1 Dear Editor Hannah Cloke,

2 Thanks for your and all reviewers' recommendations. We improved the
3 manuscript following the suggestions. The main changes are:

- The introduction has been revised to improve the review of soil moisture and
 surface temperature assimilation, the background of this study, etc.
- 6 2. The order of figures has been changed, the Fig. 6, Fig. 7 and Fig. 8 have been7 combined and Table 3 has been deleted.
- 8 3. The discussion on bias estimation, observation error, definition of the state vector,
 9 COSMIC model and COSMOS has been extended,
- 10

11 Editor comments:

Thank you for your author responses. As you are aware, the reviewers have raised a number of concerns. I invite you to submit a revised manuscript which incorporates your suggested comments to address these reviewer concerns. Please take special care with the clarity of your manuscript so it is always entirely clear what you are undertaking. Where necessary this could involve a further sentence or two explaining background work/references of importance.

18 Response: the corresponding changes have been made following the reviewer19 comments.

20

21 **Reviewer 1:**

General comment: The major contribution of this work is to improve CLM 22 performances by assimilating cosmic-ray data and LST data over irrigated site with 23 24 Local Ensemble Transform Kalman Filter method. Basically, the idea is good. It is impressive to update soil moisture and temperature by jointly assimilation of 25 cosmic-ray data and LST. Moreover, the turbulent heat fluxes are improved 26 significantly. However, the manuscript is lacking in detail in a few areas and I'd not 27 recommend the paper for publication unless substantial improvements are made to 28 29 address the following concerns.

30 Response: thanks for the recommendation. We handled your comments, see below.

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32 Major comments:

1. The introduction section needs to be carefully revised. The aim of this paper is to 33 correct biases in CLM forcing, and improve model performances (e.g. soil 34 moisture profile, ET) by assimilating cosmic-ray data and LST. However, the 35 authors pay less attention on soil moisture and LST assimilation; only two 36 sentences focus on soil moisture and temperature assimilation progresses were 37 38 stated in the introduction part. The progresses should be enhanced in this part. Moreover, on page 9031, "In CLM, the surface fluxes are calculated based on the 39 Monin-Obukhov similarity theory. The sensible heat flux is formulated as a 40 function of temperature and leaf area index, and the latent heat flux is formulated 41 as a function of the temperature and leaf stomatal resistances. The leaf stomatal 42 resistance is calculated from the Ball-Berry conductance model (Collatz et al., 43 1991). The surface fluxes are therefore sensitive to the surface and soil 44 temperature." this sentence looks wired, why surface fluxes are sensitive to soil 45 temperature, the previous sentences cannot lead to this conclusion. Then why 46 calibrate LAI? It is stated abrupt. Any other persons focus on LAI calibration to 47 improve ET? I recommend authors rewrite the introduction part to describe more 48 49 logically.

Response: We improved the introduction in the revision for the soil moisture and LST assimilation. (line 116-134)

"The positive impact of soil moisture data assimilation was shown in several 52 studies. Importantly, surface soil moisture could be used to obtain better 53 54 characterization of the root zone soil moisture (Barrett and Renzullo, 2009; Crow et al., 2008; Das et al., 2008; Draper et al., 2011; Li et al., 2010). It was also 55 shown that the assimilation of soil moisture observations can be used to correct 56 rainfall errors (Crow et al., 2011; Yang et al., 2009). Often a systematic bias 57 58 between measured and modelled soil moisture content can be found; soil moisture estimation can be significantly improved using joint state and bias estimation (De 59 Lannoy et al., 2007; Kumar et al., 2012; Reichle et al., 2008). Also studies on data 60

61 assimilation of remotely sensed land surface temperature products show a positive impact on the estimation of soil moisture, latent heat flux and sensible heat flux 62 63 (Ghent et al., 2010; Xu et al., 2011). Also in these studies it was found that bias, in these cases soil temperature bias, of land surface models can be removed with 64 land surface temperature assimilation (Bosilovich et al., 2007; Reichle et al., 65 2010). Other studies updated both land surface model states and parameters with 66 67 soil moisture and land surface temperature data (Bateni and Entekhabi, 2012; Han et al., 2014a; Montzka et al., 2013; Pauwels et al., 2009). The assimilation of 68 measured cosmic-ray neutron counts in a land surface model was successfully 69 70 tested, but these studies focused on state updating alone (Rosolem et al., 2014; Shuttleworth et al., 2013)." 71

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73 The update of soil temperature is defined as:

- $\Delta T_{soil} = f(h) / -\lambda$
- 75 where λ is the thermal conductivity.

The heat flux h into the soil surface from the overlying atmosphere is defined as:

 $h = \vec{S}_{soil} + \vec{L}_{soil} - H_{soil} - \lambda E_{soil}$

79 \vec{S}_{soil} is the solar radiation absorbed by top soil, \vec{L}_{soil} is the longwave 80 radiation absorbed by soil, H_{soil} is the sensible heat flux from soil, λE_{soil} is the 81 latent heat flux from soil.

82 The update of vegetation temperature is defined as:

83
$$\Delta T_{v} = \frac{\vec{S}_{v} - \vec{L}_{v} - H_{v} - \lambda_{vap}E_{v}}{\frac{\partial \vec{L}_{v}}{\partial T_{v}} + \frac{\partial \overline{H}_{v}}{\partial T_{v}} + \frac{\partial \overline{\lambda}E_{v}}{\partial T_{v}}}$$

84 \vec{S}_{v} is the solar radiation absorbed by the vegetation, \vec{L}_{v} is the net longwave 85 radiation absorbed by vegetation, H_{v} and $\lambda_{vap}E_{v}$ are the sensible and latent 86 heat fluxes from vegetation.

87

The above equations show the sensitivity of vegetation temperature to the

surface heat fluxes. Measured land surface temperature is composed of the land 88 surface temperature and vegetation temperature. Therefore, a mismatch of land 89 90 surface temperature is statistically linked to a mismatch of land surface fluxes. On the other hand, land surface fluxes are also sensitive to soil moisture content. 91 Therefore, land surface temperature shows a statistical correlation with soil 92 93 moisture content and allows to update soil moisture content. In various papers, land surface temperature assimilation served to improve the estimation of surface 94 95 fluxes (Ghent et al., 2010; Meng et al., 2009; Reichle et al., 2010; Xu et al., 2011). The relation between the soil temperature / vegetation temperature and surface 96 fluxes has been explained in the revision. (line 162-174) 97

"In CLM, land surface fluxes are calculated based on the Monin-Obukhov 98 similarity theory. The sensible heat flux is formulated as a function of 99 100 temperature and LAI, and the latent heat flux is formulated as a function of the temperature and leaf stomatal resistances. The leaf stomatal resistance is 101 calculated from the Ball-Berry conductance model (Collatz et al., 1991). The 102 103 updates of soil temperature and vegetation temperature are derived based on the solar radiation absorbed by top soil (or vegetation), longwave radiation absorbed 104 by soil (or vegetation), sensible heat flux from soil (or vegetation) and latent heat 105 106 flux from soil (or vegetation). Measured land surface temperature is composed of the ground temperature and vegetation temperature. Therefore a difference 107 between measured and calculated land surface temperature can be adjusted by 108 109 changing land surface fluxes. As land surface fluxes are sensitive to soil moisture content, land surface temperature is sensitive to soil moisture content." 110

- Ghent, D., Kaduk, J., Remedios, J., Ardo, J., and Balzter, H.: Assimilation of
 land surface temperature into the land surface model JULES with an
 ensemble Kalman filter, J Geophys Res-Atmos, 115, 2010.
- 114 2) Meng, C. L., Li, Z. L., Zhan, X., Shi, J. C., and Liu, C. Y.: Land surface
 115 temperature data assimilation and its impact on evapotranspiration estimates
 116 from the Common Land Model, Water Resour Res, 45, 2009.
- 117 3) Reichle, R. H., Kumar, S. V., Mahanama, S. P. P., Koster, R. D., and Liu, Q.:

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Assimilation of Satellite-Derived Skin Temperature Observations into Land Surface Models, J Hydrometeorol, 11, 1103-1122, 2010.

4) Xu, T. R., Liu, S. M., Liang, S. L., and Qin, J.: Improving Predictions of
Water and Heat Fluxes by Assimilating MODIS Land Surface Temperature
Products into the Common Land Model, J Hydrometeorol, 12, 227-244,
2011.

Our study was also based on the conclusions of Schwinger, J., et al., 2010: 124 125 "results confirm that soil texture and LAI are key parameters that have a dominant influence on modeled LE under specific environmental conditions in 126 CLM4." More works have studied the sensitivity of land surface models to the 127 leaf area index (Ghilain et al., 2012; Jarlan et al., 2008; Schwinger et al., 2010; 128 van den Hurk et al., 2003; Yang et al., 1999). Moreover, we used the MODIS 129 130 LAI in CLM, whereas the MODIS products usually underestimate the LAI compared with field measurements, as was found in validation studies by the 131 NASA (http://landval.gsfc.nasa.gov): the underestimation by the MODIS LAI 132 product is 0.66 * LAI (MODIS) for all biomes and 0.5 * LAI (MODIS) except for 133

"Soil moisture, land surface temperature and LAI influence the estimation of 135 latent and sensible heat fluxes (e.g., Ghilain et al., 2012; Jarlan et al., 2008; 136 Schwinger et al., 2010; van den Hurk et al., 2003; Yang et al., 1999), and 137 therefore this study focuses in addition on the calibration of LAI with help of the 138 139 assimilation of land surface temperature. However, there are large discrepancies between the remotely retrieved LAI and measured values, and the MODIS LAI 140 product underestimates in situ measured LAI by 44% on average 141 (http://landval.gsfc.nasa.gov/), and therefore the LAI is also calibrated by data 142 assimilation." 143

broadleaf forests. We improved the introduction in the revision. (line 180-188)

Schwinger, J., et al. "Sensitivity of Latent Heat Fluxes to Initial Values and
 Parameters of a Land-Surface Model." <u>Vadose Zone Journal</u> 9(4): 984-1001,
 2010.

147 2) Ghilain, N., Arboleda, A., Sepulcre-Canto, G., Batelaan, O., Ardo, J., and

- Gellens-Meulenberghs, F.: Improving evapotranspiration in a land surface
 model using biophysical variables derived from MSG/SEVIRI satellite,
 Hydrology and Earth System Sciences, 16, 2567-2583, 2012.
- Jarlan, L., Balsamo, G., Lafont, S., Beljaars, A., Calvet, J. C., and Mougin, E.:
 Analysis of leaf area index in the ECMWF land surface model and impact on
 latent heat and carbon fluxes: Application to West Africa, J Geophys
 Res-Atmos, 113, 2008.
- 4) Schwinger, J., Kollet, S. J., Hoppe, C. M., and Elbern, H.: Sensitivity of
 Latent Heat Fluxes to Initial Values and Parameters of a Land-Surface Model,
 Vadose Zone J, 9, 984-1001, 2010.
- van den Hurk, B. J. J. M., Viterbo, P., and Los, S. O.: Impact of leaf area
 index seasonality on the annual land surface evaporation in a global
 circulation model, J Geophys Res-Atmos, 108, 2003.
- 161 6) Yang, Z. L., Dai, Y., Dickinson, R. E., and Shuttleworth, W. J.: Sensitivity of
 162 ground heat flux to vegetation cover fraction and leaf area index, J Geophys
 163 Res-Atmos, 104, 19505-19514, 1999.
- 164
- 165 2. In section 3, LAI was updated by assimilating LST and soil moisture, I'm not
 166 certain if it is correct to do this. Does LST and soil moisture are strong correlated
 167 to LAI? Please state their relationship clearly.
- 168 Response: the LST was used to update the LAI, not soil moisture or Cosmic-ray.
 169 This has been clarified in the revision (line 183-184). Details can be found in our
- response to question 1. The introduction in the revision has been improved.
- 171
- In this study, the soil moisture related instrument, the cosmic-ray, is a ground
 measurement instrument. It can be used to measure soil moisture at plot scale
 about 600 m. it is hard and expensive to be applied at the continent scales.
 However, MODIS LST can be easily obtained globally. Thus, the limitation of
 assimilating cosmic-ray data should be discussed.
- 177 Response: the Cosmic-ray Soil Moisture Observing System (COSMOS) has been

designed as a continental scale network by installing 500 COSMOS probes across
the USA (Zreda et al., 2012). Nevertheless, it is true that there are still some
disadvantages of COSMOS compared with remote sensing. COSMOS is also
expensive for extensive deployment to measure the continental/regional scale soil
moisture. This discussion has been added in the revision. (line 642-647)

"Although the Cosmic-ray Soil Moisture Observing System (COSMOS) has been
designed as a continental scale network by installing 500 COSMOS probes across
the USA (Zreda et al., 2012), there are still some disadvantages of COSMOS
compared with remote sensing. COSMOS is also expensive for extensive
deployment to measure the continental/regional scale soil moisture."

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E., and Rosolem, R.: COSMOS: the COsmic-ray Soil Moisture Observing System, Hydrology and Earth System Sciences, 16, 4079-4099, 2012.

1) Zreda, M., Shuttleworth, W. J., Zeng, X., Zweck, C., Desilets, D., Franz, T.

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192 Minor comments

 On page 9040, the augmentation method was used to update surface temperature, ground temperature, vegetation temperature and 10 layers of soil temperature by assimilating LST. However, surface temperature and vegetation temperature are diagnostic variables in CLM. To change them at the current time step may not influence model estimates in next time step. It is wasting time to add them as the updated variables. Remove them in the vectors.

199 Response: Thanks for the suggestion. CLM needs the initial state of the ground temperature, vegetation temperature and 15 layers of soil temperature. For 200 example, the calculation of vegetation temperature in CLM is: $T_n^{n+1} = T_n^n + \Delta T_n$. 201 Only the surface temperature is the diagnostic variable. Because we calculated 202 the surface temperature with help of an observation operator for assimilation 203 204 purpose only, it is the right state to be assimilated. In order to calculate the 205 Kalman gain, we need the surface temperature to compare with the MODIS LST. For reasons of technical simplicity, we calculated the surface temperature out of 206 Kalman filter and transferred the calculated surface temperature into Kalman 207

- filter through the state vector. It means the identity matrix was used as theobservation operator *H* in the Kalman filter.
- 210
- 211 2. In section 2.2, please state what meteorology parameters are used as the forcing212 data in CLM, and how long is the time step of CLM run?
- 213 Response: The incident longwave radiation, incident solar radiation, precipitation,
- air pressure, specific humidity, air temperature and wind speed were used in
- 215 CLM. The time step of CLM was hourly. (line 238-240)
- 216
- 3. The forcing data were perturbed by set of noises, what are the observation errorsof cosmic-ray data and MODIS LST? How to perturb them?
- Response: The observation data were not perturbed in LETKF because it is a
 square root Kalman filter. Only the classical ensemble Kalman filter (EnKF)
 needs to perturb the observations. The variance of Cosmic-ray was the measured
 neutron count value (Zreda, M., et al., 2012) and the variance of MODIS LST
 was assumed to be 1 K (Wan, Z. and Z. L. Li, 2008), and the error of MODIS
 LST has been verified (<u>http://landval.gsfc.nasa.gov</u>) by many studies. (line
 460-464)
- "The variance of the instantaneous measured neutron intensity is equal to the
 measured neutron count intensity (Zreda et al., 2012) and smaller for temporal
 averaging for daily or sub-daily applications. The instantaneous neutron intensity
 was assimilated in this study. The variance of MODIS LST was assumed to be 1
 K (Wan and Li, 2008)"
- 231
- Zreda, M., et al. (2012). "COSMOS: the COsmic-ray Soil Moisture
 Observing System." Hydrology and Earth System Sciences 16(11):
 4079-4099.
- 235 2) Wan, Z. and Z. L. Li (2008). "Radiance based validation of the V5 MODIS
 236 land surface temperature product." International Journal of Remote Sensing
 237 29(17-18): 5373-5395.

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239	4.	The captain of figure 4 can be change as "Same as figure 3 but for 50 cm and 80
240		cm"
241		Response: thanks, changed.
242		
243	5.	The figures 6, 7, and 8 can be combined into one figure, as they are all turbulent
244		heat fluxes.
245		Response: thanks, changed.
246		
247	6.	The ignorance of energy imbalance problem for eddy covariance system may
248		cause some error in producing ET observation. This should be discussed.
249		Response: the discussion has been added in the revision. (line 526-528)
250		"The true evapotranspiration is therefore likely larger, but not much larger as the
251		energy balance gap was limited (3.7%)."
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254 **Reviewer 2:**

255 General comments

The paper provides an important contribution to the research on data assimilation in 256 257 land surface modelling. The paper considers assimilation of cosmic-ray soil moisture data and land surface temperature in the Community Land Model (CLM). 258 Assimilation of the data sources individually and jointly as well as in combination 259 with estimation of leaf area index are evaluated with respect to soil moisture, 260 evapotranspiration, and latent and sensible heat flux. The paper is, in general, well 261 written and technically sound. However, some elaborations are needed; especially on 262 the Kalman filter setup and evaluation (see detailed comments below). 263

264 Response: Thanks for your recommendation. We have improved the manuscript265 according to the responses below.

266

267 Detailed comments

Page 9031, line 10-13. Not clear. Inclusion of bias in the Kalman filter is usually
 defined either as a bias in the system equation or a bias in the observation
 equation. The specific source of error need not be known.

Response: Before we estimate the bias, we should determine whether the bias 271 comes from the model, observation, or both. If the source of bias is not attributed 272 to the right source, model predictions cannot be improved. In the Kalman filter 273 equation, the model bias and the observation bias are handled differently: the 274 model bias is removed in the model forecast $x^b = x^b - bias_{model}$; the 275 observation bias is removed from the innovation part $K \times (y_{obs} - bias_{obs} - x^b)$. 276 In summary, the source of the bias should be defined before estimation. A 277 278 comprehensive overview of bias estimation is given by Dee (2005). According to the description, "By design, bias-aware assimilation requires assumptions about 279 280 the nature of the biases: first, the attribution of a bias to a particular source, and second, a characterization of the bias in terms of some well-defined set of 281 parameters". In this paper, no explicit model for observation bias or model bias 282 was assumed, and no explicit bias estimation was done for simplicity. 283 Nevertheless, the model states were corrected by the observations. We have 284 clarified this part in the revision. (line 154-160) 285

²⁸⁶ "The bias can be attributed to the model structure, model parameters, atmospheric ²⁸⁷ forcing or observation data, and the bias-aware assimilation requires the ²⁸⁸ assumption that the bias comes from a particular source. If the source of bias is ²⁸⁹ not attributed to the right source, model predictions cannot be improved (Dee, ²⁹⁰ 2005). Therefore bias-blind assimilation in which the bias estimation was not ²⁹¹ handled explicitly was used for safety. Instead, it was investigated whether ²⁹² neutron counts measured by cosmic-ray probe were able to correct for the bias."

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 Dee, D. P. (2005). "Bias and data assimilation." Quarterly Journal of the Royal Meteorological Society 131(613): 3323-3343.

296

297 2. Page 9031, line 13. Not clear what is meant by 'bias blind assimilation' and why

this is applied for 'safety'.

Response: The bias blind assimilation is the traditional data assimilation without 299 bias estimation. Dee et al. (2005) wrote: "If the source of a known bias is 300 uncertain, bias-blind assimilation may be the safest option. The main scientific 301 challenge is to correctly attribute a detected bias to its source, and then to develop 302 a useful model for the bias. When different sources produce similar biases, the 303 assimilation may correct the wrong source." Because the study area is a very 304 305 heterogeneous irrigated farmland, both the observation and model could be biased. In CLM, the main bias came from the atmospheric forcing input due to the lack of 306 307 irrigated water amount, but the bias could also came from wrong soil properties (e.g. sand fraction, clay fraction and organic matter density) and other vegetation 308 parameters (e.g. leaf area index, Vcmax). For example, three papers studied the 309 310 sensitivity of the latent heat flux and sensible heat flux to the hydraulic parameters (Hou, et al., 2012) and vegetation parameters Vcmax (Bonan, et al., 2011) in 311 CLM4, and soil moisture and leaf area index (Schwinger, et al., 2010) in CLM4. 312 In each of these studies, the assumption was made that the other sensitive 313 parameters were defined properly. In this study, we focused on the model bias 314 introduced by the forcing data and the leaf area index, and neglected the other 315 sources of bias. We have clarified the discussion in the revision. (see response to 316 earlier reviewer question) 317

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Hou, Z. S., et al. (2012). "Sensitivity of surface flux simulations to hydrologic
 parameters based on an uncertainty quantification framework applied to the
 Community Land Model." Journal of Geophysical Research-Atmospheres
 117.

323 2) Bonan, G. B., et al. (2011). "Improving canopy processes in the Community
324 Land Model version 4 (CLM4) using global flux fields empirically inferred
325 from FLUXNET data." Journal of Geophysical Research-Biogeosciences 116.
326 3) Schwinger, J., et al. (2010). "Sensitivity of Latent Heat Fluxes to Initial
327 Values and Parameters of a Land-Surface Model." Vadose Zone Journal 9(4):

984-1001.

329

330 3. Page 9031, line 17. Define 'CLM'.

Response: CLM is Community Land Model, was included in the revision.

332

4. Page 9036, line 8-10. Are the measured data at the station in Switzerlandrepresentative for the Chinese case study?

Response: The data are used to remove temporal (secular or diurnal) variations caused by the sunspot cycle. We follow the standard approach applied by the COSMOS network globally, discussed in detail by Zreda et al. (2012). This reference is appropriately mentioned in the revision. (line 302-303)

339 "The temporal (secular or diurnal) variations caused by the sunspot cycle could be
340 removed after this correction (Zreda et al., 2012)."

341

Zreda, M., et al. (2012). "COSMOS: the COsmic-ray Soil Moisture
 Observing System." Hydrology and Earth System Sciences 16(11):
 4079-4099.

345

5. Page 9036, line 24-26. Soil moisture from 10 soil layers (does this correspond to
the top 10 cm of the soil?) in CLM is used as input to COSMIC. The effective
measurement depth of the cosmic-ray probe depends on soil moisture, so why is a
fixed depth used here? I expect this will introduce a bias in the simulated soil
moisture for comparison with the measurements.

Response: The thickness of top 10 soil layers in CLM is about 3.8 m. Because the effective measurement depth of cosmic-ray probe is between 12 and 76 cm, it is unlikely that anything beyond 1 m deep will substantially impact the results. The COSMIC model assumes a more detailed soil profile. In COSMIC, the soil moisture information from the 10 layers from CLM was interpolated to information for 300 layers based on the soil layer depth for stable numerical solution. The contribution of each soil layer to the measured neutron flux changes

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temporally depending on the soil moisture condition. Therefore the effective
measurement depth of the cosmic ray probe also changes temporally. The
explanation in the manuscript was improved. (line 317-328)

"The simulated soil moisture content for 10 CLM soil layers (3.8 m depth) was 361 used as input to COSMIC in order to simulate the corresponding neutron count 362 363 intensity and compare it with the measured neutron count intensity. It should be mentioned that it is unlikely that anything beyond 1 m deep will substantially 364 365 impact the results because the effective measurement depth of the cosmic-ray probe is between 12 and 76 cm. The COSMIC model assumes a more detailed soil 366 profile. COSMIC interpolates the soil moisture information from the ten CLM soil 367 layers to information for 300 soil layers of depth 1cm. The contribution of each 368 soil layer to the measured neutron flux will change temporally depending on the 369 370 soil moisture condition. Therefore the effective measurement depth of the cosmic ray probe will also change temporally. COSMIC calculates the vertically weighted 371 soil moisture content based on the vertical distribution of soil moisture content." 372

373

Bage 9039, line 1. Definition of state vector not clear. Why soil moisture from 10
layers (see previous comment) and soil temperature for 15 layers?

Response: These are the standard CLM layout for soil moisture and soil temperature. The hydrology calculations are done over the top 10 layers, and the bottom 5 layers are specified as bedrock. The lower 5 layers are hydrologically inactive layers. Temperature calculations are done over all layers. The manuscript has been revised to include this explanation. (line 422-426)

381 "The 10 layers of soil moisture and 15 layers of soil temperature are the standard
382 CLM layout for both soil moisture and soil temperature. The hydrology
383 calculations are done over the top 10 layers, and the bottom 5 layers are specified
384 as bedrock. The lower 5 layers are hydrologically inactive layers. Temperature
385 calculations are done over all layers (Oleson et al., 2013)"

386

387 7. Page 9040, line 17-20. How is the leaf area index represented in the augmented

388 system equation? As a persistence model?

Response: the leaf area index was treated as a parameter and updated with help of 389 390 the augmented state vector approach, but only changed after each update. For the 391 calibration of the LAI, the state vector was augmented with surface temperature, ground temperature, vegetation temperature, soil temperature for 15 layers and 392 393 LAI if only the land surface temperature observations were assimilated without soil moisture update. This resulted then in a state dimension of 19. (line 380-384) 394 395 "For the calibration of the LAI, the state vector was augmented with surface temperature, ground temperature, vegetation temperature, soil temperature for 15 396 CLM-layers and LAI if only the land surface temperature observations were 397 398 assimilated without soil moisture update. This resulted then in a state dimension of 19." 399

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401 8. Page 9041, line 1-15. The Kalman filter settings are not sufficiently discussed. They seem rather arbitrarily chosen. It is not clear how the standard deviations, 402 403 spatial and temporal correlations, and cross correlations given in Table 1 are determined. Has sensitivity analysis been applied to analyse the sensitivity of 404 ensemble size and model error statistics on the assimilation results? You can 405 406 analyse the prediction uncertainty provided by the Kalman filter to evaluate the Kalman filter settings by comparing measurements with predicted confidence 407 bands or analyse the statistical properties of the model innovations. Definition of 408 409 measurement uncertainty is not described.

Response: the values of standard deviations and temporal correlations in Table I 410 411 were chosen based on commonly used values in previous catchment scale and regional scale data assimilation studies (Kumar et al., 2009; Reichle et al., 2010; 412 De Lannoy et al., 2012). In the 3D-EnKF, the imposed spatial correlation on 413 414 forcing data is very important for the assimilation (Reichle and Koster, 2003; De 415 Lannoy et al., 2009). In 1D-EnKF and LETKF (which we used), no horizontal correlation among model grid cells is calculated, so the imposed spatial 416 correlation of forcing data will not influence the assimilation. The impacts of 417

horizontal spatial correlation on the assimilation can be included through the
localization technique (Reichle and Koster, 2003; De Lannoy, et al., 2009). The
selection of the ensemble size was based on the results of Han et al., 2014, who
reported that for more than 30~40 ensemble members, the assimilation results
could not be improved too much. Therefore 50 ensemble members were used in
this study. (line 443-446)

424 "The values of standard deviations and temporal correlations in Table 1 were
425 chosen based on previous catchment scale and regional scale data assimilation
426 studies (De Lannoy et al., 2012; Kumar et al., 2012; Reichle et al., 2010)."

The observation standard deviation of cosmic-ray probes is equal to the square root of the measured neutron counts (Zreda, et al., 2012) and the observation standard deviation of MODIS land surface temperature was here equal to 1 K (Wan and Li, 2008). We added this information in the revised version of the manuscript. (line 460-464)

432 "The variance of the instantaneous measured neutron intensity is equal to the
433 measured neutron count intensity (Zreda et al., 2012) and smaller for temporal
434 averaging for daily or sub-daily applications. The instantaneous neutron intensity
435 was assimilated in this study. The variance of MODIS LST was assumed to be 1
436 K (Wan and Li, 2008)"

437

- 438 1) Kumar, S. V., et al. (2009). "Role of Subsurface Physics in the Assimilation
 439 of Surface Soil Moisture Observations." Journal of Hydrometeorology 10(6):
 440 1534-1547.
- 2) Reichle, R. H., et al. (2010). "Assimilation of Satellite-Derived Skin
 Temperature Observations into Land Surface Models." Journal of
 Hydrometeorology 11(5): 1103-1122.
- 444 3) De Lannoy, G. J. M., et al. (2012). "Multiscale assimilation of Advanced
 445 Microwave Scanning Radiometer-EOS snow water equivalent and Moderate
 446 Resolution Imaging Spectroradiometer snow cover fraction observations in
 447 northern Colorado." Water Resources Research 48.

- 448 4) Reichle, R. H. and R. D. Koster (2003). "Assessing the impact of horizontal
 449 error correlations in background fields on soil moisture estimation." Journal
 450 of Hydrometeorology 4(6): 1229-1242.
- 451 5) De Lannoy, G. J. M., et al. (2009). "Satellite-Scale Snow Water Equivalent
 452 Assimilation into a High-Resolution Land Surface Model." Journal of
 453 Hydrometeorology 11(2): 352-369.
- 454 6) Han, X., et al. (2014). "Soil moisture and soil properties estimation in the
 455 Community Land Model with synthetic brightness temperature observations."
 456 Water Resources Research 50(7): 6081-6105.
- 457 7) Wan, Z. and Z. L. Li (2008). "Radiance based validation of the V5 MODIS
 458 land surface temperature product." International Journal of Remote Sensing
 459 29(17-18): 5373-5395.
- 460 8) Zreda, M., et al. (2012). "COSMOS: the COsmic-ray Soil Moisture
 461 Observing System." Hydrology and Earth System Sciences 16(11):
 462 4079-4099.
- 463
- 464 9. Page 9043, line 4. How is measured soil moisture estimated?
- Response: the soil moisture for the CRS footprint scale was calculated from the
 arithmetic mean of the 23 SoilNet soil moisture observations. This information
 has been included in the manuscript. (line 304-305)
- 468 "In this study, the soil moisture for the CRS footprint scale was calculated from469 the arithmetic mean of the 23 SoilNet soil moisture observations."
- 470
- 471 10. Page 9045, line 4. Same information shown in Figs. 6-8 and Table 3. All results472 can be included in the table and figures omitted.
- 473 Response: thanks for the suggestion. Table 3 was removed in the revision.
- 474

11. Page 9045, line 3-25. It is stated that the results for latent and sensible heat flux
correspond to the results obtained for soil moisture. However, there are some
notable differences that should be elaborated. The effect of inclusion of parameter

estimation of LAI on latent and sensible heat flux depends on the type of data
being assimilated. For LST assimilation an increase in RMSE is obtained when
LAI estimation is included. With assimilation of both LST and CRS lower RMSE
is obtained with LAI estimation. In addition, assimilation of LST provides better
results than assimilation of both LST and CRS.

- Response: thanks, in the scenario of only LST assimilation without LAI update,
 the latent heat flux could not be improved. The univariate assimilation of LST did
 not give any improvement for this case. The joint soil moisture and LAI update
 scenario of LST_Feedback_Par_LAI was worse than the single soil moisture
 update scenario of LST_Feedback in this case. This part has been improved in the
 discussion section of the revision. (line 509-514)
- Without assimilation of cosmic-ray probe neutron counts, the soil moisture simulation cannot be improved (scenario Only_LST). However, the scenarios of LST_Feedback and LST_Feedback_Par_LAI improve the soil moisture profile characterization, which shows that explicitly using LST to update soil moisture content in the data assimilation routine gives better results than using LST only to update soil moisture by the model equations."
- "The scenario where soil moisture and LAI jointly updated 495 are 496 (LST_Feedback_Par_LAI) gave worse results than the scenario of LST_Feedback." 497
- 498
- 12. Figure 5. Explain numbers in lower-right corner in figure caption.
- Response: these are the accumulated ET amounts during the study period; this has
 been corrected in this revision. (line 523-524)
- 502

503

504	Correction of Systematic Model Forcing Bias of CLM using
505	Assimilation of Cosmic-Ray Neutrons and Land Surface
506	Temperature: a study in the Heihe Catchment, China
507	
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546 Abstract

The recent development of the non-invasive cosmic-ray soil moisture sensing 547 548 technique fills the gap between point scale soil moisture measurements and regional scale soil moisture measurements by remote sensing. A cosmic-ray probe measures 549 soil moisture for a footprint with a diameter of ~600 m (at sea level) and with an 550 effective measurement depth between 12 cm to 76 cm, depending on the soil humidity. 551 In this study, it was tested whether neutron counts also allow to correct for a 552 systematic error in the model forcings. Lack of water management data often cause 553 554 systematic input errors to land surface models. Here, the assimilation procedure was tested for an irrigated corn field (Heihe Watershed Allied Telemetry Experimental 555 Research - HiWATER, 2012) where no irrigation data were available as model input 556 557 although for the area a significant amount of water was irrigated. In the study, the <u>Mm</u>easured cosmic-ray neutron counts and Moderate Resolution Imaging 558 Spectroradiometer (MODIS) land surface temperature (LST) products were jointly 559 assimilated into the Community Land Model (CLM) with the Local Ensemble 560 Transform Kalman Filter. Different data assimilation scenarios were evaluated, with 561 assimilation of LST and/or cosmic-ray neutron counts, and possibly parameter 562 estimation of leaf area index (LAI). The results show that the direct assimilation of 563 cosmic-ray neutron counts can improve the soil moisture and evapotranspiration (ET) 564 estimation significantly, correcting for lack of information on irrigation amounts. The 565 566 joint assimilation of neutron counts and LST could improve further the ET estimation, but the information content of neutron counts exceeded the one of LST. Additional 567

improvement was achieved by calibrating LAI, which after calibration was also closer to independent field measurements. It was concluded that assimilation of neutron counts was useful for ET and soil moisture estimation even if the model has a systematic bias like neglecting irrigation. However, also the assimilation of LST helped to correct the systematic model bias introduced by neglecting irrigation and LST could be used to update soil moisture with state augmentation.

574 Keywords: Cosmic-ray neutron counts, Land surface temperature, Evapotranspiration,

575 Land data assimilation, Parameter estimation

576 **1. Introduction**

Soil moisture plays a key role for crop and plant growth, water resources 577 578 management and land surface-atmosphere interaction. Therefore accurate soil moisture retrieval is important. Point scale measurements can be obtained by methods 579 like time domain reflectometry (TDR) (Robinson et al., 2003) and larger scale, coarse 580 soil moisture information from remote sensing sensors (Entekhabi et al., 2010; Kerr et 581 al., 2010). Wireless Sensor Networks (WSN) allow characterization of soil moisture at 582 the catchment scale with many local connected sensors at separated locations (Bogena 583 584 et al., 2010). TDR only measures the point scale soil moisture and the maintenance of WSN is expensive. Recently, neutron count intensity measured by above-ground 585 cosmic-ray probes was proposed as alternative information source on soil moisture. 586 587 Neutron count intensity is measured non-invasively at an intermediate scale between the point scale and the coarse remote sensing scale (Zreda et al., 2008). A network of 588 cosmic-ray sensors (CRS) has been set-up over N-America (Zreda et al., 2012). 589

Cosmic rays are composed of primary protons mainly. The fast neutrons 590 generated by high-energy neutrons colliding with nuclei lead to "evaporation" of fast 591 neutrons and the generated and moderated neutrons in the ground can diffuse back 592 into the air where their intensity can be measured by the cosmic-ray soil moisture 593 probe. Soil moisture affects the rate of moderation of fast neutrons, and controls the 594 neutron concentration and the emission of neutrons into the air. Dry soils have low 595 moderating power and are highly emissive; wet soils have high moderating power and 596 are less emissive. The neutrons are mainly moderated by the hydrogen atoms 597

contained in the soil water and emitted to the atmosphere where the neutrons mix 598 instantaneously at a scale of hundreds of meters. The measurement area of a 599 600 cosmic-ray soil moisture probe represents a circle with a diameter of ~600 m at sea level (Desilets and Zreda, 2013) and the measurement depth decreases non-linearly 601 from ~76 cm (dry soils) to ~12 cm (saturated soils) (Zreda et al., 2008). The measured 602 cosmic-ray neutron counts show an inverse correlation with soil moisture content. The 603 cosmic-ray neutron intensity could be reduced to 60% of surface cosmic-ray neutron 604 intensity if the soil moisture was increased from zero to 40% (Zreda et al., 2008). The 605 606 soil moisture estimation on the basis of cosmic-ray probe based neutron counts over a horizontal footprint of hectometers received considerable attention in scientific 607 literature during the last years (Desilets et al., 2010; Zreda et al., 2008; Zreda et al., 608 609 2012).

Hydrogen atoms are present as water in the soil, lattice soil water, below ground 610 biomass, atmospheric water vapor, snow water, above ground biomass, intercepted 611 water by vegetation and water on the ground. These additional hydrogen sources 612 contribute to the measured neutron intensity. The role of these additional hydrogen 613 sources should be included in the analysis of the cosmic-ray measurements in order to 614 isolate the main contribution from soil moisture. Formulations for handling water 615 vapor (Rosolem et al., 2013), for lattice water and organic carbon (Franz et al., 2013) 616 and for a litter layer present on the soil surface (Bogena et al., 2013) have been 617 618 developed.

619

It was shown that the assimilation of soil moisture observations could be used to

620	correct the rainfall errors ; the soil moisture estimation can be significantly improved
621	using the joint state and bias estimation. The positive impact of soil moisture data
622	assimilation was shown in several studies. Importantly, surface soil moisture could be
623	used to obtain better characterization of the root zone soil moisture (Barrett and
624	Renzullo, 2009; Crow et al., 2008; (Barrett and Renzullo, 2009; Crow et al., 2008; Das
625	et al., 2008; Draper et al., 2011; Li et al., 2010)-Das et al., 2008; Draper et al., 2011;
626	Li et al., 2010). It was also shown that the assimilation of soil moisture observations
627	can be used to correct rainfall errors (Crow et al., 2011; Yang et al., 2009)(Crow et al.,
628	2011; Yang et al., 2009). Often a systematic bias between measured and modelled soil
629	moisture content can be found; soil moisture estimation can be significantly improved
630	using joint state and bias estimation (De Lannoy et al., 2007; Kumar et al., 2012;
631	Reichle, 2008)(De Lannoy et al., 2007; Kumar et al., 2012; Reichle et al., 2008). Also
632	studies on data assimilation of remotely sensed land surface temperature products
633	show a positive impact on the estimation of soil moisture, latent heat flux and sensible
634	heat flux (Ghent et al., 2010; Xu et al., 2011)(Ghent et al., 2010; Xu et al., 2011).
635	Also in these studies it was found that bias, in these cases soil temperature bias, of
636	land surface models can be removed with land surface temperature assimilation
637	(Bosilovich et al., 2007; Reichle et al., 2010)(Bosilovich et al., 2007; Reichle et al.,
638	2010). Other studies updated both land surface model states and parameters with soil
639	moisture and land surface temperature data (Bateni and Entekhabi, 2012; Han et al.,
640	2014a; Montzka et al., 2013; Pauwels et al., 2009)(Bateni and Entekhabi, 2012; Han
641	et al., 2014a; Montzka et al., 2013; Pauwels et al., 2009). The assimilation of

	642	measured cosmic-ray neutron counts in a land surface model was successfully tested,
	643	but these studies focused on state updating alone (Rosolem et al., 2014b; Shuttleworth
	644	et al., 2013)(Han et al., 2014b; Rosolem et al., 2014; Shuttleworth et al., 2013).; the
	645	surface soil moisture could be used to obtain better characterization of the root zone
	646	soil moisture . The studies of data soil moisture measurements are useful for
	647	improving the soil moisture profile estimation in land surface models or hydrologic
	648	models. Aassimilation of remotely sensed land surface temperature products also
	649	improves the estimation of evapotranspirationshow the positive impacts on land
	650	surface states estimation: the soil moisture, latent heat flux and sensible heat flux
	651	could be improved by assimilating the remote sensed land surface temperature ; the
	652	soil temperature bias of land surface model could be removed using the land surface
	653	temperature assimilation The joint state and parameter estimation in land surface
	654	model with soil moisture and land surface temperature also shows the success. The
	655	assimilation of measured cosmic ray neutron counts in a land surface model has been
	656	tested. In this paper we focus on the assimilation of measured cosmic-ray neutron
	657	counts for improving soil moisture content characterization at the field scale. The
	658	assimilation of measured cosmic-ray neutron counts in a land surface model has been
	659	tested-(Han et al., 2014b; Rosolem et al., 2014a; Shuttleworth et al., 2013)–This paper
I	660	focuses on the case that model input is biased. Land surface models still are affected
	661	by limited knowledge on water resources management and for regions in China (and
	662	elsewhere) typically no information on irrigation amounts is available as irrigation is
	663	mainly by the flooding system. We analyse whether measured neutron counts are able

to correct for such biases. This case is not only relevant for neglecting irrigation in 664 China, but also for other water resources management issues (e.g., groundwater 665 pumping) which are neglected in the simulations. Neglecting irrigation in land surface 666 models results in a large bias in the simulated soil moisture content because of a lack 667 of water input. The bias in soil moisture content also results in a too small latent heat 668 flux and too high sensible heat flux. We hypothesize that data assimilation also can 669 play an important role for removing such biases in data deficient areas. One possible 670 strategy in data assimilation studies for handling this type of bias, which is not 671 672 followed in this paper, is to calibrate the simulation model (e.g., land surface model) prior to data assimilation to remove biases (Kumar et al., 2012) and use the corrected 673 674 simulation model in the context of sequential data assimilation. A different strategy is 675 was followed in this paper and no a priori bias correction is-was carried out because this type of problem (neglecting water resources management) does not allow for such 676 an a priori bias correctiondoes not allow for such an a priori bias correction. The bias 677 678 can be contributed to the model structure, model parameter, atmospheric forcing or 679 observation data, and the bias-aware assimilation requires the assumption that the bias comes from a particular source. If the source of bias is not attributed to the right 680 source, model predictions cannot be improved Because tThe bias could can be 681 682 contributed to the model structure, model parameter, atmospheric forcing or observation data, and the bias-aware assimilation requires the assumption that the bias 683 684 comes from a particular source_(Dee, 2005). Therefore bias-blind assimilation in which the bias estimation was not handled explicitly was used for safety. Instead, it 685

was investigated whether neutron counts measured by cosmic-ray probe were able to
correct for the bias. So <u>Therefore</u> the bias blind assimilation was used for safety.
Instead, it is investigated whether neutron counts measured by cosmic ray probe are
able to correct for the bias. Aim is to improve the soil moisture profile estimation in a
crop land with seed corn as main crop type.

691 In CLM, the-land surface fluxes are calculated based on the Monin-Obukhov similarity theory. The sensible heat flux is formulated as a function of temperature and 692 leaf area indexLAI, and the latent heat flux is formulated as a function of the 693 694 temperature and leaf stomatal resistances. The leaf stomatal resistance is calculated from the Ball-Berry conductance model (Collatz et al., 1991). The updates of soil 695 temperature and vegetation temperature are derived based on the solar radiation 696 697 absorbed by top soil (or vegetation), longwave radiation absorbed by soil (or vegetation), sensible heat flux from soil (or vegetation) and latent heat flux from soil 698 (or vegetation). And the mMeasured land surface temperature is composed of the 699 700 ground temperature and vegetation temperature. Therefore a difference between measured and calculated land surface temperature can be adjusted by changing land 701 surface fluxes. As land surface fluxes are sensitive to soil moisture content, land 702 surface temperature is sensitive to soil moisture content. Therefore Tthe surface fluxes 703 704 are therefore sensitive to the surface and soilland surface temperature. Beside of the cosmic-ray neutron counts observation, Therefore, Tthe land 705

surface temperature (LST) products measured by the Moderate Resolution Imaging
 Spectroradiometer (MODIS) Terra (MOD11A1) and Aqua (MYD11A1) are also

708	assimilated jointly to improve the soil temperature profile estimation because the
709	evapotranspiration is sensitive to the soil temperature. Two Terra LST products can be
710	obtained per day at 10:30 am/pm and two Aqua LST products can be obtained per day
711	at 1:30 am/pm. Soil moisture, land surface temperature and LAI influence the
712	estimation of latent and sensible heat fluxes (Ghilain et al., 2012; Jarlan et al., 2008;
713	Schwinger et al., 2010; van den Hurk, 2003; Yang et al., 1999)-(e.g., Ghilain et al.,
714	2012; Jarlan et al., 2008; Schwinger et al., 2010; van den Hurk et al., 2003; Yang et
715	al., 1999), and therefore this study focuses in addition on the calibration of LAI with
716	help of the assimilation of land surface temperature. However, there are large
717	discrepancies between the remotely retrieved LAI and measured values, and the
718	MODIS LAI product underestimates in situ measured LAI by 44% on average
719	(http://landval.gsfc.nasa.gov/), and therefore the LAI is also calibrated by data
720	assimilation.Soil moisture, land surface temperature and leaf area indexLAI
721	contribute to the estimation of latent and sensible heat fluxes_(Ghilain et al., 2012;
722	Jarlan et al., 2008; Schwinger et al., 2010; van den Hurk, 2003; Yang et al., 1999), and
723	therefore this study focuses in addition on the calibration of leaf area indexLAI using
724	the land surface temperature assimilation. However, there are large-discrepancies
725	between the remotely retrieved LAI and measured values, and the MODIS LAI
726	product underestimates 44% of field measurement on average
727	(http://landval.gsfc.nasa.gov/), and therefore the leaf area indexLAI is also calibrated
728	by data assimilation. In summary, the novel aspects of this work are: 1) investigating
729	whether data assimilation is able to correct for missing water resources management

data without a priori bias correction; 2) joint assimilation of cosmic-ray neutron
counts, LST and updating of LAI; 3) application of this framework to real-world data
in an irrigated area with the availability of detailed verification data;...

733

734 **2. Materials and Methods**

735 **2.1 Study Area and Measurement**

The Heihe River Basin is the second largest inland river basin of China, and it is 736 located between 97.1 ° E-102.0 ° E and 37.7 ° N-42.7 ° N and covers an area of 737 approximately 143,000 km² (Li et al., 2013). In 2012, a multi-scale observation 738 experiment of evapotranspiration with a well-equipped superstation (Daman 739 superstation) to measure the atmospheric forcings and soil moisture at 2 cm, 4 cm, 10 740 741 cm, 20 cm, 40 cm, 80 cm, 120 cm and 160 cm depth (Xu et al., 2013), was carried out from June to September in the framework of the Heihe Watershed Allied Telemetry 742 Experimental Research (HiWATER) (Li et al., 2013). SoilNet wireless network nodes 743 744 (Bogena et al., 2010) were deployed to measure soil moisture content and soil temperature at four layers (4 cm, 10 cm, 20 cm and 40 cm). One cosmic-ray soil 745 moisture probe (CRS-1000B) was installed (Han et al., 2014c) with 23 SoilNet nodes 746 (Jin et al., 2014; Jin et al., 2013) in the footprint (Fig. 1). The main crop type within 747 the footprint of the cosmic-ray probe is seed corn. The irrigation is applied through 748 channels using the flooding irrigation method. Exact amounts of applied irrigation are 749 750 therefore not available.

751

The measured cosmic-ray neutron count data were processed to remove the

outliers according to the sensor voltage (≤ 11.8 Volt) and relative humidity ($\geq 80\%$). 752 The surface fluxes were measured using the eddy covariance technique, and data were 753 754 processed using EdiRe (http://www.geos.ed.ac.uk/abs/research/micromet/EdiRe) software, in which the anemometer coordinate rotation, signal lag removal, frequency 755 756 response correction, density corrections and signal de-spiking were done for the raw data. The energy balance closure was not considered in this study. The leaf area 757 indexLAI was measured by the LAI-2000 scanner during the field experiment, there 758 759 are 17 samples collected in 14 days of 3 months.

760 [Insert Figure 1 here]

761

762 2.2 Land Surface Model and Data

The Community Land Model (CLM) was used to simulate the spatio-temporal distribution of soil moisture, soil temperature, land surface temperature, vegetation temperature, sensible heat flux, latent heat flux and soil heat flux of the study area. The coupled water and energy balance are modeled in CLM, and the land surface heterogeneity is represented by patched plant functional types and soil texture (Oleson et al., 2013).

The soil properties used in CLM were from the soil database of China with 1 km spatial resolution (Shangguan et al., 2013). The MODIS 500 m resolution plant functional type product (MCD12Q1) (Sun et al., 2008) which was resampled by nearest neighbor interpolation to 1 km resolution and MODIS <u>leaf area indexLAI</u> product (MCD15A3) with 1 km spatial resolution (Han et al., 2012) were used as

input. Due to a lack of measurement data, two atmospheric forcing data sets were 774 used: the Global Land Data Assimilation System reanalysis data (Rodell et al., 2004) 775 776 was interpolated using the National Centers for Environmental Prediction (NCEP) bilinear interpolation library iplib in spatial and temporal dimensions and used in the 777 CLM for the spin-up period 778 (http://www.nco.ncep.noaa.gov/pmb/docs/libs/iplib/ncep_iplib.sht- ml). For the three 779 months data assimilation period, hourly forcing data (incident longwave radiation, 780 incident solar radiation, precipitation, air pressure, specific humidity, air temperature 781 782 and wind speed) from the Daman superstation of HiWATER were available and used.

783

784 2.3 Cosmic-Ray Forward Model

785 In this study, the new developed COsmic-ray Soil Moisture Interaction Code (COSMIC) model (Shuttleworth et al., 2013) was used as the cosmic-ray forward 786 model to simulate the cosmic-ray neutron count rate using the soil moisture profile as 787 788 input. The effective measurement depth of the cosmic-ray soil moisture probe ranges from 12 cm (wet soils) to 76 cm (dry soils) (Zreda et al., 2008), within which 86% of 789 the above-ground measured neutrons originate. COSMIC also calculates the effective 790 sensor depth based on the cosmic-ray neutron intensity and the soil moisture profile 791 values (Franz et al., 2012; Shuttleworth et al., 2013). 792

COSMIC makes several assumptions to calculate the number of fast neutrons reaching the cosmic-ray soil moisture probe (N_{COSMOS}) at a near-surface measurement location, and the soil layer with a depth of 3 meters for the complete soil profile, was discretized into 300 layers for the integration of Eq. 2 in COSMIC. The number of fast neutrons reaching the cosmic-ray probe N_{COSMOS} is formulated as (Shuttleworth et al., 2013):

799
$$N_{COSMOS} = N \int_{0}^{\infty} \left\{ A(z) [\alpha \rho_s(z) + \rho_w(z)] \exp\left(-\left[\frac{m_s(z)}{L_1} + \frac{m_w(z)}{L_2}\right]\right) \right\} dz \qquad (1)$$

800
$$A(z) = \left(\frac{2}{\pi}\right) \int_{0}^{\pi/2} \exp\left(\frac{-1}{\cos(\theta)} \left[\frac{m_s(z)}{L_3} + \frac{m_w(z)}{L_4}\right]\right) d\theta$$
(2)

801
$$\alpha = 0.405 - 0.102 \times \rho_s$$
 (3)

802
$$L_3 = -31.76 + 99.38 \times \rho_s$$
 (4)

803 where N is the high energy neutron intensity (counts/hour), z denotes the soil layer depth (m), ρ_s denotes the dry soil bulk density (g/cm³), ρ_w denotes the total 804 water density, including the lattice water (g/cm³) and α denotes the ratio of fast 805 806 neutron creation factor. L_1 is the high energy soil attenuation length with value of 162.0 g/cm², and L_2 denotes the high energy water attenuation length of 129.1 807 g/cm². In equation (2) θ is the angle between the vertical below the detector and the 808 809 line between the detector and each point in the plane-, $m_s(z)$ and $m_w(z)$ are the integrated mass per unit area of dry soil and water (g/cm²), respectively. L_3 denotes 810 the fast neutron soil attenuation length (g/cm²) and L_4 stands for the fast neutron 811 water attenuation length with value of 3.16 g/cm^2 . 812

The cosmic-ray neutron intensity reaching the land surface is influenced by air pressure, atmospheric water vapor content and incoming neutron flux. In order to isolate the contribution of soil moisture content to the measured neutron density, it is important to take these effects into account and the calibrated neutron count <u>intensity</u> 817 can be derived as follows:

818
$$N_{Corr} = N_{Obs} \times f_P \times f_{wv} \times f_i$$
(5)

819 where N_{Corr} represents corrected neutron counts and N_{Obs} the measured 820 neutron counts. f_p is the correction factor for air pressure, f_{wv} the correction 821 factor for atmospheric water vapor and f_i the correction factor for incoming neutron 822 flux.

823 The correction factor for air pressure f_P can be calculated as 824 factor for air pressure f_P can be calculated as (Zreda et al., 2012):

825
$$f_P = \exp(\frac{P - P_0}{L}) \tag{6}$$

where *P* (mbar) is the local air pressure, P_0 (mbar) the average air pressure during the measurement period and *L* (g/cm²) is the mass attenuation length for high-energy neutrons; the default value of 128 g/cm² was used for in this study (Zreda et al., 2012).

830 The correction factor f_{wv} for atmospheric water vapor is calculated as (Rosolem 831 et al., 2013):

832
$$f_{wv} = 1 + 0.0054 \times (\rho_{v0} - \rho_{v0}^{ref})$$
(7)

833 where $\rho_{\nu 0}$ (k/gm³) is the absolute humidity at the measurement time and $\rho_{\nu 0}^{ref}$ 834 (kg/m³) is the average absolute humidity during the measurement period.

Fluctuations in the incoming neutron flux should be removed because the cosmic-ray probe is designed to measure the neutron flux based on the incoming background neutron flux. The correcting factor f_i for the incoming neutron flux is calculated as:

$$F_i = \frac{N_m}{N_{avg}} \tag{8}$$

where N_m is the measured incoming neutron flux and N_{avg} is the average 840 incoming neutron flux during the measurement period. The measured data at the 841 Jungfraujoch station in Switzerland at 3560 m (http://cosray.unibe.ch/) was used to 842 calculate N_m and N_{avg} . The temporal (secular or diurnal) variations caused by the 843 sunspot cycle could be removed after this correction (Zreda et al., 2012). 844 In this study, the soil moisture for the CRS footprint scale was calculated from the 845 arithmetic mean of the 23 SoilNet soil moisture observations. In this study, the soil 846 moisture at for the CRS footprint scale was calculated from the arithmetic mean of the 847 23 SoilNet soil moisture observations. The calibration of the high energy neutron 848 intensity parameter N in equation (1) was done using the measured cosmic-ray 849 neutron counts rate and averaged soil moisture content at the CRS footprint scale. 850 Because lattice water was unknown for this site, a value of 3% was assumed in this 851 study (Franz et al., 2012). Hourly soil moisture measurements for a period of 2.5 852 months were used for COSMIC calibration. Inside the cosmic-ray probe footprint, the 853 amount of applied irrigation was spatially variable due to the different management 854 practice of each farmer. The gradient search algorithm L-BFGS-B (Zhu et al., 1997) 855 was used to minimize the root mean square error of the differences between simulated 856 cosmic-ray neutron counts (using measured soil moisture by SoilNet as input to 857 COSMIC) and the measured neutron counts N_{Corr} . The optimized parameter value of 858 859 N was 615.96 counts/hour in this case.

860 The simulated soil moisture content for 10 CLM soil layers (3.8 m depth) was

861	used as input to COSMIC in order to simulate the corresponding neutron count
862	intensity and compare it with the measured neutron count intensity. It should be
863	mentioned that it is unlikely that anything beyond 1 m deep will substantially impact
864	the results because the effective measurement depth of the cosmic-ray probe is
865	between 12 and 76 cm. The COSMIC model assumes a more detailed soil profile.
866	COSMIC interpolates the soil moisture information from the ten CLMCOSMIC,
867	interpolates the soil moisture information from the ten CLM soil layers to information
868	for 300 soil layers of depth 1cm. The contribution of each soil layer to the measured
869	neutron flux will change temporally depending on the soil moisture condition.
870	Therefore the effective measurement depth of the cosmic ray probe will also change
871	temporally. COSMIC calculates the vertically weighted soil moisture content based
872	on the vertical distribution of soil moisture content. For the data assimilation, the
873	simulated soil moisture content for 10 soil layers (3.8 m depth) in CLM was used as
874	the input to COSMIC in order to simulate the corresponding cosmic ray neutron
875	counts and compare it with the measured neutron counts. It should be mentioned that
876	it is unlikely that anything beyond 1 m deep will substantially impact the results
877	because the effective measurement depth of cosmic-ray probe is between 12 and 76
878	cm. The COSMIC model assumes a more detailed soil profile. In COSMIC, the soil
879	moisture information from the 10 layers from CLM was interpolated to information
880	for 300 layers based on the soil layer depth for stable numerical solution. The
881	contribution of each soil layer to the measured neutron flux will change temporally
882	depending on the soil moisture condition. So the effective measurement depth of the

883 <u>cosmic ray probe will also change temporally.</u> COSMIC calculates as output also the
884 neutron count rate and the vertically weighted soil moisture content, which is
885 calculated with help of the effective sensor depth obtained from COSMIC based on
886 the vertical distribution of soil moisture contents <u>at different depth.</u>

887

888 2.4 Two Source Formulation - TSF

The land surface temperature products of MODIS are composed of a ground 889 temperature and vegetation temperature component, which are however unknown. 890 891 CLM models the ground temperature and vegetation temperature separately, but does not model the composed land surface temperature as seen by MODIS. The 892 corresponding land surface temperature of CLM should therefore be modelled for 893 894 data assimilation purposes. The two source formulation (Kustas and Anderson, 2009) was used in this study to calculate the land surface temperature from the MODIS view 895 angle using ground temperature and vegetation temperature simulated by CLM: 896

897
$$T_s = [F_c(\Phi)T_c^4 + (1 - F_c(\Phi)T_e^4)]^{1/4}$$
(9)

where $T_s(K)$ is the composed surface temperature as seen by the MODIS sensor, $F_c(\Phi)$ is the fraction vegetation cover observed from the sensor view angle Φ (radians), $T_c(K)$ is the vegetation temperature and $T_g(K)$ is the ground temperature. (Kustas and Anderson, 2009):

902
$$F_c(\Phi) = 1 - \exp\left(\frac{-0.5\Omega(\Phi)LAI}{\cos\Phi}\right)$$
(10)

903 where *LAI* is the leaf area index, $\Omega(\Phi)$ is a clumping index to represent the 904 nonrandom leaf area distributions of farmland or other heterogeneous land surfaces 905 (Anderson et al., 2005), and is defined as:

906
$$\Omega(\Phi) = \frac{0.49\Omega_{\text{max}}}{0.49 + (\Omega_{\text{max}} - 0.49)\exp(k\theta^{3.34})}$$
(11)

907
$$\Omega_{\text{max}} = 0.49 + 0.51(\sin \Phi)^{0.05}$$
 (12)

908
$$k = -\{0.3 + [1.7 * 0.49 * (\sin \Phi)^{0.1}]^{14}\}$$
 (13)

909

910 2.5 Assimilation Approach

The Local Ensemble Transform Kalman Filter (LETKF) was used as the assimilation algorithm, which is one of the square root variants of the ensemble Kalman filter (Evensen, 2003; Hunt et al., 2007; Miyoshi and Yamane, 2007). The model uncertainties are represented using the ensemble simulation of model states and LETKF derives the background error covariance using the model state ensemble members. LETKF uses the non-perturbed observations to update all the ensemble members of model states at each assimilation step.

In this study, $x_1^b, ..., x_N^b$ denote the model state ensemble members; \bar{x}^b is the ensemble mean of $x_1^b, ..., x_N^b$; *N* is the ensemble size; $y_1^b, ..., y_N^b$ denote the mapped model state ensemble members; \bar{y}^b is the ensemble mean of $y_1^b, ..., y_N^b$; *H* is the observation operator (COSMIC for soil moisture or the two source function for land surface temperature). The analysis step of LETKF can be summarized as follows:

923 Prepare the model state vector
$$X^b$$
:

924
$$X^{b} = [x_{1}^{b} - \bar{x}^{b}, \dots, x_{N}^{b} - \bar{x}^{b}]$$
(14)

where \bar{x}^b is composed of one vertically weighted soil moisture content and soil moisture content for 10 CLM-layers, resulting in a state dimension equal to 11 if only

927	the neutron count observation was assimilated the neutron counts observations were
928	assimilated; and \bar{x}^b is composed of surface temperature, ground temperature,
929	vegetation temperature and soil temperature for 15 CLM-layers if only the land
930	surface temperature observations were assimilated without soil moisture update,
931	giving a state dimension of 18. The water and energy balance are coupled, and in
932	CLM the energy balance is firstly solved, then the derived surface fluxes are used in
933	for updating the soil moisture content. So tThe cross correlation between the soil
934	temperature and soil moisture could-can be calculated using the ensemble prediction
935	in LETKF, and this makes the updating of soil moisture by assimilating land surface
936	temperature possible. We also used the land surface temperature to update the soil
937	moisture profile, in this case the soil moisture vector was augmented to the LETKF
938	state vector of land surface temperature assimilation, and resulting in a state
939	dimension of 28. For the calibration of the LAI, the state vector was augmented with
940	surface temperature, ground temperature, vegetation temperature, soil temperature for
941	15 CLM-layers and LAI if only the land surface temperature observations were
942	assimilated without soil moisture update. This resulted then in a state dimension of
943	19.For the calibration of the LAI, the state vector was augmented as surface
943 944	19.For the calibration of the LAI, the state vector was augmented as surface temperature, ground temperature, vegetation temperature, soil temperature for 15
944	temperature, ground temperature, vegetation temperature, soil temperature for 15
944 945	temperature, ground temperature, vegetation temperature, soil temperature for 15 CLM layer and LAI if only the land surface temperature observations were

948 operator:

949
$$\mathbf{y}_i^b = H(\mathbf{x}_i^b) \tag{15}$$

950
$$Y^{b} = \left[y_{1}^{b} - \bar{y}^{b}, \dots, y_{N}^{b} - \bar{y}^{b} \right]$$
(16)

951 The following analysis is looped for each model grid cell to calculate the update 952 of model state ensemble members:

953 Calculate analysis error covariance matrix P^a :

954
$$P^{a} = [(N-1)I + Y^{bT}R^{-1}Y^{b}]$$
(17)

955 The perturbations in ensemble space are calculated as:

956
$$W^a = [(N-1)P^a]^{1/2}$$
(18)

957 Calculate the analysis mean \overline{w}^a in ensemble space and add to each column of 958 W^{*a*} to get the analysis ensemble in ensemble space:

959
$$\overline{w}^a = P^a Y^{bT} R^{-1} (y^o - \overline{y}^b)$$
 (19)

960 Calculate the new analysis:

961
$$X^a = X^b [\bar{w}^a + W^a] + \bar{x}^b$$
 (20)

962 where *R* is the observation error covariance matrix, y^o is the observation vector 963 and X^a contains the updated model ensemble members.

The LETKF method can also be extended to do parameter estimation using a state augmentation approach (Bateni and Entekhabi, 2012; Li and Ren, 2011; Moradkhani et al., 2005; Nie et al., 2011). Alternative strategies for parameter estimation are a dual approach (Moradkhani et al., 2005) with separate updating of states and parameters. Vrugt et al. (2005) also proposed a dual approach with parameter updating in an outer optimization loop using <u>a</u> Markov Chain Monte Carlo methods, and state updating in an inner loop. The a priori calibration of model parameters is also an option (Kumar et

971	al., 2012). With the augmentation approach, the state vector of LETKF can be
972	augmented by the parameter vector including soil properties (sand fraction, clay
973	fraction and organic matter density) and vegetation parameters (leaf area indexLAI,
974	etc.). In a preliminary sensitivity study it was found that for this site simulation results
975	were more sensitive to the leaf area indexLAI than to soil properties. Soil texture is
976	also quite well known for this site from measurements. Therefore in this study, only
977	the leaf area indexLAI was in some of the simulation scenarios calibrated. In the
978	different scenarios of land surface temperature assimilation, the LETKF state vector
979	was also augmented to include leaf area indexLAI as calibration target. As a
980	consequence, the augmented state vector contains surface temperature, ground
981	temperature, and vegetation temperature, 15 layers of soil temperature and leaf area
982	indexLAI, making up a state dimension equal to 19 for the scenarios of land surface
983	temperature assimilation without soil moisture update; for the scenarios of land
984	surface temperature with soil moisture update, the state dimension is 29 for the
985	scenarios of land surface temperature with soil moisture update, the state dimension
986	will be changed to 29. The 10 layers of soil moisture and 15 layers of soil temperature
987	are the standard CLM layout for both soil moisture and soil temperature. The
988	hydrology calculations are done over the top 10 layers, and the bottom 5 layers are
989	specified as bedrock. The lower 5 layers are hydrologically inactive layers.
990	Temperature calculations are done over all layers (Oleson et al., 2013).
991	

3. Experiment Setup

993 Firstly the 50 ensemble members of CLM with perturbed soil properties and atmospheric forcing data were driven from the 1st of Jan. 2012 to the 31st of May 2012 994 to do the CLM spin-up; secondly an additional assimilation period of cosmic-ray 995 neutron counts was done from the 1st of Jun. 2012 to the 30th Aug. 2012 to reduce the 996 spin-up error. Then the final CLM states on 30th Aug. 2012 were used as the initial 997 states for the following data assimilation scenarios. Perturbed soil properties were 998 generated by adding a spatially uniform perturbation sampled from a uniform 999 distribution between -10% and 10% to the values extracted from the Soil Database of 1000 1001 China for Land Surface Modeling (1 km spatial resolution). The LAI was perturbed with multiplicative uniform distributed random noise in the range of [0.8 - 1.2]. The 1002 003 perturbations added to the model forcings show correlations in space and timeThe leaf .004 area index was perturbed with multiplicative uniform distributed random noise in the range of [0.8~1.2]. The model forcings were perturbed by adding a perturbation, .005 1006 showing correlations in space and time. The spatial correlation was induced by a Fast 1007 Fourier Transform and the temporal correlation by a first-order auto-regressive model (Han et al., 2013; Kumar et al., 2009; Reichle et al., 2010). The statistics on the 1008 1009 perturbation of the forcing data are summarized in Table 1. The values of standard deviations and temporal correlations in Table 1 were chosen based on previous 1010 catchment scale and regional scale data assimilation studiesdata assimilation (De 1011 Lannoy et al., 2012; Kumar et al., 2012; Reichle et al., 2010). 1012

1013[Insert Table 1 here]

1014 The cosmic-ray neutron intensity was assimilated every 3 days at 12Z from the 1st

of June 2012 onwards, because we found that the difference between daily 1015 assimilation and 3 days assimilation was small (Entekhabi et al., 2010; Kerr et al., 1016 1017 2010). The measured neutron count intensity showed large temporal fluctuations in time and these fluctuations were not corresponding to the temporal variations of soil 1018 1019 moisture. Therefore the measured neutron count intensity was smoothed with the Savitzky-Golay filter using a moving average window of size 31 hours and a 1020 polynomial of order 4 (Savitzky and Golay, 1964). The originally measured neutron 1021 counts and smoothed neutron counts are plotted in Fig. 2. The assimilation frequency 1022 1023 of MODIS LST products of MOD11A1 and MYD11A1 was up to 4 times (maximum) per day depending on the data availability. There are 230 observation data (including 1024 1025 cosmic-ray probe neutron counts, MODIS LST, MOD11A1 and MYD11A1 LST) in 1026 the whole assimilation window. The variance of the instantaneous measured neutron intensity wasis equal to the measured neutron count intensity (Zreda et al., 2012) and 1027 smaller for temporal averaging for daily or sub-daily applications.(Zreda et al., 2012) 1028 1029 The instantaneous neutron intensity was assimilated in this study. and tThe variance 1030 of MODIS LST was assumed to be 1 K (Wan and Li, 2008) (Wan and Li, 2008). The variance of Cosmic-ray was the measured neutron counts value (Zreda et al., 2012) 031 1032 and the variance of MODIS LST was assumed to be 1 K. 1033 The 4 days MODIS leaf area indexLAI product was aggregated and used as the CLM leaf area indexLAI parameter. Because the leaf area indexLAI from MODIS is .034 035 usually lower than the true value (compared with the field measured leaf area

036 indexLAI in the HiWATER experiment) and because the surface flux and surface

temperature are sensitive to the leaf area indexLAI, two additional scenarios were
investigated where leaf area indexLAI was calibrated to study the impact of leaf area
indexLAI estimation on surface flux estimation within the data assimilation
framework.

1041 The following assimilation scenarios were compared: (1) CLM: open loop simulation without assimilation; (2) Only_CRS: only the measured neutron counts 1042 were assimilated; (3) Only_LST: only the MODIS LST products were assimilated. 1043 The quality control flags of LST products were used to select the data with good 1044 1045 quality for assimilation; (4) CRS_LST: the measured neutron counts and MODIS LST products were assimilated jointly. In the above scenarios, the neutron count data was 1046 1047 used to update the soil moisture and the LST data were used to update the ground 1048 temperature, vegetation temperature and soil temperature. (5) LST_Feedback: We also evaluated the scenario of assimilating the LST measurements to update the soil 1049 1050 moisture profile. (6) CRS_LST_Par_LAI: the leaf area indexLAI was included as 1051 variable to be calibrated, otherwise the scenario was the same as CRS_LST. (7) 1052 LST Feedback Par LAI: the leaf area indexLAI was included as variable to be 1053 calibrated, otherwise the scenario was the same as LST_Feedback. (8) 1054 CRS LST True LAI: the in situ measured leaf area indexLAI during the HiWATER experiment was used in the model simulation. 1055

1056 [Insert Figure 2 here]

1057

1058 **4. Results and Discussion**

In order to evaluate the assimilation results for the different scenarios outlined in
section 3, the Root Mean Square Error (RMSE) was used:

1061
$$RMSE = \sqrt{\frac{\sum_{n=i}^{N} (Estimated - Measured)^2}{N}}$$
(21)

where "*Estimated*" is the ensemble mean without assimilation or the ensemble mean after assimilation, "*Measured*" is measured soil moisture content evaluated at the SoilNet nodes (or latent heat flux, sensible heat flux or soil heat flux). *N* is the number of time steps. For the soil moisture analysis in this study, *N* is equal to 2184. The smaller the RMSE value is, the closer assimilation results are to measured values, which is in general considered to be desirable.

The temporal evolution of soil moisture content at 10, 20, 50 and 80 cm depth for 1068 1069 different scanarios scenarios is plotted in Fig. 3 and Fig. 4. The RMSE values for 1070 different scenarios are summarized in Table 2. Assimilating the land surface temperature could improve the soil moisture profile estimation in the scenario of 1071 LST_Feedback_Par_LAI; the soil moisture results are better than the open loop run at 1072 all depths. With the assimilation of CRS neutron counts, the soil moisture RMSE 1073 (scenarios CRS LST Par LAI and CRS LST True LAI) decreased 1074 values significantly. The RMSE values for the scenarios Only_CRS and CRS_LST (not 1075 shown) are similar to CRS LST Par LAI, which indicates that the main 1076 improvement for the soil moisture profile characterization is achieved by neutron 1077 count assimilation; and land surface temperature assimilation and leaf area indexLAI 1078 079 estimation play a minor role. Without assimilation of cosmic-ray probe neutron counts, the soil moisture simulation cannot be improved (scenario Only_LST). However, the .080

1081 scenarios of LST_Feedback and LST_Feedback_Par_LAI improve the soil moisture profile characterization, which shows that explicitly using LST to update soil moisture 1082 .083 content in the data assimilation routine gives better results than using LST only to update soil moisture by the model equations. Without assimilation of cosmic-ray probe .084 neutron counts, the soil moisture simulation cannot be improved in the scenario 1085 Only_LST. However, the scenarios of LST_Feedback and LST_Feedback_Par_LAI .086 improve the soil moisture profile characterization, which shows that explicitly using 1087 LST to update soil moisture content in the data assimilation routine gives better 1088 1089 results than using LST only to update soil moisture over the model equations. Results of LST_Feedback and LST_Feedback_Par_LAI are similar; therefore only results for 1090 LST_Feedback_Par_LAI are shown in Fig. 3 and Fig. 4. This implies that the 1091 1092 improved soil moisture characterization due to LAI calibration is low. The results for the cosmic-ray probe neutron count assimilation proved that the cosmic-ray probe 1093 sensor can be used to improve the soil moisture profile estimation at the footprint 1094 1095 scaleThe results for the cosmic-ray probe neutron count assimilation proved the 1096 cosmic-ray probe sensor can be used to improve the soil moisture profile estimation at 1097 the footprint scale.

1098 [Insert Figure 3 here]

- 1099 [Insert Figure 4 here]
- 1100 [Insert Table 2 here]

Fig. 5 depicts the scatter plots of measured ET versus modelled ET for different scenarios, and the accumulated ET for all scenarios are summarized in the lower-right

1103 corner of Fig. 5.- The EC measured evapotranspiration (ET) is 384.7 mm for the assimilation period, without energy balance closure correction. The true 1104 evapotranspiration is therefore likely larger, but not much larger as the energy balance 1105 gap was limited (3.7%). The CLM estimated ET, without data assimilation, using only 1106 precipitation as input is 223.7 mm and is much smaller than the measured value as 1107 applied irrigation is not considered in the model. This open loop simulated value 1108 would imply water stress and a limitation of canopy transpiration and soil evaporation 1109 due to low soil moisture content. Assimilation of land surface temperature only 1110 1111 (Only_LST) hardly affected the estimated ET and was not able to correct for the artificial water stress condition. However, if land surface temperature was used to 1112 update soil moisture directly, taking into account correlations between the two states 1113 1114 in the data assimilation routine, the ET estimates improved to 336.8 mm and 354.8 mm for the scenarios of LST_Feedback and LST_Feedback_Par_LAI respectively. 1115 The assimilation of land surface temperature of MODIS with soil moisture update 1116 1117 results in significant improvements of ET.

The different neutron count assimilation scenarios also resulted in significantly 1118 improved estimates of ET. Univariate assimilation of cosmic-ray neutron data 1119 (Only CRS) resulted in 301.9 mm ET. This shows that the impact of neutron count 1120 assimilation to correct evapotranspiration estimates is little smaller than the impact of 1121 land surface temperature with soil moisture update. Joint assimilation of land surface 1122 temperature data and cosmic-ray neutron data (CRS_LST) gave a slightly larger ET of 1123 310.6 Only_CRS. Scenarios CRS_LST_Par_LAI mm than of and 1124

1125 CRS_LST_True_LAI gave the best ET estimates (360.5 mm and 349.3 mm). This 1126 shows that correcting the biased LAI-estimates from MODIS by in situ data or 1127 calibration helped to improve model estimates.

1128 [Insert Figure 5 here]

1129 The RMSE values of latent heat flux, sensible heat flux and soil heat flux for all 1130 scenarios are summarized in Fig. 6, Fig. 7, Fig. 8 and Table 3. It is obvious that the 1131 RMSE values are very large for both the latent heat flux (123.9 W/m^2) (Fig. 6) and sensible heat flux (80.5 W/m^2) (Fig. 7) for the open loop run and all other scenarios 1132 where the soil moisture was not updated. If the land surface temperature was 1133 assimilated to update the soil moisture, the latent heat flux RMSE decreased to 60.5 1134 W/m² (LST_Feedback) and 62.5 W/m² (LST_Feedback_Par_LAI). The scenario 1135 1136 where soil moisture and LAI are jointly updated (LST_Feedback_Par_LAI) gave worse results than the scenario of LST_Feedback. The joint soil moisture and LAI 1137 update scenario of LST_Feedback_Par_LAI was worse than the single soil moisture 1138 update scenario of LST_Feedback in this case. Again, the assimilation of neutron 1139 counts also resulted in a strong RMSE reduction for the latent heat flux (76.5 W/m^2 1140 for Only_CRS). If in addition land surface temperature was assimilated and leaf-area 1141 indexLAI optimized, the RMSE value of latent heat flux further decreased to 56.1 1142 W/m^2 (70.7 W/m^2 without LAI optimization). If the field measured LAI was used 1143 instead in the assimilation (CRS_LST_True_LAI), the RMSE was 61.0 W/m². These 1144 results are in correspondence with the ones discussed before for soil moisture 1145 characterization. Evidently, the combined assimilation of cosmic-ray probe neutron 1146

1147 counts and land surface temperature, and calibration of leaf area indexLAI (or use of field measured leaf area indexLAI as model input) shows the strongest improvement 1148 1149 for the estimation of land surface fluxes. The soil heat flux did not show a clear improvement related to assimilation and showed only some improvement in case LAI 1150 1151 was calibrated (Fig. 8). For the scenario of land surface temperature assimilation 1152 without soil moisture update (Only_LST), estimates of latent and sensible heat flux are not improved. It means that under water stress condition, the improved 1153 characterization of land surface temperature (and soil temperature) does not contribute 1154 1155 to a better estimation of land surface fluxes.

1156 <u>[Insert Table 3 here]</u>

[Insert Figure 6 here]

158[Insert Figure 7 here]

1159 [Insert Figure 8 here]

The updated leaf area indexLAI for scenarios of LST_Feedback_Par_LAI and 1160 1161 CRS_LST_Par_LAI is shown in Fig. 97. The MODIS leaf area indexLAI product was used as input for CLM and time series are plotted as blue line in Fig. 9-71162 1163 (Background). The leaf area indexLAI was also measured in the HiWATER experiment, and the measured values are shown as green star (Observation). 1164 1165 Ens_Mean represents the mean leaf area indexLAI of all ensemble members 1166 (Ensembles). It is obvious that MODIS underestimates the leaf area indexLAI 1167 compared with the observations. With the assimilation of land surface temperature, the leaf area indexLAI could be updated and be closer to the observations, but there is 1168

still a significant discrepancy between the measured <u>leaf area indexLAI</u> and the updated one. The <u>leaf area indexLAI</u> values for the scenario with <u>leaf area indexLAI</u> calibration (CRS_LST_Par_LAI) are close to the measured <u>leaf area indexLAI</u> values (CRS_LST_True_LAI), which is an encouraging result. The calibrated <u>leaf area</u> indexLAI shows some unrealistic increases and decreases during the assimilation period, which is inherent to the data assimilation approach. A smoothed representation of the <u>leaf area indexLAI</u> might provide a more realistic picture.

Insert Figure 7 here

1177 This study illustrates that for an irrigated farmland, the measured cosmic-ray probe neutron counts can be used to improve the soil moisture profile estimation 1178 significantly. Without irrigation data, CLM underestimated soil moisture content. The 1179 1180 cosmic-ray neutron count data assimilation can be used as an alternative way to retrieve the soil moisture content profile in CLM. The improved soil moisture 1181 simulation was helpful for the characterization of the land surface fluxes 1182 characterization. The univariate assimilation of land surface temperature without soil 1183 moisture update is not helpful for the estimation of <u>land</u> surface fluxes and even 1184 1185 worsened the sensible heat flux characterization (Fig. 76). However, in a multivariate data assimilation framework where land surface temperature was assimilated together 1186 with measured cosmic-ray probe neutron counts, the land surface temperature 1187 assimilation contributed significantly to an improved ET estimation. The simulated 1188 1189 canopy transpiration in CLM was in general too low, even when the water stress condition was corrected by assimilating neutron counts, which was related to small 1190

values of the leaf area indexLAI. The additional estimation of leaf area indexLAI
 through the land surface temperature assimilation resulted in an increase of the leaf
 area indexLAI yielding an increase of estimated ET.

In general, land surface models need to be calibrated before use in land data 1194 1195 assimilation, especially if there is an apparent large bias in the model simulation (Dee, 2005). The simulation of soil moisture and surface fluxes was biased in our study, 1196 mainly due to the lack of irrigation water as input. This bias cannot be corrected a 1197 priori without exact irrigation data, which are not available in the field. The data 1198 1199 assimilation was proven to be an efficient way to remove the model bias in this case. We also calculated the equivalent water thickness to analyze the equivalent irrigated 1200 water after each step of soil moisture update. For the scenarios of CRS_LST_Par_LAI 1201 1202 and CRS_LST_True_LAI, the equivalent irrigation in three months was 693.6 mm and 607.6 mm, respectively. Because the irrigation method is flood irrigation, it is not 1203 easy to evaluate the true irrigation applied in the field. From the results we see 1204 1205 however that the applied irrigation (in the model) is much larger than actual ET 1206 (~600-700mm vs ~400mm)(~700mm vs ~400mm). This could indicate that the 1207 amount of applied irrigation in the model is too large, but irrigation by flooding is also inefficient and results in excess runoff and infiltration to the groundwater, because it 1208 cannot be controlled so well as sprinkler irrigation or drip irrigation. Therefore, the 1209 calculated amount of irrigation could be realistic, but might also be too large if soil 1210 1211 properties are erroneous in the model.

1212 The soil moisture content measured by the cosmic-ray probe represents the depth

between 12 cm (very humid) and 76 cm (extremely dry case) depending on the 1213 amount of soil water (soil moisture content and lattice water). Therefore the effective 1214 1215 sensor depth of the cosmic-ray probe will change over time. In order to model the variable sensor depth and the relationship between the soil moisture content and 1216 neutron counts, the new developed COSMIC model was used as the observation 1217 operator in this study. Additionally the influences of air pressure, atmospheric vapor 1218 pressure and incoming neutron counts were removed from the original measured 1219 neutron counts. Because there is still some water in the crop which also affects the 1220 1221 cosmic-ray probe sensor, the COSMIC observation operator could be improved to include vegetation effects. Several default parameters proposed by (Shuttleworth et al., 1222 2013) were used in the COSMIC model, these parameters probably need further 1223 1224 calibration following the development of the COSMIC model.

The spatial distribution of soil moisture for the study area was very 1225 heterogeneous due to the small farmland patches and different irrigation periods for 1226 1227 the different farmlands. Therefore the soil moisture content inferred by SoilNet may not represent the true soil moisture content of the cosmic-ray probe footprint, which is 1228 1229 a further limitation of this study. Although the Cosmic-ray Soil Moisture Observing System (COSMOS) has been designed as a continental scale network by installing 1230 500 COSMOS probes across the USA (Zreda et al., 2012), there are still some 1231 disadvantages of COSMOS compared with remote sensing. COSMOS is also 1232 expensive for extensive deployment to measure the continental/regional scale soil 1233 moisture.there are still some disadvantages of COSMOS compared with remote 1234

1235 sensing. The land surface is heterogeneous and COSMOS only samples part of this heterogeneity. COSMOS is also expensive for extensive deployment. Although the 1236 1237 Cosmic-ray Soil Moisture Observing System (COSMOS) has been designed as a continental scale network by installing 500 COSMOS probes across the USA (Zreda 1238 et al., 2012). But there are still some disadvantages of COSMOS compared with the 1239 remote sensing. Because the land surface is heterogeneous and COSMOS only catch 1240 the heterogeneity of local footprint scale, and COSMOS is expensive for extensive 1241 1242 deployment.

1243 **5. Summary and Conclusions**

In this paper, we studied the univariate assimilation of MODIS land surface 1244 temperature products, the univariate assimilation of measured neutron counts by the 1245 1246 cosmic-ray probe, the bivariate assimilation of land surface temperature and neutron count data, and the additional calibration of leaf area indexLAI for an irrigated 1247 farmland at the Heihe catchment in China, where data on the amount of applied 1248 1249 irrigation were lacking. The most important objective of this study was to test whether data assimilation is able to correct for the absence of information on water resources 1250 1251 management as model input, a situation commonly encountered in large scale land surface modelling. For the specific case of lacking irrigation data, no a priori bias 1252 correction is possible. The bias blind assimilation without explicit bias estimation was 1253 used. We focused on the model bias introduced by the forcing data and the LAI, and 1254 neglected the other sources of bias. In case leaf area indexLAI was calibrated, this 1255 was done at each data assimilation step of land surface temperature. The data 1256

assimilation experiments were carried out with the Community Land Model (CLM)
and the data assimilation algorithm used was the Local Ensemble Tranform Kalman
Filter (LETKF). A likely further model bias, besides missing information on irrigation,
is the underestimation of LAI by MODIS, which was used to force the model.

The results show that the direct assimilation of measured comic-ray neutron 1261 counts improves the estimation of soil moisture significantly, whereas univariate 1262 assimilation of land surface temperature without soil moisture update does not 1263 improve soil moisture estimation. However, if the land surface temperature was 1264 1265 assimilated to update the soil moisture profile directly with help of the state augmentation method, the evapotranspiration and soil moisture could be improved 1266 significantly. This result suggests that the land surface temperature remote sensing 1267 1268 products are needed to correct the characterization of the soil moisture profile and the evapotranspiration. The improved soil moisture estimation after the assimilation of 1269 neutron counts resulted in a better ET estimation during the irrigation season, 1270 correcting the too low ET of the open loop simulation. The joint assimilation of 1271 neutron counts and MODIS land surface temperature improved the ET estimation 1272 1273 further compared to neutron count assimilation only. The best ET estimation was obtained for the joint assimilation of cosmic-ray neutron counts, MODIS land surface 1274 1275 temperature including calibration of the leaf area indexLAI (or if field measured leaf area indexLAI was used as input). This shows that bias due to neglected information 1276 on water resources management can be corrected by data assimilation if a 1277 combination of soil moisture and land surface temperature data is available. 1278

We can conclude that data assimilation of neutron counts and land surface 1279 temperature is useful for ET and soil moisture estimation of an irrigated farmland, 1280 1281 even if irrigation data are not available and excluded from model input. The land surface temperature measurements are an alternative data source to improve the soil 1282 1283 moisture and land surface fluxes estimation under water stress conditions. This shows 1284 the potential of data assimilation to correct also a systematic model bias. Leaf area indexLAI optimization further improves simulation results, which is also likely 1285 related to a systematic underestimation of LAI by the MODIS remote sensing product. 1286 1287 The results of using the calibrated leaf area indexLAI are comparable to the results of using field measured leaf area indexLAI as model input. 1288

1289

1290 Acknowledgements

This work is supported by the NSFC (National Science Foundation of China) 1291 project (grant number: 41271357, 91125001), the Knowledge Innovation Program of 1292 the Chinese Academy of Sciences (grant number: KZCX2-EW-312) and the 1293 Transregional Collaborative Research Centre 32, financed by the German Science 1294 foundation. Jungfraujoch neutron monitor data were kindly provided by the 1295 Cosmic-ray Group, Physikalisches Institut, University of Bern, Switzerland. We 1296 acknowledge computing resources and time on the Supercomputing Center of Cold 1297 and Arid Region Environment and Engineering Research Institute of Chinese 1298 Academy of Sciences. 1299

List of Tables 1301

1302 Table 1 Summary of perturbation parameters for atmospheric forcing data.

1303

Table 2 Root Mean Square Error (RMSE) of soil moisture profile of open loop run 1304 (CLM), feedback assimilation of land surface temperature including LAI calibration 1305 (LST_Feedback_Par_LAI), bivariate assimilation of neutron counts and land surface 1306 temperature including LAI calibration (CRS_LST_Par_LAI) and bivariate 1307 assimilation of neutron counts and land surface temperature (CRS_LST_True_LAI). 1308 1309 1310 Table 3 Root Mean Square Error (RMSE) of latent heat flux and sensible heat flux for-

- 1311 different simulation scenarios.

Variables	Noise	Standard deviation	Time Correlation scale	Spatial Correlation Scale	Cross correlation
Precipitation	Multiplicative	0.5	24 h	5 km	[1.0,-0.8, 0.5, 0.0,
Shortwave radiation	Multiplicative	0.3	24 h	5 km	-0.8, 1.0, -0.5, 0.4,
Longwave radiation	Additive	20 W/m^2	24 h	5 km	0.5, -0.5, 1.0, 0.4,

24 h

5 km

0.0, 0.4, 0.4, 1.0]

1 K

Table 1 Summary of perturbation parameters for atmospheric forcing data

1313

Air temperature

Additive

1314

Table 2 Root Mean Square Error (RMSE) of soil moisture profile of open loop run
(CLM), feedback assimilation of land surface temperature including LAI calibration
(LST_Feedback_Par_LAI), bivariate assimilation of neutron counts and land surface
temperature including LAI calibration (CRS_LST_Par_LAI) and bivariate
assimilation of neutron counts and land surface temperature using ground-based
measured LAI as input (CRS_LST_True_LAI).

Soll Lower	$\mathbf{RMSE}\;(\mathbf{m}^{3}/\mathbf{m}^{3})$					
Soil Layer	Open Loop	LST_Feedback	CRS_LST	CRS_LST		
Depth	(CLM)	_Par_LAI	_Par_LAI	_True_LAI		
10 cm	0.202	0.137	0.085	0.086		
20 cm	0.167	0.106	0.047	0.048		
50 cm	0.193	0.112	0.112	0.119		
80 cm	0.188	0.124	0.136	0.146		

 1323
 Table 3 Root Mean Square Error (RMSE) of latent heat flux and sensible heat flux for

different simulation scenarios.

Seconomics	RMSE (W/m ²)		
<u>Scenarios</u>	Latent Heat	Sensible Heat	
Open Loop (CLM)	123.9	80.5	
LST_Feedback	60.5	34.8	
LST_Feedback_Par_LAI	62.5	37.2	
Only_CRS	76.5	4 3.3	
CRS_LST	70.7	4 0.5	
CRS_LST_Par_LAI	56.1	31.9	
CRS_LST_True_LAI	61.0	34.5	

1326 List of Figures

Figure 1. Map of the cosmic-ray probe and SoilNet Nodes in the footprint of the CRS 1327 probe positioned at the Heihe river catchment 1328 1329 1330 Figure 2. Measured and temporally smoothed CRS neutron counts 1331 Figure 3. Soil moisture at 10 cm (upper) and 20 cm (lower) depth as obtained from an 1332 open loop run (CLM), local sensors (Obs), and different simulation scenarios. For a 1333 description of the scenarios see section 3 of the paper. The CRS neutron counts were 1334 assimilated from the 1st of June 1335 1336 1337 Figure 4. Same as figure 3 but for 50 cm and 80 cm. Soil moisture at 50 (upper) cmand 80 cm (lower) depth measured and modeled according different scenarios. For a 1338 full description see Fig. 3 1339 1340 Figure 5. Evapotranspiration estimated according different scenarios for the period 1341 1342 June-August 2012. For a full description see Fig. 3.Figure 5. Evapotranspiration estimated according different scenarios for the period June August 2012. For a full 343 description see Fig. 3. 1344 1345 Figure 6. RMSE values of latent heat flux, sensible heat flux and soil heat flux for the 1346 period June-August 2012. For a description of the scenarios see section 3 of the 347 paper.Figure 6. RMSE of latent heat flux for the period June-August 2012. For a-.348 description of the scenarios see section 3 of the paper. 349 .350 351 Figure 7. RMSE of sensible heat flux for the period June August 2012. For a description of the scenarios see section 3 of the paper. 352 .353 Figure 8. RMSE of soil heat flux for the period June-August 2012. For a description 354 of the scenarios see section 3 of the paper. 1355 1356 1357 Figure 97. Leaf area indexLAI evolution for the period June-August 2012. Displayed 1358 are the measured leaf area indexLAI (Observation), default values (Background), mean of ensemble members (Ens_Mean) and ensemble members (Ensembles) for 1359 scenarios of LST_Feedback_Par_LAI (upper) and CRS_LST_Par_LAI (lower) 1360 1361

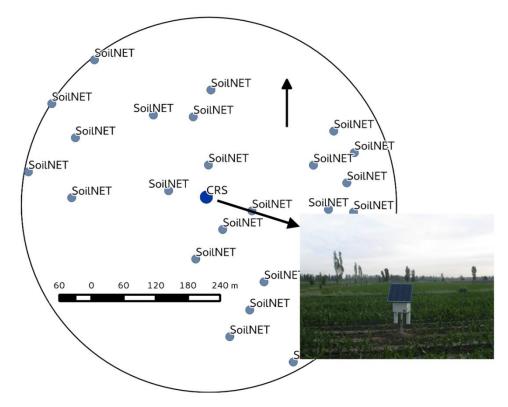
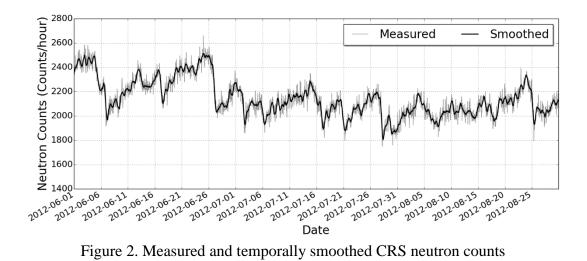


Figure 1. Map of the cosmic-ray probe and SoilNet Nodes in the footprint of the CRS
probe positioned at the Heihe river catchment





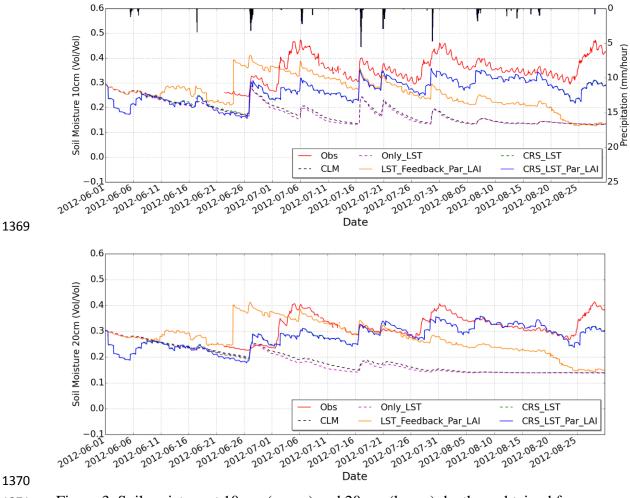
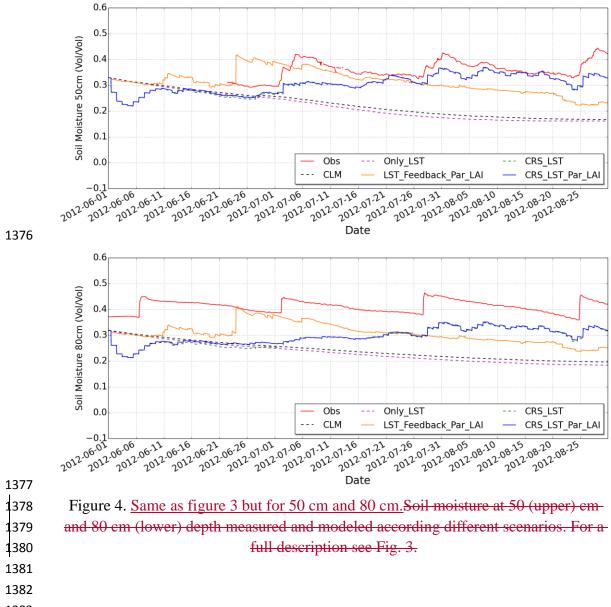
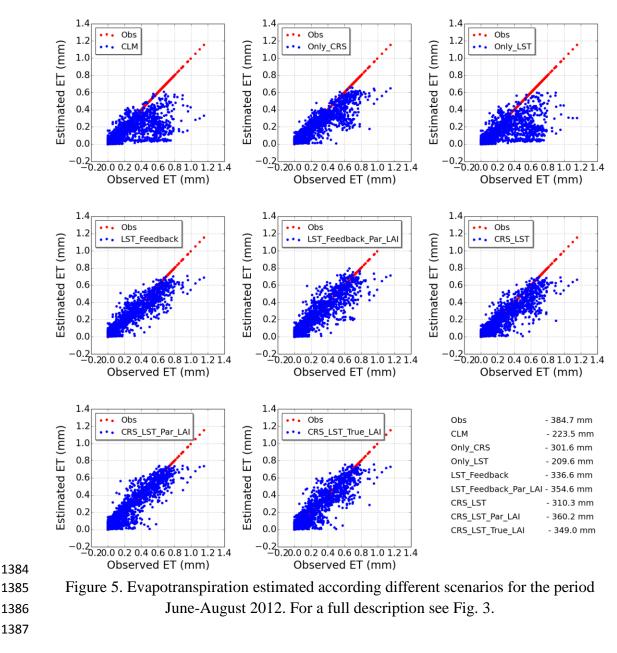
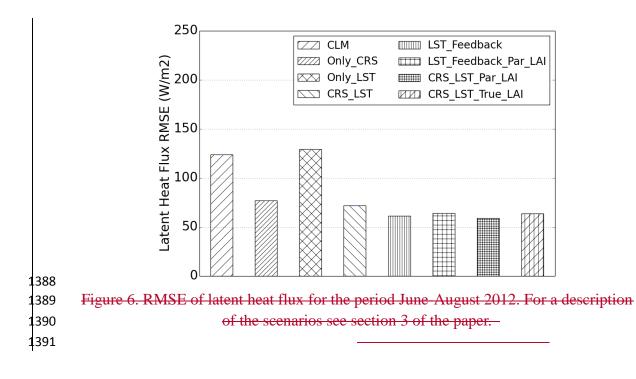
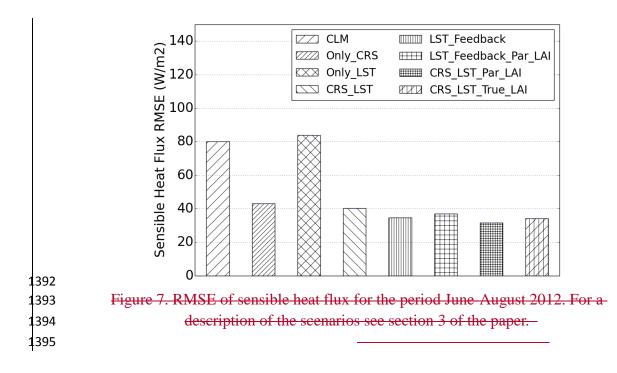


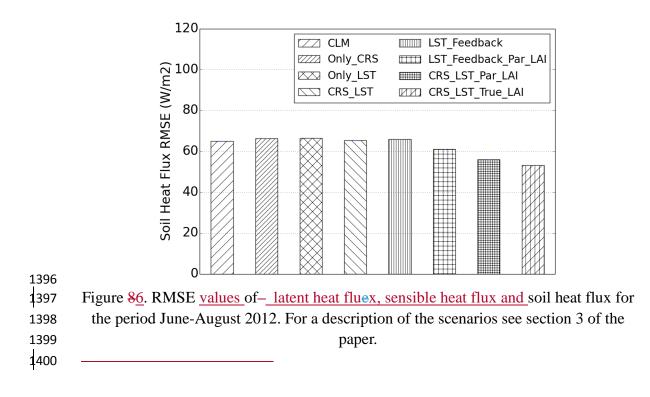
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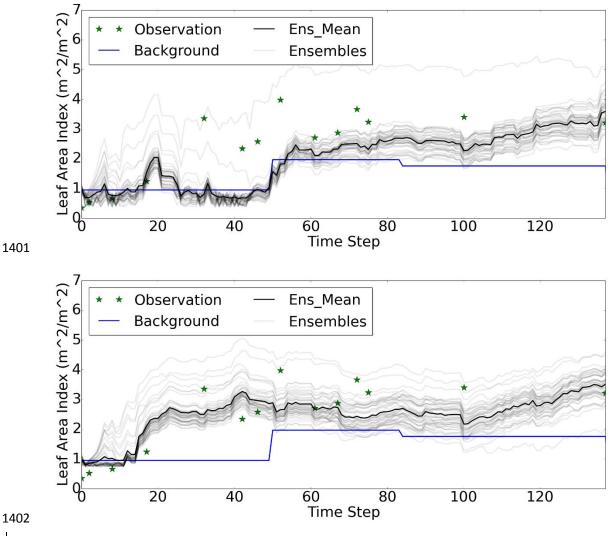


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