

Responses to comments Provided by Referee 1

Parameter optimization by MCMC method for the evapotranspiration model is one of the best solutions for improving the estimation accuracy. Zhu et al. did an interesting work on simultaneous assimilation of two different data streams: 30min evapotranspiration (ET) and daily evaporation (E), then finally gained the moderately good accordance between the simulations and the observations. The efforts proved a new feature for optimizing the canopy transpiration and soil evaporation parameters, and also brought the direction for further improvement of such ET model.

Authors' response: Thanks very much for your positive comments.

Main comments:

1. However, this paper is suffering from insufficient explanation on the optimization scheme.

Authors' response: According to your valuable suggestions, a detail explanation of the optimization scheme were added in our revised paper (Lines 303-315, Pages 14-15):

It was well recognized that efficiency of the M-H algorithm was strongly effected by the proposal distribution function. To find an effective proposal distribution $P(\mathbf{c}^{\text{new}} | \mathbf{c}^{k-1})$, a test run of the M-H algorithm with 10, 000 simulations was made by using a uniform proposal distribution (Braswell et al., 2005):

$$\mathbf{c}^{\text{new}} = \mathbf{c}^{k-1} + r(\mathbf{c}^{\text{max}} - \mathbf{c}^{\text{min}}) \quad (26)$$

where \mathbf{c}^{k-1} is the current accepted point; r is a random number uniformly distributed between -0.5 and +0.5; \mathbf{c}^{min} and \mathbf{c}^{max} are the lower and upper limits of parameter vector \mathbf{c} . Based on the test run, we then constructed a normal proposal distribution $\mathbf{c}^{\text{new}} : N(\mathbf{c}^{(k-1)}, \text{cov}^0(\mathbf{c}))$, where $\text{cov}^0(\mathbf{c})$ is the covariance matrix of the parameter vector \mathbf{c} from the initial test run (Xu et al., 2006).

In addition, a detailed flowchart representing the basic scheme of the M-H

algorithm and the Matlab code were presented in **Appendix B**.

2. ... and on the optimization of which parameter reduced the uncertainty on model simulation.

Authors' response: We thought that it may be good to explain this problem by doing a parameter sensitivity analysis. Thus, in our revised paper a sensitivity analysis was conducted (see details in **Appendix A**). The results indicated that the most sensitive parameters in the S-W model was r_{STmin} , and followed by b_1 , b_2 , k_2 and k_1 . Other parameter had almost no effect on the variability in model output. We have stated it in our revised paper (Lines 374-381, Page 18):

The global sensitivity analysis with the first-order impact ratio (FOIR) values (Appendix C) reveal the importance of input parameters in affecting total ecosystem evapotranspiration. The results indicated that total ET responded sensitively to r_{STmin} , b_1 , b_2 and k_2 with FOIR values being 54.3%, 21.9%, 10.4% and 8.5%, respectively. Other parameters exhibits relative low (<5%) FOIR values, suggesting that the variability in these parameters had almost no effect on the variability in model output.

3. and on how individual measurement data of two data steams improved your model simulation.

Authors' response: According to your suggestion, two different assimilation schemes were conducted to evaluated on how individual measurement data of two data steams improved your model simulation. The two assimilation schemes were: (1) simultaneous assimilation all data sets including half-hourly ET (λET ; $W m^{-2}$) and daily soil evaporation (E ; $mm d^{-1}$); (2) only assimilation half-hourly ET (λET ; $W m^{-2}$). The detail comparisons between the two assimilation scheme were presented in **Appendix B**.

4. The authors miss the explanations on the parameter optimization

processes and results. First, why don't you optimize other parameters for better estimation? Your former paper, Zhu et al. (2013), used g_{max} , q_{50} , d_{50} , k_q , k_a more than this study. Explain the reason why you chose 6 parameters for optimization in this study.

Authors' response: Firstly, the canopy resistance model in this two studies are different. In our former paper, the Leuning's type canopy resistance model (Leuning et al., 2008) were used. In this study, the Jarvis-type model (Jarvis, 1976) was used. Thus, the parameters were different for these two different model.

Secondly, we thought that parameters with really physical or biological meanings (e.g., K_A) should be measured in site (Sauer et al., 2007) rather than to be estimated.

Third, to avoiding the equifinality, a global sensitivity analysis was conducted to reveal the most sensitive parameters in the S-W model. The first-order impact ratio (FOIR) values for r_{STmin} , b_1 , b_2 and k_2 were 54.3%, 21.9%, 10.4% and 8.5%, respectively. While FOIR values for some parameters (T_{amin} and T_{amax}) were less than 5% (see **Appendix A**).

Thus, we chose r_{STmin} , b_1 , b_2 , and k_1-k_3 as parameters, while other from literatures.

References:

Leuning, R., Zhang, Y.Q., Rajaud, A., Cleugh, H., Tu, K., 2008. A simple surface conductance model to estimate regional evaporation using MODIS leaf area index and the Penman–Monteith equation. *Water Resour. Res.* 44, W10419. <http://dx.doi.org/10.1029/2007WR006562>.

Jarvis, P.G. 1976. The interpretation of the variations in leaf water potential and stomatal conductance found in canopies in the field. *Philos. T. R. Soc. B.*, 273, 563-610.

Sauer, T.J., Singer, J.W., Prueger, J.H., DeSutter, T.M., Hatfield, J.L. 2007. Radiation balance and evaporation partitioning in a narrow-row soybean

canopy. Agriculture and Forest Meteorology, 145, 206-214.

5. Second, how did you decide the measurement error variance, σ ?

Authors' response: In our revised paper, the method to determine the error variance were given as (Lines 271-284, Pages 13-14):

σ_i ($i=1,2$) represents the residual errors, or standard deviation about model predicted output of the i th dataset. Here, we assumed σ_i is the same over the observation time for the i th data set (Braswell et al., 2005). Traditionally, σ_i can be included into the analysis explicitly (i.e., assuming σ_i is uniform over $\log \sigma_i$; Gelman et al., 1995) and treated as one the model parameters, which yields a complete posterior distribution of σ_i . However, this method artificially increased the parameter dimension of the problem and may result in unreasonable estimations of the parameter values (Kavetski et al., 2006). In this study, σ_i was estimated by using the analytical method (Hurt and Armstrong, 1996; Braswell et al., 2005), which is to find the value of σ_i that maximizes $\log(p(\mathbf{O}_i(\cdot)|\mathbf{c}))$ for a given parameter vector. By differentiating $\log(p(\mathbf{O}_i(\cdot)|\mathbf{c}))$ with respect to σ_i , we can obtain:

$$\sigma_i^a = \sqrt{\frac{1}{n_i} \sum_{t=1}^{n_i} (e_i(t))^2} \quad (24)$$

We then used σ_i^a to replace σ_i in the equations (22).

6. Third, the arithmetic mean values from posterior parameter probability density were picked up as the optimized parameter numbers in this study. However, I think that the median values should be used for them although the mean and median would be the same if there is a perfect Gaussian probability distribution. However, normally it is not the case. So you should take the median value for the optimized parameter number.

Authors' response: According to your valuable suggestion, the median value was used as the optimized parameter (Lines 340-342, in Page 16):

, $f_i(t)$ is the simulation which was calculated using the posterior median parameter values, and other parameter vectors selected from the parameter chains generated by the MCMC iteration (van Oijen et al., 2013).

7. Fourth, you compare the range of posterior parameter values to those of other posterior parameter values. But, if you like to inter-compare the relative influence by each parameter optimization on reducing total ET error, you have to use the relative range of parameter values, by dividing the absolute parameter value range by posterior/prior parameter uncertainty value.

Authors' response: According to your suggestion, relative uncertainty reduction was added in our revised paper (Lines 370-372, Page 18):

Parameters r_{STmin} , b_1 , b_2 and k_2 showed relatively large uncertainty reductions (defined as $1 - CI_{posterior} / CI_{prior}$, where CI is the length of the 95% credible interval) (Fig. 5).

8. This study assimilated daily E in addition to 30min ET, which is already used in your previous study on the Qinghai Tibetan Plateau (Zhu et al., 2013). This is a good originality of this study. So I like to know how the estimation accuracy will change if you optimize single data (ET or E), and how the accuracy on E estimation is if only ET is assimilated, and vice versa.

Authors' response: To clearly investigate this interesting question, we compared two different assimilation scheme: (1) simultaneous assimilation all data sets including half-hourly ET (λET ; $W m^{-2}$) and daily soil evaporation (E;

mm d⁻¹); (2) only assimilation half-hourly ET (λET ; W m⁻²). (see **Appendix B**).

Comparing with the two assimilation schemes, [important differences occurred in estimates of the posterior distribution of parameters related to the soil surface resistance](#) (b_1 and b_2 ; s m⁻¹). Generally, tighter posterior distributions for parameters b_1 and b_2 were obtained by Scheme 1. For example, the values of uncertainty reduction for b_1 and b_2 in Scheme 1 (0.89 and 0.56, respectively) were higher than that in Scheme 2 (0.79 and 0.12, respectively). Thus, the daily soil evaporation data helped to well constrain estimates of b_1 and b_2 . In addition, the six calibrated parameters by Scheme 1 were not significantly inter-correlated with each other (correlation coefficients lower than 0.1), while for Scheme 2 the pairs b_1 and b_2 and r_{STmin} and b_2 tended to be constrained together with correlation coefficients being 0.84 and 0.32, respectively.

Overall, the simulations (half-hourly λET and daily soil evaporation) of the S-W model optimized by using all data sets simultaneously were comparable to the measurements (see [Fig. 6 in the Manuscript](#)). For example, the slope of regressive equation between the measured and modeled half-hourly λET values for Scheme 1 was 0.84, with MBE of 24.2 W m⁻², IA of 0.93 and EF of 0.74. A relatively good agreement between measured and estimated daily soil evaporation (E) was also obtained. The slope of regression equation was 1.01, with MBE of -0.01 mm day⁻¹, IA of 0.94 and EF of 0.76. When only EC-measured data were used (Scheme 2), the performances of the S-W model optimized by Scheme 2 on simulations of half-hourly λET were not significantly different from that optimized by Scheme 1. The regression equation between the measured λET and the estimated λET from the S-W

model optimized by Scheme 2 was 0.83, with MBE of 30.5 W m^{-2} , IA of 0.67 and EF of 0.13. However, the S-W model optimized by Scheme 2 significantly underestimated the soil evaporation (E). The slope of regression equation between the measured and the estimated E was 0.59, with MBE of 0.11 mm day^{-1} , IA of 0.67 and EF of 0.13. Thus, we can not ensure the S-W model properly partition the total ET into its different components using only the half-hourly λET data, even though the simulated values were in good agreement with measurements.

9. For advection, you concluded that the underestimation by S-W model was induced by no representation of enhanced ET by such dry air advection so-called as an oasis effect. I guess that the hot/dry airflow effect by advection could be reflected by enhanced air temperature and enhanced vapor pressure deficit, which would give higher ET estimation by S-W model to some extent.

Authors' response: Yes, when the air gets hot and dry in the absence of inversion temperature layer, a higher ET was estimated by the S-W model. However, for heterogeneous land surface such as desert and oasis, advection was often observed. In desert region, the available energy is mainly dissipated as sensible heat to warm the air; In the oases on the other hand, water is generally not limited due to irrigation and it permits evapotranspiration freely. Thus, the oasis is cooler than the regional air in which it is embedded, and there is a continual air-to-oasis inversion temperature gradient driving a downward directed heat flux. The energy used to evapotranspiration is more than available solar radiation. Oke (1978) pointed that: **this anomalous situation is explained by the fact that the atmosphere supplies sensible heat to the oasis surface**. The interaction between the oasis and nearby desert were illustrated in Fig. S1.

However, the advection process was neglected in the S-W model, and

underestimations of evapotranspiration were observed in our study in the presences of inversion temperature layer (Fig. 10 in our revised paper).

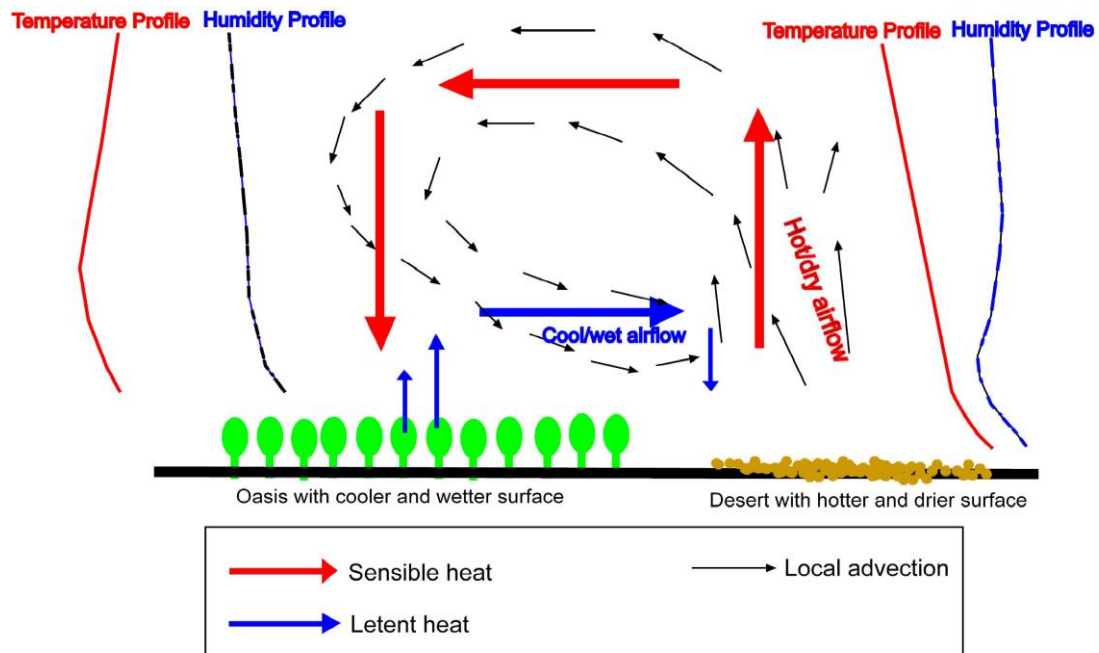


Fig. S1 The interaction between desert and oasis (modified according to Hu, 1994).

References:

Oke, T. R. Boundary layer Climates, Second ed. Mathuen, London, 1978.
 Hu, Y.Q.: Research advance about the energy budget and transportation of water vapour in the HEIFE area. Advance in Earth Science, 9(4), 30-34, 1994. (in Chinese with English abstract).

10. The S-W model is a nicely simple model to be applied for estimating ET in the sparsely-planted crop field to take into account the considerable soil evaporation, which could not be represented by widely-used Penman-Monteith model. However, the optimized S-W simulation shows that the relative contribution by soil evaporation on total ET was quite low (less than 0.1 for most of growing season), so that the S-W model is not necessarily required this time actually.

Authors' response: We fully agree with your comments. In this study, we

mainly to show that only using the EC-measured data it may be not proper in estimating model parameters, especially for parameters related the soil residence (**Appendix B**). We want that this study may be helpful to researches in doing field observations.

Minor comments:

1. Title: What does "Simultaneous parameterization" mean? Does it mean that 6 parameters are optimized concurrently? Either, do you mean that S-W model assimilates two data sets, λ ET and E, together at once? You modify the title to appeal the focal point of this research concerning such "simultaneous parameterization".

Authors' response: The title was changed as:

Simultaneously assimilating multivariate datasets into the two-source evapotranspiration model by Bayesian approach: Application to spring maize in an arid region of northwest China

2. Page 742, Line 10, "a good agreement": I do not think that the regression line's slope, 0.84, shows a good agreement.

Authors' response: "a good agreement" was changed as "a moderately good agreement"

3. Page 742, Line 11-13: This is a speculation. You should not write in this way, which strongly affirms the advection although you did not measure it directly

Authors' response: The sentence was changed as:

The causes of underestimations of ET by the S-W model was possibly attributed to the micro-scale advection.

4. Page 742, Line 14, "accounted": account?

Authors' response: The word "accounted" has been changed as "account".

5. Page 742, Line 15-16: This is a speculation again.

Authors' response: This sentence was changed as:

Also, underestimations were observed on or shortly after rainy days, which may be due to direct evaporation of liquid water intercepted in the canopy.

6. Page 743, Line 12, "has": have?

Authors' response: the word "has" was changed as "have".

7. Page 744, Line 25, "The spring wheat": How sparsely was it planted? Normally the S-W model is needed for the crop land where the crop is planted sparsely. But, you have not mentioned anything about the crop

density. You clarify it.

Authors' response: We have clarified it as (Lines 115-116, Page 6):

Stand density of the spring maize is about 37 plants m² with row spacing of 40 cm and planting spacing of 7 cm.

8. Page 745, Line 4-20: You have to address about the **estimation accuracy or energy closure for eddy flux measurement**, which could relate to the error range of assimilated data set.

Authors' response: According to your valuable suggestions, these issues were addressed (Lines 130-138, Pages 6 and 7):

About 85% energy balance closure (the sum of $H+\lambda ET$ against the available energy) was found in EC data (Liu et al., 2011). In addition, the flux uncertainties are directly related to the likelihood function of Bayesian inference (Section 2.5). Thus, determining the uncertainties is EC measurements is essential for proper parameter estimates. Recently, Wang et al. (2014) systemically studies the flux uncertainties of EC systems equipped in the HiWATER experiment. Generally, uncertainties for H ($\sigma_r(H)$; W m⁻²) by using method of Mann and Lenschow (1994) tended to be $\sigma_r(H)=0.14H+2.7$ ($R^2=0.95$), and uncertainties for λET ($\sigma_r(\lambda ET)$; W m⁻²) be $\sigma_r(\lambda ET)=0.13\lambda ET+6$ ($R^2=0.93$) (Wang et al., 2014).

9. Page 746, Line 8-9: **The position of lysimeter installation is very important to think of estimation accuracy**. If the lysimeter was installed just in the middle of rows, the soil evaporation located closer to row is missed. In this situation, when plant gets large, you may overestimate the E under the shades of leaves. It contributes to underestimate T by modeling due to adjusting the soil conductance to match the modeled E with the overestimated E by lysimeter.

Authors' response: Yes, we fully agree with your opinions. The equipment and field observation was presented in the following figure. In our revised paper, we stated as (Lines 160-161, Page 8):

....between crop rows (one in the middle of the rows and the other two close to plants on each side of the rows).

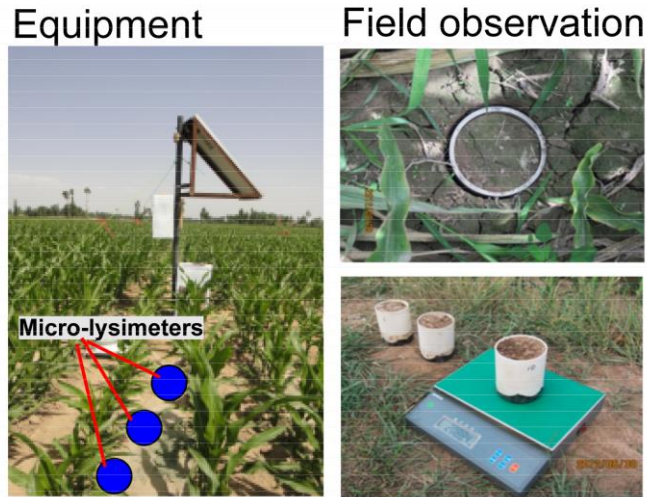


Fig. S2 The equipments and field observation during the study period

10. Page 750, Section 2.5: Add a flow chart of data calibration and evaluation steps.

Authors' response: According to your valuable suggestion, a flow chart of data calibration were presented in our revised paper. In order to save pages of the paper, we presented it in **Appendix B**. It can be easily found by the readers as shown below (Fig. S3).

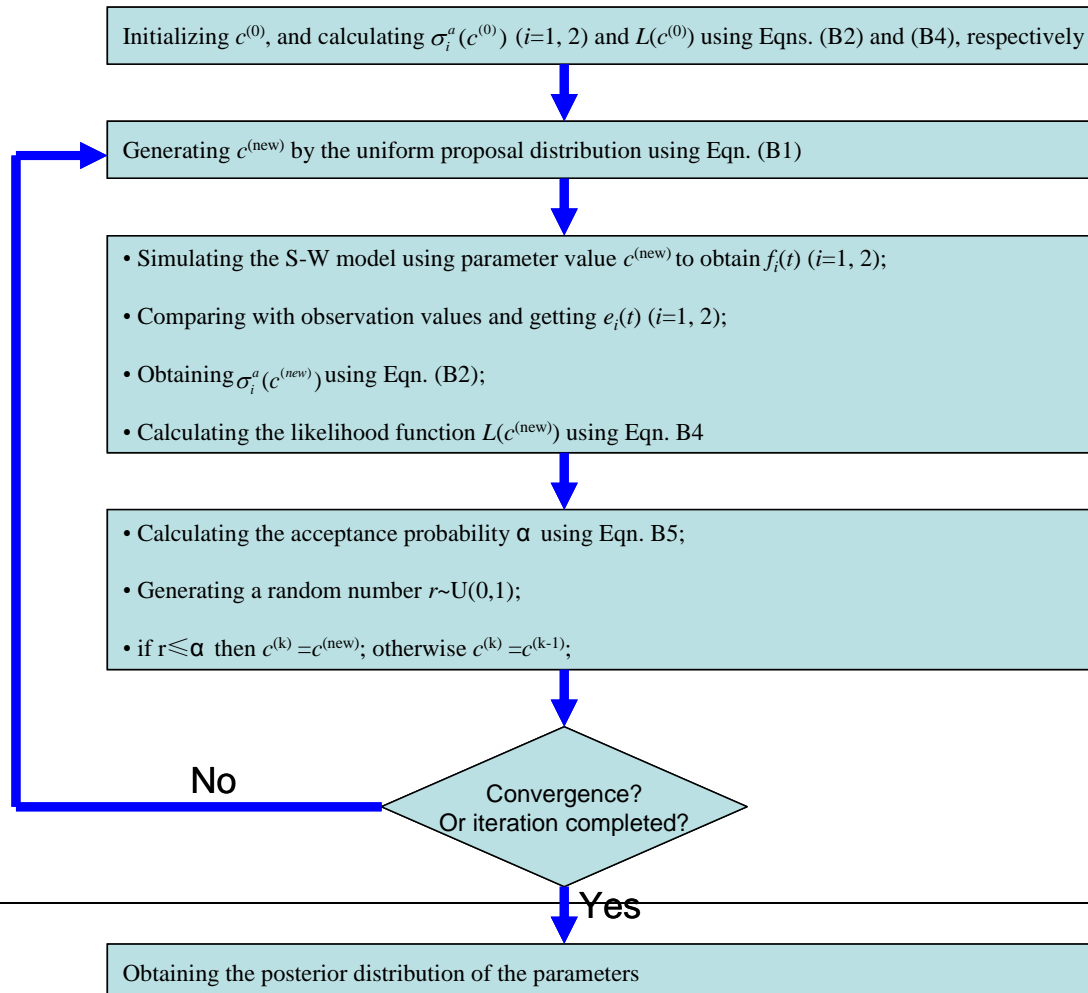


Fig. S3 Flowchart representing the basic scheme of the M-H algorithm.

11. Page 750, Line 21, “is”: are?

Authors’ response: It has been corrected

12. Page 751, Line 2, σ_i : **How did you decide this number?** It is a very important number, which decides the relative influence by each measured data in the assimilation process. So you have to write about it.

Authors’ response: According to your suggestion, a detail descriptions were given in our revised paper as (Lines 271-284, Pages 13-14):

σ_i ($i=1,2$) represents the residual errors, or standard deviation about model predicted output of the i th dataset. Here, we assumed σ_i is the same over the observation time for the i th data set (Braswell et al., 2005). Traditionally, σ_i can be included into the analysis explicitly (i.e., assuming σ_i is uniform over $\log \sigma_i$; Gelman et al., 1995) and treated as one the model parameters, which yields a complete posterior distribution of σ_i . However, this method artificially increased the parameter dimension of the problem and may result in unreasonable estimations of the parameter values (Kavetski et al., 2006). In this study, σ_i was estimated by using the analytical method (Hurtt and Armstrong, 1996; Braswell et al., 2005), which is to find the value of σ_i that maximizes $\log(p(\mathbf{O}_i(\cdot)|\mathbf{c}))$ for a given parameter vector. By differentiating $\log(p(\mathbf{O}_i(\cdot)|\mathbf{c}))$ with respect to σ_i , we can obtain:

$$\sigma_i^a = \sqrt{\frac{1}{n_i} \sum_{t=1}^{n_i} (e_i(t))^2} \quad (24)$$

We then used σ_i^a to replace σ_i in the equations (22).

13. Page 751, Line 22-23: I do not understand this sentence.

Authors’ response: The same question was also putted by the other two

referees. In our revised paper, these sentences were changed as (Lines 323-326, Pages 15 and 16):

Since the primary interest in application of the S-W model was to reproduce the pattern of water vapour fluxes from different sources (i.e., soil and vegetation) during the whole study period, we used all available data to construct the likelihood function (equation 25) and to obtain the posterior distribution of the parameters.

14. Page 751, Line 23-25: You should add the flowchart of this sequence.

Authors' response: These sentences have been deleted in our revised paper.

15. Page 753, Section 3.2: There are several problems in this subsection. You did not make the proper explanation of results in many places. For ex., how did you calculate the corr. coefficient of 0.85? From what kind of data do you calculate this corr. coeff.? Another thing is that you did not make the discussion. At the end of paragraphs, you are finishing with the mention that the optimized parameters were within reported values. Is that all to say here? This is just a report, but discussion. You have to discuss more about why the optimized parameters fell into such reported ranges. And why did k_1 and k_3 have no Gaussian distribution?

Authors' response: (1) In our revised paper, the how did we calculate the corr. coefficient were explained and a table was presented in **Appendix B**. These sentences were changed as (Lines 385-389, Pages 18 and 19):

In addition, the correlation coefficient between the posterior distribution of parameters can be used to find groups of parameters tend to be constrained together (Knorr and Kattge, 2005). In this study, the six calibrated parameters were not significantly inter-correlated with each other with correlation coefficients lower than 0.1 (Appendix B).

(2) According to the valuable suggestions from you and other referees, a Discussion section were added in our revised paper to explain the posterior distribution of optimized parameters.

- When just using EC-measured λET data, a relative wider posterior distribution of b_2 was observed (see Appendix B). Thus, the daily soil evaporation data helped to well constrain estimates of b_1 and b_2 . (Lines 395-397, Page 19);
- However, some parameters related to canopy surface resistance (i.e., k_1 and k_3) seemed to be not well updated (Fig. 4). This may be due to the fact that these parameters may be insensitive to the present available data sets. (Lines

404-407, Page 19)

- However, even with all datasets (EC-measured λET and microlysimeters-measured daily E), some parameters related to canopy surface resistance seemed to be not well updated (Fig. 4). We thought that this may be due to the insensitivities of these parameters (e.g., k_1 , k_3 , T_{amax} , T_{amin} and K_A) to the present available datasets. Thus, direct observations of plant transpiration using sap flow or stable isotope (δ^{2H} and δ^{18O}) technologies (see Williams et al., 2004), canopy temperature using infrared thermometer and continuous within- and above-canopy radiation using the four-component net radiometer (see Sauer et al., 2007) are needed in the future studies. (Lines 523-531, Page 25).

16. Page 753, Line 24-25, “while ~”: k_1 and k_3 did not have a Gaussian distribution. Then you finally could not have the proper mean or median value, which should be located in the middle of parabola of parameter histograms. So it means that the optimization did not work for those two parameters. Another thing is that it proves that Transpiration was not sensitive to R_s and D while T was sensitive to T_{air} and soil moisture.

Authors’ response: Yes, we fully agree with your comments. The posterior distributions of k_1 and k_3 seemed to be non-Gaussian. The median value may be not correct for these parameters. We explained why these parameters were not well updated as following:

- However, some parameters related to canopy surface resistance (i.e., k_1 and k_3) seemed to be not well updated (Fig. 4). This may be due to the fact that these parameters may be insensitive to the present available data sets. (Lines 404-407, Page 19)
- However, even with all data sets (EC-measured λET and microlysimeters-measured daily E), some parameters related to canopy surface resistance seemed to be not well updated (Fig. 4). We thought that this may be due to the insensitivities of these parameters (e.g., k_1 , k_3 , T_{amax} , T_{amin} and K_A) to the present available data sets. Thus, direct observations of plant transpiration using sap flow or stable isotope (δ^{2H} and δ^{18O}) technologies (see Williams et al., 2004), canopy temperature using infrared thermometer and continuous within- and above-canopy radiation using the four-component net radiometer are needed in the future studies. (Lines 523-531, Page 25)

Also, a sensitivity analysis was conducted in our revised paper (Lines 374-381, Page 18):

The global sensitivity analysis with the first-order impact ratio (FOIR) values (Appendix A) reveal the importance of input parameters in affecting total ecosystem evapotranspiration. The results indicated that total ET responded sensitively to r_{STmin} ,

b_1 , b_2 and k_2 with FOIR values being 54.3%, 21.9%, 10.4% and 8.5%,

respectively. Other parameters exhibits relative low (<5%) FOIR values, suggesting that the variability in these parameters had almost no effect on the variability in model output.

17. Page 753, Line 25-27, “Ortega-Farias et al. (2007)~”: **First, I do not understand what you are trying to say here.** Second, I assume that you mean here that 95% probability intervals narrower than your prior parameter ranges and relatively clear Gaussian distribution in rstmin show those sensitivity of rstmin, and also that relatively wider parameter ranges in b1, b2 and k2 and no Gaussan distribution in k1 and k3 show less sensitivity to uncertainties in other parameters. If my assumptions are correct, I do not agree with them. **You cannot estimate relative sensitivity of parameter only from the absolute range between max and min. You have to divide the absolute range by prior or posterior uncertainty of each parameter for comparison of relative influence by error. For ex., $(p(95\%ile)-p(5\%ile))/Unc_p$ should be applied for this comparison.**

Authors’ response: The sentences “Ortega-Farias et al. (2007)~” were deleted in our revised paper, and they were changed as (Lines 374-381, Page 18):

The global sensitivity analysis with the first-order impact ratio (FOIR) values (Appendix A) reveal the importance of input parameters in affecting total ecosystem evapotranspiration. The results indicated that total ET responded sensitively to r_{STmin} , b_1 , b_2 and k_2 with FOIR values being 54.3%, 21.9%, 10.4% and 8.5%, respectively. Other parameters exhibits relative low (<5%) FOIR values, suggesting that the variability in these parameters had almost no effect on the variability in model output. It is worth noting that the four highest sensitive parameters (r_{STmin} , b_1 , b_2 and k_2) also corresponded to the greatest degree of updating in the Bayesian inference.

According to your suggestions, a relative uncertainty reductions of parameters were used in our revised paper (Lines 353-355, Page 17):

Parameters r_{STmin} , b_1 , b_2 and k_2 showed relatively large uncertainty reductions (defined as $1 - CI_{posterior} / CI_{prior}$, where CI is the length of the 95% credible interval) (Fig. 5).

18. Page 754, Line 1, “estimated”: optimized?

Authors’ response: Yes, it has been corrected.

19. Page 754, Line 2-4: You should explain more about the results, from which you can consider if there are the inter-correlations. In which Figure and Table can we see the corr. Coeff. Number of 0.85? And what does corr. Coefficient mean? There is no proper information about the corresponding results written here. You cannot confirm the inter-correlations without calculating the covariance in errors in each combination of two parameters.

Authors' response: According to your suggestion, we explained the results as (Lines 385-389, Pages 18 and 19):

In addition, the correlation coefficient between the posterior distribution of parameters can be used to find groups of parameters tend to be constrained together (Knorr and Kattge, 2005). In this study, the six calibrated parameters were not significantly inter-correlated with each other with correlation coefficients lower than 0.1 (Appendix B).

20. Page 754, Line 13, "plantshave": plants have?

Authors' response: Yes, it has been corrected.

21. Page 754, Line 20, "was": were?

Authors' response: Yes, it has been corrected.

22. Page 754, Line 22, "were": was?

Authors' response: Yes, it has been corrected.

23. Page 754, Line 23, "predicate": predict?

Authors' response: Yes, it has been corrected.

24. Page 755, Line 21, "daily ET was": daily ETs were?

Authors' response: Yes, it has been corrected.

25. Page 756, Subsection 3.4: There should be great uncertainty in eddy flux measurement for ET and lysimeter measurement for E. So in this subsection you also have to discuss the possibility of containing the great unc. by the errors in measurement data.

Authors' response: According to your suggestion, the uncertainties of EC measurements were added in our revised paper:

- In addition, the flux uncertainties are directly related to the likelihood function of Bayesian inference (Section 2.5). Thus, determining the uncertainties is EC measurements is essential for proper parameter estimates. Recently, Wang et al. (2014) systemically studies the flux uncertainties of EC systems equipped in the HiWATER experiment. Generally, uncertainties for

H ($\sigma_r(H)$; W m^{-2}) by using method of Mann and Lenschow (1994) tended to be $\sigma_r(H) = 0.14H + 2.7$ ($R^2=0.95$), and uncertainties for λET ($\sigma_r(\lambda ET)$; W m^{-2}) be $\sigma_r(\lambda ET) = 0.13\lambda ET + 6$ ($R^2=0.93$) (Wang et al., 2014). (Lines 131-138, Pages 6 and 7);

- The uncertainties of H and λET increased with the flux magnitude (Fig. 8), and tended to be approximately 14% and 13%, respectively (Wang et al., 2014). The relative error for R_n was relatively small and estimated to be 1.24% (Xu et al., 2013). (Lines 450-453, Page 21)

In addition, the uncertainties of measurements were illustrated in Fig. 9.

26. Page 756, Line 9, “micro-scale advection”: Did not you measure the lateral wind speed and direction to directly probe the advection?

Authors’ response: Yes, we did not measure the lateral wind speed and direction to directly. However, this phenomenon has well been documented and measured in previous studies. For example, Oke (1978) has describe the oasis effect in his book as: *Therefore there is a continual air-to-oasis inversion temperature gradient driving a downward directed heat flux, and the process is aided by air mass subsidence over the oasis.* (Page 166); Hu (1994) had constructed the interaction between desert and oasis. In our revised paper these references were given, so readers can obtain the basic information about the oasis effect.

27. Page 756, Line 18, “representing”: represent?

Authors’ response: Yes, it has been corrected.

28. Page 757, Line 20, “when micro-scale advection occurred”: You cannot conclude it yet.

Authors’ response: The words ‘micro-scale advection’ was changed as ‘oasis-effect’.

29. Page 769, Fig. 3: you have to add the signs “(a)” to “(f)” in panels and legends to identify the variable.

Authors’ response: According to your valuable suggestion, the signs “(a)” to “(f)” in panels and legends to identify the variable were added in the figure.

30. Page 775, Fig. 9: The color assignment of RH is not intuitive. I prefer that the red is dry and the blue is wet.

Authors’ response: The color assignment of RH has been corrected according to your suggestion.

Responses to comments Provided by Referee 2

General comments and overall evaluation: Bayesian statistics, based on probability theory, is a logical choice for model calibration; it provides parameter estimates by quantifying the uncertainties in the data and model structure. The authors employ Bayesian method to calibrate the Shuttleworth-Wallace model, using eddy-covariance evapotranspiration measurements and daily soil evaporation. The work is interesting but some technical aspects should be clarified and additional analyses should be carried out.

Authors' response: Thanks very much for your positive comments.

General Comments:

1. In order to test model performances the authors split the dataset in two parts by taking alternate measurements and using one sub-dataset for model calibration and the other for model evaluation. The authors claim that the sub-datasets are independent, but for an independent validation of the model data from different site should be used. If that is not possible, model evaluation would be more rigorous if the first half of the data is used for calibration and the second half for model validation, i.e. defining the sub-dataset using subsequent measurements and not alternate measurements. Finally parameter estimates reported in Table 1 and Figure 4 should be obtained using the whole dataset, i.e. a new calibration should be carried out using all the available data.

Authors' response: The same question has been proposed by Referee 3. In our revised paper, these sentences were changed as (Lines 323-326, Pages 15 and 16):

Since the primary interest in application of the S-W model was to reproduce the pattern of water vapour fluxes from different sources (i.e., soil and vegetation) during

the whole study period, we used all available data to construct the likelihood function (equation 25) and to obtain the posterior distribution of the parameters.

- Results from the Gelman and Rubin test should be reported at least in the text. By observing the marginal posterior distribution of parameter k_1 , k_2 and k_3 it seems that convergence was not reached.

Authors' response: According to your valuable suggestion, the G-R test was reported in **Appendix C**. The figure below showed that the parameters tend to converge after 5000 iterations.

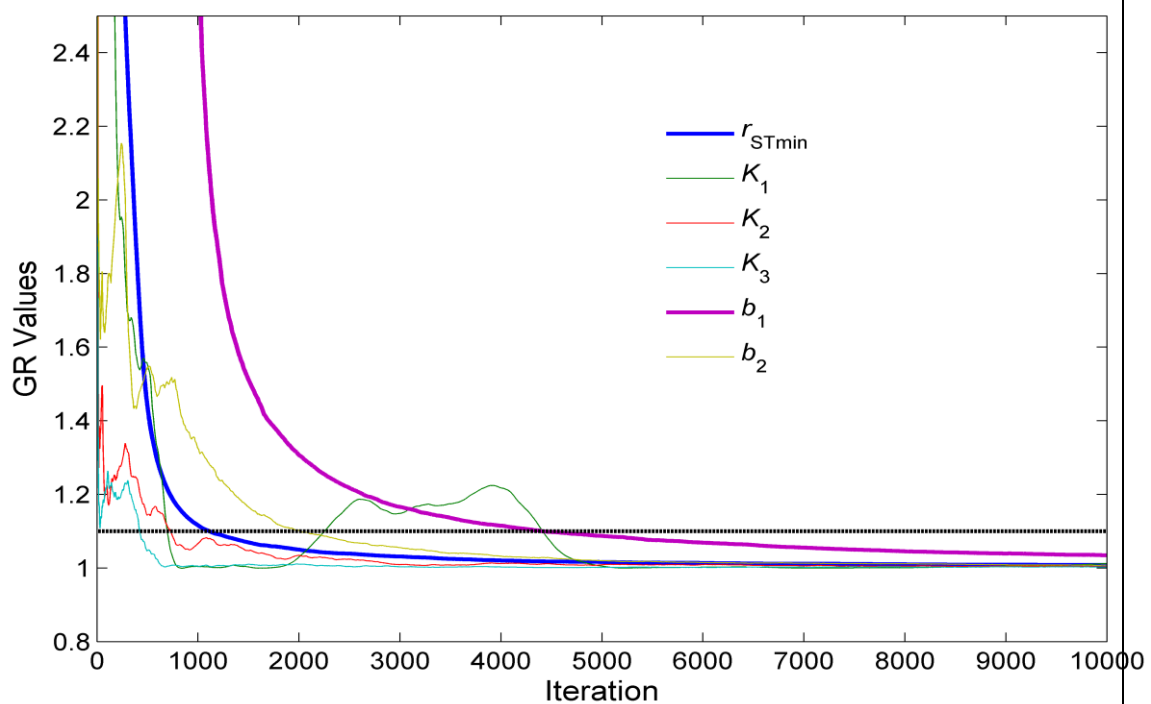


Fig. B1 The evolution of GR diagnostic of convergence of MCMC. Four parallel chains with different initial values were used to calculate GR values.

- lines 318- 321. Sensitivity analysis are always conditional to the parameter space and the input data used in the analysis. I strongly suggest you to carry out a global sensitivity analysis (such as the Morris method) using the prior parameter ranges to understand which are the key parameters of the model in your case study.

Authors' response: According to your valuable suggestion, the global

sensitivity was conducted in **Appendix A**. The results indicated that the most sensitive parameters in the S-W model was r_{STmin} , and followed by b_1 , b_2 , k_2 and k_1 . Other parameter had almost no effect on the variability in model output (Fig. B2).

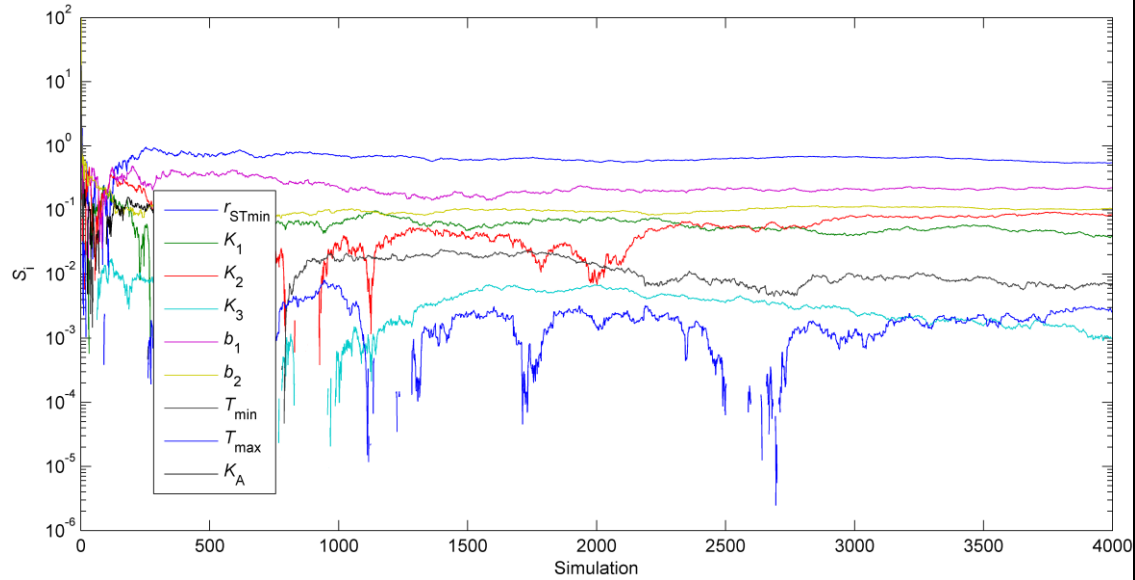


Fig. B2 The evolution of the first-order sensitivity indices.

4. Which prior do you use? I suppose you were using a uniform prior with the minimum and maximum values of Table 1. Please, state it more clearly in the manuscript.

Authors' response: The chose of prior distribution was stated as (Lines 252-253, Page 12):

, which are chosen as uniform distributions with specified allowable ranges (Table 1).

5. Uncertainty in the data is really important when using a Bayesian approach. How did you define the measurement errors of equation 22?

Authors' response: In our revised paper, the calculation of errors in equation 22 were stated as (Lines 271-284, Pages 13 and 14):

σ_i ($i=1,2$) represents the residual errors, or standard deviation about model predicted output of the i th dataset. Here, we assumed σ_i is the same over the observation time for the i th data set (Braswell et al., 2005). Traditionally, σ_i can be

included into the analysis explicitly (i.e., assuming σ_i is uniform over $\log \sigma_i$; Gelman et al., 1995) and treated as one the model parameters, which yields a complete posterior distribution of σ_i . However, this method artificially increased the parameter dimension of the problem and may result in unreasonable estimations of the parameter values (Kavetski et al., 2006). In this study, σ_i was estimated by using the analytical method (Hurtt and Armstrong, 1996; Braswell et al., 2005), which is to find the value of σ_i that maximizes $\log(p(\mathbf{O}_i(\cdot)|\mathbf{c}))$ for a given parameter vector. By differentiating $\log(p(\mathbf{O}_i(\cdot)|\mathbf{c}))$ with respect to σ_i , we can obtain:

$$\sigma_i^a = \sqrt{\frac{1}{n_i} \sum_{t=1}^{n_i} (e_i(t))^2} \quad (24)$$

We then used σ_i^a to replace σ_i in the equations (22).

6. Why did you include 6 parameters in the calibration and not the whole parameter vector? And which values did you assign to the parameters not included in the calibration? Please provide the references.

Authors' response: According to your suggestion, a global sensitivity analysis was conducted in our revised paper (**Appendix C**). The most sensitive parameters were selected to optimized. Other parameter (K_A , $T_{a,\min}$, $T_{a,\max}$) were cited form previous studies, and the references were provided:

- in which K_A is the extinction coefficient of light attenuation. It can be measured on *site* (see Sauer et al., 2007), and was set to be approximately 0.41 for spring maize (Mo et al., 2000).(Lines 208-210, Page 10)
- $T_{a,\min}$ and $T_{a,\max}$ are the lower and upper temperatures limits ($^{\circ}\text{C}$), respectively, which are T_a values when $F_2(T_a) = 0$ and are set at values of 0

and 40 °C (Harris et al., 2004) (Lines 231-233)

7. Which parameter vector did you use to generate model outputs? You should use the maximum a posteriori parameter vector.

Authors' response: The median value of the parameter vector was used to generate model output.

8. Bayesian statistics allows to quantify uncertainties. Was the calibration effective in reducing uncertainties of model predictions? [The posterior uncertainty of simulated ET and E are not shown and discussed.](#)

Authors' response: Thanks for your valuable suggestions. The posterior uncertainty of simulated ET and E were presented in our revised paper. Please see Fig. 8 and Fig. 9. We also discussed in the paper:

- Also, the 95% posterior prediction intervals of simulated soil E was narrow. (Lines 433-434, Page 21);
- that the estimated daily ET generally fluctuated tightly with the measured values with relative narrow uncertainties (95% posterior prediction intervals) (Lines 436-438, Page 21);
- However, there are 12 days during the study period (111 days) with observations beyond the upper bounder of the 95% posterior prediction intervals (Fig. 8) (Lines 440-442, Page 21);
- simulated λ ET and E were comparable to the measurements with relatively narrow uncertainties (95% posterior prediction intervals) (Lines 506-507, Page 24).

9. The manuscript is relatively well written, but in my opinion the [Results and discussion session should be slitted in two parts](#) in order to provide more clear take-home messages.

Authors' response: According to your suggestion, a **Discussion** section was

added in our revised paper (Lines 281-548, Pages 23-26).

Minor Comments:

1. Abstract. Line: 31-33. “The posterior distributions...intervals.” This phrase is not clear [what do you mean for well updated?](#)

Authors’ response: This sentence was changed as (Lines 31-33, Page 2):

4 of the six main parameters were showed relatively larger uncertainty reductions (>50%), and their posterior distributions became approximately symmetric with distinctive modes

2. Introduction. Line: 79-81. The main advantage of Bayesian method is that uncertainties can be properly quantified. Optimization algorithms can also be used to optimize parameters in the light of multiple data sources.

Authors’ response: According to your suggestion, the sentence was changed as (Lines 78-81, Page 4):

Secondly, as far as the parameterization method is concerned, abundant evidence has shown that the Bayesian method provides a powerful new tool to simultaneously optimize many or all model parameters against all available measurements, and to quantify the influences of uncertainties.

3. Materials and methods. Line: 106-107. [Which dryness index](#) was used. Line: 136. “Air temperature and relative humidity”: Air temperature, relative humidity Line: 199. “Eqns.(1)-(3) is calculated”: Eqns.(1)-(3) are calculated

Authors’ response: The sentence was changed as:

the dryness index according to the World Atals of Desertification (UNEP, 1992) is 15.9

Other errors have been corrected according to your suggestions.

4. Line: 256-264. Which MCMC algorithm did you use? From the description it seems to be the Metropolis algorithm and not the Metropolis-Hastings.

Authors' response: The detail of MCMC algorithm was presented in Appendix A. The M-H algorithm was used in our study. Because the prior distribution was selected as uniform distribution, the M-H algorithm was indeed the same as the Metropolis algorithm.

5. Results and discussion Line: 359. "In this case, a good agreement ...": A good agreement Line: "On the other hand, the diurnal variation": On the other hand must go after on one hand.

Authors' response: The words 'On the other hand' were deleted in our revised paper.

Responses to comments Provided by Referee 3

1. This is in general a well thought out and methodologically sound piece of work and the authors make a sufficient case that the work is novel for it to warrant publication.

Authors' response: Thanks very much for your positive comments.

2. While there are no fundamental issues with the work there are a number of ways in which it could be improved. These are mainly regarding key pieces of information that are currently missing from the manuscript.

The authors go to the trouble of conducting a Bayesian Calibration on six of the model parameters which is excellent since rather than employing an optimisation routine to merely 'tune' the model parameters they estimate the full conditional probability of the parameters being probable given the ET and E data. However, once the calibration is made only a single parameter vector is selected and all the subsequent analysis versus the data is based on results of that single vector. This is an opportunity missed since they already have all the information they need to report the influence of posterior parameter uncertainty on model outputs. This could be done by calculating the 5th and 95th quantiles from their 3000 member parameter sample for example. This would make for a far superior analysis of model-measurement differences since the model output can now be represented by the full calibrated posterior distribution not just a single run.

Authors' response: Thanks for your valuable suggestions. In our revised paper, model-measurement differences were analysed using the 5th and 95th quantiles from their 3000 member parameter sample. Please see Fig. 8 and Fig. 9. We also discussed in the paper:

- Also, the 95% posterior prediction intervals of simulated soil E was narrow. (Line 422, Page 20);
- that the estimated daily ET generally fluctuated tightly with the measured values with relative narrow uncertainties (95% posterior prediction

intervals) (Lines 425-426, Page 20);

- However, there are 12 days during the study period (111 days) with observations beyond the upper bounder of the 95% posterior predication intervals (Fig. 8) (Lines 428-430, Page 20);
- simulated λET and E were comparable to the measurements with relatively narrow uncertainties (95% posterior predication intervals) (Lines 495-496, Page 23).

3. The choice of an MCMC algorithm to sample the posterior is generally good one although assessing convergence requires special care as it is too easy to be fooled into believing that convergence has been obtained when in fact only a local maxima has been found. For this reason the manuscript is too light on details of the Gelman-Rubin numbers that were obtained that convinced the authors that the MCMC had converged. This should be reported especially since fig 4. k_1 , k_2 , k_3 might suggest that convergence has not yet been reached.

Authors' response: According to your valuable suggestion, the G-R test was reported in **Appendix C**. The figure below showed that the parameters tend to converge after 5000 iterations.

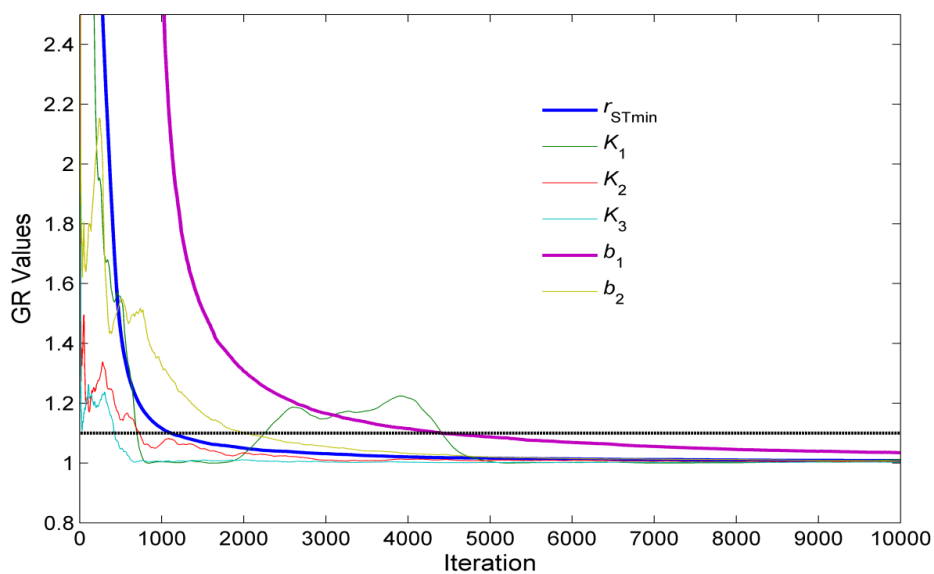


Fig. C1 The evolution of GR diagnostic of convergence of MCMC. Four parallel

chains with different initial values were used to calculate GR values.

- The authors should give details of why they chose the 6 parameters that they did to be calibrated. Ideally a calibration should include all model parameters and if a subset is selected perhaps for reasons of computational practicality then an objective method such as Morris should be used to select the most important parameters.

Authors' response: According to your valuable suggestion, the global sensitivity was conducted in **Appendix A**. The results indicated that the most sensitive parameters in the S-W model was r_{STmin} , and followed by b_1 , b_2 , k_2 and k_1 . Other parameter had almost no effect on the variability in model output (Fig. C2).

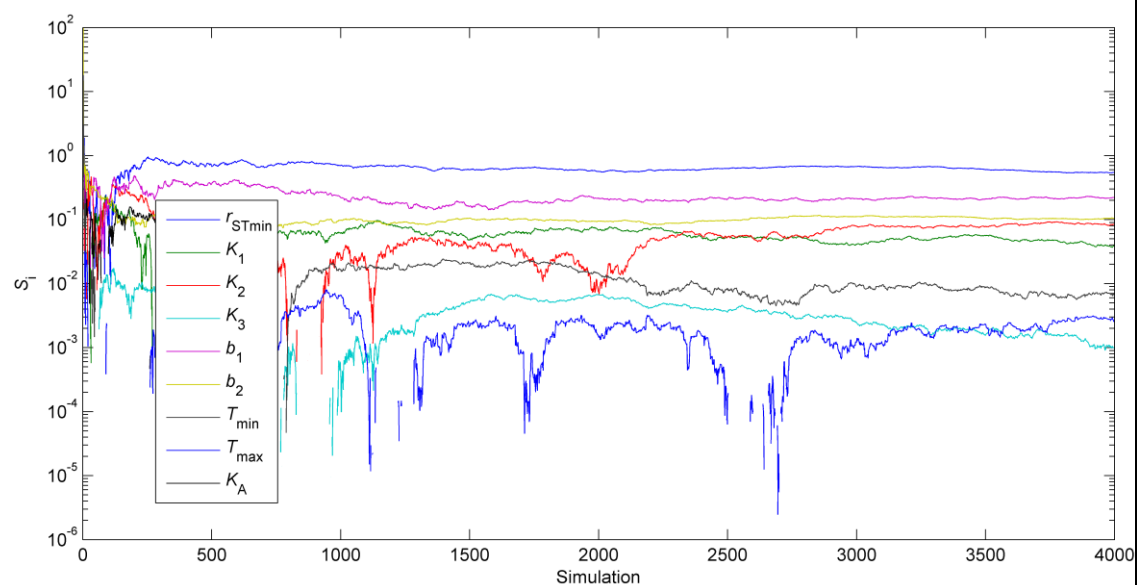


Fig. C2 The evolution of the first-order sensitivity indices.

- In Bayesian Calibration the choice of the prior distribution is also important and should be discussed but this is currently missing.

Authors' response: According to your valuable suggestion, the influence of prior distribution on the simulation results was conducted in our revised paper (see **Appendix A**). As expected the simulated values of daily evapotranspiration and soil evaporation both showed larger uncertainties. Thus, there is a need to update the parameters based on observation

datasets. In our revised paper, the following sentences were stated (Lies 252-258, Page 12):

where $p(c)$ represents prior probability distributions of parameters c , which is chosen as uniform distributions with specified allowable ranges (Table 1). In general, the parameter ranges were wide enough to include the actual parameter values and to give the optimization freedom (Sack et al., 2006). In the test study, we run the S-W model using 4000 parameter vectors which were sampled from the prior distribution using Latin Hypercube Sampling (LHS) method (Iman and Helton, 1998), and found that the observed data in most case were in the range of predicted values (Appendix A).

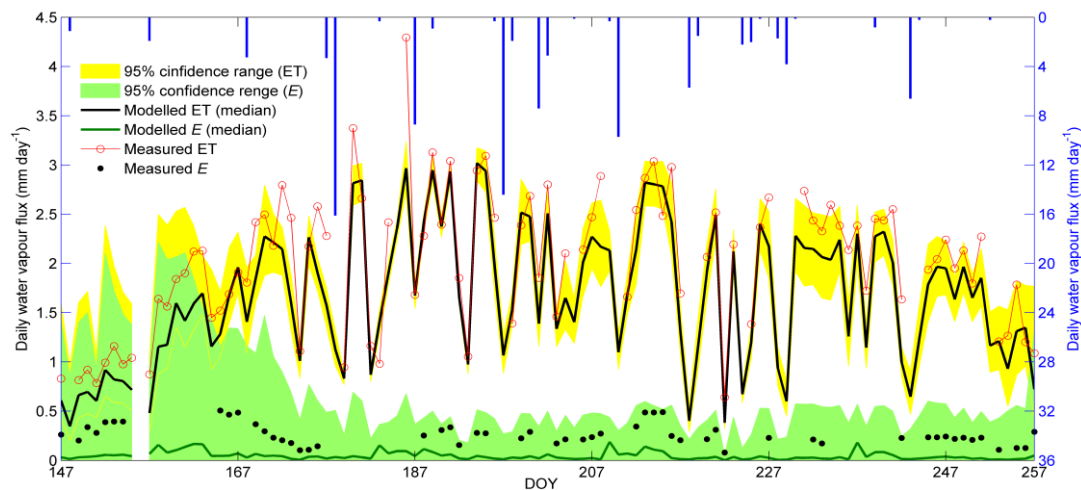


Fig. C3 Seasonal variation in daily evapotranspiration (ET; mm d^{-1}) and soil evaporation (E ; mm day^{-1}) measured by the EC system and modeled by the S-W model using the prior distribution of parameters. Gap in the time series is caused either by the absence of flux measurements or missing ancillary data.

6. The manuscript is also lacking details on the errors were used in the likelihood calculation to represent the random errors that were assigned to the measurements. This is gain an important omission as these errors should be discussed and justified on the asis of analyses or from literature.

Authors' response: In our revised paper, the calculation of errors were stated as (Lines 262-275, Page 13):

σ_i ($i=1,2$) represents the residual errors, or standard deviation about model predicted output of the i th dataset. Here, we assumed σ_i is the same over the observation time for the i th data set (Braswell et al., 2005). Traditionally, σ_i can be included into the analysis explicitly (i.e., assuming σ_i is uniform over $\log \sigma_i$; Gelman et al., 1995) and treated as one the model parameters, which yields a complete posterior distribution of σ_i . However, this method artificially increased the parameter dimension of the problem and may result in unreasonable estimations of the parameter values (Kavetski et al., 2006). In this study, σ_i was estimated by using the analytical method (Hurtt and Armstrong, 1996; Braswell et al., 2005), which is to find the value of σ_i that maximizes $\log(p(\mathbf{O}_i(\cdot)|\mathbf{c}))$ for a given parameter vector. By differentiating $\log(p(\mathbf{O}_i(\cdot)|\mathbf{c}))$ with respect to σ_i , we can obtain:

$$\sigma_i^a = \sqrt{\frac{1}{n_i} \sum_{t=1}^{n_i} (e_i(t))^2} \quad (24)$$

We then used σ_i^a to replace σ_i in the equations (22).

Detailed Comments:

1. Throughout the manuscript the authors refer to "multiple measuring datasets". This doesn't work in English perhaps "multivariate datasets" might convey what the authors want?

Authors' response: Thanks for your detailed helps to us. According to your valuable suggestion, the words "multiple measuring datasets" were changed as "multivariate datasets" in our revised paper.

2. Abstract: accounted -> account

Authors' response: It has been corrected.

3. p743 line4 has good performances -> performs well

Authors' response: It has been changed.

4. p744 line8 in arid -> in the arid

Authors' response: It has been corrected.

5. p745 line18 synchronously -> synchronous

Authors' response: It has been corrected.

6. p746 line2 were-> was

Authors' response: It has been corrected.

7. line7 delete was

Authors' response: It has been deleted

8. p747 line13 coefficient -> coefficients

Authors' response: It has been corrected.

9. line18 is -> are

Authors' response: It has been corrected.

10. p748 line16 is -> are

Authors' response: It has been corrected.

11. p750 line8 parameters needed -> parameters that needed

Authors' response: It has been corrected.

12. line13 dataset -> datasets

Authors' response: It has been corrected (Line 286 in our revised paper).

13. line17 The difference between the model and the observations should not

be called model error as if the observations are 'truth'. A better description is model data mismatch recognising that both the model and the data contain errors. Also see above you need to discuss how the observational random error is obtained.

Authors' response: According to your suggestion, the 'model error' was changed as 'model-data mismatch'.

The observational error was studied by Wang et al. (2014). In our revised paper, these errors were stated as (Lines 131-138, Pages 6 and 7):

In addition, the flux uncertainties are directly related to the likelihood function of Bayesian inference (Section 2.5). Thus, determining the uncertainties in EC measurements is essential for proper parameter estimates. Recently, Wang et al. (2014) systemically studies the flux uncertainties of EC systems equipped in the HiWATER experiment. Generally, uncertainties for H ($\sigma_r(H)$; W m^{-2}) by using method of Mann and Lenschow (1994) tended to be $\sigma_r(H) = 0.14H + 2.7$ ($R^2=0.95$), and uncertainties for λET ($\sigma_r(\lambda ET)$; W m^{-2}) be $\sigma_r(\lambda ET) = 0.13\lambda ET + 6$ ($R^2=0.93$) (Wang et al., 2014)

References:

Wang, J.M., Zhuang, J.X., Wang, W.Z., Liu, S.M., Xu, Z.W.: Assessment of Uncertainties in Eddy Covariance Flux Measurement Based on Intensive Flux Matrix of HiWATER-MUSOEXE. IEEE Geosciences and Remote Sensing Letters, 2014, (under review).

14. Line22 "assuming the model error follows a Gaussian" no this is not a correct interpretation of likelihood. The likelihood is formally the "chance of getting the observations given the parameters". Therefore the Gaussian in the likelihood represents the errors in the observation rather than the model. The idea here is that random observational error (as quantified by the sigma and the Gaussian) is stopping us from always obtaining the

observations from the parameters. The errors in the parameters are represented in the prior and as it stands this calibration estimates the probability of the parameters being correct given the observations assuming that this is the correct model. That is to say an assumption of the calibration is that the model is correct. We know this is wrong but the Bayesian Calibration does not explicitly represent this. Of course the model data mismatch in the likelihood does implicitly quantify both model and data errors but this is not the formal understanding of the likelihood. Indeed later on you go on to suggest possible model improvements. As future work I would advocate creating a new version of the model with those improvements and formally quantifying whether the new model is more likely using Bayesian analysis. See Bayesian Model Comparison in Van Oijen, M.; Reyer, C.; Bohn, F.J.; Cameron, D.R.; Deckmyn, G.; Flechsig, M.; Härkönen, S.; Hartig, F.; Huth, A.; Kiviste, A.; Lasch, P.; Mäkelä, A.; Mette, T.; Minunno, F.; Rammer, W.. 2013 Bayesian calibration, comparison and averaging of six forest models, using data from Scots pine stands across Europe. *Forest Ecology and Management*, 289. 255-268. 10.1016/j.foreco.2012.09.043.

Authors' response: Thanks for your clear interception of the definition of the likelihood function. Also, thanks very much for your guides to us for the future studies. We will conduct some model comparison studies of different ET model in typical ecosystems (i.e., alpine grassland, alpine forest, arid farmland, and arid forest) in northwest China. According to your suggestion, the sentence was changed as (Lines 261-263, Pages 12 and 13):

Assuming the model-data mismatch $e_i(t)$, which represents a relative “goodness-of-fit” measure for each possible parameter vector (van Oijen et al., 2011, 2013)

References:

van Oijen, M., Cameron, D.R., Butterbach-Bahl, K., Farahbakhshazad, N., Jansson, P.E., Kiese, R., Rahn, K.H., Werner, C., Yeluripati, J.B.: A Bayesian framework for model calibration, comparison and analysis: application to four models for the biogeochemistry of a Norway spruce forest. *Agric. For. Meteorol.*, 151(12),

1609-1621, 2011.

van Oijen, M., Reyer, C., Bohn, F.J., Cameron, D.R., Deckmyn, G., Flechsig, M., Härkönen, S., Hartig, F., Huth, A., Kiviste, A., Lasch, P., Mäkelä A., Mette, T., Minunno, F., Rammer, W.: Bayesian calibration, comparison and averaging of six forest models, using data from Scots pine stands across Europe. *Forest Ecol. Manag.*, 289, 255-268, 2013.

15. p751 line10 formally I believe you are using the Metropolis algorithm rather than Metropolis-Hastings

Authors' response: The detail of MCMC algorithm was presented in Appendix B. The M-H algorithm was used in our study. Because the prior distribution was selected as uniform distribution, the M-H algorithm was indeed the same as the Metropolis algorithm.

16. line14 Which distribution are you using for the proposal density (multivariate normal?)

Authors' response: In our revised paper, the proposal function was presented more clear (Lines 303-315, Pages 14 and 15):

It was well recognized that efficiency of the M-H algorithm was strongly effected by the proposal distribution function. To find an effective proposal distribution $P(\mathbf{c}^{\text{new}} | \mathbf{c}^{k-1})$, a test run of the M-H algorithm with 10, 000 simulations was made by using a uniform proposal distribution (Braswell et al., 2005):

$$\mathbf{c}^{\text{new}} = \mathbf{c}^{k-1} + r(\mathbf{c}^{\text{max}} - \mathbf{c}^{\text{min}}) \quad (26)$$

where \mathbf{c}^{k-1} is the current accepted point; r is a random number uniformly distributed between -0.5 and +0.5; \mathbf{c}^{min} and \mathbf{c}^{max} are the lower and upper limits of parameter vector \mathbf{c} . Based on the test run, we then constructed a normal proposal

distribution $\mathbf{c}^{\text{new}} : N(\mathbf{c}^{(k-1)}, \text{cov}^0(\mathbf{c}))$, where $\text{cov}^0(\mathbf{c})$ is the covariance matrix of the parameter vector \mathbf{c} from the initial test run (Xu et al., 2006). The detailed description on MCMC sampling procedure and the code written in Matlab were presented in Appendix B.

17. line22 I don't think you need to split the datasets in this way. Indeed the calibration would benefit from the inclusion of all of the data. The comparison against data that you make later on would be just as valid since this is more about identifying weaknesses in the structure of the model i.e. missing processes rather than parametrisation.

Authors' response: According to your valuable suggestion, these sentences were changed as (Lines 323-326, Pages 15 and 16):

Since the primary interest in application of the S-W model was to reproduce the pattern of water vapour fluxes from different sources (i.e., soil and vegetation) during the whole study period, we used all available data to construct the likelihood function (equation 25) and to obtain the posterior distribution of the parameters.

18. line23 dataset -> datasets

Authors' response: This sentence has been deleted.

19. line24 optimised -> calibrated

Authors' response: This sentence has been deleted.

20. p752 line11 posterior expectancy? Assume you mean the expectation of the posterior (i.e. the mean). See comments above about representing the full posterior in your analysis rather than just one parameter vector.

Authors' response: Yes, it is the posterior median values of the parameters. The full posterior were also included in our analysis in the revised paper.

Please see Figs. 8 and 9.

21. p753 line4 was -> are

Authors' response: It has been corrected.

22. p754 line8 contents -> content

Authors' response: It has been corrected.

23. line13 split plantshave

Authors' response: It has been split.

24. line22 were -> are

Authors' response: It has been corrected.

25. line23 predicate -> predict

Authors' response: It has been corrected.

26. line25 reword: something like "However, significant differences exist between measured and modeled half-hourly ET values for the spring maize in the arid desert oasis."

Authors' response: Thanks, it has been corrected.

27. line27 regressive -> the regression

Authors' response: It has been corrected.

28. p755 line10 was -> is

Authors' response: It has been corrected.

29. line17 observed -> observe

Authors' response: It has been corrected.

30. line20 5 -> on the 5th of

Authors' response: It has been corrected.

31. line22 needed -> needs

Authors' response: It has been corrected.

32. p756 line4 was -> is

Authors' response: It has been corrected.

33. line10 on the 5th of July

Authors' response: It has been corrected.

34. line11 no gaps in time i.e. 12:00 20:00

Authors' response: The gaps in time were added in our revised paper.

35. line17 flows do not -> flows that do not

Authors' response: It has been corrected.

36. line18 representing -> represent

Authors' response: It has been corrected.

37. line19 attentions -> attention

Authors' response: It has been corrected.

38. Figure8: The text in this figure is currently too small

Authors' response: The size of this figure was 18cm x 8cm.

Finally, we want to express our deep appreciations to you for your patient helps in improving the quality of our paper. Thanks very much!

Appendix A

A.1 Global Sensitivity Analysis

To identify the key parameters that being responsible for most of the variability of the model outputs, a global sensitivity analysis were performed. Following Saltelli et al. (2008), the first-order sensitivity index S_i and total effect sensitivity index S_{Ti} are given as:

$$S_i = \frac{\text{Var}_{c_i}}{\text{Var}(Y)} = \frac{\text{Var}[E(Y | c_i)]}{\text{Var}(Y)} \quad (\text{B1})$$

$$S_{Ti} = S_i + \sum_{j \neq i} S_{ij} + L = \frac{E[\text{Var}(Y | c_{\sim i})]}{\text{Var}(Y)} \quad (\text{B2})$$

where Var_{c_i} is the partial variance of c_i on output Y and given by $\text{Var}_{c_i} = \text{Var}[E(Y | c_i)]$; $\text{Var}(Y)$ is the total unconditional output variance; S_{ij} is the contribution to the total variance by the interactions between parameters c_i and c_j ; $c_{\sim i}$ denotes variation on all input parameters but c_i ;

A.2 Monte Carlo Simulations

The Monte Carlo method was used to calculate $\text{Var}(Y)$, S_i and S_{Ti} . The procedure are listed as below (Saltelli et al., 2010):

Step 1:

Generate two independent input parameter sampling matrices A and B with dimension $N \times d$, where N is the sample size and d is the number of input parameters;

Step 2:

Build another $N \times d$ matrix A_B^i ($i = 1, 2, \dots, d$) such that the i th column of A_B^i is equal to the i th column of B , and the remaining columns are from A ;

Step 3:

Calculate $\text{Var}(Y)$, S_i and S_{Ti} using the following estimators:

$$\hat{f}_0 = \frac{1}{N} \sum_{j=1}^N f(A)_j$$

$$\text{Var}(\hat{f}) \Rightarrow \frac{1}{N} \sum_{j=1}^N f(A_j)^2 - \hat{f}_0^2$$

$$S_i = \frac{1}{N} \sum_{j=1}^N \frac{f(B)_j - \hat{f}_0}{\text{Var}(\hat{f})}$$

$$S_{Ti} = \frac{1}{2N} \sum_{j=1}^N \frac{(f(A_j) - f(A_B^i))^2}{\text{Var}(\hat{f})}$$

where $\hat{\dots}$ denotes the estimate; \hat{f}_0 is the estimated value of model output; The matrices A and B are generated using the Latin Hypercube Sampling technique (Iman and Helton, 1988).

A.3 Matlab Code for Global Sensitivity Analysis

```
function [A,B]=LHSSample(N,d, interval)
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% Using the Latin Hypercube Sampling (LHS) technique (Iman and Helton, 1988)
% to generate matrices A and B
% Authors   : Zhu Gaofeng
% Date      : March 19, 2014
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% Description:
% N         :   number of sample
% d         :   dimension of parameter vector
% Interval  :   interval of prior distribution of paramter being d*2 matrix
% A        :   matrix A being N*d
% B        :   matrix B being N*d

interval=[interval;interval];

% Generates a LHS M1 containing N samples and 2*d dimension
M1=lhsdesign(N,2*d);

for j=1:size(M1,2)
    int=interval(j,:);
    for i=1:size(M1,1)
        %transform to parameter space
        M(i,j)=unifinv(M1(i,j),int(1),int(2));
```

```

    end
end
A=M(:,1:d);           % the first d columns were designed to matrix A
B=M(:,d+1:end);       % the last d columns were designed to matrix B
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%% End of the sub-model

function
LET=SWSA(rstmin,k1,k2,k3,b1,b2,Tamin,Tamax,KA,flag,F4,G,Rn,S,LAI,Ta,r
ho,D,SWC_2,delta,gamma,raa,ras,rac)

% calculate rss
thetas=0.45;          % saturated water content at the 20 cm depth in [m3 m-3];

rss=exp(b1-b2*SWC_2./thetas);

% calculated rsc
F1=(eps+S)*(1055+k1)/(1055*(S+k1));          % S:short wave radiation W m-2

tao=(Tamax-k2)/(k2-Tamin);
numerator=(Ta-Tamin).*(Tamax-Ta).^tao;
denominator=(k2-Tamin).*(Tamax-k2).^tao;
F2=numerator./denominator;
F3=1-k3*D;
rsc=rstmin./(2*LAI.*F1.*F2.*F3.*F4);

% S-W model
% specific heat capacity of the dry air in kJ/kg/K;
Cp=1.013;
Ra=(delta+gamma).*raa;
Rs=(delta+gamma).*ras+gamma.*rss;
Rc=(delta+gamma).*rac+gamma.*rsc;

Cs=1./(1+Rs.*Ra./(Rc.*(Rs+Ra)));
Cc=1./(1+Rc.*Ra./(Rs.*(Rc+Ra)));

Rns=Rn.*exp(-KA.*LAI);

A=Rn-G;
As=Rns-G;

ETs=(delta.*A+(rho.*Cp.*D-delta.*ras.*(A-As))./(raa+ras))./(delta+gam
ma.*(1+rss./(raa+ras)));

```

```

ETc=(delta.*A+(rho.*Cp.*D-delta.*rac.*As)./(raa+rac))./(delta+gamma.*
(1+rsc./(raa+rac)));
LE=Cs.*ETs;
LT=Cc.*ETc;
LET=LE+LT;

D0=D+(delta.*A-(delta+gamma).*LET).*raa./(rho.*Cp);
E=(delta.*As+rho.*Cp.*D0./ras)./(delta+gamma.*(1+rsc./ras));
T=(delta.*(A-As)+rho.*Cp.*D0./rac)./(delta+gamma.*(1+rsc./rac));
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%% End of the sub-model

```

% Main Program

```

clc
clear
Nss=4000; % Sample numbers

% Prior parameter interval for rstmin, k1,k2,k3,b1,b2,Tamax,Tamin,KA
interval=[1 80
          0 500
          20 40
          0 .1
          4 15
          0 8
          0 5
          40 45
          .2 .8];
dem=size(interval,1); % dimension of parameter vector

% Generate matrices A and B using the LHS technique
[Am,Bm]=LHSSample(Nss,dem,interval);

% input meteorological data, Here we used the daily average data
data=[108.1539915 125.3973438 -3.675183507 0.871684028 13.78421875
64.39277778 844.5503472 17.07349201 26.71506701 2.832 256.97255
253.5320313];

% Variables
ET = data(1); % w m-2
Rn = data(2); % w m-2
G = data(3); % w m-2
u = data(4); % m s-1

```



```

Ta = data(5);           % oC
RH = data(6)/100;      % humidity
P = data(7)/10;        % kPa
SWC_2= data(8)/100;    % m3 m-3
SWC_r= data(9)/100;    % m3 m-3
LAI = data(10);        % m2 m-2;
hc = data(11)/100;    % canopy height in m
z = 3;                 % reference height in m
S = data(12);          % solar radiation

% calculate wind speed at canopy height
z0 = 0.13*hc;          % roughness length
d = 0.67*hc;           % zero plane displacement
uh = u.*log((hc-d)./z0)./log((z-d)./z0);

% Calculate meteorologic variables
lambda=2500.78-2.3601*Ta;

% saturated vapour pressure in kPa
es=.6108*exp(17.27*Ta./(Ta+237.3));
% slope of pressure to temperature
delta=4098*es./(Ta+237.3).^2;

%air density
Rd=287/1000;           % the gas constant in kJ/kg/K
ea=es.*RH;
D=es-ea;
rho=P./(Rd*(Ta+273.14).*(1+.378*ea./P));

%
Cp=1.013;              %specific heat capacity of the dry air in kJ/kg/K;
epsilong=.622;         %the ratio between the mplecular weight of water
vapor and air

gamma=Cp*P./(lambda*epsilong);

% calculate raa
k=0.41;                % von K rm n constant
z0h=0.1*z0;           % roughness length to the
heat flux in [m];
n=2.5;                 % parameter in SW model
% LAI >4
raa_inf=log((z-d)./z0)./(k*k*(u+eps)).*(log((z-d)/(hc-d))+hc./(n*(hc

```

```

-d)).*(exp(n*(1-(d+z0)./hc))-1));
% for bare surface
z0s=0.01;
ras0=log(z/z0s).*log((d+z0)/z0s)./(k*k*(u+eps));
raa_bare=(log(z/z0s).*log(z/z0s))./(k*k*(u+eps))-ras0;    % bare
surface

raa=.25*LAI.*raa_inf+.25*(4-LAI).*raa_bare;

% calculate ras
% LAI >4
ras_inf=log((z-d)./z0)./(k*k*(u+eps)).*hc./(n*(hc-d)).*(exp(n)-exp(n*
(1-(d+z0)./hc)));

% for bare surface
z0s=0.01;
ras_bare=log(z/z0s).*log((d+z0)/z0s)./(k*k*(u+eps));

ras=.25*LAI.*ras_inf+.25*(4-LAI).*ras_bare;

% calculate rac
% method 1
rb=50;
rac=rb./(2*LAI);

% calculalte F4 in canopy resistance model
thetas=.45;                % saturated SWC
thetacr=0.75*thetas;
thetaw=.11;
for i=1:length(SWC_r)
    if SWC_r(i)>thetacr
        F4(i,1)=1;
    elseif SWC_r(i)>thetaw
        F4(i,1)=(SWC_r(i)-thetaw)./(thetacr-thetaw);
    else
        F4(i,1)=eps;
    end
end

% calculate the sensitivity index
sa1=0;
sb1=0;
ss1=zeros(1,dem);

```

```

st1=zeros(1,dem);
AB=zeros(1,dem);

for j=1:Nss

ETA=SWSA(Am(j,1),Am(j,2),Am(j,3),Am(j,4),Am(j,5),Am(j,6),Am(j,7),Am(j,8),Am(j,9),flag,F4,G,Rn,S,LAI,Ta,rho,D,SWC_2,delta,gamma,raa,ras,rac);

sal=sal+ETA;
sbl=sbl+ETA^2;

bfo(j,1)=sal/j;
VY(j,1)=sbl/j-bfo(j,1)^2;

ETB=SWSA(Bm(j,1),Bm(j,2),Bm(j,3),Bm(j,4),Bm(j,5),Bm(j,6),Bm(j,7),Bm(j,8),Bm(j,9),flag,F4,G,Rn,S,LAI,Ta,rho,D,SWC_2,delta,gamma,raa,ras,rac);

for i=1:dem
AB=Am(j,:);
AB(i)=Bm(j,i);

ETAB=SWSA(AB(1),AB(2),AB(3),AB(4),AB(5),AB(6),AB(7),AB(8),AB(9),flag,F4,G,Rn,S,LAI,Ta,rho,D,SWC_2,delta,gamma,raa,ras,rac);
ss1(i)=ETB*(ETAB-ETA)+ss1(i);
Si(j,i)=ss1(i)/(j*VY(j,1));
st1(i)=st1(i)+(ETA-ETAB)^2;
ST(j,i)=st1(i)/(2*j*VY(j,1));
end
end

% Create figure
figure1 = figure('PaperType','a4letter','PaperSize',[20.98 29.68]);

% Create axes
axes1 = axes('Parent',figure1,'YScale','log','YMinorTick','on');
box('on');
hold('all');

% Create multiple lines using matrix input to semilogy
semilogy1 = semilogy(Si);
set(semilogy1(1),'DisplayName','{\it r}_{STmin}');
set(semilogy1(2),'DisplayName','{\it K}_1');

```

```

set(semilogy1(3), 'DisplayName', '\itK_2');
set(semilogy1(4), 'DisplayName', '\itK_3');
set(semilogy1(5), 'DisplayName', '\itb_1');
set(semilogy1(6), 'DisplayName', '\itb_2');
set(semilogy1(7), 'DisplayName', '\iT_{min}');
set(semilogy1(8), 'DisplayName', '\iT_{max}');
set(semilogy1(9), 'DisplayName', '\itK_A');

% Create xlabel
xlabel('Simulation');

% Create ylabel
ylabel('\itS_{i}');

% Create legend
legend1 = legend(axes1, 'show');
set(legend1, 'Position', [0.7141 0.3258 0.1121 0.2881]);

% Create textbox
annotation('textbox', 'String', {'August'}, 'FontSize', 14, ...
    'EdgeColor', 'none', ...
    'Position', [0.1387 0.8208 0.393 0.1009], ...
    'FitHeightToText', ...
    'on');

save Si

```

A.4 First-order sensitivity indices

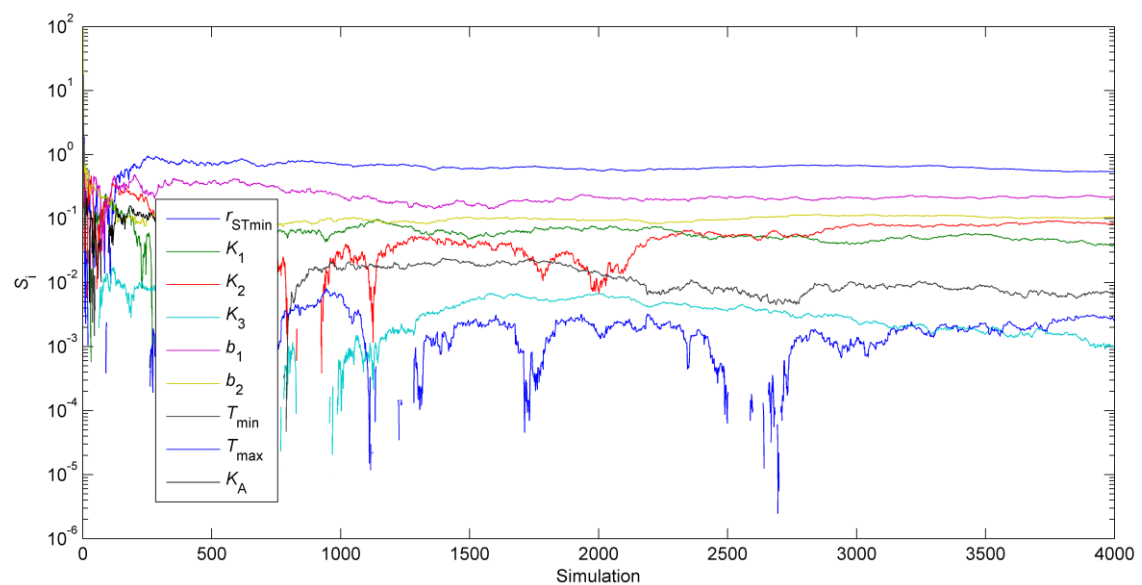


Fig. A1 The evolution of the first-order sensitivity indices.

Table A1 The first-order sensitivity index S_i for different parameters

Parameter	S_i (%)	Order
r_{STmin}	54.3	1
k_1	4.2	5
k_2	8.5	4
k_3	0	9
b_1	21.9	2
b_2	10.4	3
T_{amin}	0.3	7
T_{amax}	0.12	8
K_A	2.84	6

From Fig. A1 and Table A1, we can see that the most sensitive parameters in the S-W model was r_{STmin} , and followed by b_1 , b_2 , k_2 and k_1 . Other parameters with S_i less than 5% had almost no effect on the variability in model output. In addition, we thought that some parameter such as K_A (the extinction coefficient of light attenuation) has obviously physical meaning and should be measured directly on *site* (see [Sauer et al., 2007](#)). Thus, in our study, only six parameters were selected to be estimated in order to avoid equifinality or over-parameterization.

Overall, the key parameters in the S-W model are r_{STmin} , b_1 and b_2 with the values of S_i larger than 10%. Thus, proper estimations of these parameters have great influences in reducing the uncertainty on model simulation.

A.5 Prior Uncertainty Quantification

To derive from that the prior predictive uncertainty, 4000 parameter vectors were sampled from the prior uniform distribution using Latin Hypercube Sampling (LHS) method. The results indicated that the both simulated daily (ET; mm d^{-1}) and soil evaporation (E ; mm day^{-1}) showed larger uncertainties (Fig. C2). Thus, there is an urgent need to optimize the parameters based on available datasets.

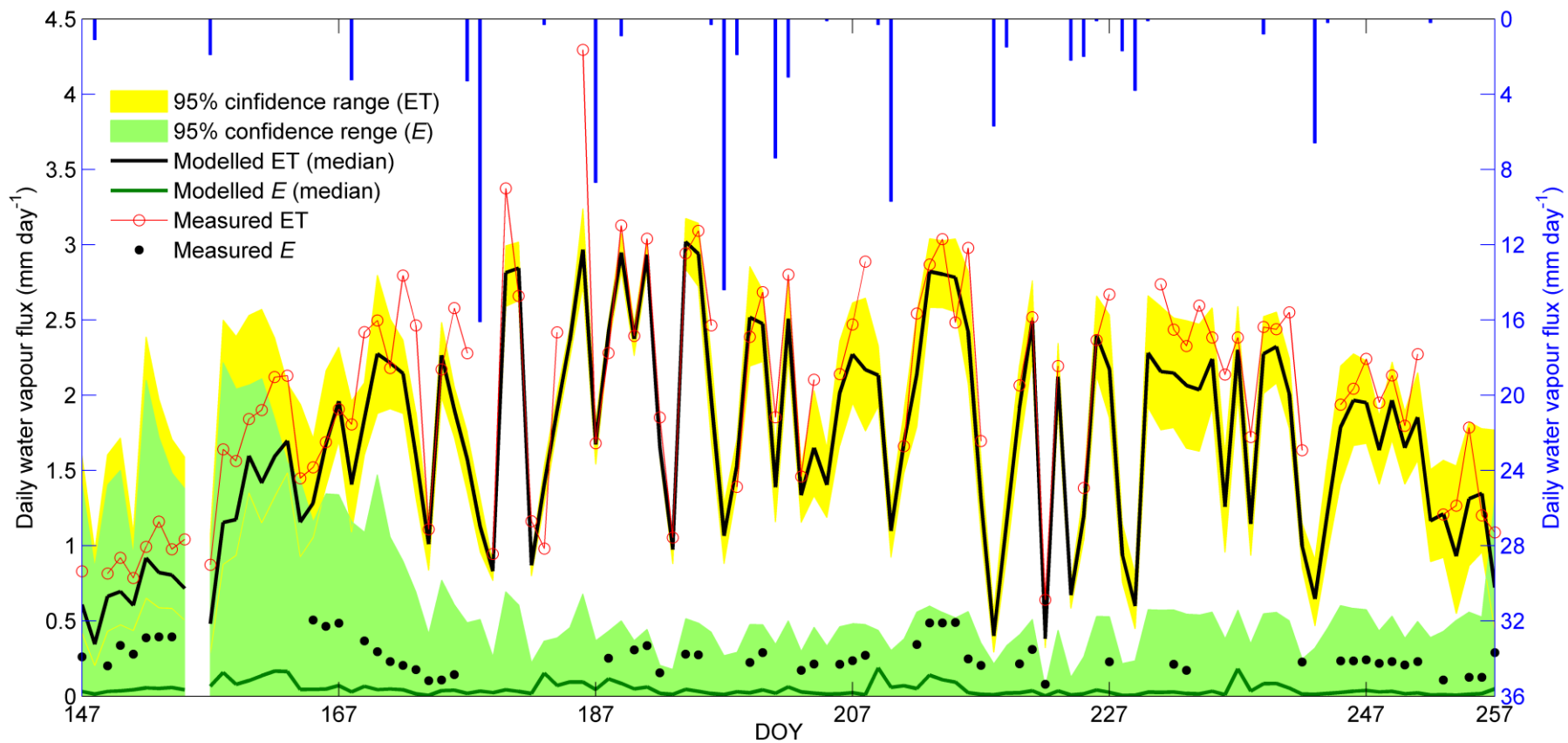


Fig. A2 Seasonal variation in daily evapotranspiration (ET; mm d^{-1}) and soil evaporation (E ; mm day^{-1}) measured by the EC system and modeled by the S-W model using the prior distribution of parameters. Gap in the time series is caused either by the absence of flux measurements or missing ancillary data.

Reference:

Iman, R.L., Helton, J.C.: An investigation of uncertainty and sensitivity analysis techniques for computer models. *Risk Analysis* 8(1): 71-90, 1988.

Saltelli, A., Annoni, P., Azzini, I., Campolongo, F., Ratto, M., Tarantola, S.: Variance based sensitivity analysis of model output. Design and estimator for the total sensitivity index. *Comput. Phys. Commun.* 181, 259-270, 2010.

Saltelli, A., Ratto, M., Andres, T., Campolongo, F., Cariboni, J., Gatelli, D., Saisana, M., Tarantola, S.: *Global Sensitivity Analysis: The Primer*. John Wiley & Sons, Ltd. 2008.

Sauer, T.J., Singer J.W., Prueger, J.H., DeSutter, T.M., Hatfield, J.L.: Radiation balance and evaporation partitioning in a narrow-row soybean canopy. *Agric. For. Meteorol.*, 145, 206-214, 2007.

Appendix B

Contents:

Part 1: Baye's Theorem

Part 2: Multi-Source Data Set Optimization Scheme

1.1 Metropolis-Hasting (M-H) Algorithm:

1.2 Matlab Code for the M-H Algorithm:

1.3 Results

Part 3: Single Data Set Optimization Scheme

2.1 Metropolis-Hasting (M-H) Algorithm:

2.2 Matlab Code for the M-H Algorithm:

2.3 Results

Part 4: Comparisons Between Two Optimization Schemes

This appendix show:

(1) Description of Bayes' Theorem

(2) the optimization scheme of M-H algorithm using multi-source data set (Part 1) and single data set (Part 2);

(2) The Matlab Code of the M-H algorithm using different assimilation scheme;

(3) The differences between the two different assimilation schemes;

The code can be used and tested freely. I would be great appreciations if you can cited our paper when using the code.

Zhu GF, Li X, Su YH, et al., 2014. Simultaneous parameterization of %% the two-source evapotranspiration model by Bayesian approach: application to spring maize in an arid region of northwest China. *Geosci. Model Dev. Discuss.*, 7, 741–775.

PART 1: The Bayes' Theorem

A general description of the Bayesian probabilistic inversion is given by Bayes' theorem (Box and Tiao, 1973) in a form of:

$$p(c|O) = \frac{p(O|c)p(c)}{\int p(O|c)p(c)dc} \propto p(O|c)p(c) \quad (\text{B1})$$

in which $p(c)$ is the prior probability density function (PDF) representing prior knowledge about parameter c ; $p(O|c)$ is the likelihood function, which defines the fit to the data for particular parameter set and also reflects the influence of the data on parameter identification; $\int p(O|c)p(c)dc$ is the probability of observations O , and $p(c|O)$ is the posterior PDF of parameter c . Thus, the inverse problem can be related to the forward problem through a set of measurements and prior knowledge about the probability of the parameters.

PART 2: Multi-Source Data Set Optimization Scheme

2.1 Metropolis-Hasting (M-H) Algorithm:

In practice, except for situations where $p(c|Z)$ have very simple forms, it is not always possible to draw samples directly from $p(c|Z)$. In such cases, the Markov Chain Monte Carlo (MCMC) method can be used to investigate the parameter space in the search for the posterior distribution (Geman et al., 1993; Gelfand and Smith, 1990). The basic idea for the MCMC sampling is to design a Markov chain with $p(c|Z)$ as the targeted stationary distribution. Once the chain has simulated for sufficiently long period samples in the chain will follow the stationary distribution, then one can collect the samples from the simulation and calculate various statistics associated with the posterior PDF from them. The Metropolis-Hastings (M-H)

algorithm (Metropolis et al., 1953; Hastings, 1970) is a type of MCMC technique that approximately obtains samples from the posterior distribution. A simple computational implementation of the M-H algorithm consists of the following steps:

Step 1:

Chose an arbitrary initial point $c^{(0)}$ in the parameter space.

Setp 2:

Propose a candidate point c^{new} according to a proposal distribution $q(c | c^{(k-1)})$;

In this study, the candidate parameter is generated by a uniform proposal distribution as:

$$c^{new} = c^{(k-1)} + \gamma(c^{max} - c^{min}) / D \quad (A1)$$

where c^{max} and c^{min} specify the prior range of the parameter vector c ; γ is a random number uniformly distributed between -0.5 and +0.5; D is a value controlling the proposing step size and was set to be 5.

Step 3:

3.1 Calculate σ_i for a given parameter vector:

For a given parameter vector c , we can simulate half-hourly λET ($W m^{-2}$) and daily E ($mm day^{-1}$) using equations (1) and (9) in the manuscript, which is labeled as $f_i(t)$ ($i=1$ and 2), respectively. Form previous analysis, we can calculate σ_i as:

$$\sigma_i^a(c) = \sqrt{\frac{1}{n_i} \sum_{t=1}^{n_i} e_i^2(t)} \quad (A2)$$

$$e_i(t) = O_i(t) - f_i(t) \quad (A3)$$

where $O_i(t)$ is observed values of the i th dataset [observed half-hourly λET

($W m^{-2}$) and daily E ($mm day^{-1}$), respectively] at time t ; n_i is the number of observations of the i th dataset.

3.2 Calculate the likelihood function

$$L(c) = \prod_{i=1}^m \prod_{t=1}^{n_i} \frac{1}{\sqrt{2\pi}\sigma_i^a(c)} e^{-\frac{(e_t - \hat{e}_t)^2}{2\sigma_i^a(c)^2}} \quad (A4)$$

where m is the number of dataset (= 2 in this study);

Step 4:

Calculate the acceptance probability:

$$\alpha = \min \left\{ \frac{L(c^{new}) q(c^{(k-1)} | c^{new})}{L(c^{(k-1)}) q(c^{new} | c^{(k-1)})} \right\} \quad (A5)$$

The ratio of likelihood is calculated under the candidate value of parameter to that calculated under preciously accepted value of parameter.

Step 5:

Generate a random number r form the uniform distribution $U[0,1]$.

If $r \leq \alpha$, accept the proposal and set $c^{(k)} = c^{new}$; otherwise set $c^{(k)} = c^{(k-1)}$;

Step 6:

Repeat steps 2 and 5 until enough samples are obtained.

The flowchart of the M-H algorithm was illustrated in [Fig. B1](#).

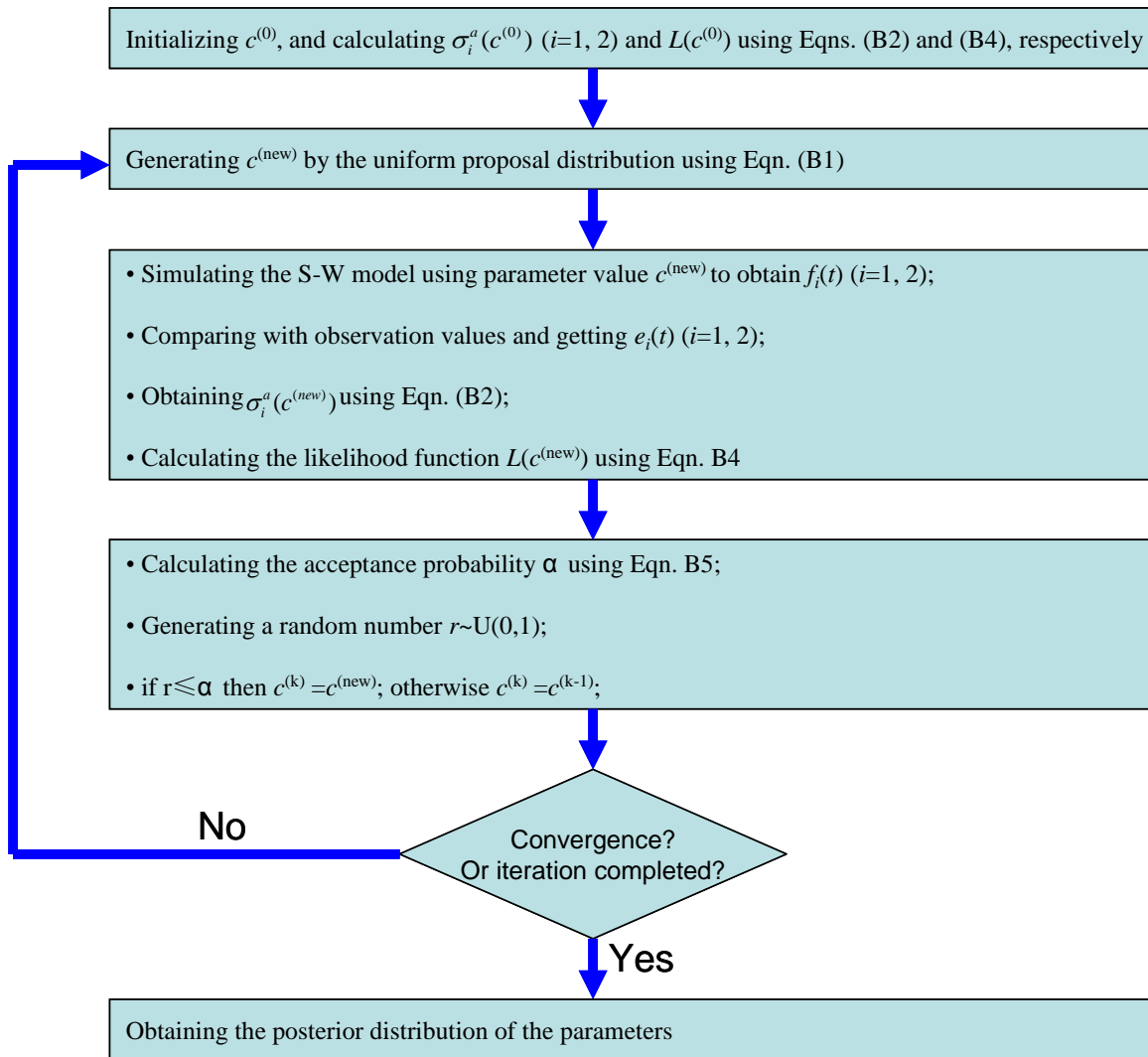


Fig. B1 Flowchart representing the basic scheme of the M-H algorithm.

2.2 Matlab Code for the M-H Algorithm:

```

%% Matlab Code of two source evapotranspiration model
function
[LET, Emd]=SW(rstmin, k1, k2, k3, b1, b2, flag, F4, G, Rn, S, LAI, Ta, rho, D, SWC_2,
delta, gamma, raa, ras, rac)
%% %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%% Author:    Gaofeng Zhu; Xin Li et al
%% Date:      March 17, 2014
%% Address:   Lanzhou University
%%
%% If there is a need for using the code, please cite the paper of the %%
authors as:
%% Zhu GF, Li X, Su YH, et al., 2014. Simultaneous parameterization of %%
the two-source evapotranspiration model by Bayesian approach:

```

```

%% application to spring maize in an arid region of northwest China.
Geosci. %% Model Dev. Discuss., 7, 741-775

```

```

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

```

```

%% Descriptions:

```

```

%% Output variables

```

```

%% LET      simulated half-hourly evapotranspiration in [w m-2]

```

```

%% Emd      simulated daily soil evaporation in [mm d-1]

```

```

%% parameter in resistance sub-model

```

```

%% rstmin   minimal stomatal resistance in [s m-1]

```

```

%% k1       parameter in eqn. 16 in the manuscript with unit [w m-2]

```

```

%% k2       unit [oc]

```

```

%% k3       unit [kPa-1]

```

```

%% b1       parameter in soil surface resistance in [s m-1]

```

```

%% b2       parameter in soil surface resistance in [s m-1]

```

```

%% input driving variables

```

```

%% F4       see eqn. (19) in the manuscript

```

```

%% G        soil heat flux in [W m-2]

```

```

%% Rn       net solar radiation in [W m-2]

```

```

%% S        short-wave solar radiation in [W m-2] (Rs in eqn.16)

```

```

%% LAI      leaf area index in [m2 m-2]

```

```

%% Ta       air temperature in reference height in [oc]

```

```

%% rho      air density in [kg m-3]

```

```

%% D        air water vapor pressure deficit in [kPa]

```

```

%% SWC_2    soil water content at the surface layer [m3 m-3]

```

```

%% delta    slope of the saturation vapor pressure versus temperature
            curve [kPa K-1]

```

```

%% gamma    psychrometric constant [kPa K-1]

```

```

%% raa      aerodynamic resistances in [s m-1]

```

```

%% ras      aerodynamic resistances in [s m-1]

```

```

%% rac      aerodynamic resistances in [s m-1]

```

```

%% Code of S-W model  %%

```

```

%% calculate rss in [s m-1]

```

```

thetas=0.45; % saturated water content at the 20 cm depth in [m3 m-3];

```

```

rss=exp(b1-b2*SWC_2./thetas);

```

```

%% calculated rsc in [s m-1]

```

```

F1=(eps+S)*(1055+k1)./(1055*(S+k1)); % S:short wave radiation W m-2

```

```

Tamin=0;

```

```

Tamax=40;

```

```

tao=(Tamax-k2)/(k2-Tamin);
numerator=(Ta-Tamin).*(Tamax-Ta).^tao;
denominator=(k2-Tamin).*(Tamax-k2).^tao;
F2=numerator./denominator;
F3=1-k3*D;
rsc=rstmin./(2*LAI.*F1.*F2.*F3.*F4);

%% S-W model
Cp=1.013; % specific heat capacity of the dry air in kJ/kg/K;
Ra=(delta+gamma).*raa;
Rs=(delta+gamma).*ras+gamma.*rss;
Rc=(delta+gamma).*rac+gamma.*rsc;

Cs=1./(1+Rs.*Ra./(Rc.*(Rs+Ra)));
Cc=1./(1+Rc.*Ra./(Rs.*(Rc+Ra)));
KA=.41;
Rns=Rn.*exp(-KA.*LAI);

A=Rn-G;
As=Rns-G;

ETs=(delta.*A+(rho.*Cp.*D-delta.*ras.*(A-As))./(raa+ras))./(delta+gamma.*
(1+rss./(raa+ras)));
ETc=(delta.*A+(rho.*Cp.*D-delta.*rac.*As))./(raa+rac))./(delta+gamma.*
(1+rsc./(raa+rac)));

LE=Cs.*ETs;
LT=Cc.*ETc;
LET=LE+LT; % total half-hourly ET in [W m-2]

% air water vapor pressure deficit at the canopy height in [kPa]
D0=D+(delta.*A-(delta+gamma).*LET).*raa./(rho.*Cp);

% half-hourly soil evaporation in [W m-2]
E=(delta.*As+rho.*Cp.*D0./ras)./(delta+gamma.*(1+rss./ras));

% half-hourly canopy transpiration in [W m-2]
T=(delta.*(A-As)+rho.*Cp.*D0./rac)./(delta+gamma.*(1+rsc./rac));

%% convert units of evaporation and transpiration from [W m-2] to [mm m-2]
lambda=2500.78-2.3601*Ta;
Em=E./lambda;
Tm=T./lambda;

```

```

%% calculate the daily accumulative soil evaporation and transpiration %%
in [mm day-1]
for i=1:length(E)/48
    Emd(i,1)=sum(Em((i-1)*48+1:i*48));
    Tmd(i,1)=sum(Tm((i-1)*48+1:i*48));
end
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%% End of the S-W model

```

% Main Code

```

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%
%% The main code used to calculate the posterior distribution of parameters
%% Authors :      Gaofeng Zhu, Xin Li
%% Date      :      March 17, 2014
%% Address   :      Lanzhou University
%% Purpose   :      using the M-H algorithm to explore the posterior
%%                  distribution parameters in the S-W model
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

```

```

clc
clear
format long
% load meteorological and biological driving data
load data
% ET Rn Gs_1 WS_3m Ta_3m RH_3m Press Ms_2cm Ms_10cm LAI h S
% Variables
ET      = data(:,1);           % w m-2
Rn      = data(:,2);           % w m-2
G       = data(:,3);           % w m-2
u       = data(:,4);           % m s-1
Ta      = data(:,5);           % oC
RH      = data(:,6)/100;       % humidity
P       = data(:,7)/10;        % kPa
SWC_2   = data(:,8)/100;       % m3 m-3
SWC_r   = data(:,9)/100;       % m3 m-3
LAI     = data(:,10);          % m2 m-2;
hc      = data(:,11)/100;      % canopy height in m
z       = 3;                   % reference height in m
S       = data(:,12);          % solar radiation

load Edaily                     % measured soil evaporation in mm day-1

```

```

% calculate wind speed at canopy height
z0 = 0.13*hc;           % roughness length
d = 0.67*hc;           % zero plane displacement
uh = u.*log((hc-d)./z0)./log((z-d)./z0);

% Calculate meteorological variables
lambda=2500.78-2.3601*Ta; % the latent heat of evaporation in J kg-1

% saturated vapor pressure in kPa
es=.6108*exp(17.27*Ta./(Ta+237.3));

% slope of pressure to temperature
delta=4098*es./(Ta+237.3).^2;

% air density
Rd=287/1000;           % the gas constant in kJ/kg/K
ea=es.*RH;            % actual vapor pressure in kPa
D=es-ea;              % air vapor pressure deficit in kPa

% air density in kg m-3
rho=P./(Rd*(Ta+273.14).*(1+.378*ea./P));

Cp=1.013;             %specific heat capacity of the dry air in kJ/kg/K;
epsilong=.622;        %the ratio of water vapor and air
gamma=Cp*P./(lambda*epsilong); % psychrometric constant (kPa K-1)

% calculate raa using equations from Shuttleworth and Wallace (1985)
k=0.41;               % von Karman constant
% z0h=0.1*z0;         % roughness length to the heat flux in [m];
n=2.5;               % parameter in SW model
% LAI >4
raa_inf=log((z-d)./z0)./(k*k*(u+eps)).*(log((z-d)./(hc-d))+hc./(n*(hc-d))).*(exp(n*(1-(d+z0)/hc))-1));
% for bare surface
z0s=0.01;
ras0=log(z/z0s).*log((d+z0)/z0s)./(k*k*(u+eps));
raa_bare=(log(z/z0s).*log(z/z0s))./(k*k*(u+eps))-ras0;
%
raa=.25*LAI.*raa_inf+.25*(4-LAI).*raa_bare;

% calculate ras
% LAI >4
ras_inf=log((z-d)./z0)./(k*k*(u+eps)).*hc./(n*(hc-d)).*(exp(n)-exp(n*

```



```

(1-(d+z0)./hc));
% for bare surface
z0s=0.01;
ras_bare=log(z/z0s).*log((d+z0)/z0s)./(k*k*(u+eps));
%
ras=.25*LAI.*ras_inf+.25*(4-LAI).*ras_bare;

% calculate rac
% method 1
rb=50;
rac=rb./(2*LAI);

% method 2
% w=6/100; % leaf width in m
% rb=(100/n)*(w./u)*(1-exp(-n/2));
% rac=rb./(2*LAI);

% calculate F4 in canopy resistance model
thetas=.45; % saturated SWC
thetacr=0.75*thetas;
thetaw=.11;
for i=1:length(SWC_r)
    if SWC_r(i)>thetacr
        F4(i,1)=1;
    elseif SWC_r(i)>thetaw
        F4(i,1)=(SWC_r(i)-thetaw)./(thetacr-thetaw);
    else
        F4(i,1)=eps;
    end
end

% Calculate observed daily ET
ETo=ET./lambda;
for i=1:length(ET)/48
    ETdaily(i,1)=sum(ETo((i-1)*48+1:i*48,1));
end

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%% M-H iteration procedure

% Parameter ranges of rsmin,k1,k2,k3,b1,b2,
cmin(1)=0;cmin(2)=0;cmin(3)=30;cmin(4)=0;cmin(5)=4;cmin(6)=0;
cmax(1)=80;cmax(2)=500;cmax(3)=40;cmax(4)=.1;cmax(5)=15;cmax(6)=8;

```

```

% initialize parameter
for i=1:length(cmin)
    co(i)=cmin(i)+rand.*(cmax(i)-cmin(i));    % Initial parameters
end

[LETo,Emdo]=SW(co(1),co(2),co(3),co(4),co(5),co(6),[],F4,G,Rn,S,LAI,Ta,
rho,D,SWC_2,delta,gamma,raa,ras,rac);

e1=LETo-ET;
e2=Emdo-Edaily;
sigma1=sqrt(sum(e1.^2)/length(LETo));
sigma2=sqrt(sum(e2.^2)/length(Emdo));

logL1=-length(LETo)*log(sigma1)-sum(e1.^2/(2*sigma1^2));
logL2=-length(Emdo)*log(sigma2)-sum(e2.^2/(2*sigma2^2));
logL=logL1+logL2;

nsim=30000;    % iteration length
parameter=zeros(nsim,length(cmin));
sigma=zeros(nsim,2);

% begin to iterate
for i=1:nsim
    % generate new parameter vector
    rr=-.5+rand(1,length(cmin));
    cnew=co+rr.*(cmax-cmin)/5;

    % simulate using new parameter vector
    [LETo,Emdo]=SW(cnew(1),cnew(2),cnew(3),cnew(4),cnew(5),cnew(6),[],F4,
G,Rn,S,LAI,Ta,rho,D,SWC_2,delta,gamma,raa,ras,rac);

    % calculate model error for different data set
    e1=LETo-ET;
    e2=Emdo-Edaily;

    % estimate sigma of different data set
    sigma1=sqrt(sum(e1.^2)/length(LETo));    % Eqn.24
    sigma2=sqrt(sum(e2.^2)/length(Emdo));    % Eqn.24

    % calculate the log-likelihood of different data set
    logL1=-length(LETo)*log(sigma1)-sum(e1.^2/(2*sigma1^2));
    logL2=-length(Emdo)*log(sigma2)-sum(e2.^2/(2*sigma2^2));

    % calculate the total log-likelihood

```

```

logLnew=logL1+logL2; % Eqn.23

% draw a rand number form uniform distribution
r=log(rand);

if r<=logLnew-logL
    parameter(i,:)=cnew; % save parameter vales used to draw statistics
    logL=logLnew;
    co=cnew;
else
    parameter(i,:)=co; % save parameter vales used to draw statistics
end
sigma(i,:)=[sigma1,sigma2]; % save sigma
end
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%% End of the Main program

```

The proposing efficiency of $q(c^{new} | c^{(k-1)})$ affects the efficiency of the algorithm, and hence should be properly designed to ensure a moderate sample acceptance rate. A rate of 23% is sometimes an optimal acceptance rate (Robert and Rosenthal, 1998). **In our test study, the accepting rate using the uniform proposal function is generally low (~10%).** Based on the test run, we constructed a normal distribution $N(0, cov(c))$, where $cov(c)$ is the diagonal matrix of the parameter with its diagonal being set to the estimated variances of the parameter c from the initial test run and zeros elsewhere. Then, we adopted the following proposal distribution:

$$c^{new} = c^{(k-1)} + N(0, cov(c)) \quad (A6)$$

Using this proposal distribution, the general acceptance rate can achieve between 20-50%. The Matlab code was shown as following:

```

function y=Generate(co,transT,eigV,cmin,cmax)
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% Purpose : using normal distribution to generate candidate
% Author  : Gaofeng Zhu, Xin Li, et al.,
% Date    : March 17, 2014
% the original code was developed by Xu et al., 2007;

```

```

% Please cited as:
% Xu T., White L., Hui DF., Luo YQ. Global Biogeochemical Cycle, 20, GB2007,
% doi:10.109/2005GB002468, 2006
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
co=co';
while(true)
% 6: the number of parameter
cT=randn(6,1).*[sqrt(eigV(1,1));sqrt(eigV(2,2));sqrt(eigV(3,3));sqrt(
eigV(4,4));sqrt(eigV(5,5));sqrt(eigV(6,6))];

%generate a new configuration based on the estimated covariance matrix
c_new =transT*(transT'*co+cT);
if c_new(1)>cmin(1)&c_new(1)<cmax(1)...
    &c_new(2)>cmin(2)&c_new(2)<cmax(2)...
    &c_new(3)>cmin(3)&c_new(3)<cmax(3)...
    &c_new(4)>cmin(4)&c_new(4)<cmax(4)...
    &c_new(5)>cmin(5)&c_new(5)<cmax(5)...
    &c_new(6)>cmin(6)&c_new(6)<cmax(6)...
    break
end
end
y=c_new';
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%% End of the sub-model

```

% Main Code

```

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%
%% The main code used to calculate the posterior distribution of parameters
%% Authors: Gaofeng Zhu, Xin Li
%% Date:    March 17, 2014
%% Adress:  Lanzhou University
%% Purpose: using the M-H algorithm to explore the posterior distribution
%%           parameters in the S-W model
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

clc
clear
format long
% load meteorological and biological driving data
load data
% ET Rn Gs_1 WS_3m Ta_3m RH_3m Press Ms_2cm Ms_10cm LAI h S
% Variables
ET    = data(:,1);          % w m-2

```

```

Rn      = data(:,2);           % w m-2
G       = data(:,3);           % w m-2
u       = data(:,4);           % m s-1
Ta      = data(:,5);           % oC
RH      = data(:,6)/100;       % humidity
P       = data(:,7)/10;        % kPa
SWC_2   = data(:,8)/100;       % m3 m-3
SWC_r   = data(:,9)/100;       % m3 m-3
LAI     = data(:,10);          % m2 m-2;
hc      = data(:,11)/100;      % canopy height in m
z       = 3;                   % reference height in m
S       = data(:,12);          % solar radiation

load Edaily                     % measured soil evaporation in mm day-1

% calculate wind speed at canopy height
z0 = 0.13*hc;                   % roughness length
d  = 0.67*hc;                   % zero plane displacement
uh = u.*log((hc-d)./z0)./log((z-d)./z0);

% Calculate meteorological variables
lambda=2500.78-2.3601*Ta;      % the latent heat of evaporation in J kg-1

% saturated vapor pressure in kPa
es=.6108*exp(17.27*Ta./(Ta+237.3));

% slope of pressure to temperature
delta=4098*es./(Ta+237.3).^2;

% air density
Rd=287/1000;                   % the gas constant in kJ/kg/K
ea=es.*RH;                     % actual vapor pressure in kPa
D=es-ea;                       % air vapor pressure deficit in kPa

% air density in kg m-3
rho=P./(Rd*(Ta+273.14).*(1+.378*ea./P));

Cp=1.013;                      %specific heat capacity of the dry air in kJ/kg/K;
epsilong=.622;                 %the ratio of water vapor and air
gamma=Cp*P./(lambda*epsilong); % psychrometric constant (kPa K-1)

% calculate raa using equations from Shuttleworth and Wallace (1985)
k=0.41;                        % von Karman constant

```

```

% z0h=0.1*z0;           % roughness length to the heat flux in [m];
n=2.5;                 % parameter in SW model
% LAI >4
raa_inf=log((z-d)./z0)./(k*k*(u+eps)).*(log((z-d)/(hc-d))+hc./(n*(hc-d)).*(exp(n*(1-(d+z0)/hc))-1));
% for bare surface
z0s=0.01;
ras0=log(z/z0s).*log((d+z0)/z0s)./(k*k*(u+eps));
raa_bare=(log(z/z0s).*log(z/z0s))./(k*k*(u+eps))-ras0;
%
raa=.25*LAI.*raa_inf+.25*(4-LAI).*raa_bare;

% calculate ras
% LAI >4
ras_inf=log((z-d)./z0)./(k*k*(u+eps)).*hc./(n*(hc-d)).*(exp(n)-exp(n*(1-(d+z0)/hc)));
% for bare surface
z0s=0.01;
ras_bare=log(z/z0s).*log((d+z0)/z0s)./(k*k*(u+eps));
%
ras=.25*LAI.*ras_inf+.25*(4-LAI).*ras_bare;

% calculate rac
% method 1
rb=50;
rac=rb./(2*LAI);

% method 2
% w=6/100;           % leaf width in m
% rb=(100/n)*(w./u)*(1-exp(-n/2));
% rac=rb./(2*LAI);

% calcualte F4 in canopy resistance model
thetas=.45;           % saturated SWC
thetacr=0.75*thetas;
thetaw=.11;
for i=1:length(SWC_r)
    if SWC_r(i)>thetacr
        F4(i,1)=1;
    elseif SWC_r(i)>thetaw
        F4(i,1)=(SWC_r(i)-thetaw)./(thetacr-thetaw);
    else
        F4(i,1)=eps;
    end
end

```

```

    end
end

% Calculate observed daily ET
ETo=ET./lambda;
for i=1:length(ET)/48
    ETdaily(i,1)=sum(ETo((i-1)*48+1:i*48,1));
end

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%% M-H iteration procedure
% Prior estimate of covariance matrix of parameters
% it was obtained from previous uniform run

cov_c=[0.9645 -0.0219   -0.3973   -0.0015   -0.0047   0.0314
-0.0219   0.0247 -0.0852   0.0003 0.0171 0.0322
-0.3973   -0.0852   5.3166 -0.0076   -0.0279   -0.0387
-0.0015   0.0003 -0.0076   0.0003 0.0025 0.0065
-0.0047   0.0171 -0.0279   0.0025 0.2524 0.6315
0.0314 0.0322 -0.0387   0.0065 0.6315 1.6916];
[transT, eigV]=eig(cov_c);

% Parameter ranges of rsmin,k1,k2,k3,b1,b2,
cmin(1)=0;cmin(2)=0;cmin(3)=30;cmin(4)=0;cmin(5)=4;cmin(6)=0;
cmax(1)=80;cmax(2)=500;cmax(3)=40;cmax(4)=.1;cmax(5)=15;cmax(6)=8;

% initialize parameter
for i=1:length(cmin)
    co(i)=cmin(i)+rand.*(cmax(i)-cmin(i));    % Initial paramerters
end

[LETo,Emdo]=SW(co(1),co(2),co(3),co(4),co(5),co(6),[],F4,G,Rn,S,LAI,T
a,rho,D,SWC_2,delta,gamma,raa,ras,rac);

e1=LETo-ET;
e2=Emdo-Edaily;
sigma1=sqrt(sum(e1.^2)/length(LETo));
sigma2=sqrt(sum(e2.^2)/length(Emdo));

logL1=-length(LETo)*log(sigma1)-sum(e1.^2/(2*sigma1^2));
logL2=-length(Emdo)*log(sigma2)-sum(e2.^2/(2*sigma2^2));
logL=logL1+logL2;

nsim=30000;                                % iteration length

```

```

parameter=zeros(nsim,length(cmin));
sigma=zeros(nsim,2);

% begian to iterate
for i=1:nsim
    % generate new parameter vector from normal destrubution
    cnew= Generate(co,transT,eigV,cmin,cmax);

    % simulate using new parameter vector
    [LETo,Emdo]=SW(cnew(1),cnew(2),cnew(3),cnew(4),cnew(5),cnew(6),[],F4,
G,Rn,S,LAI,Ta,rho,D,SWC_2,delta,gamma,raa,ras,rac);

    % calcualte model error for different data set
    e1=LETo-ET;
    e2=Emdo-Edaily;

    % estimate sigma of different data set
    sigma1=sqrt(sum(e1.^2)/length(LETo));           % Eqn.24
    sigma2=sqrt(sum(e2.^2)/length(Emdo));           % Eqn.24

    % calclaute the log-likelihood of different data set
    logL1=-length(LETo)*log(sigma1)-sum(e1.^2)/(2*sigma1^2);
    logL2=-length(Emdo)*log(sigma2)-sum(e2.^2)/(2*sigma2^2);

    % calcualte the total log-likelihood
    logLnew=logL1+logL2;                           % Eqn.23

    % draw a rand number form uniform distribution
    r=log(rand);

    if r<=logLnew-logL
        parameter(i,:)=cnew; % save parameter vales used to draw statistics
        logL=logLnew;
        co=cnew;
    else
        parameter(i,:)=co; % save parameter vales used to draw statistics
    end
    sigma(i,:)=[sigma1,sigma2]; % save sigma
end

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%% End of the main program

```

2.3 Results of Multi-source Assimilation Scheme

The results of 10,000 evolution of MCMC using multi-source data are shown in

Fig. B2

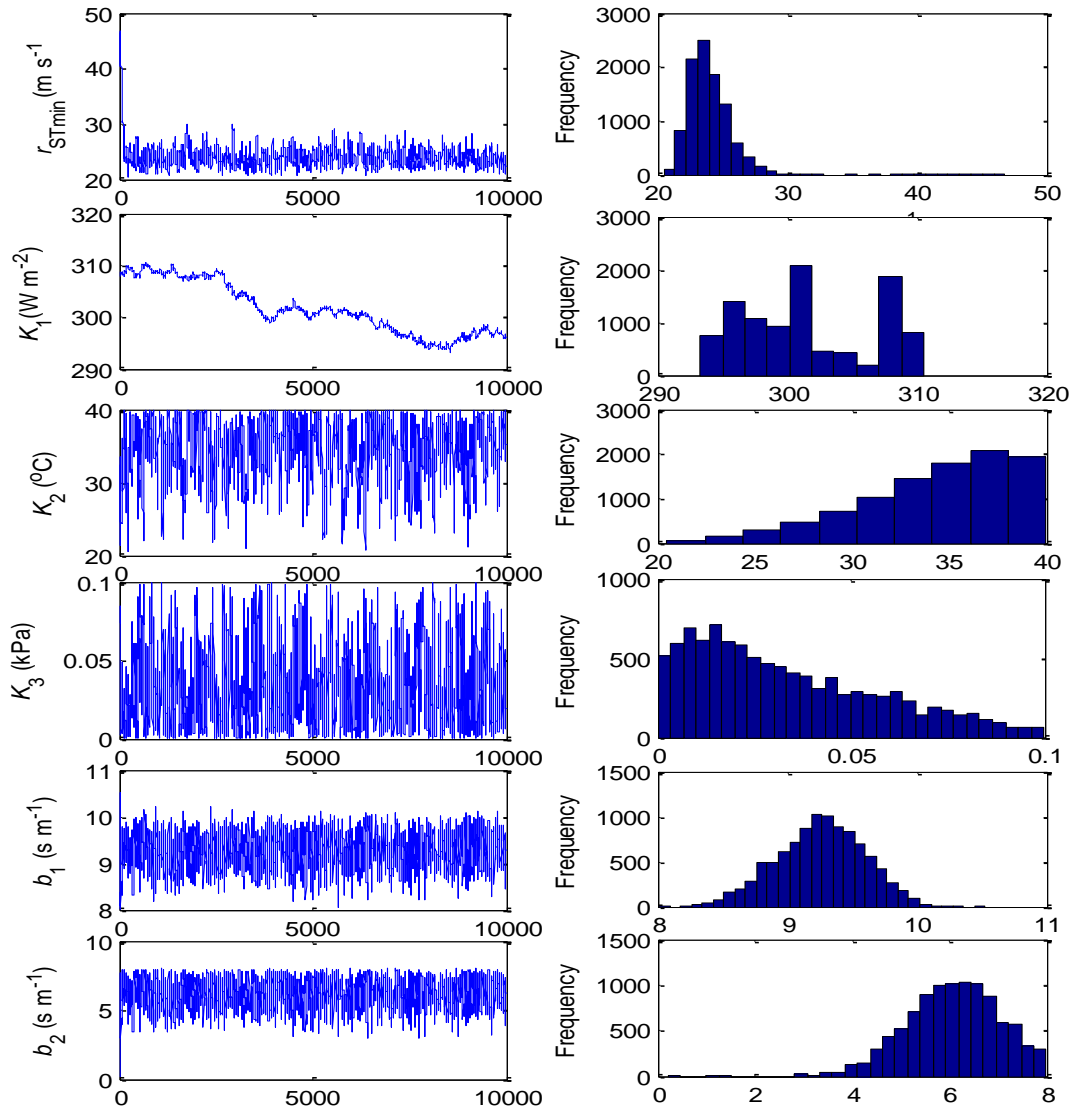


Fig. B2 The evolution of MCMC chain using the normal distribution proposal (left) and histograms of sample from posterior distribution (right) by using multi-source dataset

The comparison between observed and simulated half-hourly evapotranspiration (W m^{-2}) were illustrated in Fig. B3. The simulated values were obtained using the **median** values of the posterior parameter distribution.

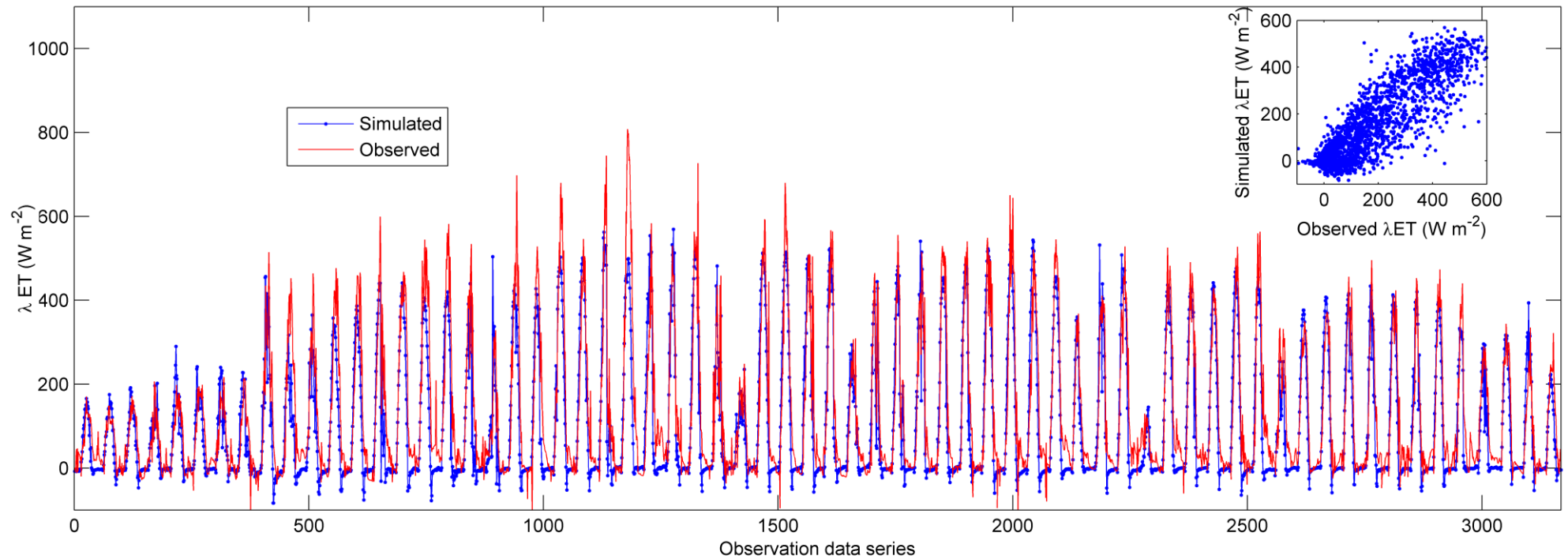


Fig. B3 Comparison between observed and simulated half-hourly evapotranspiration (W m^{-2}). The regression line between observed and simulated values was: $y=0.84x+0.18$ ($R^2=0.83$)

PART 3: Single Data Set Optimization Scheme

3.1 M-H Algorithm:

To investigate how the estimation accuracy and parameters vary, a test case was also run by using one single data set (the EC-measured half-hourly ET; W m^{-2}). In this case, the likelihood function was set as:

$$L = p(O | c) = \prod_{t=1}^n \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(e(t))^2}{2\sigma^2}} \quad (\text{A7})$$

$$e(t) = O(t) - f(t) \quad (\text{A8})$$

where $O(t)$ is EC-observed half-hourly ET (W m^{-2}); $f(t)$ is simulated ET values (W m^{-2} ; Eqn.1 in the manuscript); $e(t)$ is the model error (W m^{-2}); and σ is the standard deviation on each data point. For a given parameter vector, σ is estimated as (Braswell et al., 2005):

$$\sigma = \sqrt{\frac{1}{n} \sum_{t=1}^n (e(t))^2} \quad (\text{A9})$$

3.2 Matlab Code

```
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%
%% The main code used to calculate the posterior distribution of parameters
%% This scheme using only the EC-measured half-hourly ET data
%% Authors: Gaofeng Zhu, Xin Li
%% Date:    March 17, 2014
%% Adress:  Lanzhou University
%% Purpose: using the M-H algorithm to explore the posterior distribution
%%          parameters in the S-W model
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
clc
clear

format long
load data
% ET Rn Gs_1 WS_3m Ta_3m RH_3m P Ms_2cm Ms_10cm LAI h S
```

```

% Variables
ET = data(:,1);           % w m-2
Rn = data(:,2);           % w m-2
G = data(:,3);           % w m-2
u = data(:,4);           % m s-1
Ta = data(:,5);          % oC
RH = data(:,6)/100;      % humidity
P = data(:,7)/10;        % kPa
SWC_2= data(:,8)/100;    % m3 m-3
SWC_r= data(:,9)/100;    % m3 m-3
LAI = data(:,10);        % m2 m-2;
hc = data(:,11)/100;     % canopy height in m
z = 3;                   % reference height in m
S = data(:,12);          % solar radiation

load Edaily              % measured soil evaporation in mm day-1

% calculate wind speed at canopy height
z0 = 0.13*hc;            % roughness length
d = 0.67*hc;            % zero plane displacement
uh = u.*log((hc-d)./z0)./log((z-d)./z0);

% Calculate meteorological variables
lambda=2500.78-2.3601*Ta;

% saturated vapour pressure in kPa
es=.6108*exp(17.27*Ta./(Ta+237.3));
% slope of pressure to temperature
delta=4098*es./(Ta+237.3).^2;

%air density
Rd=287/1000;            % the gas constant in kJ/kg/K
ea=es.*RH;
D=es-ea;
rho=P./(Rd*(Ta+273.14).*(1+.378*ea./P));

%
Cp=1.013;               %specific heat capacity of the dry air in kJ/kg/K;
%the ratio between the mplecular weight of water vapor and air
epsilong=.622;

gamma=Cp*P./(lambda*epsilong);

```

```

%% calculate raa
k=0.41; % von Karman constant
% z0h=0.1*z0; % roughness length to the heat flux in [m];
n=2.5; % parameter in SW model

% LAI >4
raa_inf=log((z-d)./z0)./(k*k*(u+eps)).*(log((z-d)/(hc-d))+hc./(n*(hc-d))).*(exp(n*(1-(d+z0)/hc))-1));

% for bare surface
z0s=0.01;
ras0=log(z/z0s).*log((d+z0)/z0s)./(k*k*(u+eps));
raa_bare=(log(z/z0s).*log(z/z0s))./(k*k*(u+eps))-ras0; % bare surface

%
raa=.25*LAI.*raa_inf+.25*(4-LAI).*raa_bare;

%% calculate ras
% LAI >4
ras_inf=log((z-d)./z0)./(k*k*(u+eps)).*hc./(n*(hc-d)).*(exp(n)-exp(n*(1-(d+z0)/hc)));

% for bare surface
z0s=0.01;
ras_bare=log(z/z0s).*log((d+z0)/z0s)./(k*k*(u+eps));

ras=.25*LAI.*ras_inf+.25*(4-LAI).*ras_bare;

% calculate rac
% method 1
rb=50;
rac=rb./(2*LAI);

% w=6/100; % leaf width in m
% rb=(100/n)*(w./u)*(1-exp(-n/2));
% rac=rb./(2*LAI);

% calcualte F4 in canopy resistance model
thetas=.45; % saturated SWC
thetacr=0.75*thetas;
thetaw=.11;
for i=1:length(SWC_r)

```

```

    if SWC_r(i)>thetacr
        F4(i,1)=1;
    elseif SWC_r(i)>thetaw
        F4(i,1)=(SWC_r(i)-thetaw)./(thetacr-thetaw);
    else
        F4(i,1)=eps;
    end
end

% Calculate observed daily ET, E and T
ETo=ET./lambda;
for i=1:length(ET)/48
    ETdaily(i,1)=sum(ETo((i-1)*48+1:i*48,1));
    Edaily(i,1)=ETdaily(i,1)*FracE(i,1);
    Tdaily(i,1)=ETdaily(i,1)*FracT(i,1);
end

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%% M-H iteration procedure
% Prior estimate of covariance matrix of parameters
% it was obtained from test uniform run, which is similar to that used
% in Part 1
%
cov_c=[2.649    -11.1951    0.4698   -0.011   -0.0843   0.5416
-11.1951    12139.2934   -80.9997    0.3606   11.5584   23.4091
0.4698   -80.9997    22.3938   -0.0033   0.3244   1.6035
-0.011    0.3606   -0.0033   0.0006   0.0007   -0.0004
-0.0843   11.5584   0.3244   0.0007   0.576    1.3829
0.5416   23.4091   1.6035   -0.0004   1.3829   4.4452];

[transT, eigV]=eig(cov_c);

% Parameter ranges of rsmin,k1,k2,k3,b1,b2,
cmin(1)=0;cmin(2)=0;cmin(3)=20;cmin(4)=0;cmin(5)=4;cmin(6)=0;
cmax(1)=80;cmax(2)=500;cmax(3)=40;cmax(4)=.1;cmax(5)=15;cmax(6)=8;

% initialize parameter
for i=1:length(cmin)
    co(i)=cmin(i)+rand.*(cmax(i)-cmin(i));    % Initial parameters
end

[LETo,Emdo]=SW(co(1),co(2),co(3),co(4),co(5),co(6),[],F4,G,Rn,S,LAI,T
a,rho,D,SWC_2,delta,gamma,raa,ras,rac);

```

```

% only ET data set was used here, that is different form Part 1
e1=LETo-ET;
sigma1=sqrt(sum(e1.^2)/length(LETo));

logL=-length(LETo)*log(sigma1)-sum(e1.^2/(2*sigma1^2));

nsim=10000; % iteration length
parameter=zeros(nsim,length(cmin));
sigma=zeros(nsim,2);

% begian to iterate
for i=1:nsim
    % generate new parameter vector from normal destribution
    cnew= Generate(co,transT,eigV,cmin,cmax);

    % simulate using new parameter vector

[LETo,Emdo]=SW(cnew(1),cnew(2),cnew(3),cnew(4),cnew(5),cnew(6),[],F4,
G,Rn,S,LAI,Ta,rho,D,SWC_2,delta,gamma,raa,ras,rac);

    % calcualte model error for ET data set
    e1=LETo-ET;

    % estimate sigma of ET data set
    sigma1=sqrt(sum(e1.^2)/length(LETo)); % Eqn.24

    % calclaute the log-likelihood
    logLnew=-length(LETo)*log(sigma1)-sum(e1.^2)/(2*sigma1^2);

    % draw a rand number form uniform distribution
    r=log(rand);

    if r<=logLnew-logL
        parameter(i,:)=cnew; % save parameter vales used to draw statistics
        logL=logLnew;
        co=cnew;
    else
        parameter(i,:)=co; % save parameter vales used to draw statistics
    end
end
end
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%% End of the Main program

```

3.3 Results

The results of 10,000 evolution of MCMC using single data are shown in Fig. B4

(left). **Comparing with multi-source assimilation scheme, we can see that the posterior distribution of soil resistance parameter (b_1 and b_2) varied wider.**

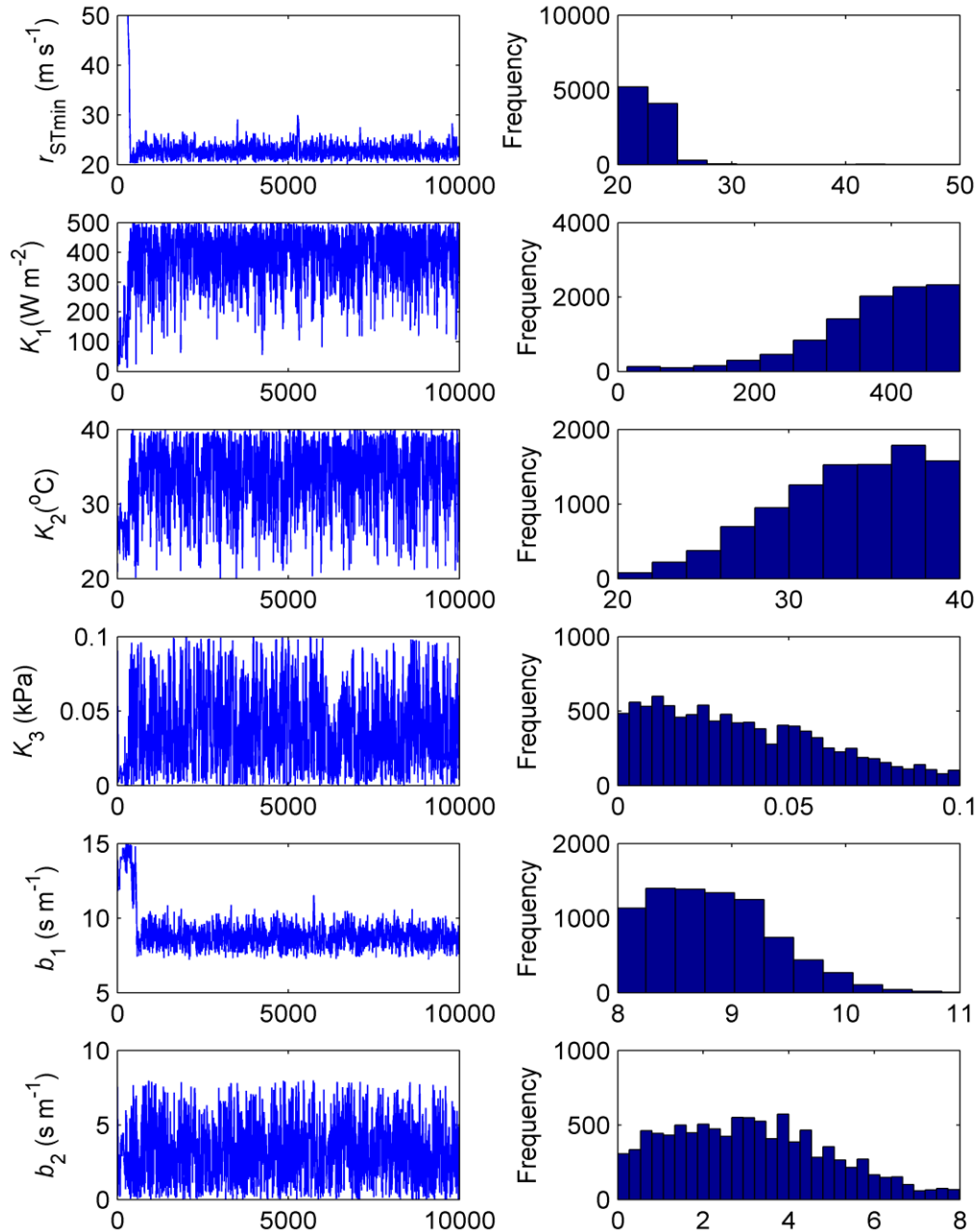


Fig. B4 The evolution of MCMC chain using the normal distribution proposal (left) and histograms of sample from posterior distribution (right) by using single dataset.

The slope (0.85) of the regression line between observed and simulated half-hourly ET for single data set assimilation scheme is slightly lower than that for multi-source data set assimilation scheme (0.86). **Thus, we can confirmed that that the multi-source data set assimilation scheme is more effective than the single data set scheme.**

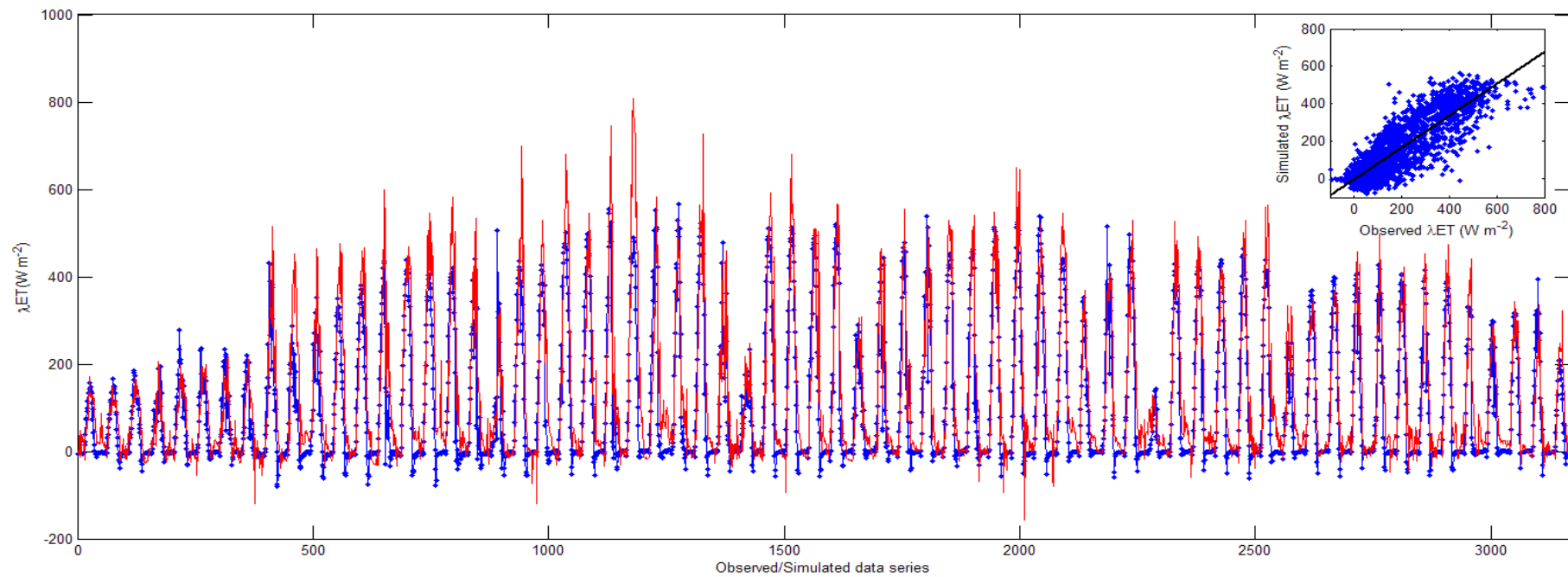


Fig. B5 Comparison between observed and simulated half-hourly evapotranspiration (W m^{-2}). The regression lion between observed and simulated values was: $y=0.83x-1.65$ ($R^2=0.75$)

PART 4: Comparisons Between Different Assimilation Schemes

4.1 Posterior distributions of parameter for different assimilation schemes

For Scheme 1 (simultaneously assimilate all data sets), r_{STmin} , b_1 , b_2 and k_2 showed relatively large uncertainty reductions (defined as $1 - CI_{posterior} / CI_{prior}$, where CI is the length of the 95% credible interval) (Fig. B6), and their posterior distributions become approximately symmetric with distinctive modes, while parameters k_1 and k_3 have relative large variability (widely spread on the prior bounds) (Fig. B7a); For Scheme 2 (only assimilate EC data), only r_{STmin} , b_1 and k_2 showed relatively large uncertainty reductions and tended to be approximately symmetric, while b_2 , k_1 and k_3 tended to span the entire prior range (Fig. B7b). Comparing with the two assimilation schemes, important differences occurred in estimates of the posterior distribution of parameters related to the soil surface resistance (b_1 and b_2 ; $s\ m^{-1}$) (Fig. B6). Generally, tighter posterior distributions for parameters b_1 and b_2 were obtained by Scheme 1. For example, the values of uncertainty reduction for b_1 and b_2 in Scheme 1 (0.89 and 0.56, respectively) were higher than that in Scheme 2 (0.79 and 0.12, respectively). Thus, the daily soil evaporation data helped to well constrain estimates of b_1 and b_2 . In addition, the six calibrated parameters by Scheme 1 were not significantly inter-correlated with each other (correlation coefficients lower than 0.1), while for Scheme 2 the pairs b_1 and b_2 and r_{STmin} and b_2 tended to be constrained together with correlation coefficients being 0.84 and 0.32, respectively (Table B1).

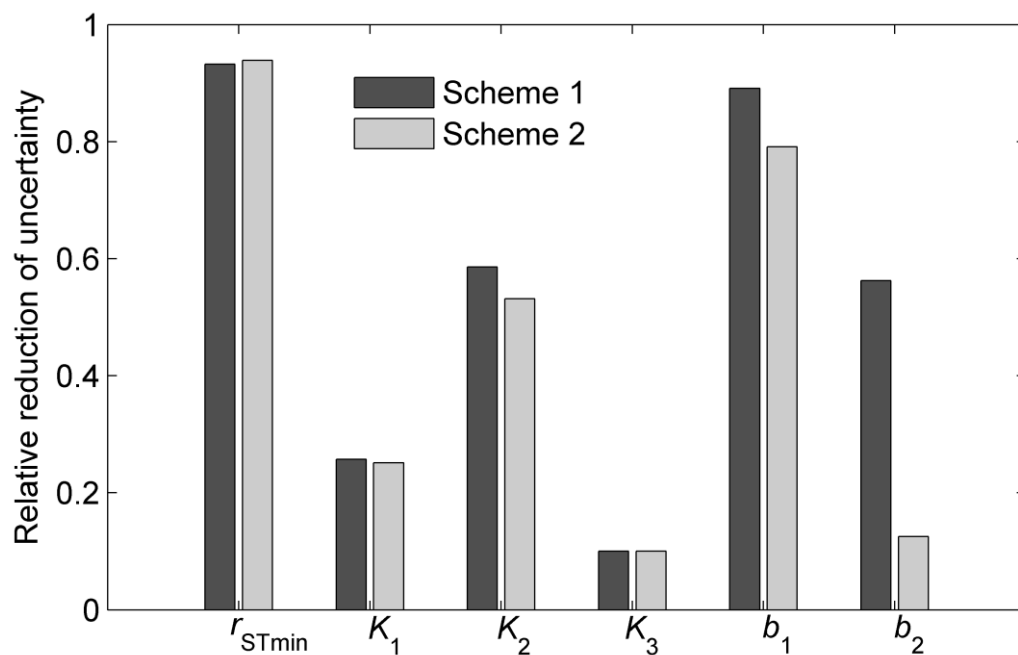


Fig. B6 Uncertainty reductions of parameters using different assimilation schemes

Table B1 The correlation coefficient, derived form the posterior distribution of parameters using different assimilation schemes.

r_{STmin}	k_1	k_2	k_3	b_1	b_2	
1	-0.004	-0.01	0.02	0.01	0.004	r_{STmin}
	1	0.05	-0.04	-0.02	0.06	k_1
		1	-0.04	-0.07	0.07	k_2
			1	0.05	-0.04	k_3
				1	0.02	b_1
					1	b_2
EC data Only						
r_{STmin}	1					
k_1	-0.13	1				
k_2	-0.13	0.06	1			
k_3	-0.15	0.02	0.01	1		
b_1	-0.09	0.05	0.04	0.02	1	
b_2	0.32	0.02	0.05	-0.03	0.84	1
	r_{STmin}	k_1	k_2	k_3	b_1	b_2

* the upper triangular matrix for Scheme 1; the lower triangular matrix for Scheme 2

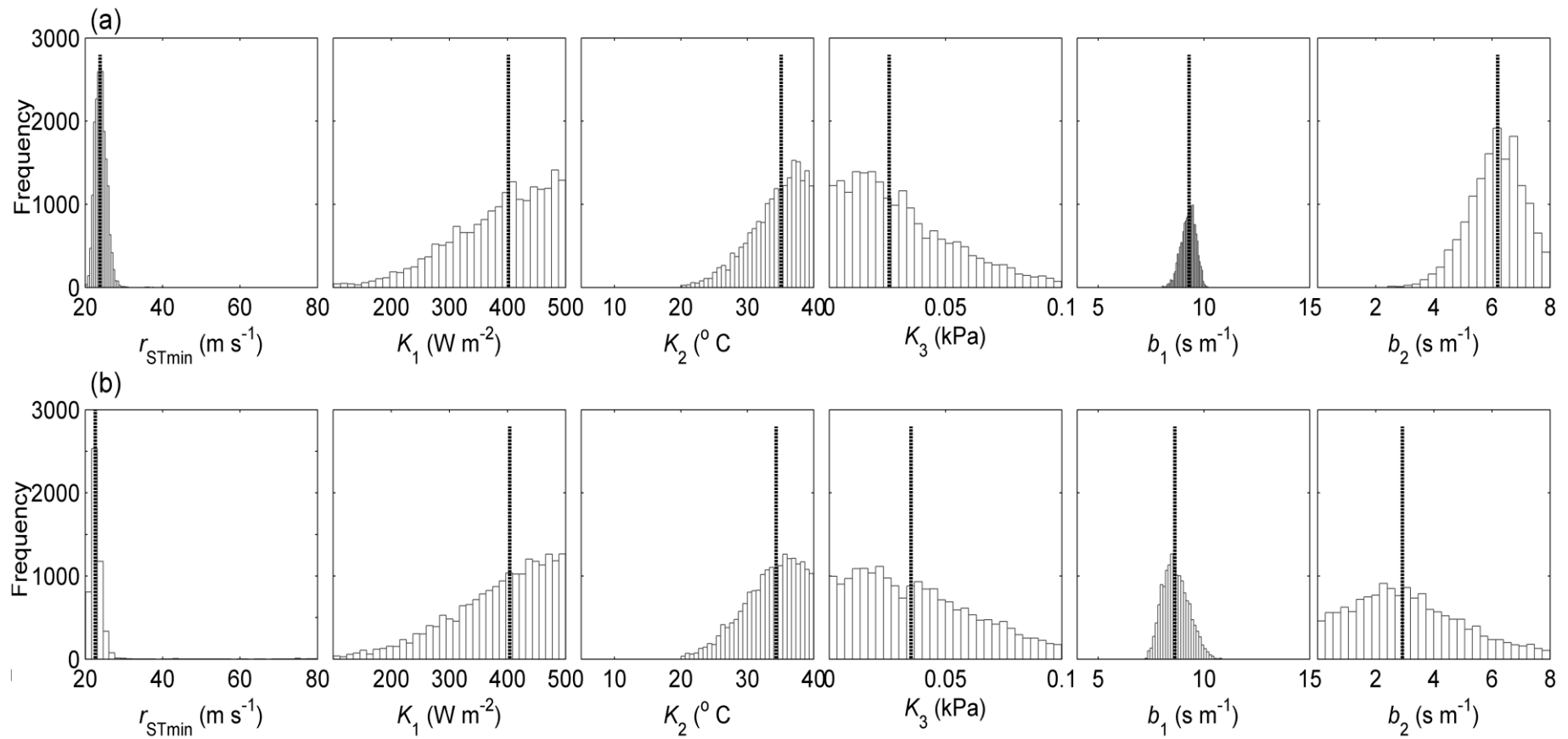


Fig. B6 Histograms of samples from the posterior distributions of the parameters. The dashed vertical lines indicate mean parameter values. (a)

Simultaneously assimilate all data sets, (b) EC-measured λET data only

4.2 Comparisons of model performance for different assimilation schemes

Having parameterized the S-W model by different assimilation schemes as described above, we ran the model to simulate the half-hourly λET (equation 1) and λE (equation 9) values ($W m^{-2}$). The daily estimations of evapotranspiration (ET ; $mm d^{-1}$) and soil evaporation (E ; $mm d^{-1}$) were obtained by summing up the half-hourly simulated values. The statistical analysis of observed versus estimated values of water vapor fluxes at different time-scales for different assimilation schemes were summarized in Table B2. Overall, the simulations (half-hourly λET and daily soil evaporation) of the S-W model optimized by using all data sets simultaneously (Scheme 1) were comparable to the measurements (see Fig. 6 in the Manuscript). For example, the slope of regressive equation between the measured and modeled half-hourly λET values for Scheme 1 was 0.84, with MBE of $24.2 W m^{-2}$, IA of 0.93 and EF of 0.74. A relatively good agreement between measured and estimated daily soil evaporation (E) was also obtained. The slope of regression equation was 1.01, with MBE of $-0.01 mm day^{-1}$, IA of 0.94 and EF of 0.76. When only EC-measured data were used (Scheme 2), the performances of the S-W model optimized by Scheme 2 on simulations of half-hourly λET were not significantly different from that optimized by Scheme 1 (Fig. B7). The regression equation between the measured λET and the estimated λET from the S-W model optimized by Scheme 2 was 0.83, with MBE of $30.5 W m^{-2}$, IA of 0.67 and EF of 0.13. However, the S-W model optimized by Scheme 2 significantly underestimated the soil evaporation (E). The slope of regression equation between the measured and the estimated E was 0.59, with MBE of $0.11 mm day^{-1}$, IA of 0.67 and EF of 0.13. Thus, we can not ensure the S-W model properly partition the total ET into its different components using only the half-hourly λET data, even though the simulated values were in good agreement with measurements.

The fluctuation of measured and estimated daily ET and E by the two different assimilation schemes was illustrated in Fig. B8. For both assimilation schemes, the simulated daily ET generally fluctuated tightly with the measured values with relative narrow uncertainties (97% posterior prediction intervals). Also, we can observed that the 97% posterior prediction interval of soil evaporation for Scheme 1 was narrower than that for Scheme 2 (Fig. B8). Thus, we thought that the soil resistance in the S-W model was properly parameterized for the spring maize by the method with the multiple data sets simultaneously assimilated.

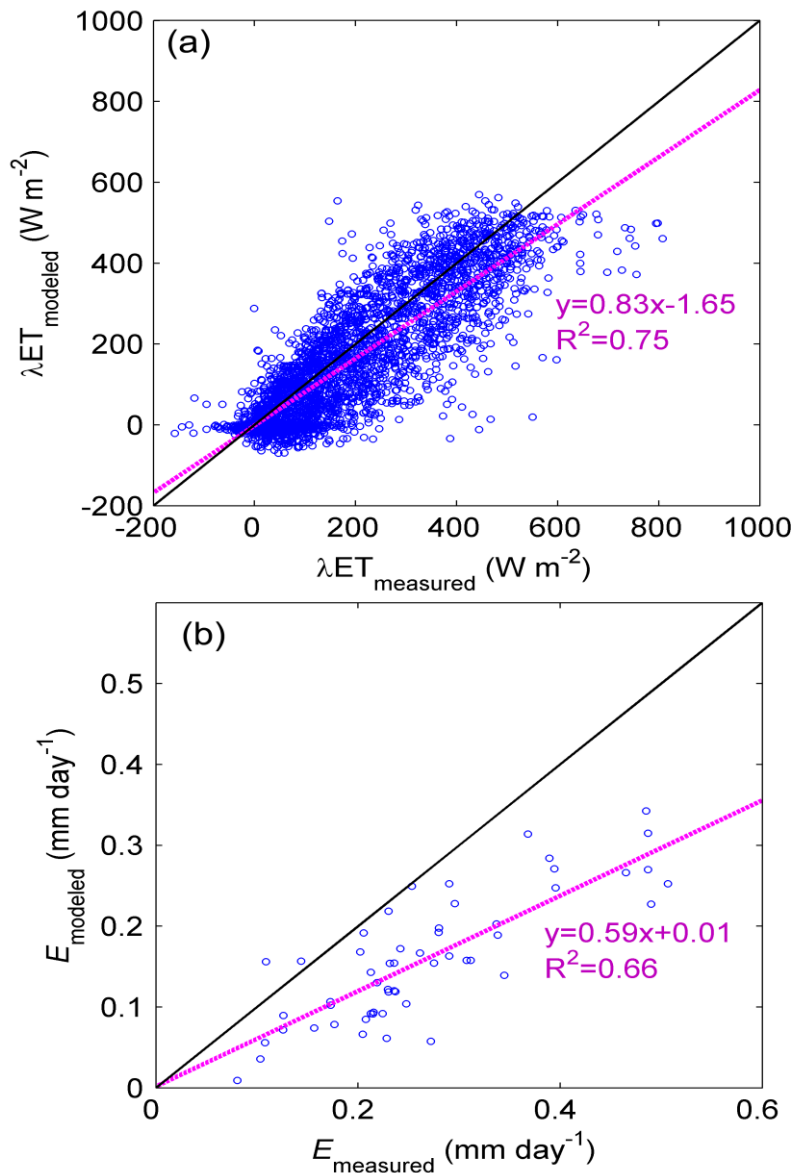


Fig. B7 Relationship between measured and estimated by Scheme 1 (a)

evapotranspiration (λET ; $W m^{-2}$), (b) daily soil evaporation (E ; $mm d^{-1}$).

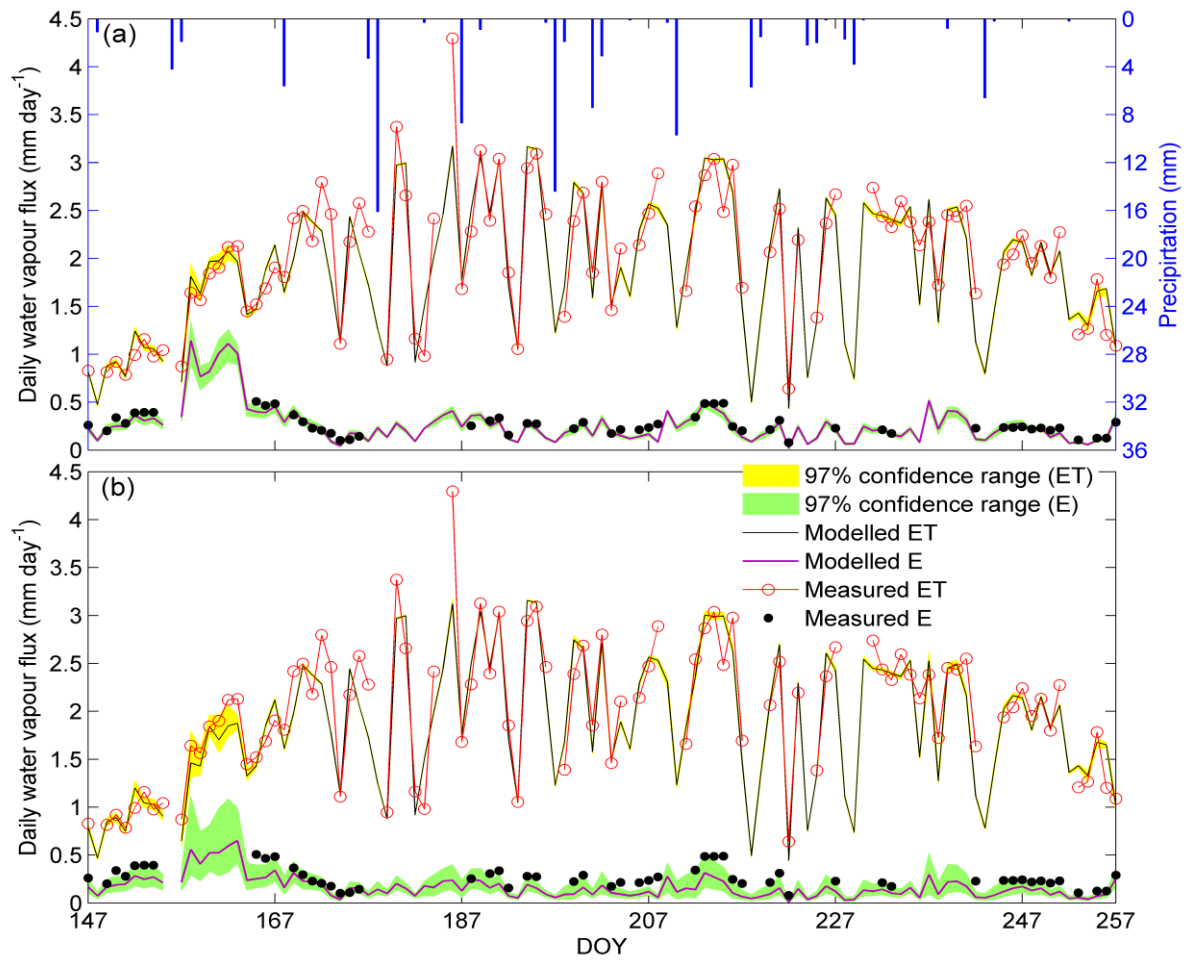


Fig. B8 Seasonal variation in daily evapotranspiration (ET; $mm d^{-1}$) and soil evaporation (E ; $mm day^{-1}$) measured by the EC system and modeled by the S-W model during the study period in Daman Oasis. Gap in the time series is caused either by the absence of flux measurements or missing ancillary data. (a) Simultaneously assimilate all data sets, (b) EC-measured λET data only.

Table B2 Statistical analysis of measured and estimated values of half-hourly evapotranspiration (λET ; $W m^{-2}$), daily soil evaporation (E ; $mm d^{-1}$), and daily evapotranspiration (ET ; $mm d^{-1}$) by different assimilation schemes for the spring maize in arid desert oasis during the study period.

	n	Regressive equation	R^2	Mean measured values	Mean simulated values	RMSE	MBE	IA	EF
Scheme 1									
λET ($W m^{-2}$)	3578	$\lambda ET_{modeled}=0.84\lambda ET_{measured}+0.18$	0.83	161.4	137.2	80.7	24.2	0.93	0.74
E ($mm d^{-1}$)	56	$E_{modeled}=1.01E_{measured} +0.01$	0.82	0.26	0.28	0.05	-0.01	0.94	0.76
ET ($mm d^{-1}$)	95	$ET_{modeled}=0.83ET_{measured} +0.19$	0.83	2.02	1.88	0.32	0.14	0.94	0.79
Scheme 2									
λET ($W m^{-2}$)	3578	$\lambda ET_{modeled}=0.83\lambda ET_{measured}-1.65$	0.75	161.4	142.4	89.1	30.5	0.90	0.70
E ($mm d^{-1}$)	56	$\lambda ET_{modeled}=0.59\lambda ET_{measured}+0.01$	0.66	0.26	0.16	0.12	0.11	0.67	0.13
ET ($mm d^{-1}$)	95	$\lambda ET_{modeled}=0.89\lambda ET_{measured}+0.15$	0.85	2.02	1.94	0.12	0.07	0.99	0.97

n =the sample number; R^2 =the determination coefficient; RMSE=root mean square error; MBE=mean bias error between measured and modeled values; IA= index of agreement; ET= model efficiency. These statistical parameters are calculated using formulas given by Legates and McCabe (1999) and Poblete-Echeverria and Ortega-Farias (2009).



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Appendix C

C.1 Convergence of MCMC

$$B_i = \frac{N}{K-1} \sum_{k=1}^K (\bar{c}_i^{..k} - \bar{c}_i^{..})$$

$$W_i = \frac{1}{N(K-1)} \sum_{k=1}^K \sum_{n=1}^N (c_i^{n,k} - \bar{c}_i^{..k})^2$$

$$GR_i = \sqrt{\frac{W_i(N-1)/N + B_i/N}{W_i}}$$

where K is the number M-H parallel chains; N is the running length of M-H algorithm; c_i is the i th component of the parameter vector c ; B_i and W_i denotes the between and within-run variances; and GR_i is the Gelman-Rubin (G-R) diagnostic of convergence of MCMC (Gelman and Rubin, 1992).

The evolution of GR diagnostic of convergence of MCMC was shown in Fig. C1. We can see that the GR values for all parameters tended to be less than 1.1 after 5000 iteration.

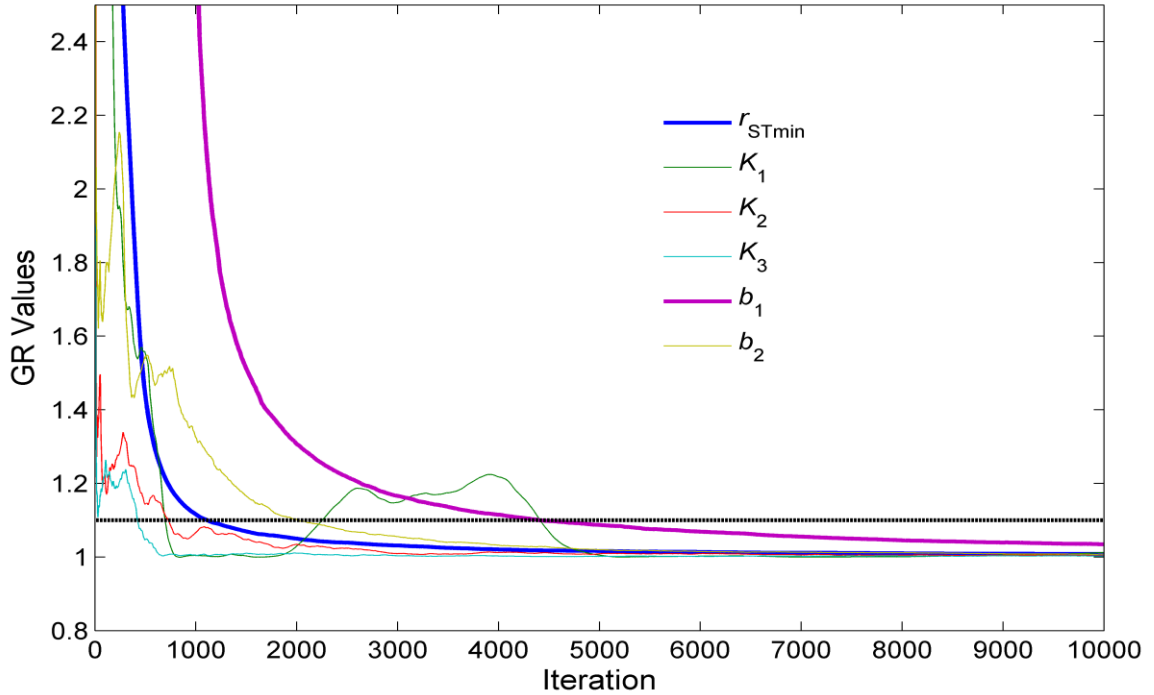


Fig. C1 The evolution of GR diagnostic of convergence of MCMC. Four parallel chains with different initial values were used to calculate GR values.

B.2 Matlab Code

```
clc
clear
load Chain
% Chain is the matrix than contain N running length, K parallel chains
% it is a N*K matrix for parameter ci

[N,K]=size(Chain);
for k=1:K
    ss=0;
    for n=1:N
        ss=ss+Chain(n,k);
        cwb(n,k)=ss/n;           %calculate c.,k
    end
end

for n=1:N
    st=0;
    for k=1:K
        st=st+cwb(n,k);
    end
    cst(n)=st/K;               % calculate c.,.
end

for n=1:N
    sb=0;
    for k=1:K
        sb=sb+(cwb(n,k)-cst(n))^2;
    end
    B(n)=n*sb/(K-1);          % calculated B
end

for k=1:K
    sw=0;
    for n=1:N
        sw=sw+(Chain(n,k)-cwb(n,k))^2;
        swc(n,k)=sw/(n-1);
    end
end

for n=1:N
    s1=0;
    for k=1:K
        s1=s1+swc(n,k);
    end
end
```

```
end
W(n,1)=s1/K; % calculated W
end

for n=1:N
GR(n,1)=sqrt((W(n)*(n-1)/n+B(n)/n)/W(n));
end
```