 1917–1919, doi:10.1126/science.1092958, <http://science.sciencemag.org/content/302/5652/1917>, 2003.
- Rosenzweig, C., Jones, J., Hatfield, J., Ruane, A., Boote, K., Thorburn, P., Antle, J., Nelson, G., Porter, C., Janssen, S., Asseng, S., Basso, B., Ewert, F., Wallach, D., Baigorria, G., and Winter, J.: The Agricultural Model Intercomparison and Improvement Project (AgMIP): Protocols and pilot studies, *Agricultural and Forest Meteorology*, 170, 166 – 182, doi:<http://dx.doi.org/10.1016/j.agrformet.2012.09.011>, <http://www.sciencedirect.com/science/article/pii/S0168192312002857>, agricultural prediction using climate model ensembles, 2013.

- Rosenzweig, C., Elliott, J., Deryng, D., Ruane, A. C., Müller, C., Arneth, A., Boote, K. J., Folberth, C., Glotter, M., Khabarov, N., et al.:
5 Assessing agricultural risks of climate change in the 21st century in a global gridded crop model intercomparison, *Proceedings of the
National Academy of Sciences*, 111, 3268–3273, 2014.
- Sacks, W. J., Deryng, D., Foley, J. A., and Ramankutty, N.: Crop planting dates: an analysis of global patterns, *Global Ecology and Biogeog-
raphy*, 19, 607–620, doi:10.1111/j.1466-8238.2010.00551.x, <http://dx.doi.org/10.1111/j.1466-8238.2010.00551.x>, 2010.
- Schlenker, W. and Roberts, M. J.: Nonlinear temperature effects indicate severe damages to U.S. crop yields under
10 climate change, *Proceedings of the National Academy of Sciences*, 106, 15 594–15 598, doi:10.1073/pnas.0906865106,
<http://www.pnas.org/content/106/37/15594.abstract>, 2009.
- Schmidhuber, J. and Tubiello, F. N.: Global food security under climate change, *Proceedings of the National Academy of Sciences*, 104,
19 703–19 708, doi:10.1073/pnas.0701976104, <http://www.pnas.org/content/104/50/19703.abstract>, 2007.
- Stackle, C. O., Donatelli, M., and Nelson, R.: CropSyst, a cropping systems simulation model, *European Journal of Agronomy*, 18,
15 289 – 307, doi:[http://dx.doi.org/10.1016/S1161-0301\(02\)00109-0](http://dx.doi.org/10.1016/S1161-0301(02)00109-0), <http://www.sciencedirect.com/science/article/pii/S1161030102001090>,
<ce:title>Modelling Cropping Systems: Science, Software and Applications</ce:title>, 2003.
- Sus, O., Heuer, M. W., Meyers, T. P., and Williams, M.: A data assimilation framework for constraining upscaled crop-
land carbon flux seasonality and biometry with MODIS, *Biogeosciences*, 10, 2451–2466, doi:10.5194/bg-10-2451-2013,
<http://www.biogeosciences.net/10/2451/2013/>, 2013.
- 20 Suyker, A., Verma, S., Burba, G., Arkebauer, T., Walters, D., and Hubbard, K.: Growing season carbon dioxide exchange in irri-
gated and rainfed maize, *Agricultural and Forest Meteorology*, 124, 1 – 13, doi:<http://dx.doi.org/10.1016/j.agrformet.2004.01.011>,
<http://www.sciencedirect.com/science/article/pii/S0168192304000188>, 2004.
- Thenkabail, P. S.: Optimal hyperspectral narrowbands for discriminating agricultural crops, *Remote Sensing Reviews*, 20, 257–291,
doi:10.1080/02757250109532439, 2001.
- 25 Tucker, C. J., Pinzon, J. E., Brown, M. E., Slayback, D. A., Pak, E. W., Mahoney, R., Vermote, E. F., and El Saleous, N.: An extended AVHRR
8 km NDVI dataset compatible with MODIS and SPOT vegetation NDVI data, *International Journal of Remote Sensing*, 26, 4485–4498,
doi:10.1080/01431160500168686, <http://www.tandfonline.com/doi/abs/10.1080/01431160500168686>, 2005.
- Von Caemmerer, S.: *Biochemical models of leaf photosynthesis*, 2, Csiro publishing, 2000.
- Wardlow, B. D., Egbert, S. L., and Kastens, J. H.: Analysis of time-series MODIS 250 m vegetation index
30 data for crop classification in the U.S. Central Great Plains, *Remote Sensing of Environment*, 108, 290–310,
<http://www.sciencedirect.com/science/article/pii/S0034425706004949>, 2007.
- Xiao, J., Zhuang, Q., Law, B. E., Baldocchi, D. D., Chen, J., Richardson, A. D., Melillo, J. M., Davis, K. J., Hollinger, D. Y., Wharton,
S., Oren, R., Noormets, A., Fischer, M. L., Verma, S. B., Cook, D. R., Sun, G., McNulty, S., Wofsy, S. C., Bolstad, P. V., Burns, S. P.,
Curtis, P. S., Drake, B. G., Falk, M., Foster, D. R., Gu, L., Hadley, J. L., Katul, G. G., Litvak, M., Ma, S., Martin, T. A., Matamala, R.,
35 Meyers, T. P., Monson, R. K., Munger, J. W., Oechel, W. C., Paw, U. K. T., Schmid, H. P., Scott, R. L., Starr, G., Suyker, A. E., and
Torn, M. S.: Assessing net ecosystem carbon exchange of U.S. terrestrial ecosystems by integrating eddy covariance flux measurements
and satellite observations, *Agricultural and Forest Meteorology*, 151, 60 – 69, doi:<http://dx.doi.org/10.1016/j.agrformet.2010.09.002>,
<http://www.sciencedirect.com/science/article/pii/S0168192310002479>, 2011.
- Ziehn, T., Scholze, M., and Knorr, W.: On the capability of Monte Carlo and adjoint inversion techniques to derive posterior parameter
uncertainties in terrestrial ecosystem models, *Global Biogeochem. Cycles*, 26, GB3025–, doi:10.1029/2011GB004185, 2012.

Table 1. Study sites. All sites correspond to eddy covariance measurement sites

Site name	Coordinates	Crop	Country	Irrigation	Reference
Mead 1	41.1651,-96.4766	Maize	United States	Irrigated	Suyker et al. (2004)
Mead 2	41.1651,-96.4766	Maize rotation	United States	Irrigated	Suyker et al. (2004)
Mead3	41.1651,-96.4766	Maize rotation	United States	Rainfed	Suyker et al. (2004)
Bondville	40.0062,-88.2904	Maize rotation	United States	Rainfed	Meyers and Hollinger (2004)
Rosemount 1	44.7217,-93.0893	Maize rotation	United States	N/A	Griffis et al. (2007)
Rosemount 3	44.7217,-93.0893	Maize rotation	United States	N/A	Griffis et al. (2007)
Fermi	41.8593,-88.2227	Maize rotation	United States	N/A	-
ARM Great Plains	36.6058,-97.4889	wheat	United States	N/A	Fischer et al. (2007)
Risbyholm	55.5303,12.0972	Wheat rotation	Denmark	Rainfed	Moors et al. (2010)
Auralde	43.5494,1.1078	Wheat rotation	France	N/A	Moors et al. (2010)
Gebesee	51.1001,10.9143	wheat rotation	Germany	Rainfed	Moors et al. (2010)
Grignon	48.844,1.9524	wheat rotation	France	Rainfed	Moors et al. (2010)
Klingenberg	50.8929,13.5225	wheat rotation	Germany	Rainfed	Moors et al. (2010)
Lonze	50.5522,4.7448	wheat rotation	Belgium	Rainfed	Moors et al. (2010)
Lutjewad	53.3833,6.3667	wheat rotation	Netherlands	Rainfed	Moors et al. (2010)

Zwart, S. J. and Bastiaanssen, W. G.: Review of measured crop water productivity values for irrigated wheat, rice, cotton and maize, *Agricultural Water Management*, 69, 115 – 133, doi:<http://dx.doi.org/10.1016/j.agwat.2004.04.007>, <http://www.sciencedirect.com/science/article/pii/S0378377404001416>, 2004.

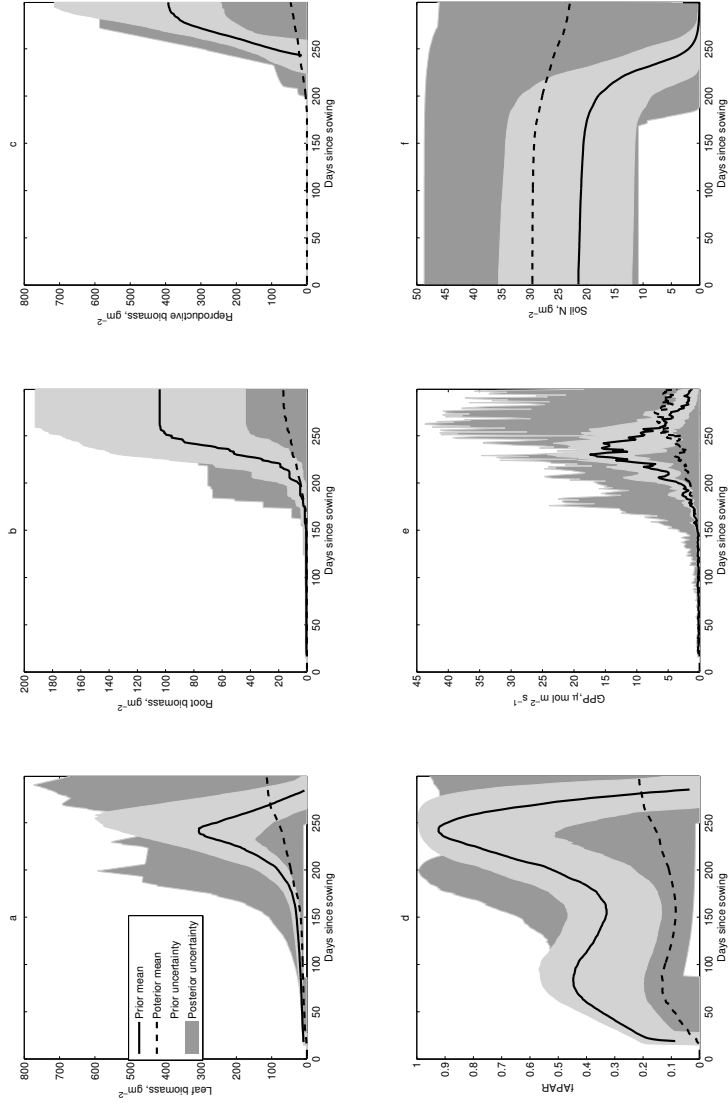


Figure 1. Comparison of prior model predictions (dark grey, dashed line) and posterior model predictions (light grey, continuous line) at one wheat (DK-Ris) site. Panels show (a) Aboveground biomass, (b) belowground biomass, (c) Reproductive biomass, (d) fAPAR, (e) GPP and (f) soil nitrogen.)

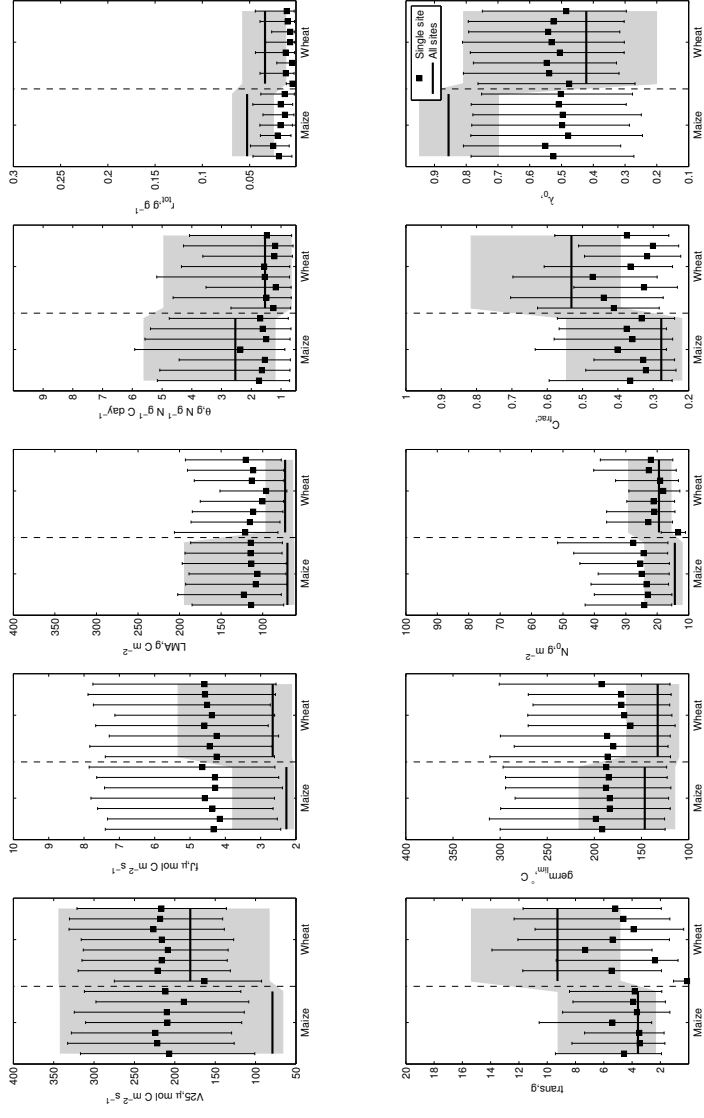


Figure 2. Estimated model parameters for all sites, fitted to individual locations (circles) and all locations combined (black line). Values are posterior medians and error bars and shaded areas represent 95th percentiles of the posterior parameter distribution for the one site and all sites parametrised respectively.

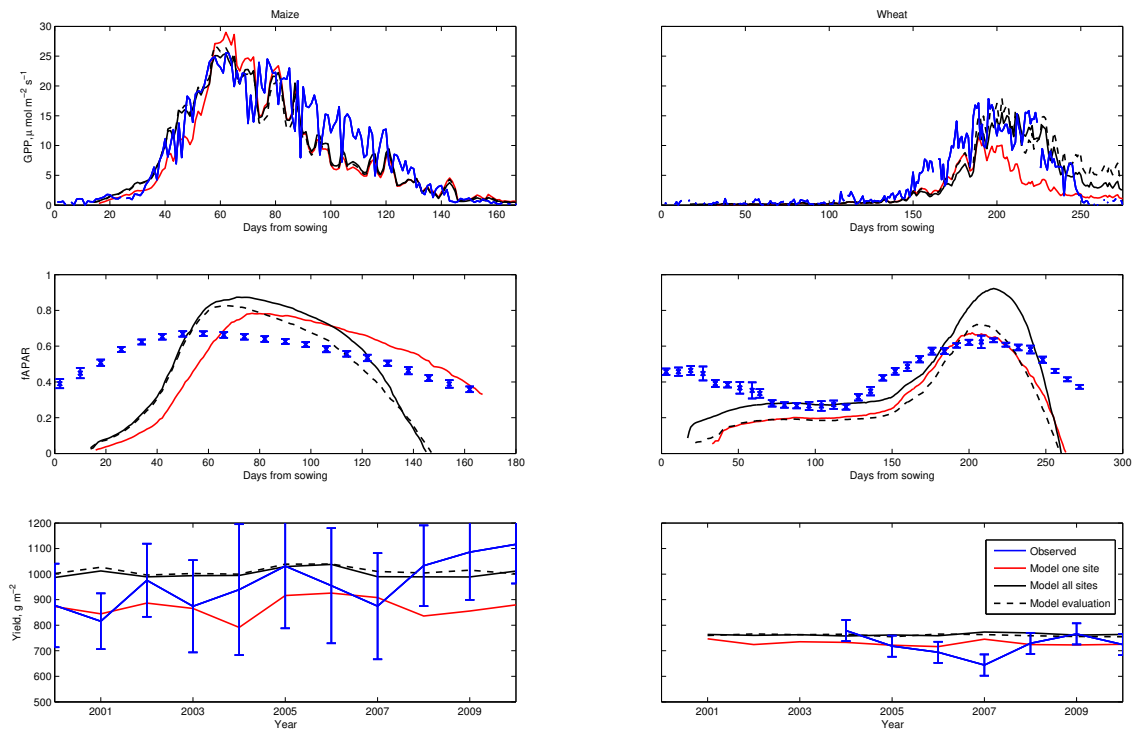


Figure 3. GPP, fAPAR and yield model predictions at one maize (US-Ro3) and one wheat (DE-Gri) site. Figure shows posterior mean predictions for the one site, all site and evaluation model fit. Neither site has been included in the evaluation fitting.

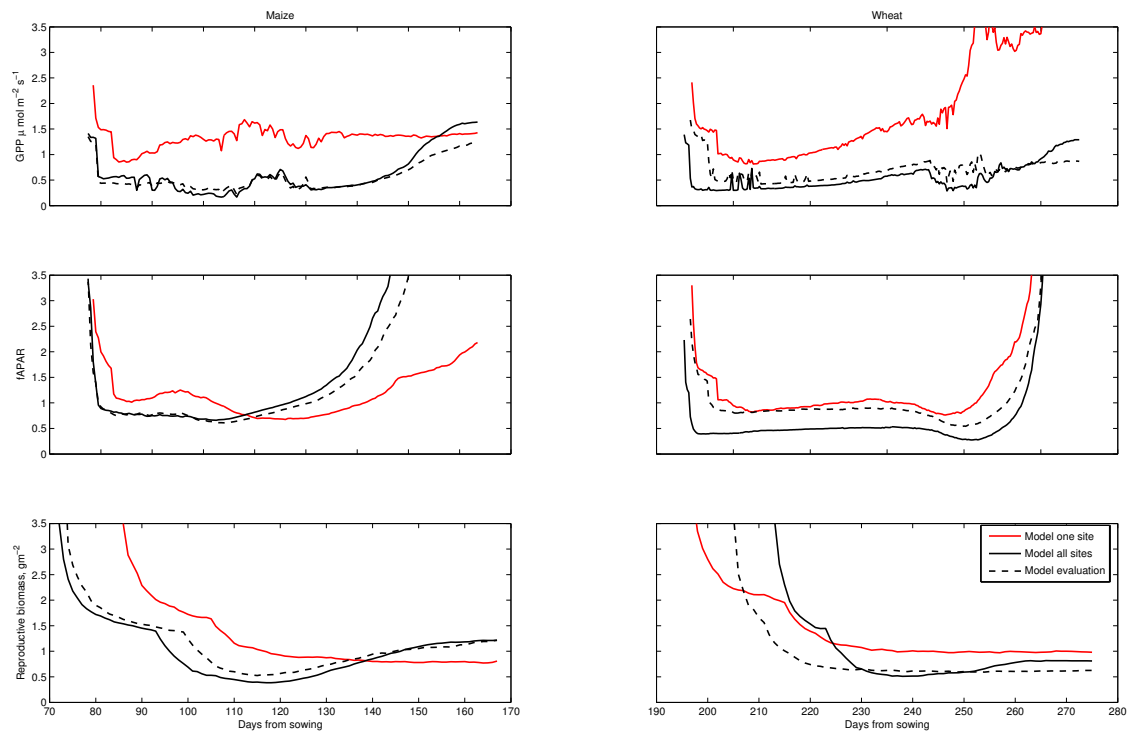


Figure 4. Normalised uncertainty for GPP, fAPAR and yield model predictions at one maize (US-Ro3) and one wheat (DE-Gri) site. Uncertainty is calculated as 95th percentile confidence bounds normalised by the posterior mean for the one site, all site and evaluation model fit. Neither site has been included in the evaluation fitting.

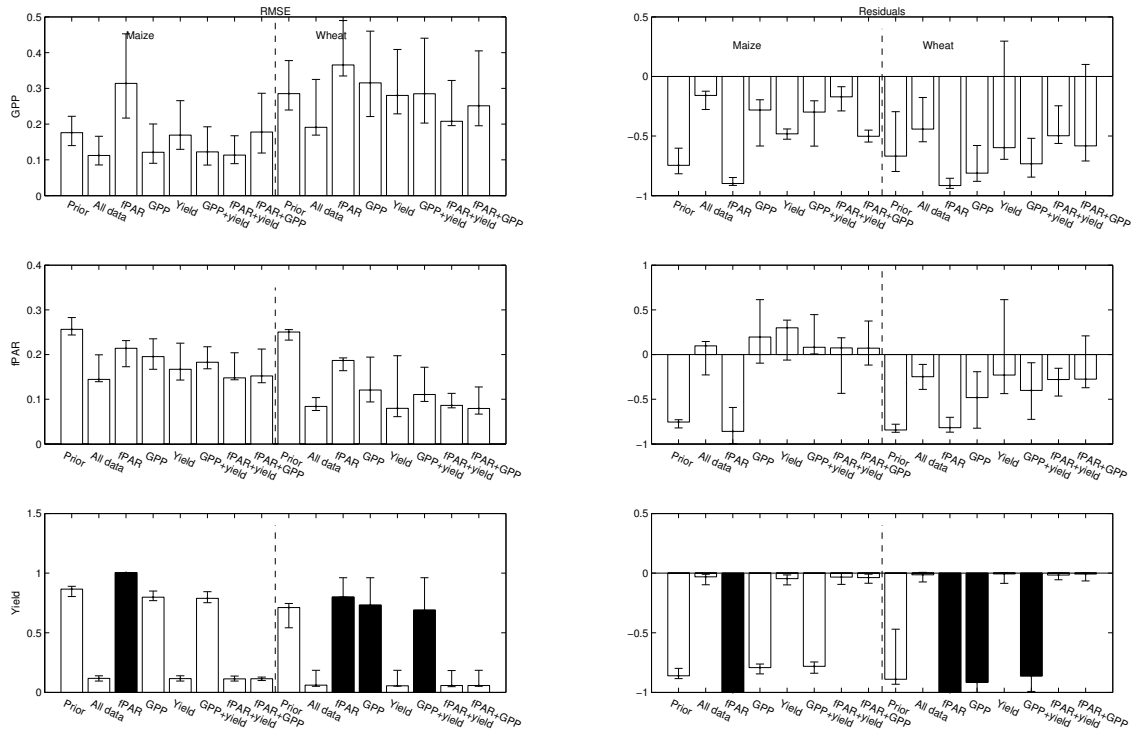


Figure 5. Model RMSE and bias for all data hold out experiments averaged over all wheat and maize sites respectively. Error bars represent variation across sites. All values have been normalised to the mean value of that variable at each site. Black bars indicate models that do not reach flowering.

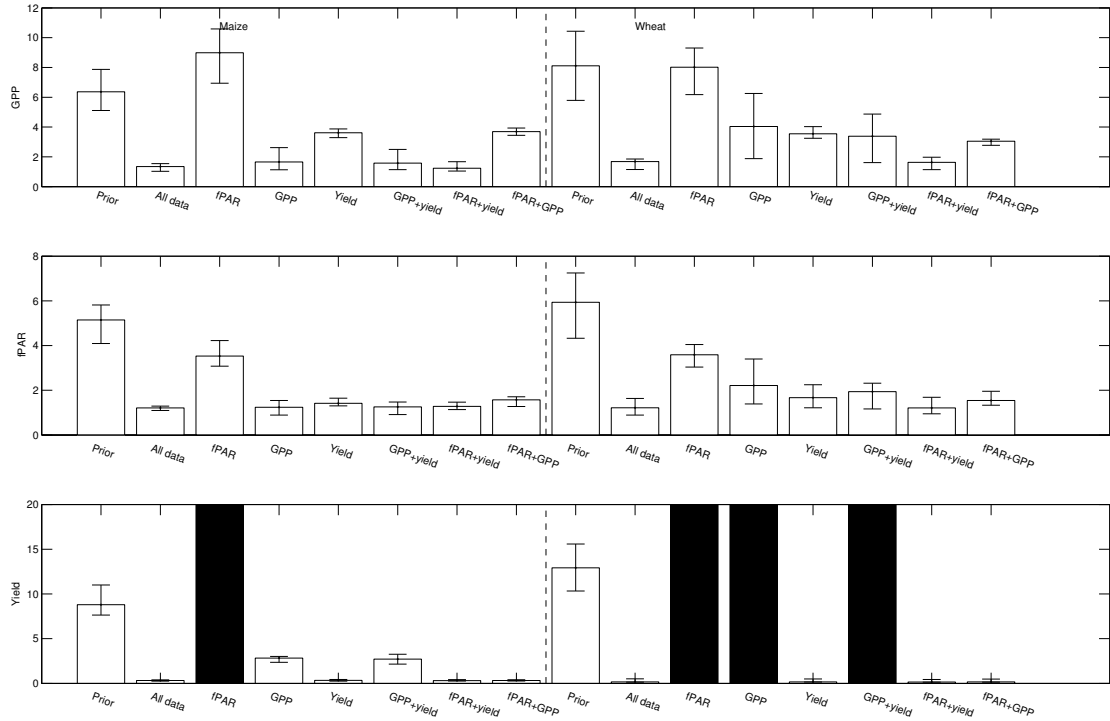


Figure 6. Model uncertainty, expressed as the difference between the upper and lower 95th confidence intervals for all model setups averaged across all wheat and maize sites. Error bars represent variation between sites. All values have been normalised. Black bars indicate models that do not reach flowering.

Table 2. Model parameters

Symbol	Units	Description
$germ_{lim}$	°C	Number of degree days required for germination
Tb_{germ}	°C	Base temperature for germination
ρ	-	Optimal carbon to nitrogen ratio in vegetative tissue
N_0	g	Initial N content of the soil
θ	$g\ N\ g^{-1}\ N\ g^{-1}\ C\ day^{-1}$	Root nitrogen extraction factor
$V25$	$\mu mol\ m^{-2}\ s^{-1}$	Photosynthetic carboxylation capacity at 25°C
λ_0	-	Ratio of atmospheric and leaf CO ₂ concentration
lma	$g\ m^{-2}$	Leaf mass per area
r_{tot}	$g\ g^{-1}$	Average plant respiration rate
m_{trans}	$g\ day^{-1}$	Mass translocation rate from vegetative to reproductive tissue
C_{frac}	-	Carbon fraction of reproductive tissue
p_{\sim}	<u>days</u>	<u>Time period for averaging environmental conditions for flowering trigger</u>

Table 3. Model RMSE, bias and uncertainty for the one site and all site parametrisation as well as the model evaluation run

	RMSE GPP	RMSE fAPAR	RMSE yield	Bias GPP	Bias fAPAR	Bias yield	Uncertainty GPP	Uncertainty fAPAR	Uncertainty yield
Maize									
Prior	0.18	0.27	0.83	-0.77	-0.79	-0.82	7.07	5.15	9.87
One site	0.11	0.14	0.12	-0.16	0.10	-0.03	1.34	1.21	0.33
All sites	0.08	0.16	0.10	-0.12	-0.04	-0.00	0.45	1.02	0.12
Evaluation	0.09	0.15	0.11	-0.10	-0.09	-0.00	0.47	1.08	0.15
Wheat									
Prior	0.27	0.25	0.67	-0.64	-0.83	-0.83	7.92	5.46	12.27
One site	0.19	0.08	0.06	-0.44	-0.25	-0.01	1.68	1.21	0.16
All sites	0.17	0.08	0.07	-0.21	0.02	0.02	0.51	0.45	0.06
Evaluation	0.17	0.09	0.07	-0.05	-0.26	0.02	0.75	0.89	0.08

Table 4. RMSE, bias and uncertainty values the data knock out experiments for wheat and maize.

Data fitted to	RMSE GPP	RMSE fAPAR	RMSE yield	Bias GPP	Bias fAPAR	Bias yield	Uncertainty GPP	Uncertainty fAPAR	Uncertainty yield
Maize									
Prior	0.18	0.26	0.85	-0.75	-0.79	-0.85	6.91	5.19	9.25
All data	0.11	0.14	0.12	-0.16	0.10	-0.03	1.34	1.21	0.33
fAPAR	0.31	0.21	1.00	-0.90	-0.86	-1.00	8.99	3.53	-
GPP	0.12	0.20	0.80	-0.28	0.20	-0.79	1.66	1.24	2.83
yield	0.17	0.17	0.12	-0.48	0.30	-0.05	3.61	1.42	0.33
GPP+yield	0.12	0.18	0.79	-0.30	0.08	-0.78	1.58	1.26	2.72
fAPAR+yield	0.11	0.15	0.11	-0.17	0.07	-0.03	1.23	1.28	0.31
fAPAR+GPP	0.18	0.15	0.11	-0.50	0.07	-0.04	3.69	1.57	0.32
wheat									
Prior	0.28	0.25	0.70	-0.66	-0.84	-0.88	8.49	5.90	12.98
All data	0.19	0.08	0.06	-0.44	-0.25	-0.01	1.68	1.21	0.16
fAPAR	0.37	0.19	0.80	-0.92	-0.82	-1.00	8.02	3.59	-
GPP	0.32	0.12	0.73	-0.81	-0.48	-0.92	4.04	2.21	-
yield	0.28	0.08	0.06	-0.60	-0.23	-0.01	3.55	1.67	0.16
GPP+yield	0.28	0.11	0.69	-0.73	-0.40	-0.86	3.38	1.94	-
fAPAR+yield	0.21	0.09	0.06	-0.50	-0.28	-0.02	1.63	1.21	0.16
fAPAR+GPP	0.25	0.08	0.06	-0.58	-0.27	-0.01	3.05	1.55	0.16

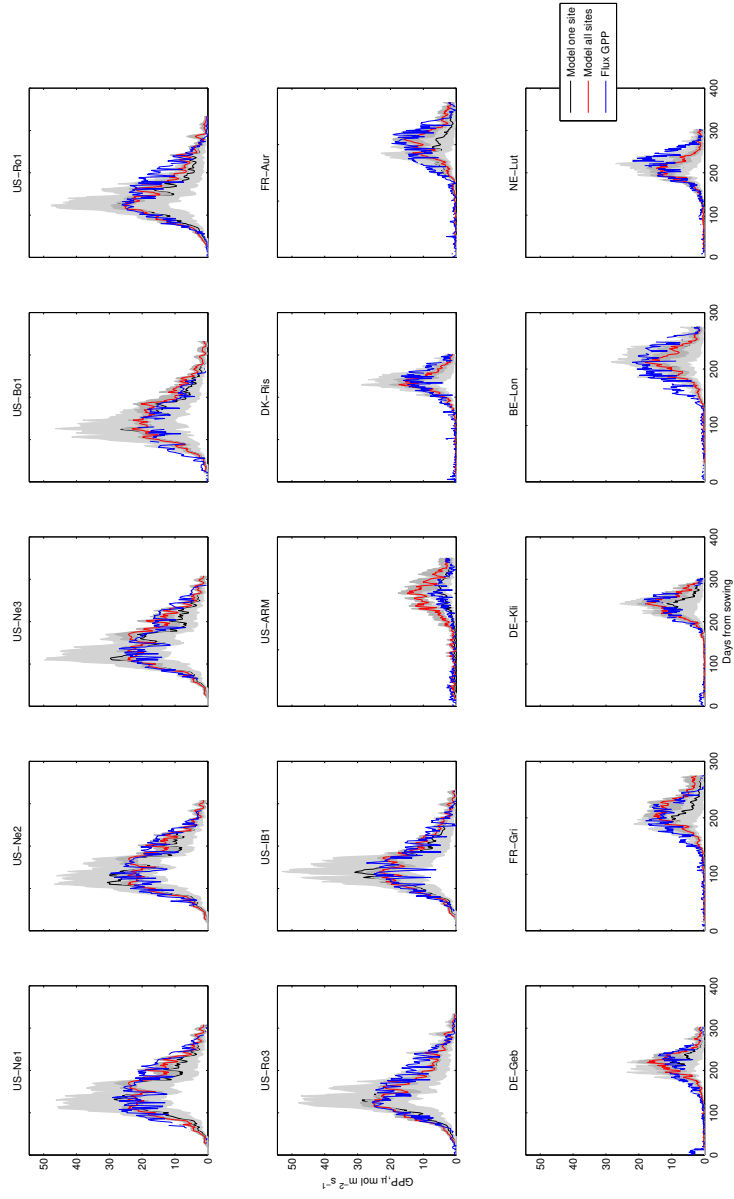


Figure A1. Gross primary production predictions for one year for all sites fitted using all available data at each individual site and at all sites together. Gray shaded areas represent 95% confidence intervals drawn from the posterior distribution.

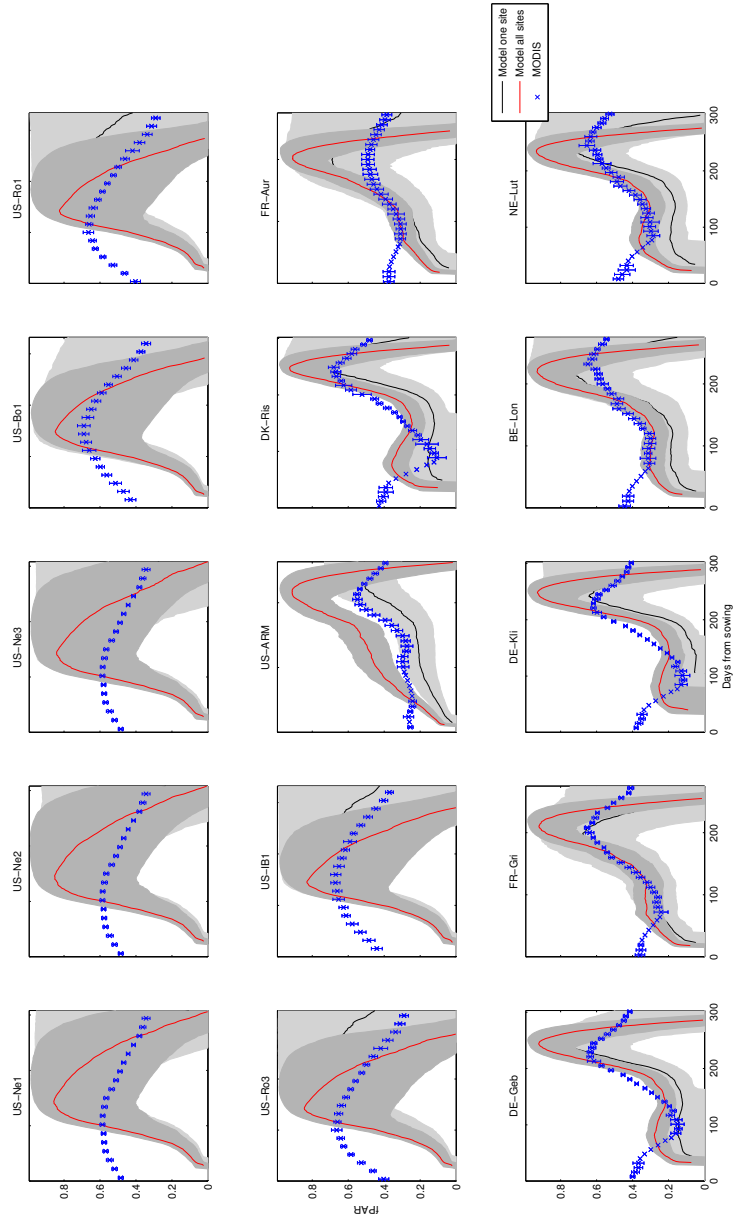


Figure A2. fAPAR predictions for one year for all sites fitted using all available data at each individual site and at all sites together. Gray shaded areas represent 95% confidence intervals drawn from the posterior distribution.

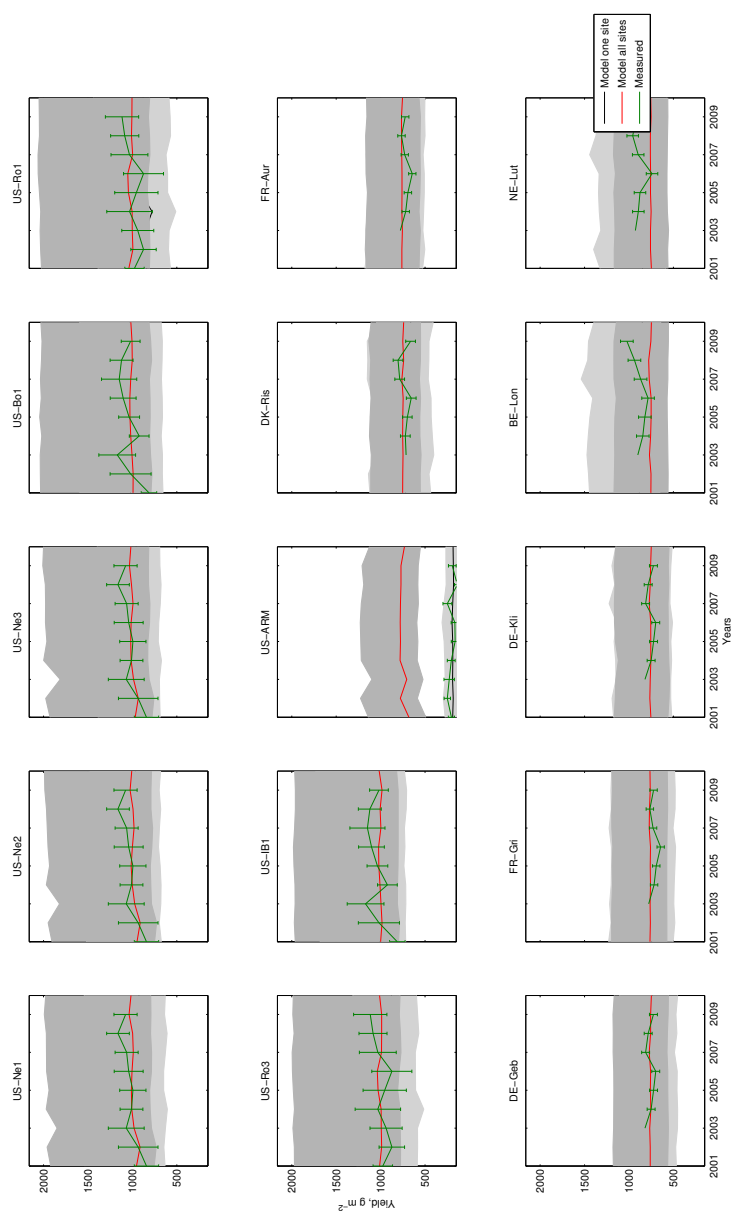


Figure A3. yield predictions for all years for all sites fitted using all available data at each individual site and at all sites together. Gray shaded areas represent 95% confidence intervals drawn from the posterior distribution.

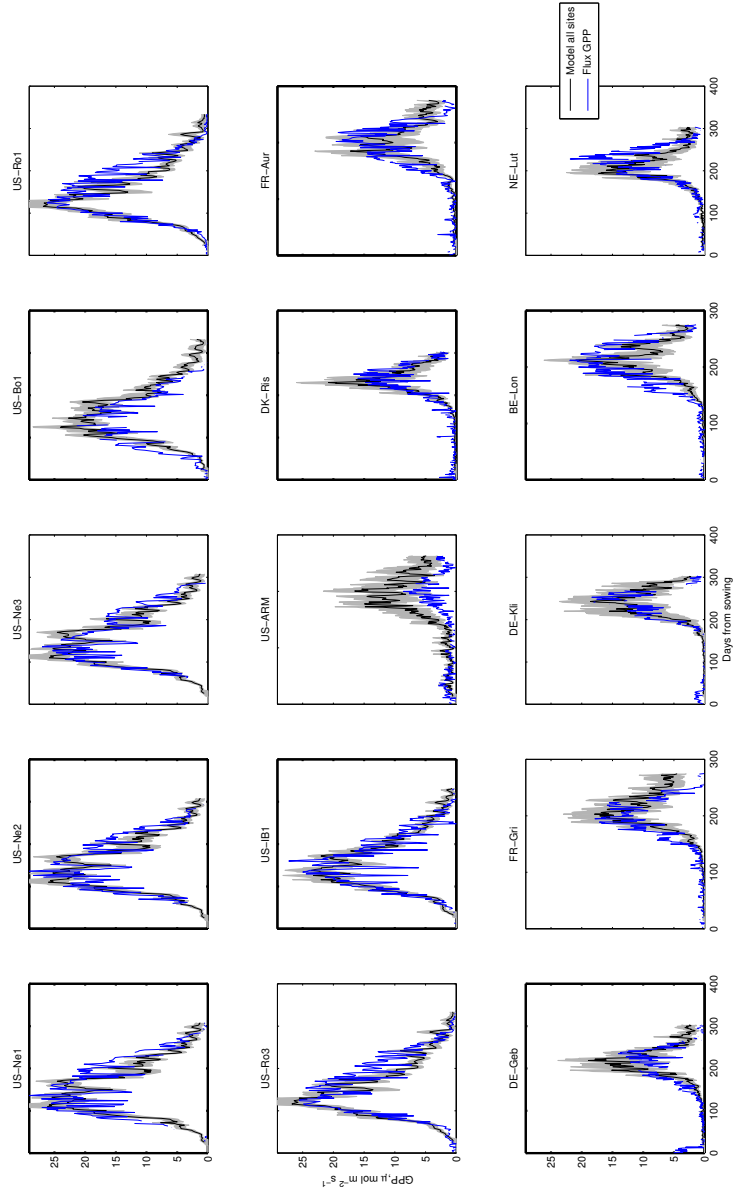


Figure A4. Gross primary production predictions for one year for all sites fitted using all available data at a subset of sites for model evaluation. Sites with black boxes have been used in the model fitting. Gray shaded areas represent 95% confidence intervals drawn from the posterior distribution.

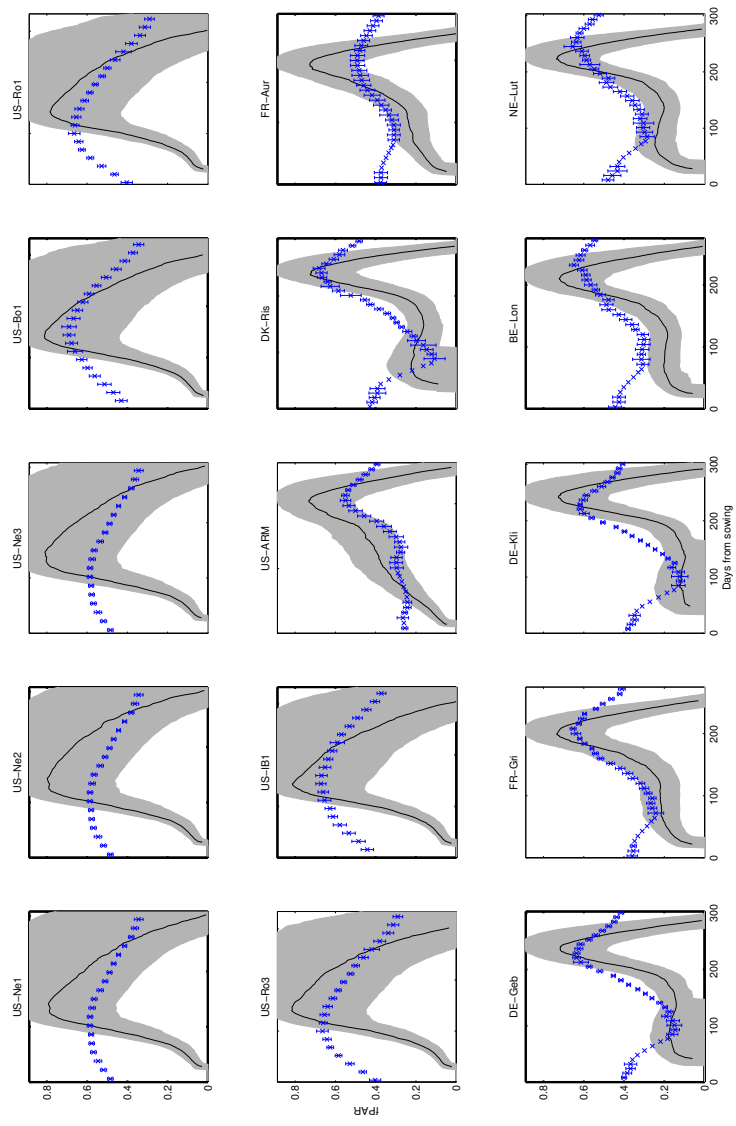


Figure A5. fAPAR predictions for one year for all sites fitted using all available data at a subset of sites for model evaluation. Sites with black boxes have been used in the model fitting. Gray shaded areas represent 95% confidence intervals drawn from the posterior distribution.

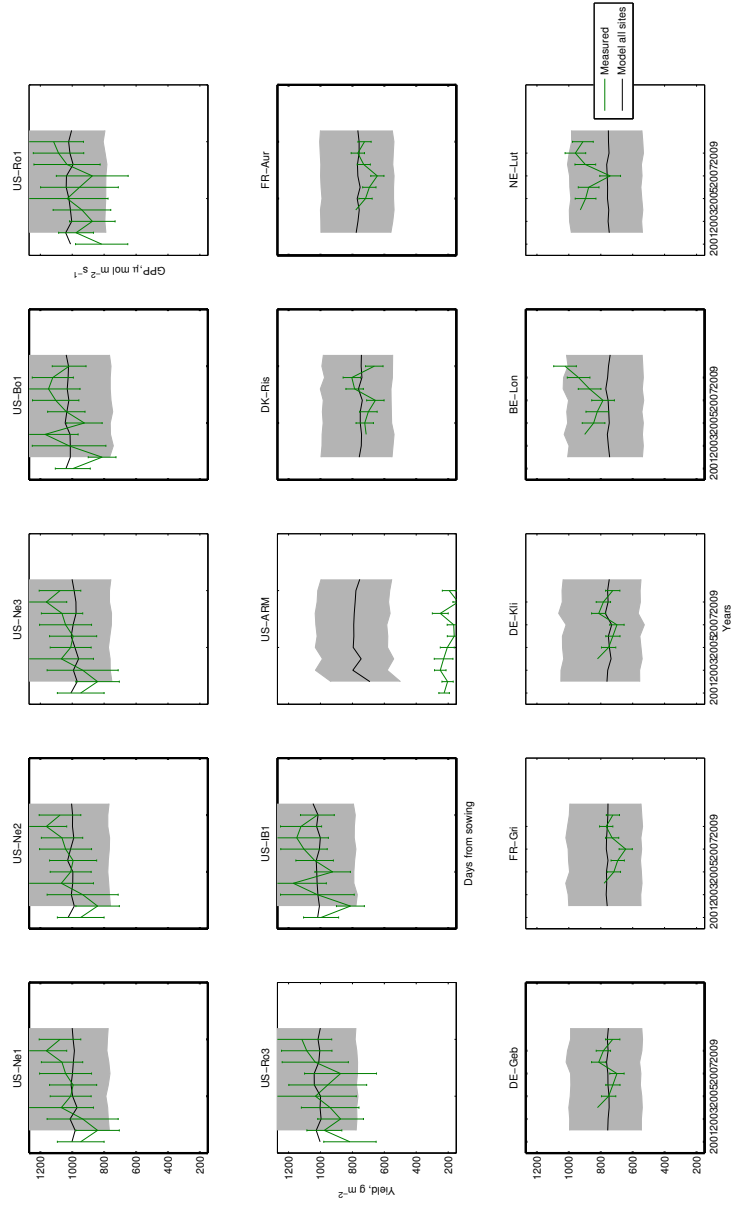


Figure A6. yield predictions for all years for all sites fitted using all available data at a subset of sites for model evaluation. Sites with black boxes have been used in the model fitting. Gray shaded areas represent 95% confidence intervals drawn from the posterior distribution.