

hess-2016-195

**“Integrated validation of assimilating satellite derived observations over France using a hydrological model”
by D. Fairbairn et al.**

New title: “*The effect of satellite-derived surface soil moisture and leaf area index land data assimilation on streamflow simulations over France*”

1 March 2017.

Dear Professor Wolfgang Wagner,

The authors’ response to the comments of the two anonymous referees have been accounted for in the revised version of the paper.

All changes relative to the previous version of the paper are detailed in the pdf of the new manuscript. They include all the response elements given by the authors in response to the reviewers’ comments: blue and red for Reviewers 1 and 2 respectively (other changes are in green).

The Discussion and Conclusion sections were re-written. Title was changed as suggested by Reviewer 1.

Five new Figures were included in the Supplement in order to address issues mentioned by Reviewer 1.

Yours sincerely,

JC Calvet, D. Fairbairn.

Response to comments from Referee 1

March 2, 2017

We would like to thank the reviewer for their constructive comments. The corrections in the revised manuscript for Referee 1 are marked in blue.

Response to major comments:

1

1.1

Referee comment - *The introduction sounds like a twisted excuse to not follow recent advances in land surface data assimilation and to get away with a suboptimal system. Please acknowledge the true state-of-the-art: a) P.2, L29: one (?) study found no advantage of 2D Kalman filtering over 1D Kalman filtering. Maybe. Yet, very many other studies use 2D/3D Kalman filtering and that is the only correct way of doing Kalman filtering if we deal with different spatial resolutions. b) The SEKF may be a preferred method at some operational centers, but in most other centers, there is a push towards the EnKF.*

Response:

The introduction was changed in response to the previous round of reviews in order to justify our use of the SEKF. As of yet we have found no evidence that the 1D EnKF performs better than the SEKF (in terms of root-zone soil moisture) for our LSM, although we have only tested the EnKF on a dozen sites (Fairbairn et al., 2015). But the reviewer is right that we should not have implied that the SEKF is superior to the EnKF, so we have given a more balanced discussion in the introduction of the revised paper. On page 3, line 2 of the revised manuscript: “The SEKF simplifies the EKF by using fixed and uncorrelated background errors at the start of each cycle. Importantly, the SEKF generates flow-dependence and implicit background-error covariances from additional model integrations in the observation operator Jacobian calculations. Draper et al. (2009) found the flow-dependence from a 24-hour assimilation window

was sufficient to enable the SEKF to perform similarly to an EKF (which cycles the background-error covariance). Likewise, Muñoz Sabater et al. (2007); Fairbairn et al. (2015) found that the SEKF and EnKF performed similarly, in spite of different linear assumptions.”

In future research, the EnKF could still be attractive as it can be designed to account for model/forcing errors and 2D background-error covariances. However, as already discussed in our paper and evidenced in the literature (e.g. Maggioni et al. (2012); Gruber et al. (2015); Fairbairn et al. (2015)), the EnKF has its own set of challenges to overcome including its own linear assumptions. Therefore we must also be cautious about recommending it. In the revised manuscript we have mentioned in the discussion and in the conclusion that we need to test the EnKF over France in the context of the SIM hydrological model. On page 17, line 28: “Fairbairn et al. (2015) found that an EnKF with a simple stochastic rainfall error estimation demonstrated similar WG2 scores to the SEKF over 12 sites in southwest France (validated using in situ observations). Both methods were also affected by nonlinearity problems. We intend to test an EnKF over France using a similar validation employed in this study.”

1.2

Referee comment - *Why did the authors continue to use the SEKF without (or w/ minimal) alterations and then run into the same problems as already reported in Draper et al. (2011)? One of the conclusions is that an EnKF and assimilation in a slightly deeper surface soil layer may alleviate the problems that are experienced in this paper: trying out these recommendations would be food for a paper, but rerunning the same problems, is not so nice.*

Response:

We use the SEKF because it is the most mature technique developed for land surface data assimilation within SURFEX. Our intention was to validate this system at a large scale by using independent streamflow observations.

The paper by Draper et al. (2011) partly motivated our experiments, but there would be no point trying to recreate their results. The novelty of our work consists of 1) assimilation of LAI and demonstration of its impact on the soil moisture fluxes and 2) validation of our experiments using streamflow observations. We also examine some issues regarding the model (and the resulting influence on the fluxes), namely the underestimated LAI minimum and a systematic overestimation of the radiative forcing. This is made clear now in the introduction (pages 3 and 4).

1.3

Referee comment *Would the EnKF really help, as suggested in the abstract? The introduction says that the EnKF and SEKF produce results with similar accuracies. (p.3 L13).*

Response:

Please see response to Question 1.1.

1.4

Referee comment *The model is run at 8 km, the ASCAT data are at 25 km, the LAI data are at 1 km resolution. Data assimilation should take care of these spatial discrepancies, especially to downscale the coarser data to the finer resolution. A priori interpolation just does not make sense: this adds unnecessary errors and the subsequent 1D assimilation wrongly assumes that spatially independent observations are assimilated, while in reality there is a perfect oversampling with perfect spatial error correlations. The latter is especially a problem when (p.7, L26) the SEKF analysis is calculated independently for each patch, with the same obs used for all patches in the grid-box.*

Response:

We agree with the reviewer that interpolation errors would be introduced regardless of the approach we employ, even if we interpolated the model gridpoints to the observation grid in the SEKF analysis. Please note that one line 5 of page 6 of the revised manuscript we have added the following sentence: “After screening, the data were projected onto the 8 km resolution model grid by averaging all the data within 0.15 degrees of each gridpoint (Barbu et al., 2014).” Then it is considered that there is not a perfect oversampling because each gridpoint uses a different set of observations, albeit with some overlap.

Also the sentence: SEKF analysis is calculated independently for each patch, with the same obs used for all patches in the grid-box. (line 14, page 8) was changed to: The SEKF analysis is calculated independently for each patch using the Jacobians for each individual patch but with one mean observation per grid box.

1.5

Referee comment *If the spatial errors are discarded, then the observation error variance should at least be increased which is done, but far too little to make any difference (i.e. from 0.050 to 0.055 m³/m³). In addition, the observation error should be adjusted in line with the rescaling and be spatially variable if the same obs is used for different vegetation classes. Yet, there is no linkage between obs errors and vegetation class in*

this paper.

Response:

We agree that the observation error variance should be increased in our case from 0.050 to 0.055 m³/m³. This reduces the WG2 analysis increments by about 10%. This has been clarified on line 21, page 8 of the revised manuscript.

One has to be aware that the vegetation class concept implies already the definition of a mean land use type. The LAI observations have an original resolution of 1 km and have been aggregated to the grid cell resolution (8 km). However, at 1km resolution, there is still a high degree of landscape heterogeneity over France. The analysis is adapted to plant functional types via the patch fractions and via the Jacobians.

1.6 Specific comments

1. **Comment:** *P.6, L28: How is it possible to assume zero (error, I assume) covariances between LAI and WG2, and at the same time derive meaningful Jacobians that calculate e.g. $dLAI/dWG2$. Isn't this a basic contradiction? Please explain.*

Response: We explain this in the revised manuscript (page 7, lines 6-10): “The SEKF simplifies the EKF by using fixed and uncorrelated background errors at the start of each cycle. Implicit background-error covariances between the layers and the prognostic variables are generated at the analysis time by the model integration in the observation operator Jacobians.”

2. *Why calculate $dLAI/dLAI$ by adding perturbations? Should this not be simply =1? Why not?*

Response: We would like to make clear this statement.

The Jacobians of the observation operator are defined on page 7 of the revised manuscript (equations 4 and 5). The perturbation is applied at the start of the window, while the finite difference from the model integrations in the Jacobian calculation is considered at the end of the window (the observation time). Therefore it depends on the model dynamics. The seasonal variability of the Jacobians was clearly demonstrated by Rüdiger et al. (2010).

3. **Comment:** *P.4, L26: Why is soil moisture rescaled, whereas LAI is not? The KF assumes unbiased innovations in either case: does this work out in the end?*

Response: Yes, we believe that it is necessary to rescale SSM observations to match the SSM model climatology because small-scale discrepancies in soil textural properties can cause very large systematic differences between the observations and the model. (Page 6, line 12 of the revised manuscript).

In order to explain our approach we have added the following sentences in the revised manuscript (page 6, lines 27-35, page 7, lines 1-5).

”When considering removing systematic differences between the model and the observations, a linear rescaling of the LAI observations to the model climatology would be problematic because the model-observation bias is linked to model deficiencies. When considering removing systematic differences between the model and the observations, a linear rescaling of the LAI observations to the model climatology would be problematic because the model-observation bias is linked to model deficiencies. For SSM, systematic errors are related to the mis-specification of physiographic parameters, such as the wilting point and the field capacity. As mentioned by several authors (e.g. Koster et al. (2009); Albergel et al. (2012)), the information content of soil moisture does not necessarily rely on its absolute magnitude but instead on its time variations. For SSM, the systematic bias between the model and the data consists mainly in their magnitude rather than their seasonal variability. Therefore this justifies the common approach used in land surface data assimilation studies for the SSM variable. Contrary to SSM, the LAI bias between the model and the data has two components: one in magnitude and the other one in timing (see e.g. Figure 6 in Barbu et al. (2014)). When compared with the satellite data, the LAI model dynamics clearly shows a shift in the seasonal cycle, mainly caused by model errors. The remote sensing LAI measurements potentially encapsulate realistic environmental features that are not or incorrectly represented by the model. Forcing the data to conform to the model climatology would result in a loss of relevant information. Therefore, in this context, a rescaling of the LAI data to the model climatology was not considered. Furthermore, Barbu et al. (2014) found that the assimilation without rescaling can cope with these model errors.”

On the other hand, systematic differences between the model and the observations can be removed by modifying the model parameters (Kumar et al., 2012), which was the motivation for correcting the LAI minimum in our study (Page 9, lines 14-16 of the revised manuscript). This substantially reduced the RMSD between the model and the observations. We repeated the cluster of experiments (NIT, LDAS1 and LDAS2) before and after correcting the systematic errors in the LAI minimum and the short-wave radiative forcing and found similar relative performances. We explained the results by analyzing the observation operator Jacobians (Section 3.3), which are not related to biases in the model.

4. **Comment:***P.6, L30: why is WG1 not part of the state vector?*

Response: We have mentioned in the revised manuscript (page 7 line 13-14): “The WG1 layer is not included in the analysis update because it is shallow layer (1 cm depth) that is driven by the atmospheric forcing rather than the initial conditions (Draper et al., 2009; Barbu et al., 2014)”. In practice it has little

bearing on the soil moisture fluxes.

5. *P.7, L2: what do you mean by a 24-hour assimilation window? A filter is used, not a smoother. Data are assimilated every 3 days for soil moisture and every 10 days for LAI.*

Response: We would like to state this clearly. The model integrations used in the observation operator Jacobians operate over a 24-hour period, otherwise the assimilation window length would be irrelevant. This is explained on page 7, line 28 of the revised manuscript.

6. *Comment: In short, the paper needs a thorough and in depth acknowledgement of all the violated assumptions in the KF: no spatial error correlations where perfect error correlations are present (and consequently, an exaggerated impact of the DA); either a relationship or none between LAI and WG2 in the setup of the background errors and the Jacobians, the choice for the observation error variance, etc. I would suggest to validate the optimality of the data assimilation system (e.g. white innovations in space and time?) and hopefully it comes out just fine: in that case, the paper could perhaps be considered for publication, otherwise it becomes hard to justify.*

Response: There is evidence in the literature that the SEKF does work effectively. The flow-dependence generated by the model integration in the observation operator Jacobians allows the SEKF to spread information between layers (SSM and WG2) and prognostic variables (WG2 and LAI). This flow-dependence is limited to the 24 hour assimilation window, but this is sufficient for the SEKF to perform as well as the EKF (Draper et al., 2009; Muñoz Sabater et al., 2007) and similarly to an EnKF (Fairbairn et al., 2015). This is explained in the introduction of the revised manuscript (page 3, lines 2-7).

As suggested by the reviewer, several figures are added to the supplement which illustrates the temporal LAI and SSM innovation evolutions (Figures S1.7 and Figure S1.8), as well as the LAI and SSM innovation distributions together with their respective Gaussian fit curves (Figure S1.4, S1.5 and S1.6). “These differences are illustrated in terms of probability distribution in Fig.S1.4 which shows the innovation histogram and the Gaussian fitting curve of the SSM product before rescaling” (page 6, lines 14-15).

In addition, in the Supplement, Fig.S15 and Fig.S1.6 show the histograms of the innovations (difference between the model-predicted observations and the data) and residual (difference between the analysis and the data). The pdf for SSM agrees very well with Kalman theory, since it closely fits the Gaussian distribution. The pdf for the LAI is not far away from its normal fit. The LAI innovations

present a left tailed distribution. As expected, the standard deviation of residuals is reduced compared to those of innovations. For an optimal filter the innovation time series should be uncorrelated in time. For both SSM and LAI the temporal evolutions of innovations are illustrated in Fig. S1.7 and in Fig. S1.8 of the Supplement, respectively.

7. Comment: *The title is not very representative: Integrated validation sets high expectations, we do expect advanced validation methods, or at least more than just only streamflow (i.e. maybe include turbulent fluxes, groundwater, in situ soil moisture,). I would rephrase it as something like The effect of [assimilation] on streamflow estimates. Secondly, the authors responded to one of the reviewers that he/she was inaccurate about referring to assimilation in a hydrological model yet, that is exactly what the title says.*

Response: We agree that this was confusing. The title “integrated validation” was meaning that we integrate a land surface model and a river routing model to perform the validation. As suggested by the reviewer the title is changed now into “The effect of satellite derived surface soil moisture and leaf area index assimilation on streamflow simulations over France”

8. Comment: *P.2, L10: observation network – observation coverage (already mentioned in earlier review, and I agree that this needs to change)*

Response: Sorry, we should have already corrected this. It is corrected in the revised manuscript.

9. Comment: *P.2, L9: instruments are subject to retrieval errors. – The *data* are subject to retrieval errors. And besides: we could assimilate raw radiance or backscatter observations and circumvent retrieval errors (but errors would be elsewhere)*

Response: It is changed in the revised manuscript.

10. Comment: *p.4, L2: integrated validation of the soil moisture fluxes. What is a soil moisture flux? Did you mean groundwater recharge, runoff, river discharge, ?*

Response: It is replaced with “integrated validation of the drainage and runoff fluxes.

11. Comment: *p.9, L13 : SIM is not a tool to validate. SIM provides model simulations which can be validated using in situ observations, and using some specific validation metrics.*

Response: It is replaced with: “The SIM hydrological model was used to validate

the drainage and runoff from ISBA-A-gs by comparing the simulated streamflow from MODCOU with observations”.

12. Comment: *p.4, L17: Draper et al. (2011) already assimilated SSM into SIM, but they did not perform the validation against streamflow, which is the whole goal of the current paper. To be complete, this paper should include a validation of these older results (Draper et al., 2011) against streamflow.*

Response: As already mentioned in the response to question 1.2 and already stated in the introduction of the revised manuscript, there is no point trying to recreate the results of the paper by (Draper et al., 2011). The novelty of our work consists of 1) assimilation of LAI and demonstration of its impact on the soil moisture fluxes and on the streamflow and 2) joint assimilation of LAI and SSM and demonstration of its impact on the soil moisture fluxes and on the streamflow.

In addition, it is difficult to reproduce Draper’s results because several modifications and improvements concerning the model and the data have been done in the meantime.

13. Comment: *P.12, section 3.2: Are all the WG1 and LAI metrics simple internal checks? I.e. comparison against data that are assimilated into the model? Please repeat that here. It would make much more sense to validate against independent soil moisture observations. What is the statistical significance level when it is stated that LDAS1 significantly improves the fit*

Response: Yes, they are internal checks, as stated in Section 2.5.1 on page 10 of the revised manuscript. We would prefer to validate WG2 rather than WG1, but WG2 cannot be validated using satellite observations. In situ measurements of WG2 are scarce and, in addition, point measurements are not necessarily representative of a coarser pixel scale, and thus are difficult to interpret when compared to model results. This is one of the reasons we are validating the drainage and runoff fluxes rather than soil moisture.

We have re-phrased “LDAS1 significantly improves the fit” to “LDAS1 substantially improves the fit”.

14. Comment: *What is the model integration time step? Since the assimilation is done at 9:00 UTC, whereas the data are taken at 9:30 UTC, I assume that there must be a very long model time step (one hour or more?). Could the long model integration time step be another cause of inferior model performance at some times?*

Response: We added the following clarification to the revised manuscript.

The model integration is performed every 15 minutes. However, the atmospheric forcing is assumed constant over hourly intervals for instantaneous measurements such as precipitation. Therefore any discrepancies in SSM are small (page 6, line 20 of the revised manuscript).

References

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Response to comments from Referee 2

March 2, 2017

We would like to thank the reviewers for their constructive comments. The corrections in the revised manuscript for Referee 2 are marked in red.

Response to major comments:

1

1.1

Referee comment *I understand how correcting the minimum LAI for an important land cover type (grassland) in the model has the desired effect of reducing streamflow overestimations. However, what is the scientific merit of replacing the minimum LAI simulation by the minimum of satellite observations? Firstly, it would be more justifiable to address these LAI shortcomings in the modeling itself, rather than replacing the values that are undesired. Alternatively, external observations can be used to correct the model LAI, but in that case, I believe it should not be restricted to only the LAI minimum for grassland. Only correcting this feature and not any other features is quite arbitrarily. Looking at Figure 3, it seems that, besides underestimating observations over grassland in winter, the model LAI is significantly larger than the observations over deciduous forest (almost the entire year) and over C3 crops in summer and fall. The latter discrepancies seem to be equally important (if not more) as the underestimation over grassland. Furthermore, looking at Table 3, correcting the grassland minimum LAI even significantly increases the average bias against the LAI observations, which feels like a counter-intuitive approach.*

Therefore, I recommend the authors to perform an additional experiment, with complete rescaling of the model LIA to the climatology of the LAI observations, and to re-evaluate the simulations of discharge, or to provide extensive scientific proof (e.g. based on other LAI products like MODIS) that the winter grasslands are really the main or only concern.

Response:

In the ISBA-A-gs model the LAI minimum is a model parameter. Using satellite data to determine the value of this parameter is relevant. The reviewer is right that simply increasing the LAI minimum parameter is not a good long term solution. It would be preferable to tackle the deficiencies in the model directly, which seem to be linked to the response of photosynthesis to temperature rather than the parameter itself, but this is a modelling problem that is beyond the scope of this paper. We have acknowledged this in the abstract/discussion/conclusions.

A thorough comparison of the ISBA-A-gs simulated LAI with both SPOT-VGT (used in our experiments) and MODIS data over south-west France was performed by Brut et al. (2009). They did notice significant discrepancies between all three data sets, suggesting that there is significant uncertainty in both the model and the observations. However, they also noticed that the modelled LAI of the C3 natural herbaceous (grasslands)/C3 crops had a delayed onset relative to both satellite products (see Figure 4 in Brut et al. (2009)). They found that this was particularly problematic for grasslands in mountainous regions. By comparing the data with in situ measurements, they found that the generic temperature response of photosynthesis used in the model is not appropriate for plants adapted to the cold climatic conditions of the mountainous areas. This problem was also linked to the reduced and prolonged LAI minimum in the model relative to the observations. Lafont et al. (2012) found similar issues when comparing the same products over France. These problems would explain the delayed onset and underestimated LAI minimum for both grasslands and C3 crops in Figure 3 in our study. Indeed, Figure 4 in our paper shows that the NIT LAI minimum was particularly underestimated in the grassland areas of the Massif Central mountains in central France, but not so much in lower regions further north. We have mentioned this in the discussion (page 16, lines 3-23).

Evidently from Figure 3 there are significant discrepancies between the model and the observations for C3 crops and deciduous forests as well as grasslands. We focused on grasslands partly because it represents the most common vegetation type over France (32%) and partly because other authors have discovered similar issues for grasslands (Brut et al., 2009; Lafont et al., 2012; Barbu et al., 2014). We have acknowledged that research is needed to improve the modelled values for the other vegetation types in the discussion. One way would be to assimilate observations at the patch scale (Response to 1.3.3 gives details).

We found that it was necessary to rescale SSM observations to match the SSM model climatology, partly because differences in the representation of the soil texture can cause very large systematic differences between the observations and the model (Page 6, line 11 of the revised manuscript). But the current ASCAT product is affected by vegetation effects (Vreugdenhill et al., 2016) and a seasonal CDF matching is needed in DA

systems assimilating ASCAT SSM. But this procedure is still sub-optimal. A solution to this problem is to go towards the implementation of an observation operator in order to assimilate the backscattering coefficients directly. In this way, the vegetation information content in the ASCAT signal could be used to analyse vegetation biomass and would also provide information for the analysis of root-zone soil moisture, in addition to the microwave soil moisture signal (page 17, lines 20-24).

A linear rescaling of the LAI observations to the model climatology would be problematic because the model-observation bias is linked to known deficiencies in the model, rather than due to specifications of the SSM physiographic parameters, such as the wilting point and the field capacity. As mentioned by several authors (e.g. Koster et al. (2009); Albergel et al. (2012)), the information content of soil moisture does not necessarily rely on its absolute magnitude but instead on its time variation. For SSM the systematic bias between the model and the data consists mainly in their magnitude rather than their seasonal variability. Therefore this common approach used in land surface data assimilation studies for the SSM variable is justified. Contrary to SSM, the LAI bias between the model and the data has two components: one in magnitude and the other one in timing. When compared with the satellite data, the LAI model dynamics clearly shows a shift in the seasonal cycle, mainly caused by model errors. The remote sensing LAI measurements potentially encapsulate realistic environmental features that are not or incorrectly represented by the model. Forcing the data to conform to the model climatology would result in a loss of important information. Therefore, in this context, a rescaling of the LAI data to the model climatology was considered inappropriate. Furthermore, Barbu et al. (2014) found that the assimilation mechanism employed without rescaling can cope with these model errors. This is now explained on page 6, lines 27-35 of the revised manuscript. Also, it does not seem consistent to us to rescale the modelled LAI to match the observations while the opposite is done for SSM (the observations are rescaled to match the WG1 climatology).

Systematic differences between the model and the observations can be removed by modifying the model parameters (Kumar et al., 2012), which was the motivation for correcting the LAI minimum in our study (Page 9, lines 14-16 of the revised manuscript). This substantially reduced the RMSD between the model and the observations. We repeated the cluster of experiments (NIT, LDAS1 and LDAS2) before and after correcting the grassland LAI minimum and the radiative forcing in the LAI minimum and the short-wave radiative forcing and found similar relative performances. We explained the results by analyzing the observation operator Jacobians (Section 3.3), which are not related to biases in the model.

1.2

Referee comment *I have some concerns regarding the choice of not correcting biases in LAI prior to the assimilation. I can see that the purpose of this experiment is to verify whether the assimilation can mediate the bias in LAI. Although being appealing, data assimilation is theoretically not designed to correct model bias. Again, as mentioned in the previous comment, such bias should actually be resolved in the model itself, or by rescaling the observations. I believe the same principle applies for LAI as for soil moisture, for which biases were appropriately removed in this study. The assimilation of biased LAI may not have had the effect that was hoped for, because of the small Jacobians in winter, but it could for instance also have disturbed the model behavior in summer, when larger Jacobians as well as large biases in LAI over crops were present. I believe this is an important issue that is not addressed in the paper. Moreover, the assimilation of (biased) LAI may also impact the climatology of the soil moisture simulations, which then again becomes biased with respect to the (previously bias-corrected) ASCAT retrievals. This could potentially be another important reason why the soil moisture assimilation, in combination with LAI assimilation, wets the lower layer and fails to improve discharge simulations.*

I suggest the authors to include an assimilation run for which the bias in LAI between model and observations is removed a priori, e.g. by rescaling the model LAI to the observations, cfr. comment 1 above. The impact of the summer bias over cropland (in combination with large Jacobians), and of deciduous forest bias need to be better addressed. Also, the impact of LAI assimilation on soil moisture bias between simulations and ASCAT retrievals requires further investigation. I believe the bias-correction of the soil moisture observations should best be done with respect to the LAI assimilation experiment.

Response:

We agree with the reviewer that DA methods are not theoretically designed to correct systematic model errors. A bias in the forecast model invalidates the assumption of bias-blind data assimilation (Dee, 2005). We admit that the DA experiments should not be motivated by correcting systematic model errors but instead DA plays an important role in correcting random errors in the initial conditions. We have now made this clear throughout the revised paper, including the abstract, introduction and conclusion. Note that this assumption does not affect the conclusions of the experiments because we repeated the cluster of experiments (NIT, LDAS1 and LDAS2) before and after correcting the systematic errors in the LAI minimum and the radiative forcing and found similar relative performances. Moreover, we explained the results in terms of the observation operator Jacobians.

We would not recommend rescaling the observed or modelled LAI (please see Section 1.3.1).

The reviewer is right that the assimilation of LAI causes a small net negative bias in LAI, which is evident in Table 2 in the paper. The bias is similar for LDAS1 and LDAS2 because it is caused by the $\frac{\partial LAI}{\partial LAI}$ Jacobian, rather than the $\frac{\partial LAI}{\partial WG2}$ Jacobian. Given that there is no significant wettening of WG2 in LDAS1, it is not possible for this bias to be causing the wettening of the WG2 layer and the resulting increase in drainage/runoff for LDAS2. The $\frac{\partial LAI}{\partial WG2}$ tends to be positive and is largest during summer/autumn (Barbu et al., 2014). There is no evidence that it leads to long term increases in WG2 or results in increased drainage/runoff for LDAS2 in winter/spring. We have mentioned this in Section 3.3 of the revised manuscript (page 14, lines 5-6). Moreover, Draper et al. (2011) assimilated only SSM observations and discovered similar issues to the LDAS2 experiment in our paper.

1.3 Specific comments

1.3.1

Referee comment *P2.L30-P3.L22: After a comment from the previous review, parts of the introduction have been rewritten to more strongly motivate the use of an SEFK relative to an ENKF. However, I feel like the text is rewritten as to actually recommend the SEFK over the ENKF. I don't believe there is really a need to defend the use of the SEFK so strongly, almost in a confrontational way with respect to the ENKF. Each has its own advantages. I would suggest to rewrite some of the phrases, making it less of a confrontation between both methods. It also feels a bit strange that the authors commend the SEFK in the introduction, whereas in the conclusion, they recommend future use of an ENKF.*

Similarly, the authors mention the study by Gruber et al. (2015) in P2.L29 to defend the choice for a 1D Kalman filter. I don't have any problem with using a 1D filter and mentioning this paper as a support, but suggest to make a more cautious statement. Theoretically one would expect a better performance with 2D systems in case of coarser-resolution observations, as they decrease the representativeness error between model forecasts and observations. As it stands, it feels like a general statement that advises the use of a 1D filter, with which I do not agree.

Response:

Indeed, the introduction was changed in response to the previous round of reviews in order to justify our use of the SEKF. As of yet we have found no evidence that the 1D EnKF performs better than the SEKF (in terms of root-zone soil moisture) for our

LSM, although we have only tested the EnKF on a dozen sites. But the reviewer is right that we should not have implied that the SEKF is superior to the EnKF, so we have given a more balanced discussion in the introduction of the revised paper. On page 3, line 2 of the revised manuscript: “The SEKF simplifies the EKF by using fixed and uncorrelated background errors at the start of each cycle. Importantly, the SEKF generates flow-dependence and implicit background-error covariances from additional model integrations in the observation operator Jacobian calculations. Draper et al. (2009) found the flow-dependence from a 24-hour assimilation window was sufficient to enable the SEKF to perform similarly to an EKF (which cycles the background-error covariance). Likewise, Muñoz Sabater et al. (2007); Fairbairn et al. (2015) found that the SEKF and EnKF performed similarly, in spite of different linear assumptions.”

In future research, the EnKF could still be attractive as it can be designed to account for model/forcing errors and 2D background-error covariances. However, as already discussed in our paper and evidenced in the literature (e.g. Maggioni et al. (2012); Gruber et al. (2015); Fairbairn et al. (2015)), the EnKF has its own set of challenges to overcome including its own linear assumptions. Therefore we must also be cautious about recommending it. In the revised manuscript we have mentioned in the discussion that we need to test the EnKF over France in the context of the SIM hydrological model. On page 16, line 19: “Fairbairn et al. (2015) found that an EnKF with a simple stochastic rainfall error estimation demonstrated similar WG2 scores to the SEKF over 12 sites in southwest France (validated using in situ observations). Both methods were affected by nonlinearity problems. We intend to test an EnKF over France using a similar validation employed in this study.”

1.3.2

Referee comment *P6.L9-11: The processing of the ASCAT data needs a little bit more explanation. How are data interpolated to the 8-km grid? Which temperature threshold was used for filtering frozen areas (zero Celsius or larger)? Have open water fractions or snow been dealt with? Why is altitude used instead of the topographic slope, or the topographic complexity flag in the ASCAT product? A plateau at high altitude seems more preferable to me than a terrain with strong slopes at low elevation, considering the backscattering mechanisms at hand. Adjusting these processing issues could be a way forward for getting improved results in future studies.*

Response:

In order to better explain the ASCAT data processing, we have added the following to Section 2.2, pages 6: “A surface-state flag is provided with the ASCAT product, which identifies frozen conditions, the presence of snow cover or temporary melting/water

on the surface. Observations are screened during frozen surface conditions or when snow-cover is present if the ASCAT flag is set to frozen. Additionally, observations with a topographic complexity flag greater than 15% and/or a wetland fraction greater than 5% (both provided with the ASCAT data) are removed. More information about ASCAT quality flags can be found in (Scipal et al., 2005).

After screening, the data were projected onto the 8 km resolution model grid by averaging all the data within 0.15 degrees of each gridpoint (Barbu et al., 2014). As in Draper et al. (2011) an additional screening step was performed to remove observations whenever frozen conditions were detected in the model using a threshold temperature of zero Celsius. In addition, observations with an altitude greater than 1500 m and with an urban fraction greater than 15% in the ECOCLIMAP database were removed.”

1.3.3

Referee comment *P7.L26: The authors assimilate the same (aggregated) LAI observation for all grid patches, which may for instance contain a forest patch and grassland patch?*

Is there any benefit of doing so? I would think this may cause very large increments that could potentially destabilize the model? Updating the aggregated grid cell LAI seems both more theoretically correct and computationally efficient to me. Please comment, and potentially modify the approach.

Response:

Taking into account the grid heterogeneity has been the justification for including vegetation patches in the model and in the assimilation scheme. The assimilation scheme uses the hypothesis that the distribution of innovations is proportional to the cover area. The analysis is adapted to plant functional types via the patch fractions and via the Jacobians. However, the assimilation of LAI has a relatively small impact on the soil moisture fluxes compared with the assimilation of SSM, partly because LAI is assimilated much less frequently (every 10 days as opposed to every 3 days on average). Moreover, it is not the primary cause of the wettening of WG2, as explained in the response to comment 1.2. These explanations are now included in the revised manuscript (page 8, lines 17-19).

1.3.4

Referee comment *P25.Table2: The assimilation of LAI only seems to flip the sign of the bias against observations, i.e. from +0.11 to -0.08. How is this possible? If the assimilation correctly balances forecast and observation errors (set equal for LAI), it should provide a result that is in-between the observations and simulations? Please*

comment.

Response:

This is linked to seasonal changes in the $\frac{\partial LAI}{\partial LAI}$ Jacobian. The behaviour of these Jacobian values was explained in Section 3.3 of the original paper. During the winter/spring the LAI observations are higher than the model, but the $\frac{\partial LAI}{\partial LAI}$ is frequently equal to zero, thus preventing any significant analysis correction. However, during the late summer/autumn the opposite is true; the observations are smaller than the model and the Jacobians are large, so the analysis correction is significantly increased. This results in a time-averaged negative bias of the LAI analysis relative to the observations (shown in Table 2). In Section 3.3 of the revised manuscript we have linked the seasonal changes in the Jacobian to the negative LAI bias in Table 2.

1.3.5

Referee comment P25.Table2: Also, the impact of the LAI assimilation seems to be very large. Is it potentially overdone? This is in large contrast with the results of the soil moisture assimilation, for which Table 3 shows almost negligible impact. Could you please comment? I was also wondering if the impacts on surface soil moisture are comparable to those observed by Draper et al. (2011)?

Response:

Table 3 in our paper shows the differences between WG1 and the observed SSM at the analysis time. Although SSM is assimilated in our experiments, it is not an analysis variable i.e. WG1 is not updated by the SEKF. Therefore WG1 is only modified indirectly during model interactions with the analysis variables (WG2 and LAI). Draper et al. (2011) updated both WG1 and WG2 with the SEKF, which explains why the assimilation of SSM had a relatively large impact on WG1 in their experiments compared to ours. We have mentioned in the revised manuscript (page 7 line 13-14): “The WG1 layer is not included in the analysis update because it is shallow layer (1 cm depth) that is driven by the atmospheric forcing rather than the initial conditions (Draper et al., 2009; Barbu et al., 2014). It has little bearing on the soil moisture fluxes.” Unfortunately it is not possible to observe WG2 with satellite observations so instead we compared WG1 with ASCAT derived SSM. The assimilation did slightly improve the fit to the observations as a result of interactions between SSM and the updated WG2.

The average magnitude of the WG2 analysis increments for our experiments was about 0.07 mm/day and the average magnitude of the WG2 analysis increment for Draper et al. (2011) was about 0.1 mm/day. The smaller size of the analysis increments for our experiments is probably a result of slightly larger observation errors prescribed

to SSM (we prescribed an average value of $0.055 \text{ m}^3/\text{m}^3$ and Draper et al. (2011) used the ASCAT SDS estimated values with a mean of about $0.050 \text{ m}^3/\text{m}^3$).

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The effect of satellite-derived surface soil moisture and leaf area index land data assimilation on streamflow simulations over France

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Abstract. This study evaluates the impact of assimilating surface soil moisture (SSM) and leaf area index (LAI) observations into a land surface model using the SAFRAN-ISBA-MODCOU (SIM) hydrological suite. SIM consists of three stages: (1) An atmospheric reanalysis (SAFRAN) over France, which forces (2) the 3-layer ISBA land surface model, which then provides drainage and runoff inputs to (3) the MODCOU hydro-geological model. The drainage and runoff outputs from ISBA are validated by comparing the simulated river discharge from MODCOU with over 500 river-gauge observations over France and with a subset of stations with low-anthropogenic influence, during several years. This study makes use of the A-gs version of ISBA that allows for physiological processes. The atmospheric forcing for the ISBA-A-gs model underestimates direct short-wave and long-wave radiation by approximately 5% averaged over France. The ISBA-A-gs model also substantially underestimates the grassland LAI compared with satellite retrievals during winter dormancy. These differences result in an underestimation (overestimation) of evapotranspiration (drainage and runoff). The excess runoff flowing into the rivers and aquifers contributes to an overestimation of the SIM river discharge. Two experiments attempted to resolve these problems: (i) a correction of the minimum LAI model parameter for grasslands, (ii) a bias-correction of the model radiative forcing. **Two data assimilation experiments were also performed, which are designed to correct random errors in the initial conditions: (iii) the assimilation of LAI observations and (iv) the assimilation of SSM and LAI observations.** The data assimilation for (iii) and (iv) was done with a simplified extended Kalman filter (SEKF), which uses finite differences in the observation operator Jacobians to relate the observations to the model variables. Experiments (i) and (ii) improved the median SIM Nash scores by about 9% and 18% respectively. Experiment (iii) reduced the LAI phase errors in ISBA-A-gs but had little impact on the discharge Nash efficiency of SIM. In contrast, experiment (iv) resulted in spurious increases in drainage and runoff, which degraded the median discharge Nash efficiency by about 7%. The poor performance of the SEKF originates from the observation operator Jacobians. These Jacobians are dampened when the soil is saturated and when the vegetation is dormant, which leads to positive biases in drainage/runoff and insufficient corrections during winter, respectively. **Possible ways to improve the model are discussed, including a new multi-layer diffusion model and a more realistic response of photosynthesis to temperature in mountainous regions. The data assimilation should be advanced by accounting for model/forcing uncertainties.**

1 Introduction

Soil moisture influences the flow of water to rivers and aquifers on weekly to monthly timescales, which makes it an important factor in hydrological models. In the last two decades there have been considerable advances in soil moisture data assimilation (DA) using remotely sensed near-surface soil moisture (Houser et al., 1998; Crow and Wood, 2003; Reichle and Koster, 2005; Draper et al., 2012; de Rosnay et al., 2013). The estimation of global-scale soil moisture states has benefited considerably from a huge expansion of the satellite coverage, namely the Advanced Scatterometer (ASCAT) instrument on board the METOP satellites (Wagner et al., 2007), the Soil Moisture and Ocean Salinity (SMOS) Mission (Kerr et al., 2001) and the Soil Moisture Active Passive (SMAP) Mission (Entekhabi et al., 2010), amongst others. However, these instruments can only indirectly observe the top 1-3 cm of soil moisture and the data are subject to retrieval errors. There are also spatial and temporal gaps in the observation coverage. The vegetation influences the soil moisture state through evapotranspiration and the vegetation coverage can be estimated by the leaf area index (LAI). This is a dimensionless quantity that represents the one-sided green leaf area per unit ground surface area (Gibelin et al., 2006). The LAI can be derived from satellite measurements in the visible range. However, over France it is available from polar-orbiting satellites at a relatively low temporal frequency (on average every 10 days) compared with soil moisture satellite observations (about every 3 days) due to cloud cover. The aim of DA methods is to combine these observations with a model forecast from the previous analysis (the background state) to provide an improved estimate of the state of the system (the analysis). DA methods are necessary to account for the errors in the observations and the model, and to spread the information through space and time.

Many studies have investigated the assimilation of surface soil moisture (SSM) and streamflow observations into hydrological models in order to improve streamflow predictions and hydrological parameters (Aubert et al., 2003; Moradkhani et al., 2005; Clark et al., 2008; Thirel et al., 2010; Moradkhani et al., 2012). For example, Thirel et al. (2010) used the Best Linear Unbiased Estimate (BLUE) method to assimilate streamflow observations into the MODCOU hydrogeological model over France, which they used to update soil moisture in the ISBA land surface model (LSM).

LSMs concern water and energy fluxes between the soil and atmosphere. Unlike hydrological models, layer-based LSMs such as the ISBA model are typically point-wise (there is no horizontal interaction between the gridpoints), which greatly reduces the computational expense. A 1D Kalman filtering approach (where observations are used to update collocated gridpoints only) is also implemented in this study, which is commonly applied to 1D LSMs (Reichle et al., 2002; Draper et al., 2009; de Rosnay et al., 2013; Barbu et al., 2014).

In large-scale land surface DA, it is common to assimilate satellite derived SSM observations and screen-level temperature and humidity observations into a LSM, in order to improve soil moisture and screen-level variables. Typically the root-zone soil moisture (WG2) (1-3 m deep) is of more interest than SSM as it has a much larger water capacity and a long memory (from weeks to months). Land surface DA is often performed using an ensemble Kalman filter (EnKF) or a simplified extended Kalman filter (SEKF).

There has been increasing interest in ensemble DA for LSMs over the last two decades (Reichle et al., 2002, 2008; Zhou et al., 2006; Muñoz Sabater et al., 2007; Draper et al., 2012; Carrera et al., 2015), partly because these methods can estimate

the “errors of the day” in the background-error covariance. The operational EnKF at Environment Canada is also motivated by coupling land surface DA with ensemble weather forecasting (Carrera et al., 2015). On the other hand, the SEKF simplifies the EKF by using fixed and uncorrelated background errors at the start of each cycle. Importantly, the SEKF generates flow-dependence and implicit background-error covariances from additional model integrations in the observation operator Jacobian calculations. Draper et al. (2009) found the flow-dependence from a 24-hour assimilation window was sufficient to enable the SEKF to perform similarly to an EKF (which cycles the background-error covariance). Likewise, Muñoz Sabater et al. (2007); Fairbairn et al. (2015) found that the SEKF and EnKF performed similarly, in spite of different linear assumptions.

Historically, the SEKF originated from a simplified 2D-Var (theoretically equivalent to an SEKF) scheme for the assimilation of screen-level temperature and humidity at the German Weather service (DWD) (Hess, 2001). An SEKF has been developed for research purposes to assimilate satellite derived soil moisture at Météo-France (Mahfouf, 2010) and the UK Met Office (Candy et al., 2012), amongst other variables. The European Centre for Medium Range Weather Forecast (ECMWF) model assimilates screen-level temperature and humidity operationally with an SEKF (de Rosnay et al., 2013) and more recently assimilates ASCAT derived SSM observations (ECMWF, 2016).

In our study, we use an SEKF to assimilate LAI and SSM observations to update LAI and WG2 in the ISBA LSM within the SAFRAN-ISBA-MODCOU (SIM) hydrological suite. This study makes use of the A-gs version of ISBA that allows for physiological processes. SIM is operational at Météo-France and its streamflow and soil moisture outputs are used as a tool by the French National flood alert services (Thirel et al., 2010). SIM consists of three stages: (1) An atmospheric reanalysis (SAFRAN) over France, which forces (2) the ISBA-A-gs land surface model, which then provides drainage and runoff inputs to (3) the MODCOU distributed hydrogeological model. The drainage and runoff outputs from ISBA-A-gs are validated by comparing the simulated streamflow from MODCOU with observations. This study is relevant to the land surface DA community because several operational centres assimilate SSM observations using an SEKF to update WG2. Many studies have demonstrated that the force-restore dynamics of the ISBA 3-layer model can effectively simulate soil moisture and propagate the increments downwards from the surface to the root-zone (Muñoz Sabater et al., 2007; Draper et al., 2009; Mahfouf et al., 2009). An integrated validation using SIM has demonstrated that the ISBA 3-layer model can skillfully simulate drainage and runoff fluxes over France (Habets et al., 2008). The dynamic vegetation model in ISBA-A-gs is also capable of modelling seasonal changes in LAI (Jarlan et al., 2008; Brut et al., 2009; Barbu et al., 2011, 2014). But relatively few studies have assessed the SEKF performance using an integrated validation of the drainage and runoff fluxes. To our knowledge, this is the first article to consider this type of validation for LAI assimilation. Furthermore, the validation is robust because it is performed using more than 500 river gauges over France during several years.

This work is partly motivated by the study of Draper et al. (2011), who investigated the influence of assimilating ASCAT derived SSM with an SEKF on SIM over France. They used a version of SIM with high quality atmospheric forcing to represent the “truth” and lower quality atmospheric forcing for the model. Although the SEKF seemed to improve the results in their study, they acknowledged that this may have been related to a bias in the SEKF rather than the assimilation accurately responding to the precipitation errors. Despite the fact that SAFRAN can be considered as a high quality atmospheric forcing, studies by Szczypta et al. (2011) and Le Moigne (2002) have found underestimations of about 5% in the direct short-wave

and long-wave radiative fluxes respectively, averaged over France. In addition to these problems with radiative forcing, we demonstrate in this study that the LSM substantially underestimates LAI for grasslands in winter (compared with satellite retrievals). The specification of the LAI minimum in the model is important because it prevents vegetation mortality and allows the regrowth of vegetation in the spring period (Gibelin et al., 2006). We use SIM to validate the impact of four experiments

5 on the drainage and runoff fluxes:

- i. Correcting the model under-estimated LAI minimum parameter;
- ii. Bias-correcting the SAFRAN radiative forcing;
- iii. Assimilating only LAI observations with an SEKF;
- iv. Assimilating SSM and LAI observations with an SEKF.

10 The first two experiments attempt to resolve systematic model issues, while experiments (iii) and (iv) assimilate data in order to correct random errors in the initial conditions.

Since Draper et al. (2011) already investigated the impact of assimilating SSM in ISBA on river discharges with MODCOU, it was not necessary to perform an experiment with the assimilation of SSM only. We validate the performance of these experiments using observations from more than 500 river gauges over France during the period July 2007 to August 2014.

15 We include an additional validation using a subset of 67 stations with low-anthropogenic influence because the MODCOU hydrogeological model only accounts for natural features. It should be noted that a bias in the forecast model invalidates the assumption of bias-blind data assimilation (Dee, 2005). We therefore repeat experiments (iii) and (iv) after applying (i) and (ii) in to explore whether the systematic model errors impact the SEKF performance.

The paper is structured as follows. The methods and materials are given in Sect. 2, which includes a description of the LSM, the assimilated observations, the DA methods, the experimental setup and the SIM validation. The results are presented in Sect. 3, including the impact of the model simulations and DA on the model state variables and the river discharge. A discussion in Sect. 4 considers potential solutions to the problems encountered in this study. Finally, the conclusions are given in Sect. 5.

2 Methods and materials

25 2.1 ISBA-A-gs land surface model

In our study, the ISBA-A-gs LSM was forced by the atmospheric variables provided by the “Système d’Analyse Fournissant des Renseignements à la Neige” (SAFRAN). The analyses of temperature, humidity, wind speed, and cloudiness are originally performed every 6 h using the ARPEGE (Action de Recherche Petite Echelle Grande Echelle) NWP (Numerical Weather Prediction) model (Courtier et al., 2001). The original precipitation analysis is performed daily at 0600 UTC, to include in

30 the analysis the numerous rain gauges that measure precipitation on a daily basis. A linear interpolation converts these values

to the hourly SAFRAN forcing values (Quitana-Ségui et al., 2008). Instantaneous variables such as precipitation are assumed constant for each 15 minute model time-step during these hourly intervals, while other variables are linearly interpolated. The SAFRAN forcing is assumed to be homogeneous over 615 specified climate zones. The forcing is interpolated from these zones to a Lambert projected grid with a horizontal resolution of 8 km (Durand et al., 1993). The delayed cut-off version of SAFRAN was employed, which uses information from an additional 3000 climatological observing stations (which report one-monthly) over France (Quitana-Ségui et al., 2008; Vidal et al., 2010) after the real-time cut-off, which makes the resulting analyses more accurate.

Version 8.0 of SURFEX was used in the experiments, which contains the “Interactions between Soil, Biosphere and Atmosphere” (ISBA) LSM (Noilhan and Mahfouf, 1996). The model uses the same horizontal grid resolution as SAFRAN of 8 km. The ISBA-A-gs version was used, which allows for the influence of physiological processes, including photosynthesis (Calvet et al., 1998). Each grid cell is split into twelve vegetation types (so called “patches”). Soil and vegetation parameters are derived from the ECOCLIMAP database (Faroux et al., 2013). The nitrogen dilution version (referred to as “NIT” hereafter) of ISBA-A-gs was applied, which dynamically simulates the LAI evolution (Gibelin et al., 2006). The NIT version allows for the effects of atmospheric conditions on the LAI, including the carbon dioxide concentrations.

The three-layer version of ISBA was adopted for this study (Boone et al., 1999). This includes the WG1 layer with depth 0-1 cm. The WG2 layer includes WG1 and is 1-3 m deep, with the depth depending on the patch type. A recharge zone exists below the WG2 layer. The model water transfers are governed by the force-restore method of Deardorff (1977). The surface and root-zone layers are forced by the atmospheric variables and restored towards an equilibrium value. The drainage and runoff outputs from ISBA-A-gs drive the MODCOU hydrogeological model. The gravitational drainage is proportional to the water amount exceeding the field capacity (the effective limit where gravitational drainage ceases) (Mahfouf and Noilhan, 1996). It is driven by the hydraulic conductivity of the soil, which depends on its texture. A small residual drainage below field capacity was introduced by Habets et al. (2008) to account for unresolved aquifers. Runoff occurs when the soil moisture exceeds the saturation value.

2.2 Assimilated observations

The SSM observations were retrieved from ASCAT C-band spaceborne radar observations, which observe at 5.255 GHz and a resolution of approximately 25 km. The radar is on board EUMETSAT’s Meteorological Operational (MetOP) satellites. The assimilation of ASCAT data was chosen because it was available throughout the analysis period. The original backscatter values were converted into a surface degree of saturation (SDS, with values between 0 and 1) using a change detection technique, which was developed at the Vienna University of Technology (Tu-Wien) and is detailed in Wagner et al. (1999); Bartalis et al. (2007). The historically lowest and highest backscatter coefficient values are assigned to dry and saturated soils respectively. The Copernicus Global Land Service then calculates a soil wetness index (SWI) by applying a recursive exponential filter to these SDS values (Albergel et al., 2008) using a time-scale that may vary between 1 and 100 days. The SWI represents the soil wetness over the soil profile and also has values between 0 (dry) and 1 (saturated). The longer the time-scale of the exponential filter, the deeper the representative soil profile. The SWI-001 version 2.0 product was used in this study, which has a one day

timescale and represents the SWI for a depth up to 5 cm. A surface-state flag is provided with the ASCAT product, which identifies frozen conditions, the presence of snow cover or temporary melting/water on the surface. Observations are screened during frozen surface conditions or when snow-cover is present if the ASCAT flag is set to frozen. Additionally, observations with a topographic complexity flag greater than 15% and/or a wetland fraction greater than 5% (both provided with the ASCAT data) are removed. More information about ASCAT quality flags can be found in (Scipal et al., 2005). After screening, the data were projected onto the 8 km resolution model grid by averaging all the data within 0.15 degrees of each gridpoint (Barbu et al., 2014). As in Draper et al. (2011) an additional screening step was performed to remove observations whenever frozen conditions were detected in the model using a threshold temperature of zero Celsius. In addition, observations with an altitude greater than 1500 m and with an urban fraction greater than 15% in the ECOCLIMAP database were removed.

In order to remove biases between model and observations, a linear rescaling to the SWI-001 data, which scales them such that the mean and standard deviations match the WG1 layer climatology (Calvet and Noilhan, 2000; Scipal et al., 2008). We found that it was necessary to rescale the SSM observations to match the SSM model climatology, partly because differences in the representation of the soil texture can cause very large systematic differences between the observations and the model. These differences are illustrated in terms of probability distribution in Figure S1.4 of the Supplement. It shows the innovation histogram and the Gaussian fitting curve of the SSM product before rescaling.

This rescaling is a linear approximation of the cumulative distribution matching technique, which uses higher order moments (Reichle et al., 2004; Drusch et al., 2005). As in Barbu et al. (2014), we applied a seasonal rescaling using a 3-month moving average over the experiment period (2007-2014). In the rescaling process the SWI-001 data are converted into the same units as the model, expressed in volumetric soil moisture (m^3/m^3). The rescaled SSM observations were assimilated into the WG1 model layer. The observations were assumed to occur at the same time as the analysis at 09:00 UTC and had a temporal frequency of about 3 days. This was a reasonable assumption since the satellite overpass is at 09:30 UTC and the atmospheric forcing is assumed constant over hourly intervals for instantaneous measurements such as precipitation. Therefore any discrepancies in SSM due to this 30 minute time difference are small.

The GEOV1 LAI product is part of the European Copernicus Global Land service. The LAI observations were retrieved from the SPOT-VGT (August 2007 to June 2014) and PROBA-V (June 2014-July 2014) satellite data. The retrieval methodology is discussed by Baret et al. (2013). Following Barbu et al. (2014), the 1 km resolution observations were interpolated to the 8 km model gridpoints, provided that observations were present for at least 32 of the observation gridpoints (just over half the maximum amount). The observations were averaged over a 10-day period and assimilated at 09:00 UTC. This assumption was reasonable given that LAI evolves slowly. When considering removing systematic differences between the model and the observations, a linear rescaling of the LAI observations to the model climatology would be problematic because the model-observation bias is linked to model deficiencies. On the other hand, for SSM, systematic errors are related to the mis-specification of physiographic parameters, such as the wilting point and the field capacity. As mentioned by several authors (e.g. Koster et al. (2009); Albergel et al. (2012)), the information content of soil moisture does not necessarily rely on its absolute magnitude but instead on its time variations. For SSM, the systematic bias between the model and the data consists mainly in their magnitude rather than their seasonal variability. Therefore this justifies the common approach used in land

surface data assimilation studies for the SSM variable. Contrary to SSM, the LAI bias between the model and the data has two components: one in magnitude and the other one in timing (see e.g. Figure 6 in Barbu et al. (2014)). When compared with the satellite data, the LAI model dynamics clearly shows a shift in the seasonal cycle, mainly caused by model errors. The remote sensing LAI measurements potentially encapsulate realistic environmental features that are not or incorrectly represented by the model. Forcing the data to conform to the model climatology would result in a loss of relevant information. Therefore, in this context, a rescaling of the LAI data to the model climatology was not considered. Furthermore, Barbu et al. (2014) found that the assimilation without rescaling can cope with these model errors.

2.3 Data assimilation

The SEKF simplifies the extended Kalman filter (EKF, (Jazwinski, 1970)) by using a fixed estimate of the background-error variances and zero covariances at the start of each cycle (Mahfouf et al., 2009). Implicit background-error covariances between the layers and the prognostic variables are generated at the analysis time by the model integration in the observation operator Jacobians. We used the same SEKF formulation as Barbu et al. (2014) for the assimilation of SSM and LAI observations over France. The prognostic variables are LAI and WG2. The WG1 layer is not included in the analysis update because it is shallow layer (1 cm depth) that is driven by the atmospheric forcing rather than the initial conditions (Draper et al., 2009; Barbu et al., 2014). The background state (\mathbf{x}^b) at time t_i is a model propagation of the previous analysis ($\mathbf{x}^a(t_{i-1})$) to the end of the 24 hour assimilation window:

$$\mathbf{x}^b(t_i) = M_{i-1}(\mathbf{x}^a(t_{i-1})), \quad (1)$$

where M is the (nonlinear) ISBA-A-gs model. The observation was assimilated at the analysis time, at 09 UTC, at the end of the 24-hour assimilation window. The analysis was calculated from the generic Kalman filter equation:

$$\mathbf{x}^a(t_i) = \mathbf{x}^b(t_i) + \mathbf{K}_i(\mathbf{y}_i^o - \mathbf{y}_i), \quad (2)$$

where \mathbf{y}^o is the assimilated observation and $\mathbf{y}_i = H(\mathbf{x}^b(t_i))$ is the model predicted value of the observation at the analysis time. The Kalman gain is defined as:

$$\mathbf{K}_i = \mathbf{B}_i \mathbf{H}_i^T (\mathbf{H}_i \mathbf{B}_i \mathbf{H}_i^T + \mathbf{R}_i)^{-1}, \quad (3)$$

where \mathbf{H} is the Jacobian matrix of the linearized observation operator, \mathbf{B} is the background-error covariance matrix and \mathbf{R} is the observation-error covariance matrix. The observation operator Jacobians were calculated using finite differences for observation k and model variable l :

$$\mathbf{H}_i^{kl} = \frac{H_i^k(M_{i-1}(\mathbf{x}(t_{i-1}) + \Delta x_{i-1}^l) - H_i^k(M_{i-1}(\mathbf{x}(t_{i-1})))}{\Delta x_{i-1}^l}, \quad (4)$$

where Δx^l is a model perturbation applied to model variable l . The WG2 and LAI perturbations were set to $1.0 \times 10^{-4} \times (w_{fc} - w_{wilt})$ and $1.0 \times 10^{-3} \times \text{LAI}$ respectively. These were within the range of acceptable perturbation sizes based on the experiments

of Draper et al. (2009) and Rüdiger et al. (2010). Equation (4) requires a 24-hour model simulation for each prognostic variable, which implicitly propagates the background-error covariance from the start of the window to the time of the observations at the end of the window. The linear assumptions in deriving the Jacobians are generally acceptable for these perturbation sizes. However, occasionally the linear assumptions can break down, especially during dry periods in summer (Draper et al., 2009; Fairbairn et al., 2015). For this reason we set an upper bound on the soil moisture Jacobians of 1.0. It is worth mentioning that in situations where the model and atmospheric forcing errors are not properly taken into account the SEKF analysis will be suboptimal even if the Jacobians are accurately computed. The Jacobian matrix derived from Eq. (4) is defined as follows:

$$\mathbf{H} = \begin{pmatrix} \frac{\partial \text{WG1}}{\partial \text{WG2}} & \frac{\partial \text{WG1}}{\partial \text{LAI}} \\ \frac{\partial \text{LAI}}{\partial \text{WG2}} & \frac{\partial \text{LAI}}{\partial \text{LAI}} \end{pmatrix}. \quad (5)$$

When assimilating just LAI, only the $\frac{\partial \text{LAI}}{\partial \text{WG2}}$ and $\frac{\partial \text{LAI}}{\partial \text{LAI}}$ terms are included. The $\frac{\partial \text{WG1}}{\partial \text{LAI}}$ is generally small, since the LAI does not substantially influence the surface layer (Barbu et al., 2014). The $\frac{\partial \text{WG1}}{\partial \text{WG2}}$ Jacobian couples WG1 with WG2 (Draper et al., 2009). The $\frac{\partial \text{LAI}}{\partial \text{WG2}}$ couples LAI with WG2 (Barbu et al., 2014). The $\frac{\partial \text{LAI}}{\partial \text{LAI}}$ Jacobian was studied by Rüdiger et al. (2010) and has a strong seasonal dependence. As we will demonstrate in Sect. 3.3, the examination of these Jacobians is essential in order to understand the performance of the SEKF.

SURFEX is implemented using the mosaic approach of Koster and Suarez (1992), where each model grid-box is split into 12 vegetation patches. The SEKF analysis is calculated independently for each patch using the Jacobians for each individual patch but with one mean observation per grid box. The analysis for the gridpoint is calculated by aggregating the analyses over the 12 patches, which are weighted according to their patch fractions (see Barbu et al. (2014) for further details). Taking into account the grid heterogeneity has been the justification for including vegetation patches in the model and in the assimilation scheme. The assimilation scheme uses the hypothesis that the distribution of innovations is proportional to the cover area. The analysis is adapted to plant functional types via the patch fractions and via the Jacobians.

Following Draper et al. (2011), the WG2 background-error standard deviation was set to $0.2(w_{fc} - w_{wilt})$, where w_{fc} is the field capacity and w_{wilt} is the wilting point. The scaling by $(w_{fc} - w_{wilt})$ assumes that there is linear relationship between the soil moisture errors and the dynamic range, which depends on soil texture (Mahfouf et al., 2009). The SSM observation error standard deviation was set to $0.65(w_{fc} - w_{wilt})$, which is about $0.055 \text{ m}^3/\text{m}^3$ averaged over France. This value is slightly larger than the median ASCAT-derived SDS error of $0.05 \text{ m}^3/\text{m}^3$ estimated by Draper et al. (2011) because it also approximates the oversampling issue i.e. the same ASCAT observation covers several gridpoints. This reduces the size of the analysis increments by approximately 10%. This value is comparable with observation errors expected for remotely sensed SSM observations (de Jeu et al., 2008; Draper et al., 2013). As in Barbu et al. (2011) the LAI background and observation error standard deviations were proportional to the LAI values themselves and a value of $0.2 \times \text{LAI}$ was used for LAI values greater than $2 \text{ m}^2/\text{m}^2$. For LAI values below $2 \text{ m}^2/\text{m}^2$ the LAI errors were fixed at $0.4 \text{ m}^2/\text{m}^2$. Both the background-error and observation-error covariance matrices of the SEKF are diagonal (zero covariances between layers), but implicit background-error covariances are derived from the \mathbf{H} matrix at the analysis time. The SEKF is a point-wise method i.e. it cannot take into account horizontal covariances between gridpoints.

2.4 Experimental setup

The main experiments in this study are summarised in Table 1. The SIM river discharge was compared with the observations from 546 stations over France. Firstly the baseline experiment (NIT) was performed, which shows the impact of the biased radiative forcing and the under-estimated LAI minimum on the SIM river discharge. Thereafter, two potential solutions to these deficiencies were investigated, as set out in the introduction: (i) NIT_m , which was equivalent to NIT but with an elevated LAI minimum of $1.2 \text{ m}^2/\text{m}^2$ for grasslands (as opposed to $0.3 \text{ m}^2/\text{m}^2$ with NIT), (ii) NIT_{bc} , which used both the elevated LAI minimum of $1.2 \text{ m}^2/\text{m}^2$ and the bias-corrected radiative forcing (+5% for direct long-wave and short-wave over France). Two data assimilation experiments were undertaken to correct random errors in the initial conditions: (iii) LDAS1, which used the SEKF to assimilate LAI only with the NIT model and (iv) LDAS2, which assimilated both LAI and SSM observations with the NIT model. **The LAI minimum parameter is required to calculate a minimum level of photosynthesis at the start of the growing season. The default model value is arbitrarily fixed at $0.3 \text{ m}^2/\text{m}^2$ for grasslands, which is low enough to account for possible fluctuations in the LAI minimum due to climatic and interannual variability over France (Gibelin et al., 2006). However, we found that over 99% of points with a high percentage of grassland (the grassland patch fraction exceeding 70%) had an observed average annual LAI minimum above $1.2 \text{ m}^2/\text{m}^2$ during the experiment period (2007-2014). But the modelled LAI is frequently kept at the prescribed LAI minimum parameter during winter dormancy and is therefore systematically underestimated over most grassland regions in winter when compared to the satellite derived observations. Similar issues were found by Brut et al. (2009); Lafont et al. (2012); Barbu et al. (2014) when comparing the model with both MODIS and SPOT-VGT satellite derived observations. Systematic differences between the model and the observations can be removed by calibrating model parameters (Kumar et al., 2012), which was the motivation for increasing the grassland LAI minimum parameter from $0.3 \text{ m}^2/\text{m}^2$ to $1.2 \text{ m}^2/\text{m}^2$ in our study.** Szczypta et al. (2011) and Le Moigne (2002) demonstrated that the direct short-wave and long-wave radiative forcing respectively are underestimated by approximately 5% averaged over France. We followed Decharme et al. (2013) in bias-correcting the direct radiative forcing by +5% for NIT_{bc} .

Three additional experiments in Table 1 explored whether SSM observation outliers, the under-estimated LAI minimum or the radiative forcing bias might impact the performance of the DA. The LDAS2_{QC} was equivalent to LDAS2 but with a strict quality control of the SSM observations. The outliers were removed by rejecting observations outside the 90% confidence interval of the model (as in Eq. (1) and (2) of Albergel et al. (2010b)) after the observations had been rescaled. The LDAS1_{bc} and LDAS2_{bc} experiments were equivalent to LDAS1 and LDAS2 respectively, except they used the NIT_{bc} model. The SSM observations for LDAS2_{bc} were rescaled such that the standard deviation and mean matched those of NIT_{bc} .

The MODCOU hydrogeological model does not account for anthropogenic water management. However, there are many parts of France where anthropogenic water management strongly influences streamflow observations, including the reservoir operations, for hydropower, irrigation, drinking water, flood and low-flow alleviation and recreation purposes. We used the reference networks of Giuntoli et al. (2012, 2013) to extract a subset of 67 river gauges with low-anthropogenic influence from the original 546 stations, valid for both low and high flows. We compared the results for these 67 stations with the 546 stations

in order to determine if the results were affected by the ability of SIM (with or without DA) to simulate anthropogenically influenced streamflow.

2.5 Performance diagnostics

2.5.1 System validation

- 5 A system validation was performed by comparing the LAI and WG1 states with the LAI and SSM observations respectively for all the simulations and data assimilation experiments. Note that this was not an independent validation of the performance of the system, for which we would have needed independent observations. The rationale was to check the effectiveness of the SEKF i.e. to examine if it improved the fit between the model simulations and the observations. The fit to the observations was determined by the root mean square difference (RMSD), the correlation coefficient (CC) and the bias.
- 10 In addition, Figure S1.5 and Figure S1.6 of the Supplement show the histograms of the innovations (difference between the model-predicted observations and the data) and residuals (difference between the analysis and the data). The SSM innovation pdf agrees very well with Kalman theory, since it closely fits the Gaussian distribution. The LAI innovation pdf is also close to its normal fit, but presents a left tailed distribution. As expected, the standard deviation of residuals is reduced compared to those of innovations. For an “optimal” filter the innovation time series should be uncorrelated in time. For both SSM and LAI
- 15 the temporal evolutions of innovations are illustrated in Figures S1.7 and S1.8 of the Supplement, respectively.

2.5.2 Validation using SIM

- The SIM hydrological model was used to validate the drainage and runoff from ISBA-A-gs by comparing the simulated streamflow from MODCOU with observations. A complete description and validation of SIM can be found in Habets et al. (2008). The first two stages of SIM are the SAFRAN atmospheric forcing and the ISBA-A-gs LSM, which were introduced
- 20 in Section 2.1. The runoff and drainage from ISBA-A-gs are fed into the MODCOU hydrogeological model (Ledoux et al., 1989), which computes the daily evolution of aquifer storages and three-hour river flow forecasts. More than 900 river gauges are simulated with areas ranging from 240 km² to 112,000 km². The temporal and spatial evolution of two aquifers in the Rhone and Seine Basins are simulated using a diffusivity equation. The interaction between the rivers and aquifers is modelled and the soil water is routed to the rivers using an isochronism algorithm. The influence of human activity, such as dams and
- 25 irrigation, is not accounted for by MODCOU. The simulated river discharge from SIM was compared with the observations from 546 river gauges that had data during the period of evaluation (2007-2014). These observations are available from the French hydrographical database (<http://www.hydro.eaufrance.fr/>, last accessed March 2016). We also analyzed the results for the subset of 67 stations with low anthropogenic influence from the original 546 stations. The fit of the average daily river discharge from MODCOU (measured in m³/m³s⁻¹) to the observations was measured using the Nash efficiency score (Nash and Sutcliffe, 1970). The Nash efficiency can range from $-\infty$ to 1, with 1 corresponding to a perfect match of the model to the observed data and a negative value implying that the model performs worse than a constant model with a value equal to the average of all the observations. Following Habets et al. (2008) we considered an efficiency of 0.6 to be a good score and 0.5 to
- 30

be a reasonable score. The median Nash scores were calculated for all the stations. The median is a more appropriate metric than the mean as it is less sensitive to extreme outliers and is a better indicator for highly skewed distributions (Moriassi et al., 2007). These issues were present in this study due to some stations being heavily affected by anthropogenic water management or unresolved aquifers, despite most stations being well simulated. The validation period extended from August 2007 to July 2014, with the hydrological year running from August to July.

The SIM domain consists of 9892 gridpoints, of which 8602 are based in France. The remaining 1290 points are based in mountainous regions bordering the French mainland, including most of Switzerland (see Figure 2 in Habets et al. (2008) for the full domain). The LSM does not model horizontal exchanges, but MODCOU takes into account horizontal streamflow. Therefore it is important to include these external points in SIM because they impact the streamflow over France, particularly in the Rhone basin in the southeast. However, we only applied the SEKF over the 8602 points in the LDAS France domain. Figure 1 shows a flowchart of SIM and how LDAS France was connected with ISBA-A-gs in SIM. Figure 2 shows the river network used by MODCOU and the 546 stations used to validate the discharge. A map of the subset of 67 stations with low anthropogenic influence can be found in Figure S1.1 of the Supplement.

3 Results

3.1 Impact of model and forcing bias-corrections on SIM

To begin with we examine the influence of the different model simulations (NIT, NIT_m and NIT_{bc}) on the LAI evolution for the four dominant vegetation patches. We can then link the hydrological performance to each simulation. Over France, the four dominant vegetation patches are grasslands (32%), C3 croplands (24%), deciduous forests (20%) and coniferous forests (12%). Figure 3 shows the monthly averaged LAI model simulations and observations for the gridpoints that contain at least 50% of the dominant vegetation types. The 50% threshold was used because no points contain more than 70% of deciduous forests, while over 1000 gridpoints contain at least 50% of any vegetation type. Table 2 shows the average LAI scores over France (RMSD, CC and bias) for each of the model simulations.

Firstly we examine the LAI performance for the NIT simulation, which dynamically estimates the LAI evolution. Figure 3 shows that the NIT simulation is close to the observations for the deciduous forests (Figure 3(a)). However, the growth and senescence phases are delayed for the simulated C3 crops and grasslands (Figure 3(c) and (d)) compared with the observations. Furthermore, the grassland LAI is **substantially** underestimated by NIT in winter. It is clear in Figure 3 that imposing this higher minimum LAI value (NIT_m) increases the LAI for grasslands in winter and improves the fit to observations. This is reflected by better scores for NIT_m , reducing (increasing) the RMSD (CC) by about 4% compared with NIT. Figure 4 shows the average annual LAI minimum over France for the original simulation (NIT), the new simulation (NIT_m) and the GEOV1 data. Figure 4 emphasizes that the LAI minimum is underestimated (compared to the GEOV1 data) over much of France for NIT. By increasing the grassland LAI minimum from $0.3 \text{ m}^2/\text{m}^2$ to $1.2 \text{ m}^2/\text{m}^2$ the model agrees much better with the data over most regions. Finally, the benefit of the bias-correction (NIT_{bc}) on LAI is also demonstrated in Figure 3. The bias-correction has little impact on the LAI of the deciduous and coniferous forest patch types. However, it does reduce the phase errors for

both the C3 crops and grassland patches. This results in much better LAI scores, reducing (increasing) the RMSD (CC) by about 10% compared with NIT_m .

The WG1 scores for the various simulations are given in Table 3. Recall that the SSM observations are linearly rescaled such that their mean and standard deviation match the NIT model simulation of WG1, which removes any bias already present.

5 Changing the model simulation has little impact on the scores, which suggests that the LAI evolution and the radiative forcing have a relatively small influence on the moisture content of the surface layer.

Next, the Nash efficiency scores for the different model simulations are displayed in Fig. 5 (a), showing the percentage of gauging stations at efficiency scores between 0 and 1.0. For the NIT simulation, about 26% of the stations have a score above 0.6 (a good score), 42% of the stations have a score above 0.5 (a reasonable score) and 79% of the stations have a positive Nash
10 score. These scores are **substantially** improved by increasing the LAI minimum and by bias-correcting the radiative forcing. For the NIT_m (NIT_{bc}) simulation about 31% (42%) of stations reach a score of at least 0.6, 48% (58%) of stations reach a score of 0.5 or higher and 80% (83%) of the stations have a positive score. Table 4 shows the median Nash scores for each simulation. The median Nash scores for NIT are increased by about 9% for NIT_m and further increased by 18% for NIT_{bc} . The median discharge ratio between the modelled (Q_s) and observed (Q_o) discharge is also shown for each simulation. A value that
15 is greater (smaller) than 1.0 indicates a positive (negative) bias in the model. NIT has a median discharge ratio of 1.19, which indicates that the simulated streamflow is over-estimated by about 20%. This is reduced to 1.15 by applying the LAI minimum and further reduced to 1.02 by applying the bias-correction. Therefore it appears that the bias in the discharge ratio has an important impact on the Nash score, with larger biases corresponding to smaller Nash scores. This is clarified when comparing the annual median Nash scores (Figure 6(a)) with the annual median discharge ratios in (Figure 6(b)). It seems that the size
20 of the bias in the discharge ratio is negatively correlated with the Nash score, which would explain why NIT_{bc} performs so well. Figure 6(c) and (d) show the average annual temperature and rainfall respectively. There does not appear to be a strong correlation between either the temperature or rainfall and the Nash score.

The Nash efficiency for NIT for each station over France is shown in Figure 2. The river discharge is well simulated over most areas, but the southeast and northern regions have generally negative scores (shown in black). In southeast France this is
25 related to a large number of dams in the Alps, which are not simulated by MODCOU. In northern France, this is linked to a large aquifer that is also not taken into account by MODCOU (see Habets et al. (2008) for details). There are a small number of stations with negative scores elsewhere, which could also be related to anthropogenic water management. The maps show similar patterns for the other simulations (not shown). The vast majority of stations ($> 80\%$) for NIT_{bc} are improved relative to NIT, including most of the stations with negative scores. A scatter plot of the Nash efficiency scores of NIT and NIT_{bc} for
30 all the stations can be found in Figure S1.2(a) of the Supplement.

Finally, we investigate the influence of the model simulations on the evapotranspiration, drainage and runoff fluxes in order to explain the differences in SIM discharges. Figures 7(a-e) show the average monthly LAI, WG2, evapotranspiration, drainage and runoff respectively, averaged over France. The NIT_m simulation has a greater average LAI in winter than NIT because the NIT LAI minimum is under-estimated. The effect of a higher LAI minimum is to enhance evapotranspiration in winter
35 and spring, which reduces the soil moisture and therefore diminishes the drainage and runoff. The consequence of increased

radiative forcing in NIT_{bc} is to further increase evapotranspiration and lower WG2 during much of the year. This substantially reduces drainage and runoff, especially from October to June. These effects are emphasized in Figure 8(a), which shows the difference between the sum of drainage and runoff for the different simulations compared with NIT. The reduced drainage and runoff feeding into the MODCOU hydrogeological model results in less river discharge, which explains the reduced river discharge bias and superior Nash scores for NIT_m and NIT_{bc} relative to NIT in Table 4.

3.2 Impact of DA on SIM

The performance of the DA runs on the LAI and WG1 scores are shown in Tables 2 and 3 respectively. LDAS1 substantially improves the fit of the simulated LAI to the LAI observations compared to NIT. We investigate the influence of DA on the drainage and runoff fluxes in Figure 7(f-j), which is equivalent to Figure 7(a-e) except that LDAS1 and LDAS2 are compared with NIT. Figure 7(g) demonstrates that the assimilation of LAI reduces the LAI phase errors in NIT, indicating that the SEKF is working effectively during much of the year. However, the LAI assimilation with the SEKF does not address the problem of the underestimated LAI in winter, unlike NIT_m in Fig. 7(b). Figure 8(b) shows the differences between the combined drainage and runoff fluxes between NIT and the DA methods. The LAI assimilation has a relatively small influence on the drainage and runoff fluxes in Figure 8(b) compared to NIT_m in Figure 8(a). The small positive correction of LAI in spring slightly increases (reduces) evapotranspiration (drainage and runoff) which is cancelled out by the opposite effect in autumn. Overall, LDAS1 does not greatly modify the discharge ratio or the Nash scores.

The LDAS2 experiment slightly improves the WG1 scores relative to NIT (Table 3). The median Nash discharge scores are degraded by about 7% for LDAS2 compared to NIT (Fig. 5(b) and Table 4) and the positive bias in the discharge ratio is increased by about 2% (Table 4). The reason for this is that LDAS2 has a higher average WG2 relative to NIT (Figure 7(f)), which translates to increased drainage and runoff for LDAS2. This is emphasized by comparing the combined drainage and runoff for LDAS2 relative to NIT in Figure 8(b). The extra water in the rivers exacerbates the Nash discharge bias already present in NIT, resulting in degraded Nash efficiency scores. The LDAS2 scores are degraded for about 70% of the stations relative to the NIT simulation and a scatter plot of the scores for all the stations can be found in Figure S1.2(b) of the Supplement.

The neutral impact of LDAS1 and the detrimental influence of LDAS2 on the soil moisture fluxes is explained in the following section by examining the observation operator Jacobians.

3.3 Examining the SEKF Jacobians

The SEKF observation operator Jacobians are governed by the physics of the model. Their examination is important in order to understand the SEKF performance. The LAI increments for LDAS1 are mainly driven by the $\frac{\partial LAI}{\partial LAI}$ Jacobian. The behaviour of the $\frac{\partial LAI}{\partial LAI}$ Jacobian values for ISBA-A-gs was investigated by Rüdiger et al. (2010). Their behaviour can be split into three distinct types, which depend on atmospheric conditions. The type “O” Jacobian is strictly equal to zero and occurs mainly in winter when the vegetation is dormant. In this case the LAI will be kept at its default model minimum. The type “A” Jacobian represents a fraction between zero and one and is correlated with the LAI value itself. It occurs during periods of vegetation growth i.e. predominantly in spring. The type “B” Jacobian is equal to 1.0 and takes place during periods of low vegetation

growth or high mortality, which occurs mainly in autumn. The grassland Jacobians are plotted for LDAS1 in Figure 9 for a particular point in southwest France (43.35° N, 1.30° E). Also plotted in the same graph are the LAI values themselves, with the minimum indicated by the red line. Indeed, the type O Jacobians tend to occur in winter, during which time the LAI returns to its minimum value of 0.3 m²/m². The type A and B Jacobians tend to occur in spring and autumn respectively. These findings are in agreement with Figure 4 of Rüdiger et al. (2010). The LAI performance for LDAS1 can now be explained by these Jacobian values. Figure 7(g) shows that during the winter the lowest LAI values are barely corrected by LDAS1 because, as shown in Figure 9, the LAI is frequently forced back to its minimum value (type O Jacobians). During the spring there is a small correction (type A Jacobians) and during the autumn there is a much larger correction (type B Jacobians). Hence the LDAS1 is able to correct the LAI phase errors to some extent, but LDAS1 is unable to correct the LAI minimum in winter. **The seasonal imbalances in the LAI Jacobian can also explain the negative bias in Table 2.** Since most of the drainage and runoff is present in winter and spring, the assimilation of LAI has little influence on SIM.

The $\frac{\partial \text{LAI}}{\partial \text{WG2}}$ Jacobian has generally positive values, since an increase in water content in the soil generally enhances photosynthesis and plant growth (not shown). However, this term is close to zero from about November to March while the vegetation is dormant. Therefore it does not **substantially** influence the LAI minimum in winter. **There is no evidence that it leads to long term increases in WG2 or results in increased drainage/runoff for LDAS2.**

The WG2 analysis increments for LDAS2 are largely driven by the $\frac{\partial \text{WG1}}{\partial \text{WG2}}$ Jacobian. A scatter plot of these Jacobian values against the WG1 variable is shown in Figure 10 for the same point as Figure 9 in Southwest France. The density of the points is derived from the kernel density estimation of Scott (1992). There are two dense regions when WG1 is equal to 0.15 and 0.30 m³/m³, which occur because WG1 is a thin layer, and therefore most of the time it is either dry or close to saturation. The WG1 and $\frac{\partial \text{WG1}}{\partial \text{WG2}}$ values are negatively correlated, with larger values of WG1 corresponding to smaller values of $\frac{\partial \text{WG1}}{\partial \text{WG2}}$. This implies that when rain is detected in the model but not in the SSM observations, the analysis increment will be smaller than when the rain is missed by the model but detected by the observations. Indeed, the average WG2 analysis increment for a positive innovation is $0.7 \times 10^{-3} \text{ m}^3/\text{m}^3$, while the average increment for a negative innovation is $-0.5 \times 10^{-3} \text{ m}^3/\text{m}^3$. This imbalance in the analysis increments leads to a net uptake of water in WG2, which induces the positive bias in the SIM river discharge. This problem was already highlighted by Draper et al. (2011). The Jacobians exhibited similar patterns of behaviour for other vegetation types than grasslands and across other points in France, albeit with different magnitudes (not shown).

3.4 Additional experiments

Additional experiments were performed to examine whether the poor performance of the SEKF was related to other factors than the Jacobians, namely the quality control of the observations, the underestimated LAI minimum or the bias in the atmospheric forcing. It is evident in Tables 2 to 4 that applying the additional quality control of the SSM observations (LDAS2_{QC}) does not **substantially** modify the LAI, WG1 or Nash discharge scorPROVA-Bes compared to LDAS2, despite removing about 10% of the SSM observations. Figure 11(a) shows only small differences in the Nash efficiency percentages between LDAS2 and LDAS2_{QC}. As expected, the LDAS1_{bc} and LDAS2_{bc} experiments improved on the LAI scores of LDAS1 and LDAS2 (Tables 2), but did not improve on the WG1 scores in Table 3. These changes are a similar order of magnitude to the improvement of

NIT_{bc} over NIT. In terms of discharge Nash efficiency scores, LDAS1_{bc} performed similarly to NIT_{bc} and LDAS2 performed **substantially** worse than NIT_{bc} (Table 4). The Nash efficiency percentages are shown in Figure 11(b). The comparison between LDAS1_{bc} and LDAS2_{bc} with NIT_{bc} in Figure 11(b) is analogous to the comparison between LDAS1 and LDAS2 with NIT in Figure 5(b).

- 5 The scores for the subset of 67 stations with low anthropogenic influence are also shown in Table 4. The scores for this subset are improved relative to the 546 stations in Table 4, as expected. In particular, the percentage of stations with good scores (Nash efficiency > 0.6) is greatly increased. For the interested reader, scatter plots of the Nash scores for the 67 stations are shown in Figure S1.3 in the Supplement. The discharge bias is also slightly smaller for the stations with low anthropogenic influence relative to the 546 stations. This suggests that a small part of the positive bias in the discharge ratio of the NIT simulation for
- 10 the 546 stations could be attributed to abstractions not being accounted for, such as drinking water or irrigation. However, most of the discharge bias in the NIT simulation is still present with the 67 stations with low anthropogenic influence. Moreover, the relative performances of the experiments are very similar. Therefore, the conclusions of the experiments are not affected by the ability of SIM (with or without DA) to simulate anthropogenically influenced streamflow. These results confirm that the inability of the SEKF to improve the soil moisture fluxes comes mostly from the SEKF Jacobians.

15 4 Discussion

- Previous work by Muñoz Sabater et al. (2007) and Fairbairn et al. (2015) clearly demonstrated that the assimilation of SSM observations with an SEKF can improve WG2 with the 3-layer ISBA-A-gs model. Barbu et al. (2014) also demonstrated that the assimilation of LAI reduces phase errors in the modelled LAI evolution. However, in this work we showed that the SEKF has little influence on the drainage and runoff fluxes when assimilating LAI observations (LDAS1 experiment). Furthermore,
- 20 the SEKF actually degrades these fluxes when assimilating SSM and LAI observations (LDAS2 experiment). The differences in these findings are due to the nonlinear interactions in LSMs which can cause the assimilation of one state variable to be detrimental to other soil moisture processes (Walker and Houser, 2005). The poor results for LDAS1 and LDAS2 can be explained by model errors, atmospheric forcing errors and model nonlinearities near the soil moisture wilting point and field capacity thresholds, none of which are captured by the SEKF observation operator Jacobians.

25 4.1 Could LAI assimilation be improved?

- In LDAS1, the seasonal variability in the analysis LAI increments was uneven, with large negative increments in late summer/autumn and small positive increments in winter/spring. This occurred because the LAI Jacobian ($\frac{\partial \text{LAI}}{\partial \text{LAI}}$) was frequently equal to zero during winter and therefore the LAI remained at its incorrect minimum value after the analysis update. Moreover, LAI is only assimilated every 10 days so the model LAI would drift back to its underestimated minimum value between
- 30 cycles. Consequently, the average LAI analysis was negatively biased. These Jacobian values are physically sensible, since the vegetation is dependent on the atmospheric conditions and is often dormant during the winter period. The problem is related to the lack of a model error term in the SEKF.

The lowest LAI values could be corrected with a full EKF and a model error term, but it would be complicated to parameterize the model-error covariance matrix because the LAI minimum is linked to several factors concerning the atmospheric conditions and the vegetation type. A short-term solution to the underestimated LAI minimum was demonstrated in the experiments, which was to set a higher LAI minimum parameter in the model based on observations. However, it would be more sensible in the long-term to resolve the underlying issues with the model physics. A thorough comparison of the ISBA-A-gs simulated LAI with both SPOT-VGT (used in our experiments) and MODIS data over south-west France was performed by Brut et al. (2009). They did notice significant discrepancies between all three data sets, suggesting that there is significant uncertainty in both the model and the observations. However, they also noticed that the modelled LAI of the C3 natural herbaceous (grasslands)/C3 crops had a delayed onset relative to both satellite products (see Figure 4 in Brut et al. (2009)). They found that this was particularly problematic for grasslands in mountainous regions. By comparing the data with in situ measurements, they found that the generic temperature response of photosynthesis used in the model is not appropriate for plants adapted to the cold climatic conditions of the mountainous areas. This problem was also linked to a prolonged LAI minimum in the model relative to the observations. Lafont et al. (2012) found similar issues when comparing the same products over France. Indeed, Figure 4 in our study shows that the NIT LAI minimum was particularly underestimated in the grassland areas of the Massif Central mountains in central France, but not so much in lower regions further north. Finally, these problems could explain the delayed onset and underestimated LAI minimum for both grasslands and C3 crops in Figure 3 in our study.

It should be recognized that errors in the modelled LAI are not just present over grasslands, but also over other vegetation types. Figure 3 shows there are significant discrepancies between the model and the observations for C3 crops and deciduous forests as well. Given that these discrepancies vary substantially between different vegetation types, it is not optimal to assimilate a gridpoint averaged observation. This issue is currently addressed by disaggregating the LAI for each patch individually.

Finally, as already mentioned, LAI is assimilated every 10-days. LAI data availability could be improved using higher spatial and temporal resolution products in order to limit the impact of clouds.

4.2 Why does SSM assimilation degrade river discharges?

It is important to point out that it is physically sensible for WG1 to decouple from WG2 during precipitation events. The precipitation forcing leads to a saturation of the surface layer and subsequently WG1 becomes less dependent on WG2. The degradation of drainage and runoff can be caused by limitations in the SEKF, in the land surface model and in the data.

Firstly, as recognized by Draper et al. (2011), an important problem is that the SEKF is not designed to capture the uncertainty in the model and the precipitation forcing, which should increase during precipitation events and therefore compensates for the smaller Jacobians. The SAFRAN precipitation forcing performs well for a mesoscale analysis and has a higher spatial resolution than global satellite products such as ERA-interim (Quitana-Ségui et al., 2008; Vidal et al., 2010). However, by design the precipitation is assumed to be homogeneous over 615 specified climate zones. Errors are therefore introduced from the spatial heterogeneity of the precipitation, particularly in mountainous regions (Quitana-Ségui et al., 2008).

Secondly, the 3-layer ISBA model has strong nonlinearities near the soil moisture thresholds, some of which lead to unrealistic behaviours of the model Jacobians. During dry conditions in summer the SEKF $\frac{\partial \text{WG1}}{\partial \text{WG2}}$ Jacobian can be excessive. This is

linked to a rapid increase in transpiration when water is added to WG2 following dry conditions (Draper et al., 2009; Fairbairn et al., 2015). The origin of this nonlinearity is partly related to an unrealistic feature of the surface energy balance. One single surface temperature is used to represent the vegetation and the surface layer, which causes the transpiration to increase too quickly after water is added to WG2 (Draper et al., 2009; Mahfouf, 2014). This problem could be relieved to some extent by introducing the new version of ISBA with a multiple energy balance (MEB, (Boone et al., 2017)) and by using a multi-layer diffusion model (ISBA-DIF, (Decharme et al., 2011)).

Lastly, regarding observations, the current ASCAT product is affected by vegetation (Vreugdenhill et al., 2016) and a seasonal CDF matching is needed in DA systems assimilating ASCAT SSM. This procedure is however sub-optimal. A solution to this problem is to go towards the implementation of an observation operator in order to assimilate the backscattering coefficients directly. In this way, the vegetation information content in the ASCAT signal could be used to analyse vegetation biomass and would also provide information for the analysis of root-zone soil moisture, in addition to the microwave soil moisture signal.

4.3 Could more sophisticated DA methods improve SSM assimilation?

The presence of the uncertainties in the model and in the forcing could more easily be addressed with an EnKF than an SEKF because an EnKF can stochastically represent model and precipitation errors (Maggioni et al., 2012; Carrera et al., 2015). Fairbairn et al. (2015) found that an EnKF with a simple stochastic rainfall error estimation demonstrated similar WG2 scores to the SEKF over 12 sites in southwest France (validated using in situ observations). Both methods were affected by nonlinearity problems.

There are DA methods, such as particle filters, designed to handle model nonlinearities. Moradkhani et al. (2012) demonstrated that good results on a hydrological model could be achieved with a particle filter with about 200 members. However, it is substantially more computationally expensive than an EnKF, which typically requires about 20 members to overcome sampling error problems for LSMs (Maggioni et al., 2012; Carrera et al., 2015; Fairbairn et al., 2015). Therefore we intend to test an EnKF over France using the same validation framework used in this study.

5 Conclusions

This study assessed the impact on streamflow simulations of assimilating surface soil moisture (SSM) and leaf area index (LAI) observations into the ISBA-A-gs land surface model (LSM). The drainage and runoff outputs were used to force the MODCOU hydrogeological model and were validated by comparing the simulated streamflow with over 500 river-gauge observations over France during several years. To our knowledge, this is the first article to examine the impact of LAI assimilation on streamflow simulations using a distributed hydrological model. Furthermore, this study highlights the importance of systematic model/forcing deficiencies on the streamflow simulations. The validation is robust due to the large number of river gauge observations employed and the long evaluation period (2007-2014). The results from this study could also have ramifications for flood warning accuracy since SIM is used operationally by Météo-France as a tool for flood forecasting.

Increasing the LAI minimum parameter resulted in greater evapotranspiration in winter/spring and bias-correcting the radiative forcing increased evapotranspiration during much of the year. Both corrections effectively reduced the positive bias in the drainage/runoff fluxes and substantially improved the Nash efficiency scores. Although DA is not theoretically designed to correct systematic model deficiencies, it was found that assimilating only LAI observations substantially reduced the LAI phase errors in the model. However, this induced a net negative bias in the LAI analysis relative to the observations. Given that drainage and runoff occurs predominantly in late winter and spring, the LAI assimilation had negligible impact on these fluxes.

Assimilating SSM resulted in spurious increases in drainage and runoff, which degraded the SIM discharge Nash efficiency.

An issue in DA experiments was the underlying assumption made by the SEKF that the model is perfect. Allowing for model and atmospheric forcing errors could more easily be addressed with an ensemble Kalman filter (EnKF) method than the SEKF, although both methods are affected by nonlinearity issues. In the future we will test the EnKF using a similar validation employed in this study. Regarding LAI assimilation, the SEKF assimilates the LAI observations by aggregating the different vegetation patches in each gridbox. This approach is not optimal because each vegetation type exhibits unique seasonal variability. Given the high resolution of LAI observations (1 km), work is underway to disaggregate the observations.

While the ISBA LSM is well established and is used operationally at Meteo-France, this study has helped us to identify some limitations that need to be addressed. A new multi-layer diffusion model should improve representation of the coupling between the surface and root-zone soil moisture. Furthermore, a new multiple energy balance version should decouple the bare soil evaporation and the transpiration processes that lead to an unphysical link in ISBA between surface and deep soil moisture. Previous research has demonstrated that the generic temperature response of photosynthesis used in the model is not appropriate for plants adapted to the cold climatic conditions of the mountainous areas. This is consistent with the phase errors and the underestimated grassland LAI minimum in our study. Solving this problem would presumably increase the LAI minimum in winter, which would be more sensible than simply fitting the LAI minimum to observations. Finally, the LDAS should benefit from further improvement of the satellite-derived LAI and SSM. Using an observation operator for the ASCAT backscattering coefficients would permit accounting for the vegetation information content in the ASCAT signal.

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Table 1. List of experiments. The bias-correct forcing option implies an increase of the direct short-wave and long-wave radiation by 5%. The SSM outliers removal applies to SSM observations outside the 90% confidence interval of the model.

Experiment	LAI grassland min (m ² /m ²)	Bias-correct forcing	DA	SSM outliers removal
NIT	0.3	No	No	–
NIT _m	1.2	No	No	–
NIT _{bc}	1.2	Yes	No	–
LDAS1	0.3	No	LAI	–
LDAS2	0.3	No	LAI+SSM	No
LDAS1 _{bc}	1.2	Yes	LAI	–
LDAS2 _{bc}	1.2	Yes	LAI+SSM	No
LDAS2 _{QC}	0.3	No	LAI+SSM	Yes

Table 2. Scores for LAI (prognostic variable compared with observations) averaged over 2007-2014. The RMSD and CC stand for root mean square difference and correlation coefficient respectively. The closest fit to the observations is shown in bold font.

Experiment	RMSD (m^2/m^2)	CC	Bias (m^2/m^2)
NIT	1.18	0.56	0.11
NIT _m	1.14	0.58	0.25
NIT _{bc}	1.02	0.63	0.17
LDAS1	0.69	0.82	-0.08
LDAS2	0.71	0.81	-0.04
LDAS1 _{bc}	0.63	0.84	-0.04
LDAS2 _{bc}	0.66	0.83	-0.02
LDAS2 _{QC}	0.72	0.81	0.02

Table 3. Scores for WG1 (prognostic variable compared with observations) averaged over 2007-2014. The RMSD and CC stand for root mean square difference and correlation coefficient respectively. The closest fit to the observations are shown in bold font.

Experiment	RMSD (m^3/m^3)	CC	Bias (m^3/m^3)
NIT	0.051	0.77	0.00
NIT _m	0.049	0.77	0.00
NIT _{bc}	0.051	0.77	0.00
LDAS1	0.049	0.77	0.00
LDAS2	0.048	0.78	0.00
LDAS1 _{bc}	0.049	0.77	0.00
LDAS2 _{bc}	0.049	0.78	0.00
LDAS2 _{QC}	0.048	0.78	0.00

Table 4. Median Nash efficiency (NE) and discharge ratio (Qs/Qo) scores over the 546 river gauges over France and for the subset of 67 gauges with low anthropogenic influence, calculated over 2007-2014. Also shown are the percentage of stations with a Nash score above 0.6. The best scores are shown in bold font.

Experiment	NE for 546/67 sta- tions	Discharge ratio for 546/67 stations	% stations with NE > 0.6 for 546/67 stations
NIT	0.44/0.48	1.19/1.16	26%/44%
NIT _m	0.48/0.54	1.15/1.12	30%/48%
NIT _{bc}	0.56/0.60	1.02/0.99	42%/59%
LDAS1	0.44/0.48	1.18/1.15	27%/44%
LDAS2	0.41/0.45	1.21/1.18	23%/40%
LDAS1 _{bc}	0.56/0.60	1.02/1.00	42%/57%
LDAS2 _{bc}	0.53/0.54	1.08/1.06	38%/53%
LDAS2 _{QC}	0.40/0.45	1.21/1.18	21%/39%

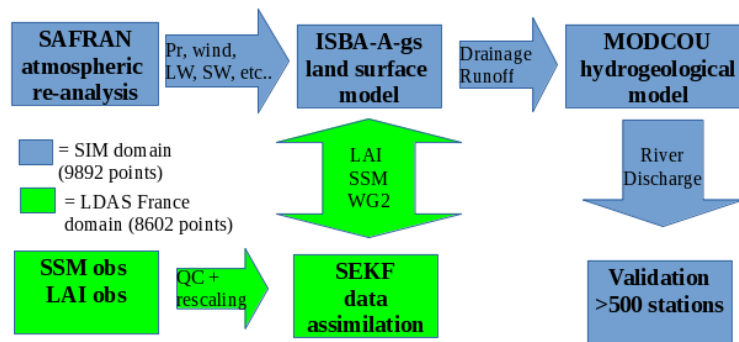


Figure 1. Flowchart of the SIM hydrological model and how LDAS France is connected with SIM.

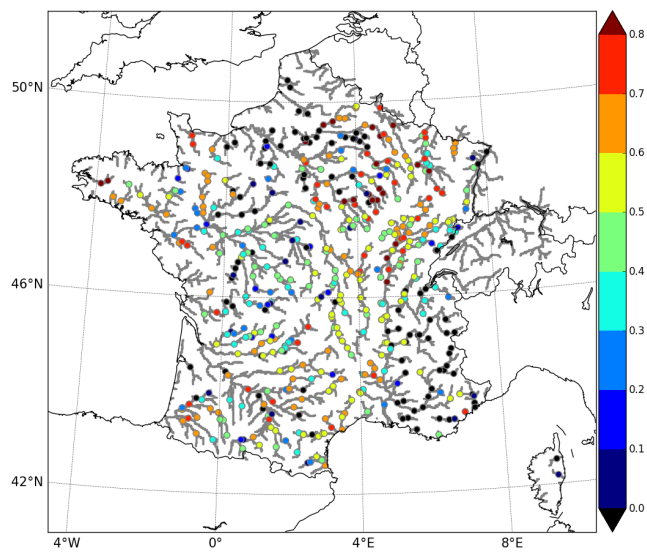


Figure 2. Nash efficiency scores for each station over France for the NIT simulation, calculated over the period 2007-2014. The river network is also shown.

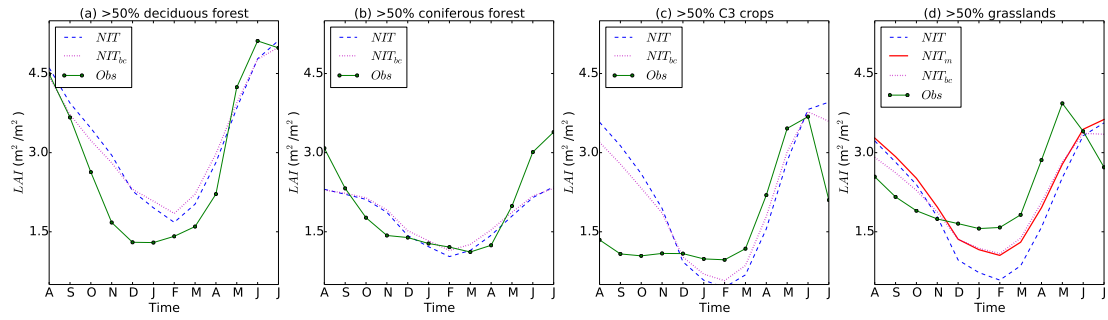


Figure 3. Monthly averaged LAI for the model simulations and for the gridpoints with at least 50% of the four dominant vegetation types, averaged over 2007-2014 and averaged over France.

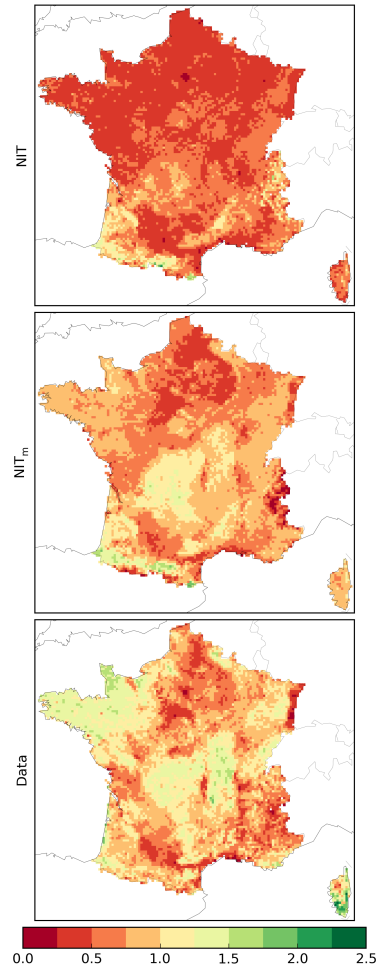


Figure 4. Map showing the average annual LAI minimum (2007-2014) for NIT, NIT_m and the GEOV1 observations (m^2/m^2) over France.

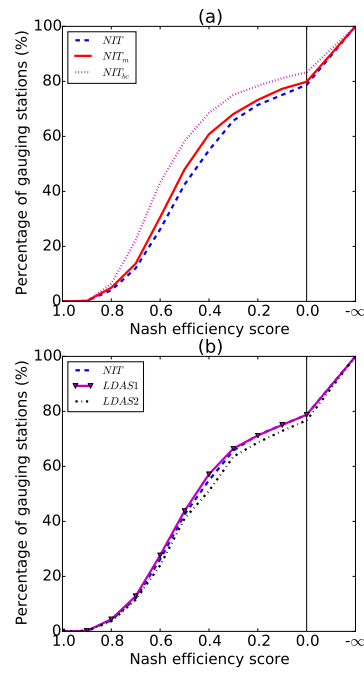


Figure 5. Nash efficiency scores over France for (a) the model simulations and (b) the DA methods, calculated over the period 2007-2014.

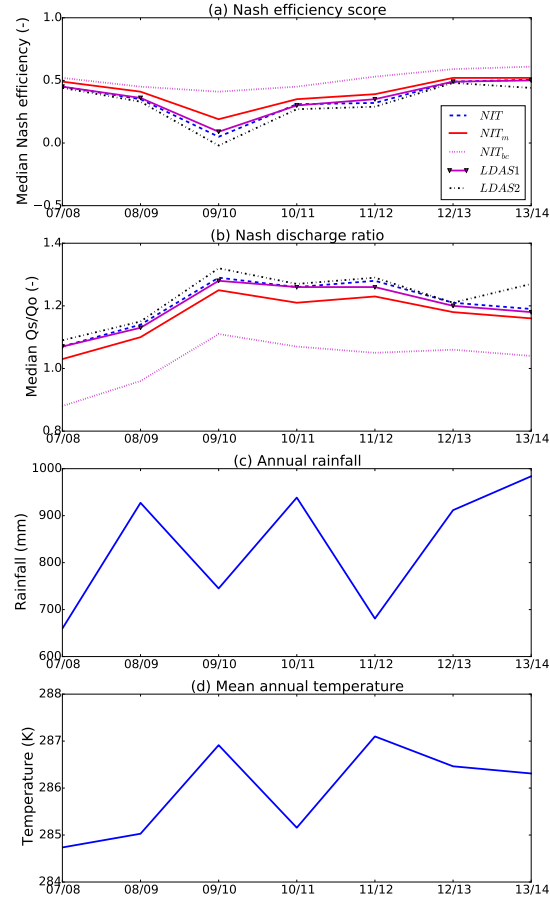


Figure 6. Median annual (a) Nash efficiency scores and (b) discharge ratio for each experiment. Average annual (c) temperature and (d) cumulated precipitation.

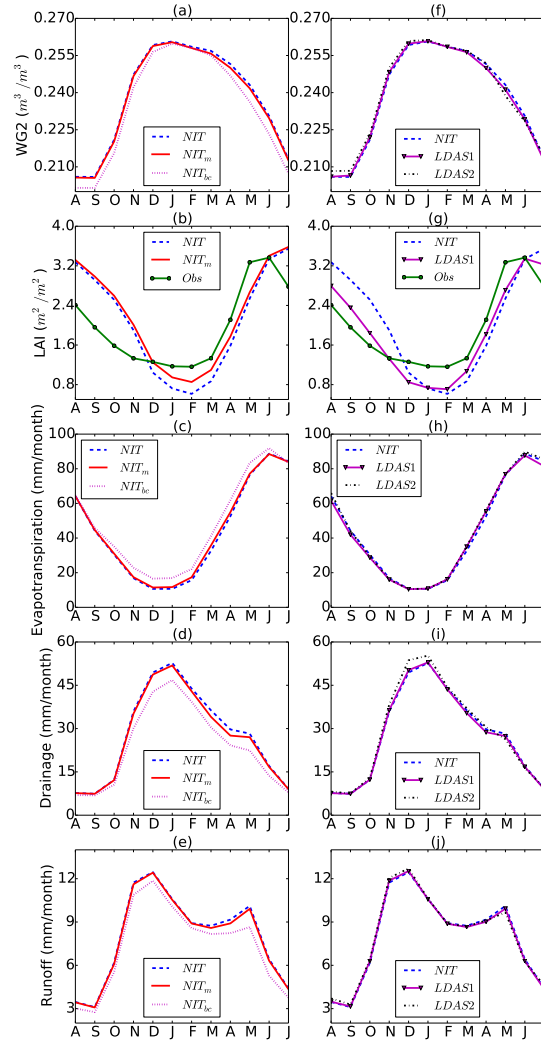


Figure 7. Average monthly (a) WG2 and (b) LAI; and monthly cumulative (c) evapotranspiration, (d) drainage and (e) runoff for NIT and the other model simulations. Plots (f-j) show NIT and the DA analyses for the equivalent variables as (a-e). Results are all averaged over the period 2007-2014 and averaged over France.

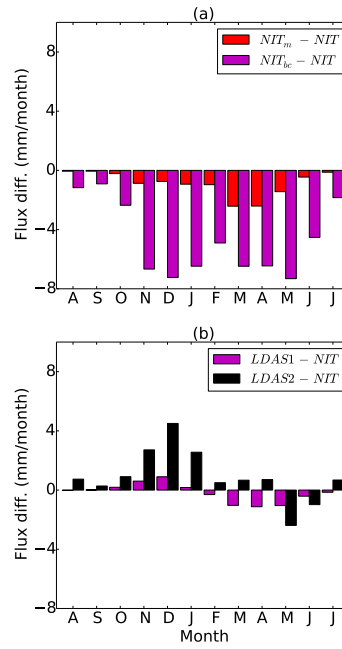


Figure 8. Monthly combined drainage+runoff flux differences between (a) NIT and the other model simulations and (b) NIT and the DA analyses averaged over the period 2007-2014 and over France.

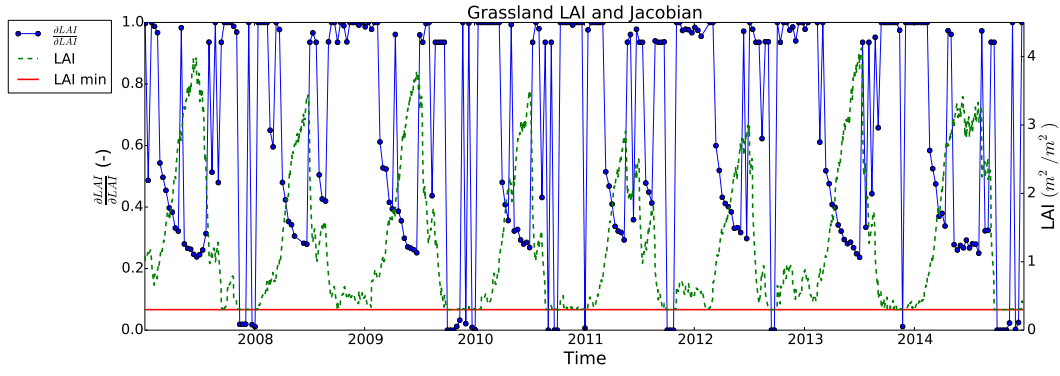


Figure 9. Time evolution of the LDAS1 $\frac{\partial LAI}{\partial LAI}$ Jacobian, together with the LAI analysis and the minimum LAI model parameter for the grassland patch at a point in southwest france (43.35° N, 1.30° E).

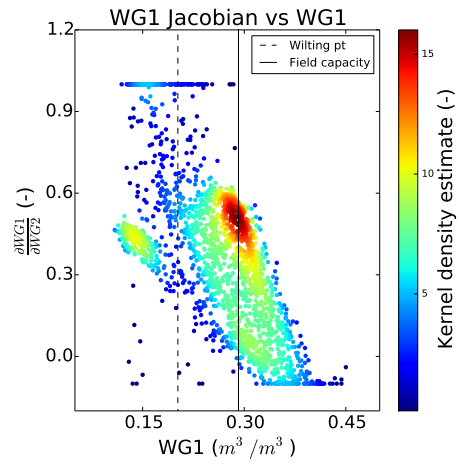


Figure 10. Scatter plot of WG1 against the LDAS2 $\frac{\partial WG1}{\partial WG2}$ Jacobian for the grassland patch at the same point as Figure 9.

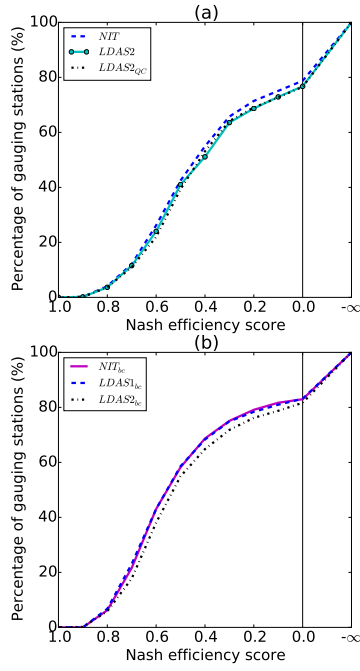


Figure 11. Average Nash efficiency scores over France for (a) the NIT, LDAS2 and LDAS2_{QC} experiments and (b) the NIT_{bc}, LDAS1_{bc} and LDAS2_{bc} experiments.

The effect of satellite-derived surface soil
moisture and leaf area index land data
assimilation on streamflow observations over
France

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Supplement

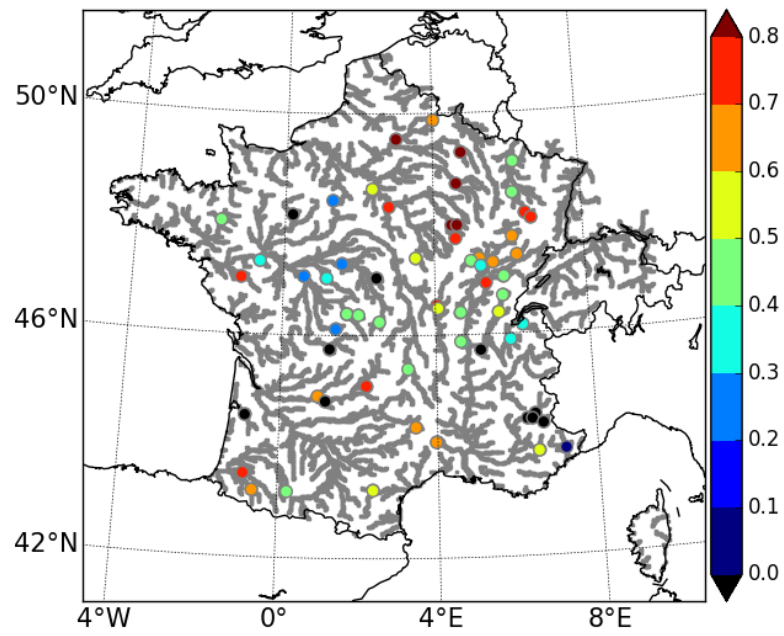


Figure S1.1: Map of the SIM discharge Nash efficiency scores for the 67 stations with low-anthropogenic influence over France for the NIT simulation, calculated over the period 2007-2014. The river network is also shown.

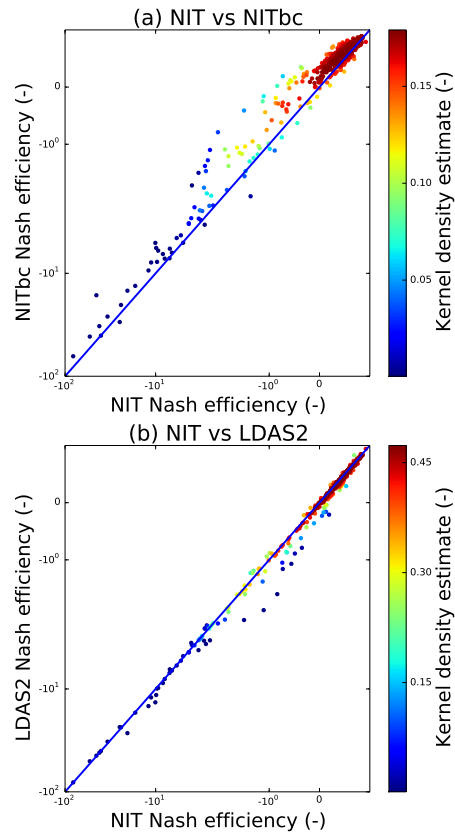


Figure S1.2: Scatter plots of the SIM discharge Nash efficiency scores for all 546 stations for (a) NIT vs NITbc and (b) for NIT vs LDAS2. The scores are calculated over 2007-2014.

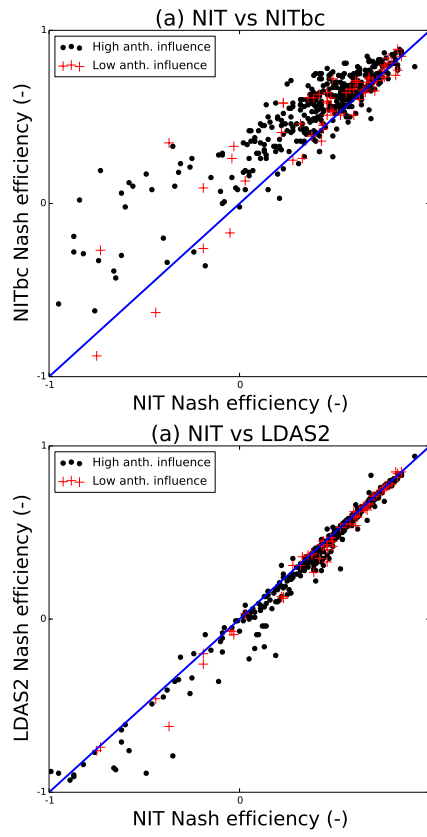


Figure S1.3: Same as Fig. S1.2, but the stations are classified with either low (67 stations) or high anthropogenic influence (479 stations). For the sake of clarity, the Nash scores are shown between -1.0 and 1.0.

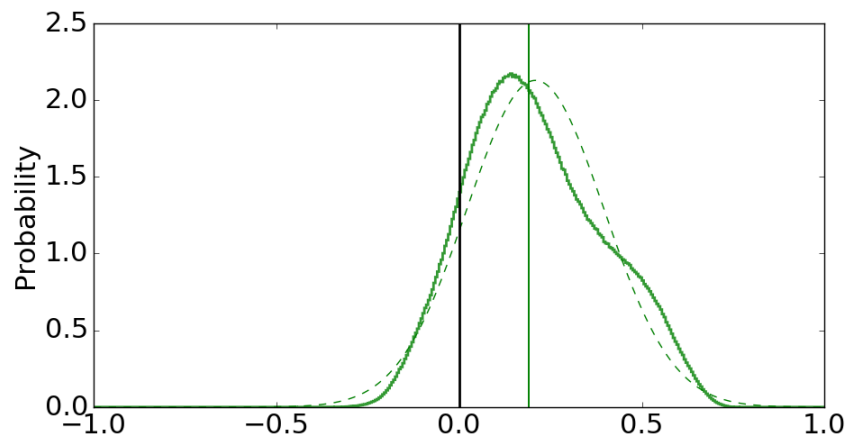


Figure S1.4: Innovation (thick line) histogram and its Gaussian fit (dashed line) for the SSM product without seasonalCDF matching.

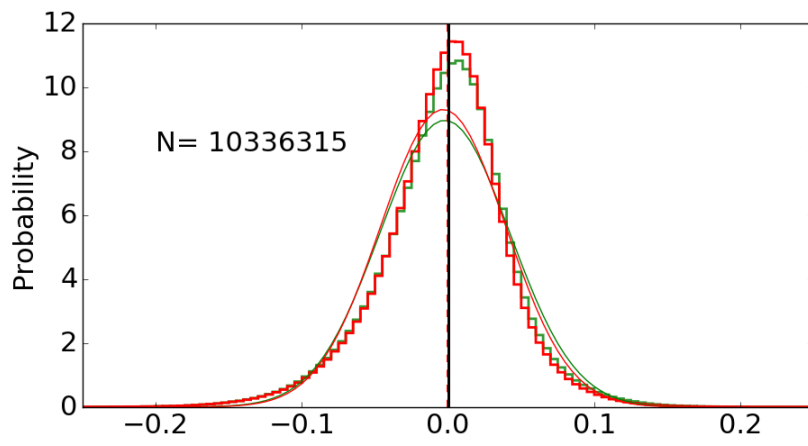


Figure S1.5: Innovation (green thick line) and residual (red thick line) histograms, as well as their Gaussian fits respectively, for the SSM product with seasonal CDF matching.

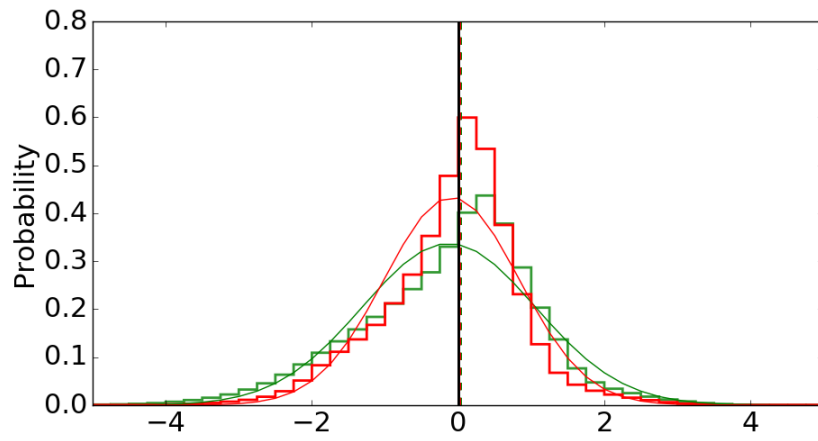


Figure S1.6: Innovation (green thick line) and residual (red thick line) histograms, as well as their Gaussian fits respectively for LAI product.

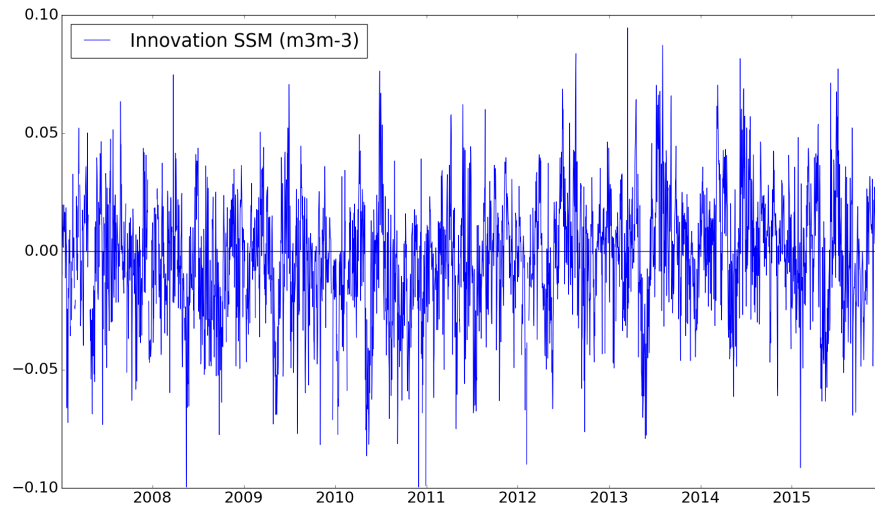


Figure S1.7: Temporal evolution of SSM innovations.

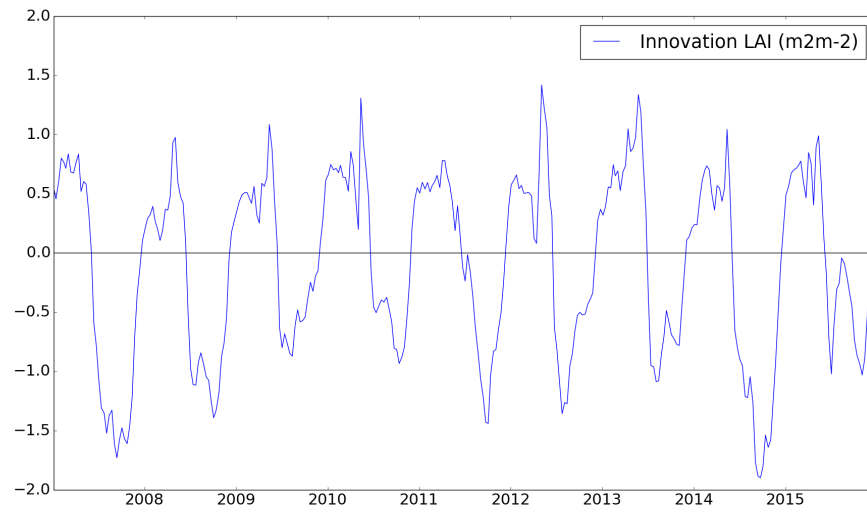


Figure S1.8: Temporal evolution of LAI innovations.