We would like to thank the reviewers for the valuable comments and suggestions that improved the manuscript. A point-by-point reply to the comments of both reviewers is provided below with the original comments shown in blue.

Reviewer #1 (anonymous)

The paper describes the addition of the bulk conductivity (BC) model into the JULES Land-surface model. The authors have implemented this very simple model in attempts to improve the simulation of chalk hydrology. The BC model is calibrated and shown to improve the simulated mass and energy fluxes over the Kennet catchment. The authors conclude by commenting on the potential suitability of this simple model for large scale land-surface modelling.

It is clear that the authors have taken the time to properly implement the comments and suggestions from the first pass of reviews which have greatly improved the manuscript. The rewording of the title and abstract highlight the strength of the simplicity of the approach, and the calibration of the BC model parameters makes for a much cleaner and more convincing study.

- We would like to thank the reviewer for the encouraging comments.

I have found the paper clunky to read in places. Some restructuring could help improve the readability of the manuscript.

- We have re-structured the manuscript as suggested by the reviewer in the "Minor Comments" section below to improve readability.

Personally I feel that the calibration step needs to be clearer. The calibration step is not mentioned in the Abstract or Introduction of the paper. The word evaluation is used in places where 'calibration' would be more relevant. The BC model is first calibrated using soil moisture data at a point scale. The calibrated model performance is assessed and compared to the performance of the default JULES parameterization. Finally it is evaluated against independent data at a catchment scale.

- We thank the reviewer for this valuable comment. We have incorporated the calibration step in the introduction of the revised manuscript (L. 75-82 in manuscript_revised.pdf):

"At the point-scale, the proposed parameterization is calibrated using observed soil moisture profile data. This is achieved by randomly sampling the parameter space and extensively running the model in order to minimize the differences between observed and simulated soil moisture variability at different depths. Finally, the proposed model is applied to the Kennet catchment in the Southern England and the fluxes and states of the hydrological cycle are simulated for multiple years. The simulation results are evaluated using observed latent heat flux (LE) and runoff data to assess the performance of the BC model in simulating land surface processes at the catchment scale."

Minor Comments

Introduction: It is worth mentioning in the introduction what default JULES does, this becomes clearer later but a sentence here to the effect: 'JULES has nothing in place for chalk' would be useful.

- We have incorporated this comment in the introduction of the revised manuscript (L. 71-74 in manuscript_revised.pdf):

"In order to test the proposed parameterization, the BC model is included in JULES (version 4.2), which, by default (i.e., uniform soil column representation using general soil database as typically applied in land surface models), does not represent any chalk feature."

Pg 4 line 65: '…relatively large number of parameters' could be worth stating how many to contrast with the three parameter model described in the paper.

- We have mentioned the number of parameters used in relevant previous studies in the revised manuscript (L. 48-52 in manuscript_revised.pdf):

"The physics-based models mentioned above were developed based on dual-continua approach and required relatively large numbers of parameters (i.e., on the order of 20-30 parameters) that were calibrated via inverse modelling using observed soil moisture and matric potential data [e.g., *Ireson et al.*, 2009; *Mathias et al.*, 2006]."

Pg 3 line 69: 'At the point-scale the BC model is evaluated using observed soil moisture data. ' maybe use calibrated instead of evaluated.

- Updated in the revised manuscript (L. 76 in manuscript_revised.pdf):

"At the point-scale, the proposed parameterization is calibrated using observed soil moisture profile data."

Pg 4 line 87: the units for Ks are inconsistent with the units found in table 3.

- We have used mmd^{-1} as the unit of K_s consistently in the revised manuscript (e.g., L. 97, L. 248-250, Table 2 and Table 3 in manuscript_revised.pdf)

Pg 5 line 105: it is not clear how Price et al.'s values of 3-5 mmd-1 for Ks imply a range of 0.8-86 mmd-1 for calibration.

- We thank the reviewer for pointing out this important issue. Note that we have chosen a different range of K_s is the revised manuscript following the suggestions of the other reviewer (Dr. Andrew Ireson). While *Ireson et al.* [2009] suggested a range of 0.2-2.0 mmd^{-1}, *Price et al.* [1993] argued that K_s is around 3-5 mmd^{-1} for most chalk soils. Therefore, we consider a range of 0.2-5.0 mmd^{-1} in the revised manuscript for K_s calibration. This updated range of K_s has been discussed in the revised manuscript (L. 248-250 in manuscript_revised.pdf):

"*Ireson et al.* [2009] suggested a range of 0.2-2.0 mmd^{-1} for K_s. On the other hand, *Price et al.* [1993] argued that in general, K_s is around 3-5 mmd^{-1} for most chalk soils. Therefore, we consider a range of 0.2-5.0 mmd^{-1} in optimizing K_s."

Pg 5 lines 112-123: Please consider moving the calibration description into the methodology.

- We have moved the description of calibration strategy to the "Methods" section (section 3.5) in the revised manuscript (L. 236-260 in manuscript_revised.pdf).

Pg 8 line 189 or Pg 10 line 223: Consider discussing the choice of using the default JULES parameters in the configuration. It is not too surprising that the calibrated parameterization of BC model would outperform an uncalibrated JULES model. The authors address this point in the first pass of reviews but I feel some of the text would benefit from being in the text. Especially since it highlights the BC model's application to a completely 'naive' model setup.

- We have explained the choice of the parameters in the *default* configuration and the fact that it represents a naïve model configuration deprived of model calibration and chalk representation in the revised manuscript (L. 217-220 in manuscript_revised.pdf):

"In this configuration, each soil column in JULES is considered to be vertically homogeneous with the soil properties defined in Table 2, which is motivated by the Met Office JULES Global Land 4.0 configuration described in *Walters et al.* [2014]."

(L. 231-234 in manuscript_revised.pdf):

"It should also be emphasized that *default* represents a "naïve" configuration deprived of model calibration. Moreover, this configuration does not represent chalk, which, according to previous studies [e.g., *Le Vine et al.*, 2016], substantially affects the hydrology of the study area considered here."

FIg 1b): The 'Bare soil', 'Needleleaf' and 'Broadleaf' colours are very similar and hard to distinguish.

- Figure 1b is updated in the revised manuscript of make the colours distinguishable.

Fig 4 (panels (b) to (c)): It would help to shade the bars of the unchanged values differently so that the changes in parameter values becomes more obvious. These panels also don't get discussed much in the main text.

- We have shaded the bars representing uncalibrated and calibrated parameter values using blue and red colours, respectively in Figure 4 of the revised manuscript. We have also enhanced the discussion on Figure 4b, c and d in the revised manuscript (L. 300-313 in manuscript_revised.pdf).

Pg 12 line 271-276: The sensitivity of So is particularly interesting and in turn the model doesn't seem sensitive to fm . I feel the sensitivity of the parameters could be further discussed. Why is it advantageous to use the macro configuration with the two optimized parameters vs the three optimized parameters?

- We have enhanced the discussion on the sensitivity of parameters on model performance in the revised manuscript (L. 282-299 in manuscript_revised.pdf). We have also discussed the benefit of reduced model complexity (i.e., reduced number of parameters for calibration) and our choice of parameters for calibration (i.e., K_s and S_o) in the revised manuscript (L. 293-299 in manuscript_revised.pdf):

"Arguably, the BC model can be implemented in other chalk regions by constraining only S_o parameter. Such result could potentially be advantageous for transferability to other regions in the UK in order to assess chalk hydrology at large-scale. However since this is the first time the BC model is introduced, we decide to take a conservative approach and select the *macro* configuration with optimized K_s and S_o ($macro_{opt}$ hereafter) to simulate chalk hydrology over the study area that ensures best overall model performance."

(L. 408-415 in manuscript_revised.pdf):

"Our results indicated that S_o is by far the most influential parameter in the model when representing water movement through a soil-chalk column. This highlights the simplicity of the proposed BC model for large-scale studies and potential ease in transferability. In comparison, K_s and f_m showed secondary (low) sensitivity on the model performance. Since this study introduces the BC model, we decided however to take a conservative approach. We optimized K_s and S_o simultaneously for our catchment scale simulations since this combination resulted in the best overall model performance."

Table 3: there seems to be a lack of consistency between Figure 4 and Table 3. In the text (line 276) '. .. we select the macro configuration with optimized Ks and S o ... ' which should mean f m remains unchanged. However in Table 3, fm 's optimized value differs for its unoptimized value. The value for f m in this table might be from optimising over this parameter alone, but then the other parameters have optimized values which differ from their single optimisation value (e.g. Ks). What optimized values are shown in this table? Surely the values used in macro opt should be represented here.

- We thank the reviewer for raising this important issue. We agree that the values presented in Table 3 of the previous manuscript were not consistent with our choice of parameters for calibration (i.e., K_s and S_o). We have updated Table 3 in the revised manuscript (P. 27 in manuscript_revised.pdf). Note that in updated Table 3, calibrated value for K_s (0.31 mmd^{-1}) and S_o (0.46) are presented, while f_m (10^5) remains uncalibrated.

A further comment on Fig.4 and Table 3: what are the units of Ks ? In figure they are of order x10 4, in the table units (md 1) and earlier in the text (mmd 1).

- We have updated Figure 4 and added units of K_s (mmd^{-1}) in the revised manuscript (P. 31 of manuscript_revised.pdf). The unit of K_s in Table 3 of the revised manuscript is also updated to mmd^{-1} (P. 27 in manuscript_revised.pdf).

Table 3: Add ranges over which the parameters were allowed to vary in calibration stage.

- Ranges are added in Table 3 of the revised manuscript (P. 27 in manuscript_revised.pdf).

Pg 13 line 196: It is worth commenting that it is still an underestimate.

- Note that this sentence along with the associated figure (i.e., Figure 6 in the previous manuscript) is removed from the revised manuscript. In manuscript_revised.pdf, we focus on the simplicity of the BC parameterization and the calibration of the model parameters to reduce the differences between observed and simulated soil moisture variability based on the comments by Dr. Andrew Ireson during the previous rounds of review. The results show that the calibrated model improves simulated key hydrological processes over the Kennet catchment compared to the *default* configuration. Therefore Figure 6 (previous manuscript) is no longer necessary because all the relevant information (i.e., the comparison between observed and simulated soil moisture variability) is shown in Figure 5 of manuscript_revised.pdf.

Pg 16 line 375: Two parameters vs the three referenced in the rest of the paper... is K s no longer considered a parameter in the conclusion?

- We would like to thank the reviewer for pointing out this issue. This discussion on the model parameters is clarified in the revised manuscript (L. 403-415 in manuscript_revised.pdf):

"The proposed BC model is a single continuum approach of modelling preferential flow [e.g., *Beven and Germann*, 2013] that involves only 3 parameters, namely the saturated hydraulic conductivity of chalk matrix (K_s), macroporosity factor (f_m) and relative saturation threshold (S_o). Initially, these parameters were estimated from existing literature to assess the performance of the uncalibrated BC model. Finally, the BC model parameters were optimized to minimize the differences between observed and simulated soil moisture variability. Our results indicated that S_o is by far the most influential parameter in the model when representing water movement through a soil-chalk column. This highlights the simplicity of the proposed BC model for large-scale studies and potential ease in transferability. In comparison, K_s and f_m showed secondary (low) sensitivity on the model performance. Since this study introduces the BC model, we decided however to take a conservative approach. We optimized K_s and S_o simultaneously for our catchment scale simulations since this combination resulted in the best overall model performance."

Fig 6: Consider adding vertical lines between the bins to highlight the fact the boxplots are of the same depth. This is not immediately clear and I've noticed that reviewer 3 also mentioned the slight confusion caused by this figure.

- As mentioned above, this figure is removed from the revised manuscript.

Reviewer #2 (Dr. Andrew Ireson)

The paper is much improved, and I think that this is a useful contribution. However, there is a lingering problem that really should be addressed before the paper can be published. The authors have misinterpretted the hydraulic conductivity in the LeVine Paper (cited in the manuscript), which was a bulk hydraulic conductivity and not a matrix conductivity. Moreover, in the optimisation of K, the authors have not sampled K on a log-scale (unless they have and have neglected to say this), meaning that the optimized K is biased towards higher values. As a result, I believe the authors still have a matrix K which is unrealistically large compared with other published estimates. In my opinion, this is important and should be corrected before this paper can be published, which unfortunately means re-running the models.

- We would like to thank the reviewer for his valuable suggestions. In the revised manuscript, we have selected a different range for K_s calibration based on relevant previous studies. While *Ireson et al.* [2009] suggested a range of 0.2-2.0 mmd^{-1}, *Price et al.* [1993] argued that K_s is around 3-5 mmd^{-1} for most chalk soils. Therefore, we consider a range of 0.2-5.0 mmd^{-1} in the revised manuscript for K_s calibration. This updated range of K_s has been discussed in the revised manuscript (L. 248-250 in manuscript_revised.pdf):

"*Ireson et al.* [2009] suggested a range of 0.2-2.0 mmd^{-1} for K_s. On the other hand, *Price et al.* [1993] argued that in general, K_s is around 3-5 mmd^{-1} for most chalk soils. Therefore, we consider a range of 0.2-5.0 mmd^{-1} in optimizing K_s."

Another significant error, though easily fixed, is that the revised manuscript still does not include a plot of runoff for the catchment scale application. Such a plot was included in the response to reviewers (Figure R2 in the response), so should be incorporated into the manuscript. I think that the performance in this figure was reasonable. They should also show the default model performance.

- We thank the reviewer for highlighting this positive result from our study. As suggested, we have incorporated the comparison between observed and simulated runoff (for both *default* and $macro_{opt}$) in the revised manuscript (Figure 8b, L. 360-368 in manuscript_revised.pdf).

If this can be quickly addressed, this will be a nice paper.

I have also identified some minor errors to be corrected, below:

L 65 - "numbers of parameters"

- Corrected in the revised manuscript (L. 50 in manuscript_revised.pdf):

L 80 - to be rigorous you should also show what "K_sb" is when S <= S_0.

- Updated in the revised manuscript (L. 90 in manuscript_revised.pdf)

L 87 - I believe the authors have misinterpretted the LeVine paper, which has a bulk saturated hydraulic conductivity of 16 mm/d, and not a matrix hydraulic conductivity. This number is at least an order of magnitude too high (see e.g. Ireson et al 2009, Price et al 1993, Price et al 2000, Brouyere 2006, all cited in the manuscript).

- As discussed earlier, we have selected a different range for K_s calibration (0.2-5.0 mmd^{-1}) based on relevant previous studies as suggested by the reviewer (L. 248-250 in manuscript_revised.pdf):

"*Ireson et al.* [2009] suggested a range of 0.2-2.0 mmd^{-1} for K_s. On the other hand, *Price et al.* [1993] argued that in general, K_s is around 3-5 mmd^{-1} for most chalk soils. Therefore, we consider a range of 0.2-5.0 mmd^{-1} in optimizing K_s.".

Table 2 & 3 should probably use the same units for hydraulic conductivity - m/d is good.

- Updated in the revised manuscript (P. 27 in manuscript_revised.pdf).

Figure 1 c) has 5 colours, while only 3 legend items.

- Updated in the revised manuscript (Figure 1 in manuscript_revised.pdf).

Figure 4 - Need to label the units of K - and what are these? Not mm/d or m/s as far as I can tell - maybe mm/s? Better to use m/d.

- Unit (mmd^{-1}) is added in the revised manuscript (Figure 4 in manuscript_revised.pdf).

L 106 - the range in Ks considered is good, though I would expect the true value to be right at the bottom of this range. Did you sample Ks in log-space? I assume not - which is a problem as it will bias your sampling to the higher values. This is important - you need to sample in log-space. I think your default and optimized Ks are still too high (i.e. values in Figure 4). Other than this, the optimization approach is good.

- We have sampled K_s in log space in the revised manuscript (L. 256-257 in manuscript_revised.pdf):

"Note that for the K_s parameter, the random sampling was performed from a logarithmic distribution [*Ireson et al.*, 2009]."

Towards a simple representation of chalk hydrology in land surface modelling

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Abstract

Modelling and monitoring of hydrological processes in the unsaturated zone of chalk, a porous medium with fractures, is important to optimize water resources assessment and management practices in the United Kingdom (UK). However, incorporating the processes governing water movement through chalk unsaturated zone in a numerical model is complicated mainly due to the fractured nature of chalk that creates high-velocity preferential flow paths in the subsurface. In general, flow through chalk unsaturated zone is simulated using dual-porosity concept, which often involves calibration of relatively large number of model parameters, potentially undermining applications to large regions. ~~Therefore, this approach may be not be suitable for large-scale land surface modelling applications.~~ In this study, a simplified parameterization, namely the Bulk Conductivity (BC) model is proposed for simulating hydrology in chalk unsaturated zone. This new parameterization introduces only two additional parameters (namely the macroporosity factor and the soil wetness threshold parameter for fracture flow activation) and uses the saturated hydraulic conductivity from chalk matrix. The BC model is implemented in the Joint UK Land Environment Simulator (JULES) and applied to a study area encompassing the Kennet catchment in the Southern UK. This parameterization is further calibrated at a point-scale using soil moisture profile observations. The performance of calibrated BC model in JULES is assessed and compared against the performance of both the default JULES parameterization and the uncalibrated version of BC model implemented in JULES. Finally, the model performance at the catchment-scale is evaluated against independent data sets ~~The simulation results are evaluated using field measurements and satellite remote sensing observations of various fluxes and states of the hydrological cycle~~ (e.g., ~~soil moisture,~~ runoff and latent heat flux)~~ at two distinct spatial scales (i.e., point and catchment).~~. The results demonstrate that the inclusion of the BC model in JULES improves simulated land surface mass and energy fluxes over the chalk-dominated Kennet catchment. Therefore, the simple approach described in this study may be used to incorporate the flow processes through chalk unsaturated zone in large-scale land surface modelling applications.

Keywords: Chalk hydrology, macroporosity, land surface model, bulk conductivity model.

1. Introduction

Chalk can be described as a fine-grained porous medium traversed by fractures [*Price et al.*, 1993]. Previous studies showed that the unsaturated zone of the chalk aquifers plays an important role on groundwater recharge in the UK [e.g., *Lee et al.*, 2006; *Ireson et al.*, 2009]. Therefore, both monitoring [e.g., *Bloomfield*, 1997; *Ireson et al.*, 2006] and modelling [e.g., *Bakopoulou*, 2015; *Brouyère*, 2006; *Ireson and Butler*, 2011, 2013; *Sorensen et al.*, 2014] strategies have been adapted previously to understand the governing hydrological processes in the chalk unsaturated zone.

In chalk, the matrix provides porosity and storage capacity, while the fractures greatly enhance permeability [*Van den Daele et al.*, 2007]. Water movement through chalk matrix is slow due to its relatively high porosity (0.3-0.4) and low permeability (10^{-9}-10^{-8} ms^{-1}). A fractured chalk system, in contrast, conducts water at a considerably higher velocity because of relatively high permeability (10^{-5}-10^{-3} ms^{-1}) and low porosity (of the order 10^{-4}) of fractures [*Price et al.*, 1993].

Simulating water flow through the matrix-fracture system of chalk has been the subject of research for some time. Both conceptual [e.g., *Price et al.*, 2000; *Haria et al.*, 2003] and physics-based [e.g., *Mathias et al.*, 2006; *Ireson et al.*, 2009] models have been proposed previously to describe water flow through chalk unsaturated zone. The physics-based models mentioned above were developed based on dual-continua approach and required relatively large numbers of parameters (i.e., on the order of 20-30 parameters) that were calibrated via inverse modelling using observed soil moisture and matric potential data [e.g., *Ireson et al.*, 2009; *Mathias et al.*, 2006].

In recent years, representation of chalk has gained attention in land surface modelling. For example, *Gascoin et al.* [2009] applied the Catchment Land Surface Model (CLSM) over the Somme River basin in northern France. A linear reservoir was included in the TOPMODEL based runoff formulation of CLSM to account for the contribution of chalk aquifers to river discharge. *Le Vine et al.* [2016] applied the Joint UK Land Environment Simulator (JULES [*Best et al.*, 2011]) over the Kennet catchment in southern England to evaluate the hydrological limitations of land surface models. In that study, two intersecting Brooks and Corey curves were proposed, which allowed a dual curve soil moisture retention representation for the two distinct flow domains of chalk (i.e., matrix and fracture) in the model. Considering this dual Brooks and Corey curve, a three-dimensional groundwater flow model (ZOOMQ3D [*Jackson and Spink*, 2004]) was coupled to JULES to demonstrate the strong influence of representing chalk hydrology and groundwater dynamics on simulated soil moisture and runoff.

The above mentioned studies illustrate the importance of representing chalk in land surface modelling. However, including chalk hydrology in large-scale land surface modelling using the contemporary dual-porosity concept can be complicated due to ~~because this approach generally involves relatively~~ large numbers~~s~~ of additional parameters. In this context, we propose a new parameterization, namely the Bulk Conductivity (BC) model as a first step towards a simple chalk representation suitable for land surface modelling. In order to test the proposed parameterization, the ~~The~~ BC model is included in JULES (version 4.2), which, by default (i.e., uniform soil column representation using general soil database as typically applied in land surface models), does not represent any chalk feature. In this study, the BC model (included in JULES) is ~~and~~ applied ~~evaluated~~ at two distinct spatial scales (i.e., point and catchment). At the point-scale, the proposed ~~BC model~~ parameterization is calibrated ~~evaluated~~ using observed soil moisture profile data. This is achieved by randomly sampling the parameter space and extensively running the model in order to minimize the differences between observed and simulated soil moisture variability at different depths. Finally, the ~~The~~ proposed model is ~~then~~ applied to the Kennet catchment in the Southern England and the fluxes and states of the hydrological cycle are simulated for multiple years. The simulation results are evaluated using observed latent heat flux (LE) and runoff data to assess the performance of the BC model in simulating land surface processes at the catchment scale.

2. A model of flow through chalk unsaturated zone

In this study, the *Bulk Conductivity* (BC) model based on the work by *Zehe et al.* [2001] is incorporated in JULES to represent the flow of water through the fractured chalk unsaturated zone. According to this approach, if the relative saturation (S) exceeds a certain threshold (S_0) at a soil grid, the saturated hydraulic conductivity of chalk matrix (K_s) is increased to a bulk saturated hydraulic conductivity (K_{sb}) as follows

$$K_{sb} = K_s + K_s f_m \frac{S-S_0}{1-S_0} \qquad \text{if } S > S_0 \qquad (1)$$

$$K_{sb} = K_s \qquad \text{if } S <= S_0 \qquad (2)$$

with $S = \frac{\theta-\theta_r}{\theta_s-\theta_r}$

where f_m is a macroporosity factor (-), θ is soil moisture (m^3m^{-3}), θ_s is soil moisture at saturation (m^3m^{-3})~~,~~ and θ_r is the residual soil moisture (m^3m^{-3}). Note that S ranges from zero in case of completely dry soils to one for fully wet soils.

At the first step of evaluation, the K_s, S_0 and f_m parameters are estimated based on existing literature to assess the performance of the uncalibrated BC model.~~ In this uncalibrated BC model, K_s for chalk matrix is 16 mmd^{-1} according to *Le Vine et al.* [2016] for the catchment investigated in this study (Figure 1)~~ For the matrix saturated hydraulic conductivity (K_s), we use K_s = 1.0 mmd^{-1} following *Mathias et al.* [2006]. In addition, Equation 1 indicates that the onset of water flow through the fracture system of chalk is controlled by the threshold S_0. According to *Wellings and Bell* [1980], water flow through fractures dominates over matrix flow in chalk when the pressure head in soil becomes higher than -0.50 mH_2O. We consider a value of S_0 = 0.80 for the uncalibrated BC model, which is based on observed soil moisture-matric potential relationship in the study area~~ (Figure S1)~~.

Finally, In *Zehe et al.* [2001], f_m was defined as the ratio of the saturated water flow rate in all macropores in a model element to the corresponding value in soil matrix, which can be determined based on the density and length of fractures at small scales. In addition, f_m has also been considered as a calibration parameter previously [e.g., *Blume*, 2008; *Zehe et al.*, 2013]. In this study, we define f_m as a characteristic soil property reflecting the influence of fractures on soil water movement [*Zehe and Blöschl*, 2004]~~,~~ and estimate it from the relative difference of permeability between chalk matrix and fractured chalk system that can be of the order 10^4-10^6 according to *Price et al.* [1993~~9~~]. Consequently, we consider a macroporosity factor of $f_m = 10^5$ for the uncalibrated BC model. In the following step, the BC model is calibrated to minimize the differences between the variability of observed and simulated soil moisture at individual depths. The calibration strategy will be discussed elaborately in section 3.5.

~~In the following step, the BC model parameters are optimized to minimize the differences between the variability of observed and simulated soil moisture. Price et al. [1999] argued that the K_s for chalk matrix is generally around 3-5 mmd^{-1} (3.5-5.8x10^{-5} mms^{-1}). In order to optimize the BC model performance, we consider a range of K_s = 0.8-86 mmd^{-1} (10^{-5}-10^{-3} mms^{-1}) for chalk matrix in this study. As mentioned earlier, S is zero for completely dry soils and one in case of fully wet soils. Therefore, we consider a range of 0-1.0 for S_0 to optimize the BC model. For f_m, a range of 10^4-10^6 is considered, which, as discussed earlier, is consistent with the relative difference between the permeability of fractured chalk and chalk matrix according to *Price et al* [1999].~~

~~We use the Root Mean Squared Error (RMSE) as the objective function to optimize the BC model parameters [e.g., *Ireson et al.*, 2009]~~

$$RMSE = \frac{1}{nd}\sum_{1}^{nd}\sqrt{\left(\frac{1}{nt-1}\sum_{2}^{nt}\left(\Delta\theta_{d,t}^{obs} - \Delta\theta_{d,t}^{sim}\right)^2\right)} \quad (2)$$

~~where *nd* is the number of soil layers, *nt* is the number of soil moisture observations available for a layer *d*, $\Delta\theta^{obs}$ is the observed variability of soil moisture and $\Delta\theta^{sim}$ is the simulated variability of soil moisture. Note that we consider $\Delta\theta$ for this optimization because of its relevance to the water flux and recharge through chalk unsaturated zone [e.g., *Ireson and Butler*, 2011]. Latin hypercube technique [e.g., *McKay et al.*, 2016] is used to generate 2000 random samples for each BC model parameter within the respective range discussed above. We perform simulations using these random samples and calculate model performance (Equation 2) to select the optimum parameter values for the BC model (discussed in section 4.1).~~

3. Methods

3.1. Study area

The study area encompasses the Kennet catchment located in the Southern England with an area of about 1033 km^2 (Figure 1a). Generally, Kennet is rural in nature with scattered settlements and has a maximum altitude of approximately 297 m (Above Ordnance Level). The River Kennet discharges into the North Sea through London. The major tributaries of this river are Lambourn, Dun, Enborne, and Foudry Brook. An average annual rainfall of approximately 760 mm was recorded in the catchment over a 40 year period from 1961-1990.

Solid geology of the Kennet catchment is dominated by chalk, which is overlain by thin soil layer. While lower chalk outcrops along the northern catchment boundary, progressively younger rocks are found in the southern part. In general, surface runoff production is very limited over the regions of the catchment where chalk outcrops. The flow regime shows a distinct characteristics of slow response to groundwater held within the chalk aquifer [*Le Vine et al.*, 2016]. According to *Ireson and Butler* [2013], the unsaturated zone of chalk shows slow drainage over summer and bypass flow during wet periods in this catchment.

3.2. Field measurements and remotely sensed data

Table 1 summarizes the field measurements and remote sensing data used in this study. We use *in-situ* soil moisture and runoff measurements along with remotely sensed LE data to assess model performance in simulating the mass and energy balance components of the hydrological cycle. Point scale soil moisture measurements at two adjacent sites (~20 m apart) at the Warren Farm (Figure 1) were provided by Centre for Ecology and Hydrology (CEH). A Didcot neutron probe was used at these locations to measure fortnightly soil moisture at different depths below land surface (10 cm apart down to 0.8 m, 20 cm apart between 0.8-2.2 m, and 30 cm apart between 2.2-4.0 m) [*Hewitt et al.*, 2010].

The National River Flow Archive (NRFA) coordinates discharge measurements from the gauging station networks across UK. These networks are operated by the Environmental

Agency (England), Natural Resources Wales, Scottish Environment Protection Agency, and Rivers Agency (Northern Ireland). We use discharge measurements provided by NRFA to ~~calculate the runoff ratio over the Kennet catchment in this study~~ assess model performance in simulating runoff over the Kennet catchment in this study.

The MOD16 product of the Moderate Resolution Imaging Spectroradiometer (MODIS) is a part of NASA/EOS project that provides estimation of global terrestrial LE. The LE estimation from MOD16 is based on remotely sensed land surface data [e.g., *Mu et al.*, 2007]. In this study, the 8-day and monthly LE data products from MODIS is used to evaluate the model performance in simulating land surface energy fluxes.

3.3. Land surface model

In this study, we use the Joint UK Land Environment Simulator (JULES [e.g., *Best et al.*, 2011; *Clark et al.*, 2011]) version 4.2. JULES is a flexible modelling platform with a modular structure aligned to various physical processes developed based on the Met Office Surface Exchange Scheme (MOSES [e.g., *Cox et al.*, 1999; *Essery et al.*, 2003]). Meteorological data including precipitation, incoming short- and longwave radiation, temperature, specific humidity, surface pressure, and wind speed are required to drive JULES. Each grid box in JULES can comprise nine surface types (broadleaf trees, needle leaf trees, C3 grass, C4 grass, shrubs, inland water, bare soil, and ice) represented by respective fractional coverage. Each surface type is represented by a tile and a separate energy balance is calculated for each tile.

Subsurface heat and water transport equations are solved based on finite difference approximation in JULES as described in *Cox et al.* [1999]. Moisture transport in the subsurface is described by the finite difference form of Richards' equation. The vertical soil moisture flux is calculated using the Darcy's law. While the top boundary condition to solve the Richards' equation is infiltration at soil surface, the bottom boundary condition in JULES is free drainage that contributes to subsurface runoff.

Surface runoff is calculated by combining the equations of throughfall and grid box average infiltration in JULES. In order to direct the generated runoff to a channel network, river routing is implemented based on the discrete approximation of one-dimensional kinematic wave equation [e.g., *Bell et al.*, 2007]. In this approach, river network is derived from the digital elevation model (DEM) of the study area and different wave speeds are applied to surface and subsurface runoff components and channel flows [e.g., *Bell and Moore*, 1998]. A return flow term accounts for the transfer of water between subsurface and land surface [e.g., *Dadson et al.*, 2010, 2011].

3.4. Model configurations and input data

In this study, simulations are performed at two distinct spatial scales, namely point and catchment. At the point scale, JULES is configured to simulate the mass and energy fluxes at the Warren Farm site (Figure 1a). A total subsurface depth of 5 m is considered in the model with a vertical discretization ranging from 10 cm at the land surface to 50 cm at the bottom of the model domain. Note that this discretization is consistent with the soil moisture measurement depths mentioned in section 3.2. The vegetation type is implemented as C3 grass using the default parameters in JULES. Point scale simulations were performed over 2 consecutive years from 2003-2005 at an hourly time step. Except for precipitation, hourly atmospheric forcing data to drive JULES was obtained from an automatic weather station operated by the CEH at Warren Farm. In order to estimate hourly precipitation data to run JULES, rain gauge measurements from the Met Office [*Met Office*, 2006] were used. Inverse distance interpolation technique [e.g. *Garcia et al.*, 2008; *Ly et al.*, 2013] was applied on rainfall measurements from 13 gauges closest to Warren Farm (distance varies from 25-60 km) to obtain hourly precipitation for the point scale simulations.

At the catchment scale, JULES is configured over a study area encompassing the Kennet catchment (Figure 1a) considering a uniform lateral grid resolution of 1 km with 70 x 40 cells in *x* and *y* dimensions, respectively. The total subsurface depth and vertical discretization are identical to those of the point scale simulations. Spatially distributed vegetation type information for the study area (Figure 1b) is obtained from the Land Cover Map 2007 (LCM2007) dataset [*Morton et al.*, 2011]. Simulations were performed over 5 consecutive years from 2006-2011 at the catchment scale. Note that the simulation periods of catchment and point scale (2003-2005) do~~es~~ not coincide due to the availability of soil moisture measurements described in section 3.2. Spatially distributed meteorological data from the Climate, Hydrology and Ecology research Support System (CHESS) was used to obtain the atmospheric forcing to drive JULES at the catchment scale. The CHESS data includes 1 km resolution gridded daily meteorological variables [*Robinson et al.*, 2015]. This daily data is downscaled using a disaggregation technique described in *Williams and Clark* [2014] to obtain hourly atmospheric forcing. The flow direction required for river routing is extracted from the USGS HydroSHEDS digital elevation data [*Lehner et al.*, 2008].

We estimate the soil hydraulic properties based on texture (Table 2). At the point scale, loam soil is dominant at the Warren Farm site. At the catchment scale, the Harmonized World Soil Database (HWSD) from the Food and Agricultural Organization of UNO (FAO) is used to obtain the texture of different soil types over Kennet (Figure 1c). The saturation-pressure head relationship for different soil types is described using the Van Genuchten [*Van Genuchten*, 1980] model with parameter values (Table 2) obtained from *Schaap and Leij* [1998].

~~Table 3 summarizes t~~The hydraulic properties for chalk used in this study are summarized in Table 3. These properties are obtained based on existing literature as a first step when evaluating the uncalibrated BC model. The BC model parameters are subsequently ~~optimized~~ calibrated to minimize the differences between observed and simulated $\Delta\theta$ (section 3.5) at various soil depths.

In this study, we consider two different model configurations, namely *default* and *macro* (Figure 2). The *default* configuration corresponds to the standard parameterizations of JULES that does not represent chalk hydrology in the model. In this configuration, each soil column in JULES is considered to be vertically homogeneous with the soil properties defined in Table 2, which is motivated by the Met Office JULES Global Land 4.0 configuration described in *Walters et al.* [2014]. The *macro* configuration, in contrast, explicitly represents chalk by applying the BC model starting at 30 cm below land surface to the bottom of the model domain (i.e. 500 cm). Therefore, the soil column in the *macro* configuration can be divided into topsoil (0-30 cm) and chalk (30-500 cm)~~ in *macro*~~. The topsoil depth of 30 cm ~~in the *macro* configuration~~ is defined based on several augured soil samples collected during a field campaign at Warren Farm in 2015 (Figure 2). This depth is corroborated by additional information from the British Geological Survey (BGS) operated borehole records (http://www.ukso.org/pmm/soil_depth_samples_points.html), which show that topsoil depths vary from 10-40 cm over the study area. We ~~therefore~~ apply the *macro* configuration assuming a spatially homogeneous topsoil depth of 30 cm for both point and catchment scale simulations. Note that except for this inclusion of chalk, *default* and *macro* configurations are identical in terms of model set up and input data. It should also be emphasized that *default* represents a "naïve" configuration deprived of model calibration. Moreover, this configuration does not represent chalk, which, according to previous studies [e.g., *Le Vine et al.*, 2016], substantially affects the hydrology of the study area considered here.

3.5. Calibration of the BC model

We calibrate the BC model at the point-scale to minimize the differences between observed and simulated soil moisture variability ($\Delta\theta$) at different depths. The Root Mean Squared Error (RMSE) is used as the objective function to optimize the BC model parameters [e.g., *Ireson et al.*, 2009]

$$RMSE = \frac{1}{nd}\sum_{1}^{nd}\sqrt{\left(\frac{1}{nt-1}\sum_{2}^{nt}\left(\Delta\theta_{d,t}^{obs} - \Delta\theta_{d,t}^{sim}\right)^2\right)} \qquad (3)$$

where *nd* is the number of soil layers, *nt* is the number of soil moisture observations available for a layer *d*, $\Delta\theta^{obs}$ is the observed variability of soil moisture and $\Delta\theta^{sim}$ is the simulated variability of soil moisture. Note that we consider $\Delta\theta$ for this optimization because of its relevance to the water flux and recharge through chalk unsaturated zone [e.g., *Ireson and Butler*, 2011].

Equation (1) reveals that the calibration of the BC model involves optimizing 3 parameters, namely the saturated hydraulic conductivity of chalk matrix (K_s), saturation threshold (S_0) and macroporosity factor (f_m). *Ireson et al.* [2009] suggested a range of 0.2-2.0 mmd^{-1} for K_s. On the other hand, *Price et al.* [1993] argued that in general, K_s is around 3-5 mmd^{-1} for most chalk soils. Therefore, we consider a range of 0.2-5.0 mmd^{-1} in optimizing K_s. We consider S_0 range 0-1, representing the entire physical domain for soil wetness from fully dry to fully wet, respectively. ~~As mentioned earlier, *S* is zero for completely dry soils and one in case of fully wet soils. Consequently, we consider S_0 = 0.0-1.0 in the optimization.~~ For f_m, a range of 10^4-10^6 is considered, which, as discussed earlier, is consistent with the relative difference between the permeability of fractured chalk and chalk matrix according to *Price et al* [1993]. Latin hypercube sampling technique [e.g., *McKay et al.*, 2016] is used to generate 2,000 random samples for each BC model parameter within the ranges discussed above. Note that for the K_s parameter, the random sampling was performed from a logarithmic distribution

[*Ireson et al.*, 2009]. We perform simulations using these random samples and calculate model performance (Equation 3) to select the optimum parameter values for the BC model for each possible parameter combination as discussed in details in the following section.

4. Results and discussion

4.1. Point scale simulations

At the point scale, the simulation results are evaluated using soil moisture observations at the Warren Farm site. Figure 3a compares observed and simulated soil moisture (θ) from the *default* and *macro* configurations at 2 m below land surface. Note that the *macro* configuration uses the chalk hydraulic parameters collected from existing literature (Table 3). This figure shows that the *default* configuration considerably underestimates θ throughout the simulation period, which is improved remarkably in case of *macro*. Figure 3b plots observed and simulated soil moisture variability ($\Delta\theta$) from the *default* and *macro* configurations ($\Delta\theta_{default}$ and $\Delta\theta_{macro}$, respectively) at the Warren Farm site. In general, both configurations show discrepancies with observed $\Delta\theta$ with *macro* showing relatively better model performance.

The results show that despite the *macro* configuration improves simulated θ, it shows considerable discrepancies with observed $\Delta\theta$, which is consistent throughout the whole chalk profile (results from other model layers are not shown). In order to minimize the differences between observed and modelled $\Delta\theta$ from the *macro* configuration, we calibrate ~~optimize~~ the BC model following the methodology described in section 3.5~~2~~. The optimization results are summarized in Figure 4. Note that for each combination considered in the optimization, 2,000 model runs were performed using randomly sampled parameters as discussed in section 3.5~~2~~. In addition to the *default* and *macro* cases, the calibrated cases in Figure 4 ~~presents~~

correspond to the results from the model runs yielding the lowest RMSE for each parameter combination evaluated.

The RMSE between observed and simulated $\Delta\theta$ for the model configurations considered in the optimization is shown in Figure 4a. This figure illustrates that the RMSE of the *default* configuration is larger than that of *macro*, indicating better model performance in reproducing $\Delta\theta$ for the latter (corresponding to a reduction of 15% in RMSE compared to the *default* case). Therefore, ~~it appears that~~ the uncalibrated BC model (i.e., ~~the~~ *macro* configuration) ~~is~~ better ~~in reproducing~~ reproduces the soil moisture variability compared to *default*. ~~Figure 4b, c and d presents the BC model parameter values from the model run producing the lowest RMSE for each configuration.~~ Concerning the calibration of single BC model parameters, Figure 4a shows that ~~optimizing~~ S_0 results in a 46% ~~16%~~ reduction of RMSE compared to the *macro* configuration. Calibrating ~~Optimizing~~ K_s ~~marginally improves model performance, which is observed from a slightly lower (4%) RMSE than~~ ~~*macro*~~ or f_m individually yields only about 25% reduction of RMSE compared to *macro*.

Optimizing both K_s and S_0 simultaneously shows ~~results in~~ the largest reduction (50~~24~~%) of RMSE compared to *macro* which coincides with the total RMSE reduction found when all parameters are calibrated. Arguably, the BC model can be implemented in other chalk regions by constraining only S_0 parameter. Such result could potentially be advantageous for transferability to other regions in the UK in order to assess chalk hydrology at large-scale. However since this is the first time the BC model is introduced, we decide to take a conservative approach and select the *macro* configuration with optimized K_s and S_0 (*macro*$_{opt}$ hereafter) to simulate chalk hydrology over the study area that ensures best overall model performance.

The lower three panels in Figure 4 presents the BC model parameter values for the *default* and uncalibrated *macro* cases as well as for different combinations of parameters calibrated. The red bars in Figure 4a, b and c highlight the cases in which a given parameter is constrained by optimization. In those cases, the calibrated parameter values are obtained from model runs producing the lowest RMSE. An interesting feature in Figure 4b (calibrating K_s individually) is that the optimization suggests a compensation mechanism in which K_s is increased remarkably in order to physically represent the “effective” flow through the chalk fractures in the BC model. This is not surprising and arguably the simplest way to attempt to improve model performance. For $macro_{opt}$, the values used for K_S is relatively lower than that of uncalibrated *macro* case nevertheless consistent with previous estimates [e.g., *Ireson et al.*, 2009]. Figure 4c clearly shows the dominance of S_0 in the BC model as all the relatively low RMSE bars in Figure 4a are associated with S_0 calibration (see red bars in Figure 4c). In addition, calibrated S_0 values for all cases show a consistent constraint around 0.50. Finally, Figure 4d indicates the lack of influence for f_m parameter on model performance.

~~Additionally, Figure 4 suggests that the sensitivity of S_0 on the model performance in simulating $\Delta\theta$ is substantially higher compared to K_s and f_m, which is corroborated by the sensitivity of the individual model parameters (Figure S2). Figure 4a also reveals the interesting fact that the RMSE from the configuration with optimized K_s and S_0 is identical to that of the one with all 3 parameters optimized simultaneously (i.e., K_s, S_0 and f_m). Therefore, we select the *macro* configuration with optimized K_s and S_0 ($macro_{opt}$ hereafter) to simulate chalk hydrology over the study area.~~

Figure 5 compares $\Delta\theta_{default}$, $\Delta\theta_{macro}$ and $\Delta\theta$ from the $macro_{opt}$ configuration ($\Delta\theta_{opt}$) with observed soil moisture variability ($\Delta\theta_{obs}$). As mentioned earlier, $\Delta\theta_{default}$ and $\Delta\theta_{macro}$ show considerable discrepancies with $\Delta\theta_{obs}$ while the *macro* configuration exhibits relatively better performance (Figure 3). Figure 5 illustrates that the overall agreement between observed and simulated $\Delta\theta$ improves substantially in case of *macro*$_{opt}$ compared to *default* and *macro*, which is pronounced especially in the deeper chalk layers. Therefore, this figure indicates that the performance of the BC model in simulating $\Delta\theta$ is further improved by optimizing the K_s and S_0 parameters simultaneously at the Warren Farm site.

~~In order to assess the model performance in simulating soil moisture over the entire column, the relative bias (Δμ, see Appendix) of simulated θ from the *default* and *macro*$_{opt}$ configurations at Warren Farm for various depth ranges are shown in Figure 6. In the soil layers (0-30 cm), θ from the two configurations are comparable with the *default* showsing slightly lower mean relative bias (Δμ$_{mean}$) of -0.03 than *macro*$_{opt}$ (Δμ$_{mean}$ = -0.12 -0.09). However, in the chalk layers (30-500 cm), *default* simulates substantially drier conditions, corresponding to Δμ$_{mean}$ ≤ -0.28. In contrast, the *macro*$_{opt}$ configuration considerably improves the agreement between the simulated and observed θ in the chalk layers with Δμ$_{mean}$ Δμmean ≥ -0.240.05. Therefore, the results indicate that the inclusion of the BC model in JULES improves the performance of overall soil moisture simulation (both θ and Δθ) at Warren Farm especially in the chalk layers although underestimation of θ compared to measurements was observed for both *default* and *macro*$_{opt}$ configurations.~~

As mentioned earlier, efficiently reproducing soil moisture variability over the profile is important due to the fact that $\Delta\theta$ significantly affects water flux and recharge through chalk unsaturated zone. The drainage flux through the bottom of soil column (d_b) of a land surface model can be considered as the potential recharge flux to groundwater [e.g., *Sorensen et al.*, 2014]. Figure ~~7~~ 6 compares the daily sum of d_b from the *default* and *macro*$_{opt}$ configurations at the Warren Farm site. Daily ~~The~~ rainfall at this site ~~characteristics~~ over the simulation ~~study~~ period is shown in Figure ~~7a~~6a. In Figure ~~7~~6b, the *macro*$_{opt}$ configuration shows considerable d_b during the colder months, while relatively slow drainage is observed in summer~~prevails throughout the rest of the year~~. In contrast, the *default* configuration shows relatively high d_b in summer compared to the colder months. In general, the recharge rate through chalk unsaturated zone during the warmer periods of the year is lower than that in the winter months [*Wellings and Bell*, 1980; *Ireson et al.*, 2009]. Therefore, the $macro_{opt}$ configuration appears to be more consistent with the recharge mechanism in chalk compared to *default*.

In this section, the BC model was evaluated at the point scale. The results showed that in general, the *macro* configuration outperforms the *default* case ~~relatively better in~~ in simulating ~~θ and~~ $\Delta\theta$ ~~compared to *default*~~. In order to improve the model performance even further, model parameter calibration ~~parameter optimization~~ was performed to minimize the differences between observed and simulated $\Delta\theta$ at the point scale. In the next sections, the optimized model ($macro_{opt}$) is evaluated at the catchment scale.

4.2. Catchment scale simulations

~~In the previous section, it was observed that the *default* configuration generally underestimates θ compared to $macro_{opt}$. Previous studies have demonstrated the interconnections between shallow soil moisture and LE [e.g., *Chen and Hu*, 2004].~~ At the catchment scale, simulation results from the *default* and $macro_{opt}$ configurations are compared with the observations over the Kennet catchment. In order to assess the differences between ~~the~~ LE from the *default* and $macro_{opt}$ configurations at the catchment scale, Figure ~~8~~ 7 plots spatially averaged 8-day composites of LE from MODIS (LE_{MOD}) against the LE from these configurations ($LE_{default}$ and LE_{opt}, respectively) over Kennet. The agreement between simulated LE and LE_{MOD} is evaluated using the coefficient of determination (R^2, see Appendix) and mean bias. Comparison between $LE_{default}$ and LE_{MOD} shows a coefficient of determination of $R^2_{default} = 0.78$ and a mean bias of $bias_{default} = 10.5$ Wm^{-2}. The agreement between simulated LE and LE_{MOD} improves in case of the $macro_{opt}$ configuration, which is reflected by an increased coefficient of determination of R^2_{opt} = 0.80~~0.81~~ and a reduced mean bias of $bias_{opt}$ = 7.1~~3~~ Wm^{-2}.

Figure 7~~8~~ shows considerable differences between $LE_{default}$ and LE_{opt} ~~especially~~ for relatively high LE, indicating discrepancies especially during the warmer months of the year. ~~Figure 9a presents s~~Spatially averaged time series of monthly LE_{MOD}, $LE_{default}$ and LE_{opt} is presented in Figure 8a. ~~.~~This figure shows that the differences between $LE_{default}$ and LE_{opt} increases ~~substantially~~ in summer compared to the colder months of the year, which is consistent with Figure ~~8~~7. Consequently, the *default* configuration underestimates LE in summer compared to LE_{MOD}, which is improved in case of the $macro_{opt}$ configuration. In contrast, the differences between $LE_{default}$ and LE_{opt} are negligible during the colder months of the year.

In addition, Figure ~~9~~8b compares the observed and simulated monthly average discharge from the two model configurations at the "Kennet at Theale" gauging station (Figure 1a). This figure depicts that the *default* configuration generally overestimates discharge at this gauging station, which is improved considerably in the case of $macro_{opt}$. We use the Kling-Gupta Efficiency criteri~~a~~on (KGE [*Gupta et al.*, 2009]) to compare the performance of the two model configurations in reproducing observed discharge variability. As mentioned above, the *default* configuration overestimates discharge with $KGE_{default}$ = -0.17. On the other hand, the $macro_{opt}$ configuration improves the agreement between observed and simulated discharge, which is reflected by KGE_{opt} = 0.51.

In order to summarize the results at catchment scale, Table 4 compares observed and simulated ~~daily average~~ runoff from the two model configurations over the Kennet catchment from 2006-2011. The runoff ratio (*RR*, see Appendix), which is equal to the mean volume of flow divided by the volume of precipitation [e.g., *Kelleher et al.*, 2015], assesses the partitioning of precipitation into runoff over the catchment. The *default* configuration (*RR* =

0.82) shows considerably higher *RR* compared to observation (*RR* = 0.40), indicating overestimation of runoff by the model that is consistent with Figure ~~9~~8b. Including chalk hydrology in the model remarkably improves the agreement between observed and simulated mean runoff over the Kennet catchment, which is assessed from a runoff ratio of *RR* = 0.46 ~~0.37~~ for the $macro_{opt}$ configuration which is much closer to the observed RR value than *default*.

In Table 4, the relative bias (Δμ) of 1.04 between observed and simulated runoff from the *default* configuration again indicates the overestimation by the model. In comparison, $macro_{opt}$ shows a smaller relative bias of~~(~~ Δμ = 0.12~~ 0.05)~~, indicating improved~~ment~~ agreement between observed and simulated mean runoff volume compared to *default*. The relative difference in standard deviation (Δσ, see Appendix) compares the variability of observed and simulated flow ~~runoff~~ in Table 4 relating directly to the seasonal change in runoff. This comparison shows that the *default* configuration overestimates the variability of runoff over the Kennet catchment (Δσ = 2.04), which is improved in case of *macro* (Δσ = 0.65~~0.70~~). This improvement in reproducing flow variability is also clearly observed in Figure 8b.

~~It was demonstrated previously that the *default* configuration predicts lower evapotranspiration (ET) compared to $macro_{opt}$ over the Kennet catchment due to the differences in simulated θ. In JULES, moisture from soil and canopy is depleted to meet the ET demand. Additionally, surface runoff generation depends on canopy water storage in the model [*Best et al.*, 2011]. Because of this connection between ET and surface runoff generation via canopy water storage, the differences in runoff demonstrated in Table 4 can be attributed to the disagreements between $LE_{default}$ and LE_{macro} (Figure 8) due to the relatively drier conditions simulated by *default*.~~

In this section, the BC model is evaluated using observed mass and energy fluxes over the Kennet catchment. The *default* configuration ~~showed considerably~~ suggested relatively low summertime LE over the catchment~~, which was pronounced during the warmer period of the year~~. The agreement between observed and simulated LE was improved in case of the $macro_{opt}$ configuration compared to *default*. It was also observed that the overall runoff prediction was considerably improved by $macro_{opt}$ compared to *default*. Given its simplicity, our results indicate that the proposed parameterization is suitable for use in land surface modelling applications.

5. Summary and Conclusions

In this study, we proposed a simple parameterization, namely the *Bulk Conductivity* (BC) model to simulate water flow through the matrix-fracture system of chalk in large scale land surface modelling applications. This parameterization was implemented in the Joint UK Land Environment Simulator (JULES) and applied to the Kennet catchment located in the southern UK to simulate the mass and energy fluxes of the hydrological cycle for multiple years. Two model configurations, namely *default* and *macro* were considered with the latter using the BC model to simulate chalk hydrology.

The proposed BC model is a single continuum approach of modelling preferential flow [e.g., *Beven and Germann*, 2013] that involves only 3~~2~~ parameters, namely the saturated hydraulic conductivity of chalk matrix (K_s), macroporosity factor (f_m) and relative saturation threshold (S_0). Initially, these parameters ~~along with the saturated hydraulic conductivity of the chalk matrix~~ were estimated from existing literature to assess the performance of the uncalibrated BC model. Finally, the BC model parameters were optimized to minimize the differences between observed and simulated soil moisture variability. Our results indicated that S_0 is by far the most influential parameter in the model when representing water movement through a soil-chalk column. This highlights the simplicity of the proposed BC model for large-scale studies and potential ease in transferability. ~~followed by~~ In comparison, ~~Parameters~~ K_s ~~the saturated hydraulic conductivity of chalk matrix while~~ and f_m showed secondary (low) sensitivity on the model performance. Since this study introduces the BC model, we decided however to take a conservative approach. ~~Motivated by the sensitivity analysis, we~~ We optimized K_s and S_0 simultaneously for our catchment scale simulations since this combination resulted in the best overall model performance~~in the next step that considerably improved the agreements between observed and simulated soil moisture variability. Note that calibrating the BC model involves optimizing only 2 out of 3 parameters. This reduced complexity may add considerable benefits in applying the proposed model over large areas. Hence, the parameterization is further improved by optimizing both saturated hydraulic conductivity of chalk matrix and S_0 to minimize the differences between observed and simulated soil moisture variability~~.

~~The simulation results were evaluated using observed mass and energy fluxes both at point and catchment scales. The results demonstrated that the inclusion of the BC model in JULES improves simulated soil moisture variability at the point scale compared to a model configuration that does not represent chalk in the subsurface (i.e., the *default* configuration).~~ At the catchment scale, ~~it was illustrated that~~ the proposed BC parameterization improved~~s~~ simulated latent heat flux (especially in summer) and the overall runoff compared to ~~the~~ *default* ~~configuration~~.

Note that the complexity (i.e., number of parameters) of the BC model for simulating water flow through chalk unsaturated zone is substantially lower compared to more commonly used models for this purpose (e.g., dual-porosity models). Despite its simplicity, ~~it appears that~~ the proposed parameterization considerably improves the key hydrological ~~mass and energy~~ fluxes simulated by JULES ~~over the Kennet~~ at the catchment~~-~~-scale. ~~As mentioned previously, representing chalk hydrology in land surface models using the dual-porosity concept is complicated mainly due to the relatively large number of parameters involved in such approach.~~ Therefore, the ~~simplified aspect of the~~ BC model ~~parameterization proposed in this study may~~ can potentially be useful for ~~large-scale~~ land surface modelling applications over large-scale chalk-dominated areas.

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Appendix

Definition of Statistical Metrics

Coefficient of determination (R^2) for observation y = y1, …, yn and prediction f = f1, …, fn is defined as

$$R^2 = 1 - \frac{SS_{res}}{SS_{tot}}$$

where SS_{res} is the residual sum of square and SS_{tot} is the total sum of square. SS_{res} and SS_{tot} are defined as

$$SS_{res} = \sum_{i=1}^{n}(y_i - f_i)^2 \quad \text{and}$$

$$SS_{tot} = \sum_{i=1}^{n}(y_i - \bar{y})^2 \quad \text{with } \bar{y} \text{ being the mean of y.}$$

Runoff ratio (RR) assesses the portion of precipitation that generates runoff over the catchment. RR is defined as

$$RR = \frac{\mu_{runoff}}{\mu_{rain}}$$

where μ_{runoff} is mean runoff and μ_{rain} is mean precipitation [e.g., *Kelleher et al.*, 2015].

Relative bias ($\Delta\mu$) between observed and simulated time series can be defined as

$$\Delta\mu = \frac{\mu_{mod} - \mu_{obs}}{\mu_{obs}}$$

where μ_{obs} and μ_{mod} are the mean of observed and simulated time series, respectively. While the optimal value of $\Delta\mu$ is zero, negative (positive) values indicate an underestimation (overestimation) by the model [e.g., *Gudmundsson et al.*, 2012].

Relative difference in standard deviation ($\Delta\sigma$) between observed and simulated time series can be defined as

$$\Delta\sigma = \frac{\sigma_{mod} - \sigma_{obs}}{\sigma_{obs}}$$

where σ_{obs} and σ_{mod} are the standard deviation of observed and simulated time series, respectively [e.g., *Gudmundsson et al.*, 2012].

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Tables

Table 1. Field measurements and remote sensing data.

Data	Spatial scale	Temporal extent	Frequency	Source
Soil moisture	Point[a]	2003-2005	15 day	N. Hewitt (CEH)
Latent heat flux	Global	2006-2011	8 day, 1 month	MODIS
Discharge	Point[b]	2006-2011	1 day	NRFA

[a]Measured at Warren Farm.
[b]Locations are shown in Figure 1a.

Table 2. Hydraulic properties for different soil types (refer to Figure 1c). Saturated hydraulic conductivity (K_s) and porosity data are obtained from *Rawls et al.* [1982]. The Van Genuchten parameters are acquired from *Schaap and Leij* [1998].

Texture	**K_s (mm-d^{-1})**	**Porosity (-)**	**α (m^{-1})**	**n (-)**
Loam	320	0.463	3.33	1.56
Silt loam	172	0.50	1.2	1.39
Clay	15	0.475	2.12	1.2

Table 3. Hydraulic properties of chalk

Properties	**Uncalibrated**		**Range for calibration**	**Calibrated value**
	Value	**Source**		
K_s (mm-d^{-1})	1.0	Price et al., 1993	0.2 - ~~2~~5.0	0.31
S_0 (-)	0.8	Observations	0.0 - 1.0	0.46
f_m (-)	~~1x~~10^5	Price et al., 1993	~~1x~~10^4 - ~~1x~~10^6	~~1x~~10^{5*}
α (m^{-1})	3.0	Le Vine et al., 2016	-	-
n (-)	1.4	Le Vine et al., 2016	-	-

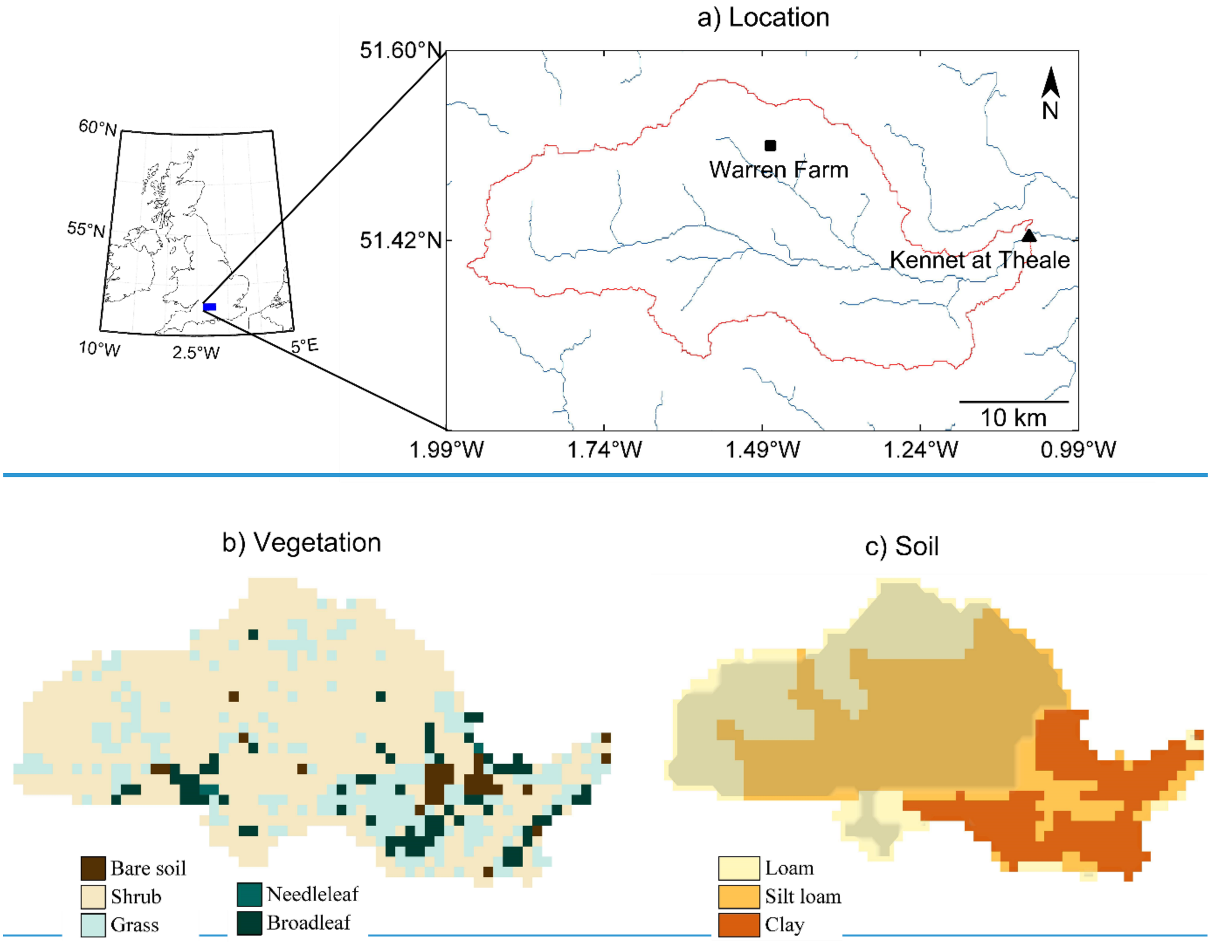
* f_m parameter not calibrated

Table 4. Comparison between observed and simulated daily average runoff from the two configurations over the Kennet catchment. Metrics include the Runoff Ratio (RR), relative bias ($\Delta\mu$), and relative difference in standard deviation ($\Delta\sigma$) (refer to appendix for further information).

Metric	Observed	Simulated (*default*)	Simulated (*macro*)
RR	0.40	0.82	0.46~~0.37~~
$\Delta\mu$	-	1.04	0.12 ~~0.05~~
$\Delta\sigma$	-	2.04	0.65~~0.70~~

Figures

Figure 1. (a) Location ~~(a)~~, (b) vegetation cover ~~(b),~~ and (c) soil texture ~~(c)~~ over the study area. The red line in (a) outlines the Kennet catchment boundary, while the river network is shown in blue. The black triangle in (a) shows the location of the discharge gauging station at the catchment outlet and ~~while~~ the black square corresponds to Warren Farm location where point-scale simulations are carried out. The black line in (c) encloses the area of the catchment where chalk is present. ~~The shaded area in (c) represents the location of chalk in the catchment.~~



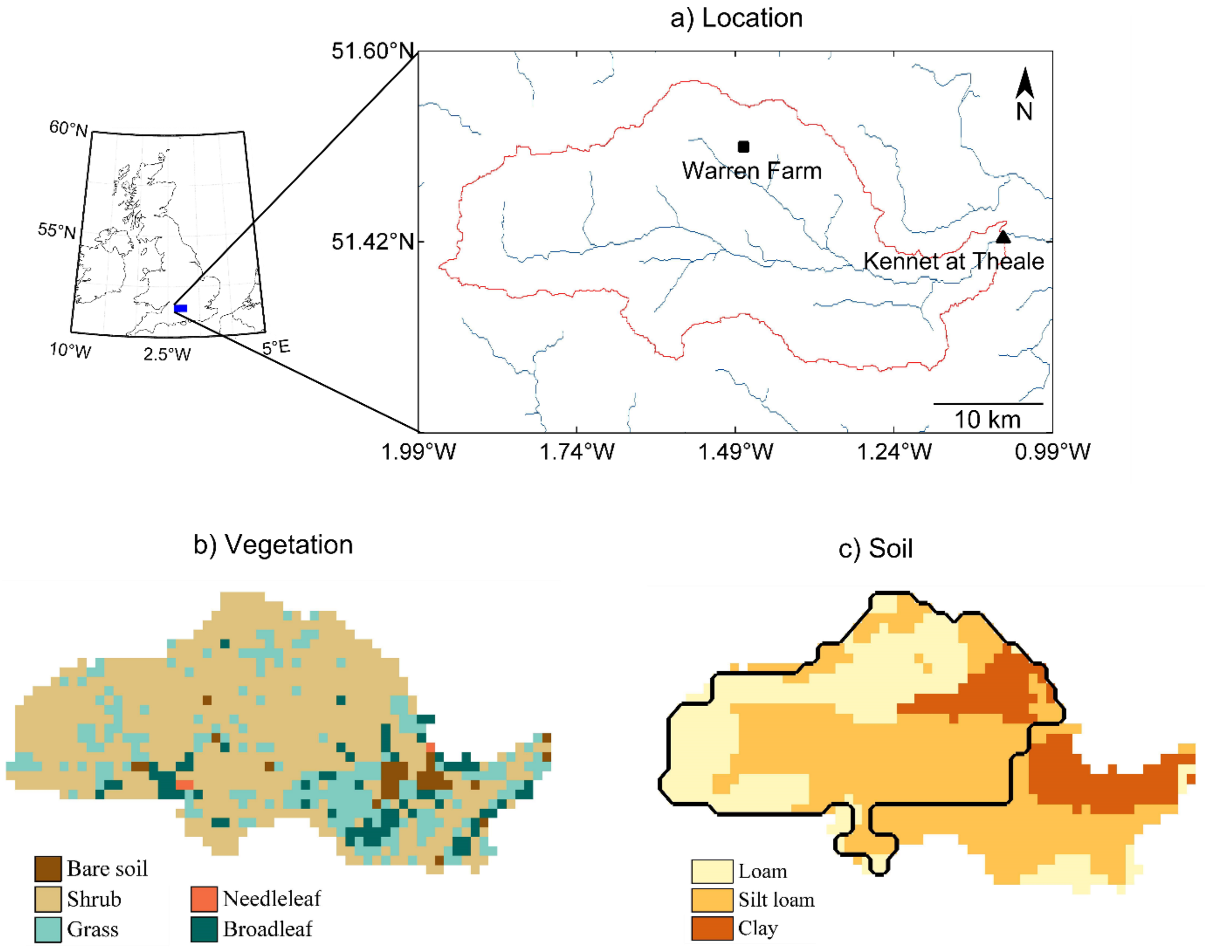


Figure 2. (a) Example of soil profiles collected at Warren Farm during a field campaign in 2015 ~~(a),~~ and (b) the two model configurations ~~(b)~~.

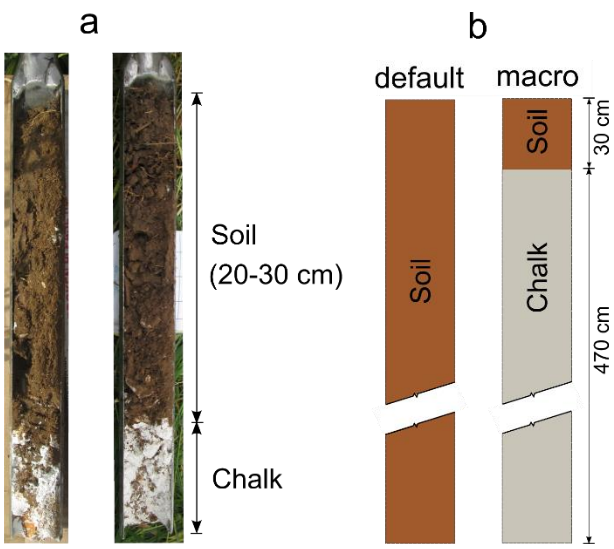
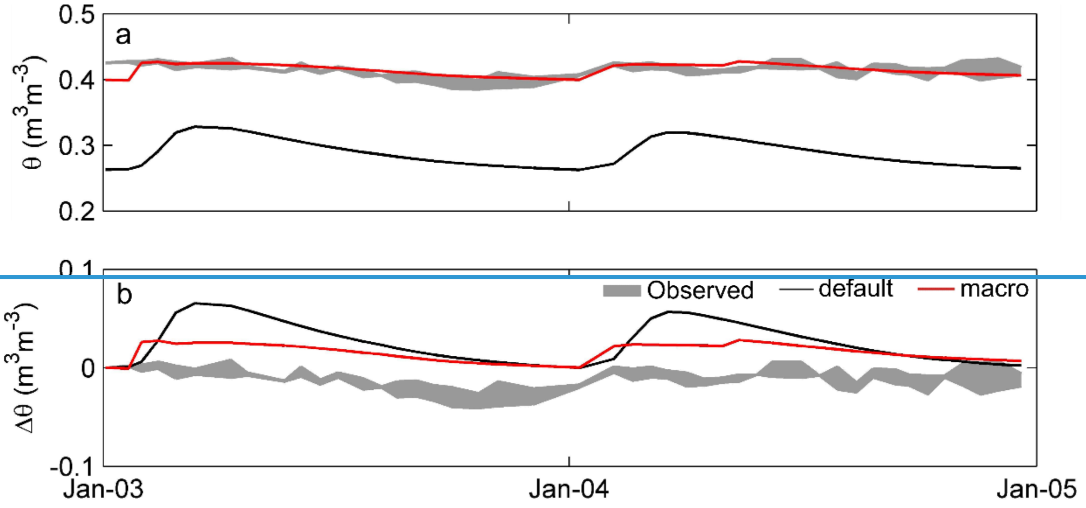


Figure 3. Comparison between observed and simulated (a) soil moisture (θ) and (b) change in soil moisture ($\Delta\theta$) from the *default* and *macro* configurations at a depth of 2 m below land

surface at the Warren Farm site. The shaded areas constructed from 2 soil moisture probes at the Warren Farm site denote the range of observed data in these plots.



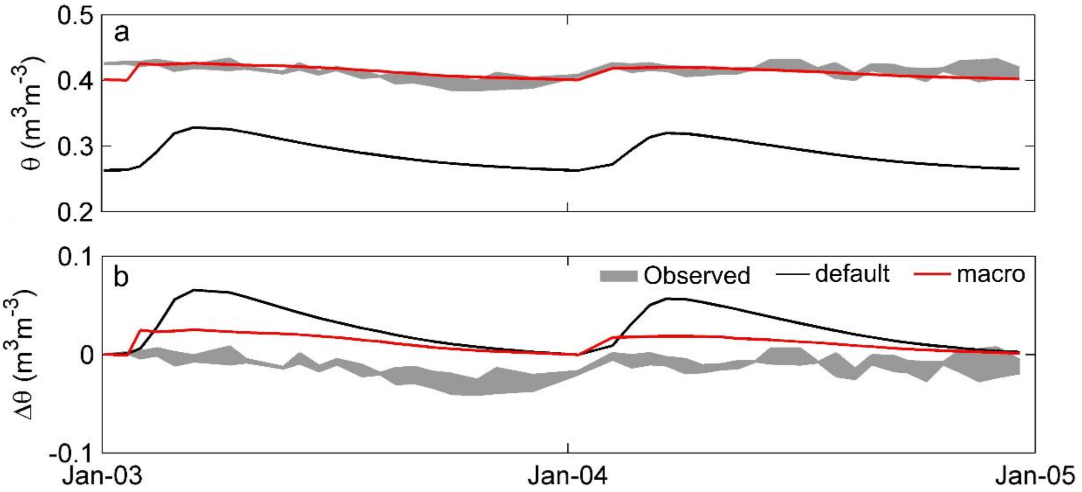
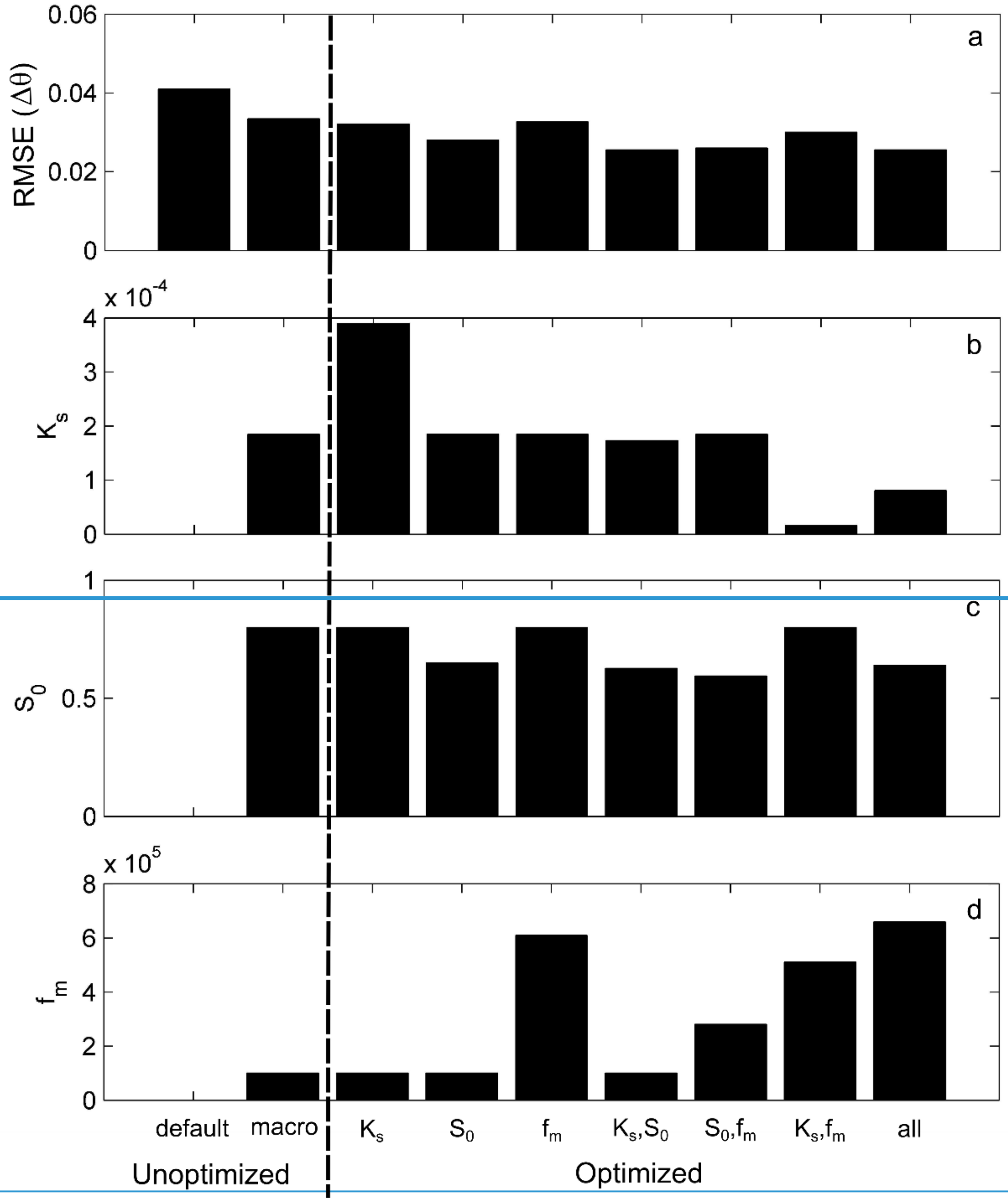


Figure 4. (a) Model performance in reproducing observed and simulated $\Delta\theta$, (b) K_s, (c) S_0 and (d) f_m for ~~various~~ different parameter combinations considered in the optimization. For each parameter (i.e., panels b, c, and d), red bars show cases in which the relevant parameter is calibrated (either individually or in combination with others); while the blue bars correspond to cases in which the selected parameter is not calibrated (i.e., fixed value according to literature as in the *macro* case)~~The uncalibrated model parameter values are shown in blue while red shows the calibrated values in b, c and d.~~ Note that except for the *default* and *macro*, the simulation yielding the lowest RMSE (out of 2,000 model runs) is presented in this plot.

766



0.06
0.04
0.02
0
RMSE (Δθ)
a
x 10^-4
4
3
2
1
0
K_s
b
1
0.5
0
S_0
c
x 10^5
8
6
4
2
0
f_m
d
default
macro
K_s
S_0
f_m
K_s,S_0
S_0,f_m
K_s,f_m
all
Unoptimized
Optimized

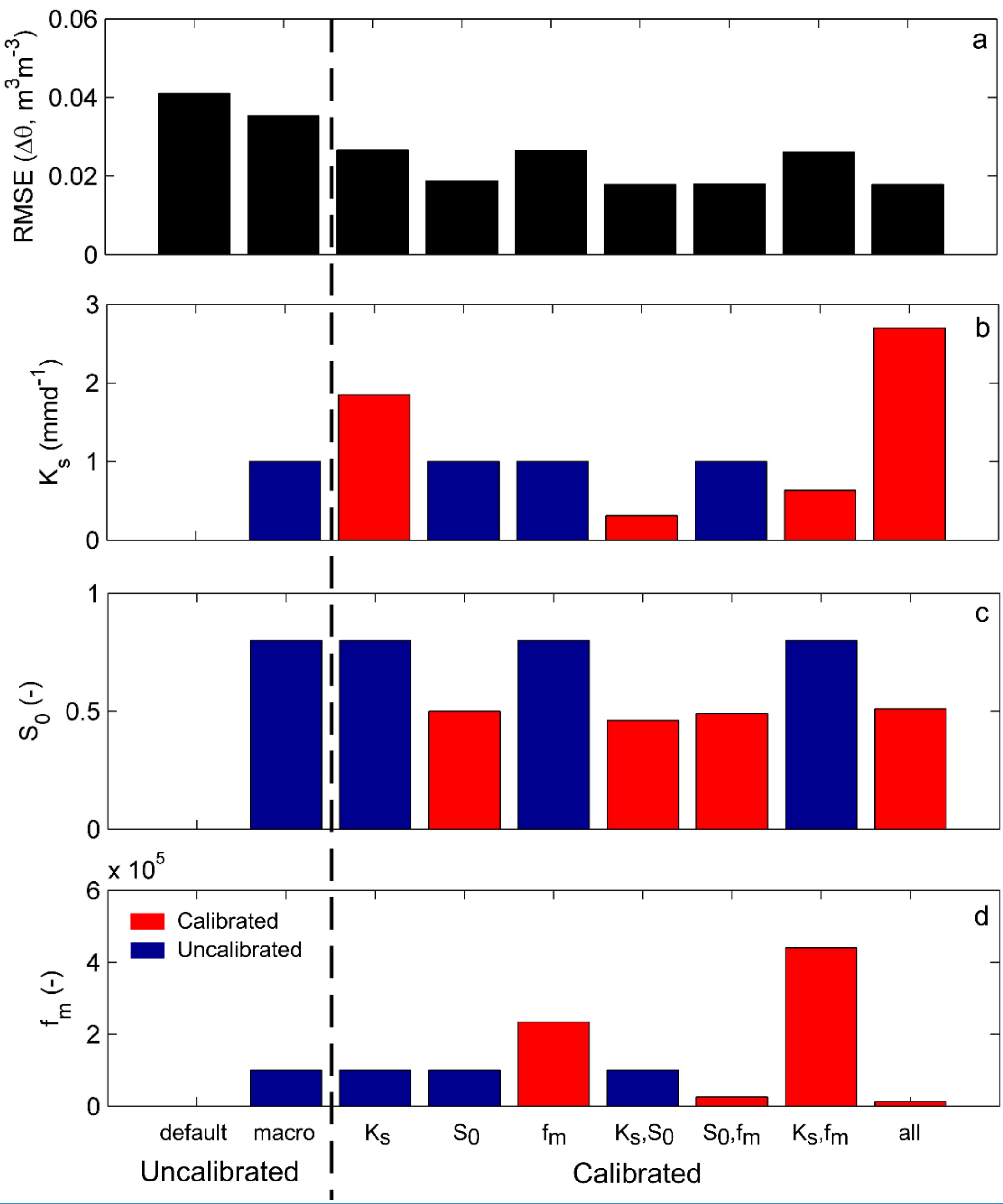
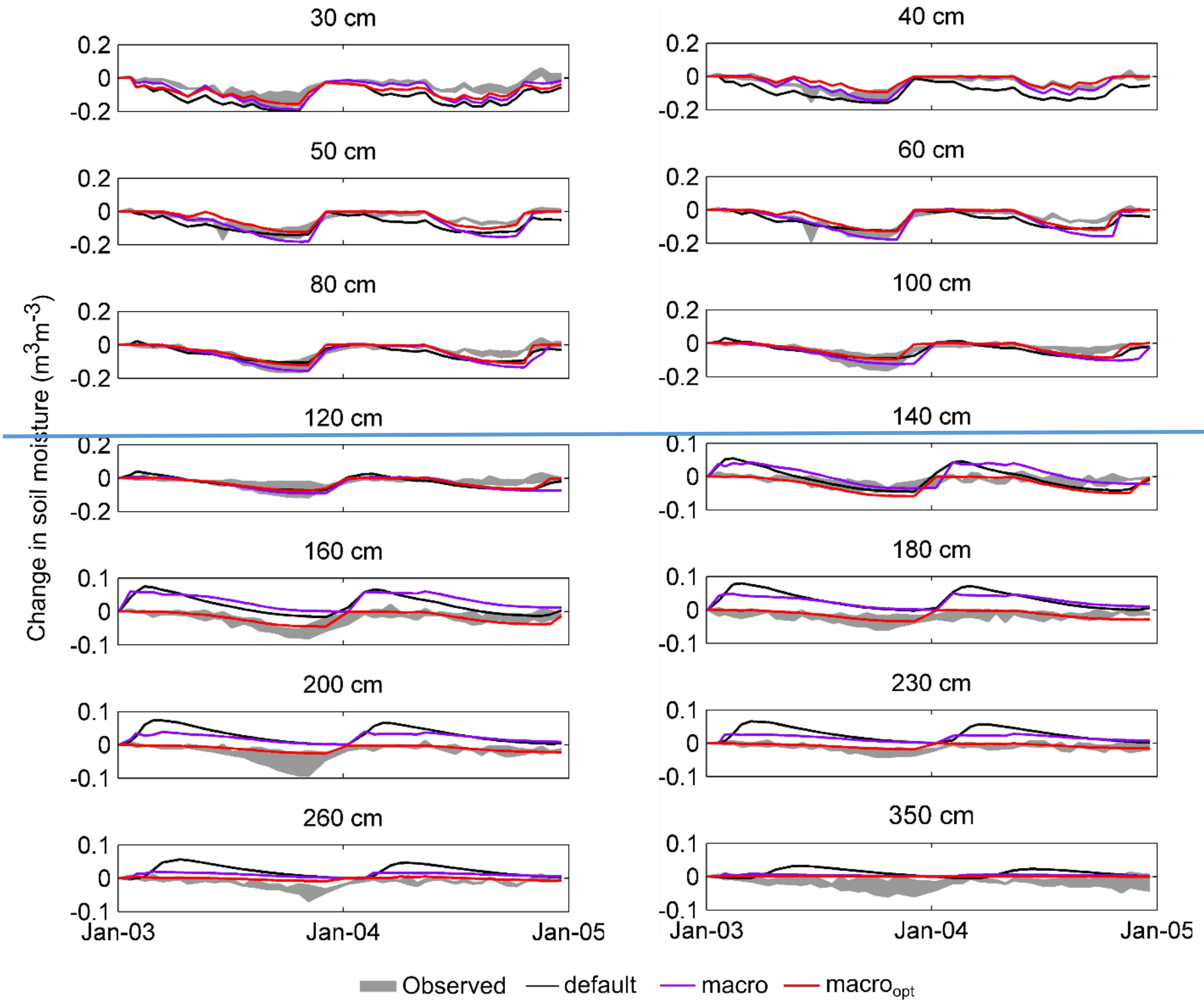
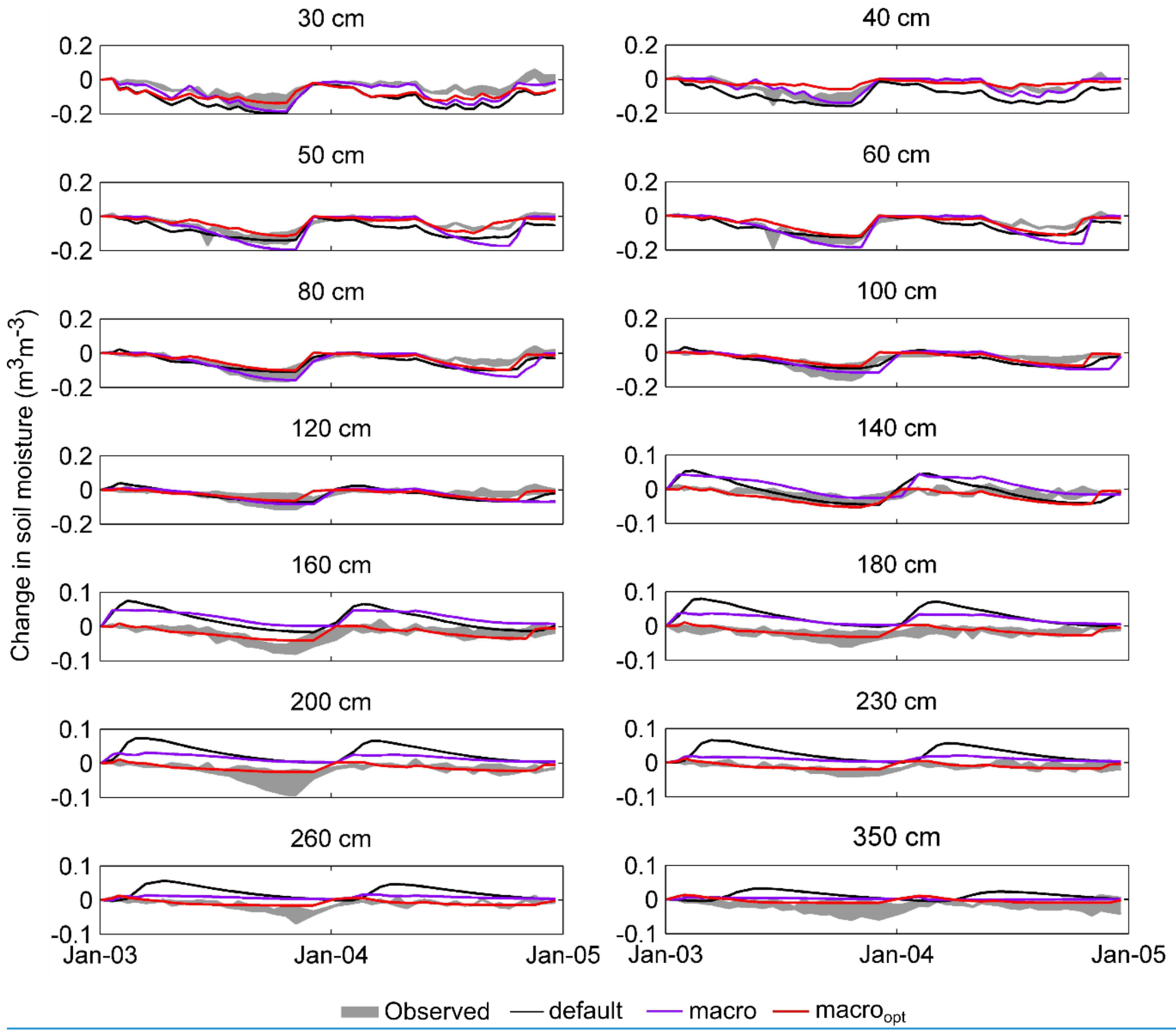


Figure 5. Comparison between observed and simulated $\Delta\theta$ from *default*, *macro* and $macro_{opt}$ configurations at various depths below land surface. The shaded areas, which are ~~is~~ constructed from 2 soil moisture probes at the Warren Farm site, denote~~s~~ the range of $\Delta\theta$.


30 cm
40 cm
50 cm
60 cm
80 cm
100 cm
120 cm
140 cm
160 cm
180 cm
200 cm
230 cm
260 cm
350 cm
Change in soil moisture (m3m-3)
Jan-03
Jan-04
Jan-05
Observed
default
macro
macroopt

772



~~Figure 6. Box plot of relative bias (Δμ) of simulated soil moisture from *default* and *macro* configurations at different depth ranges shown in individual intervals (e.g., 0-30 cm, 30-100 cm, and so on).~~

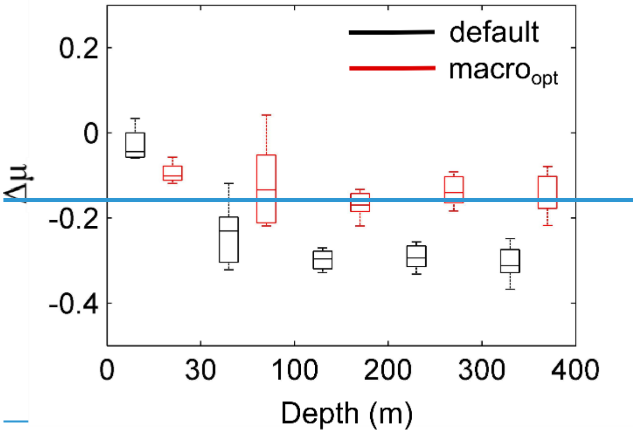
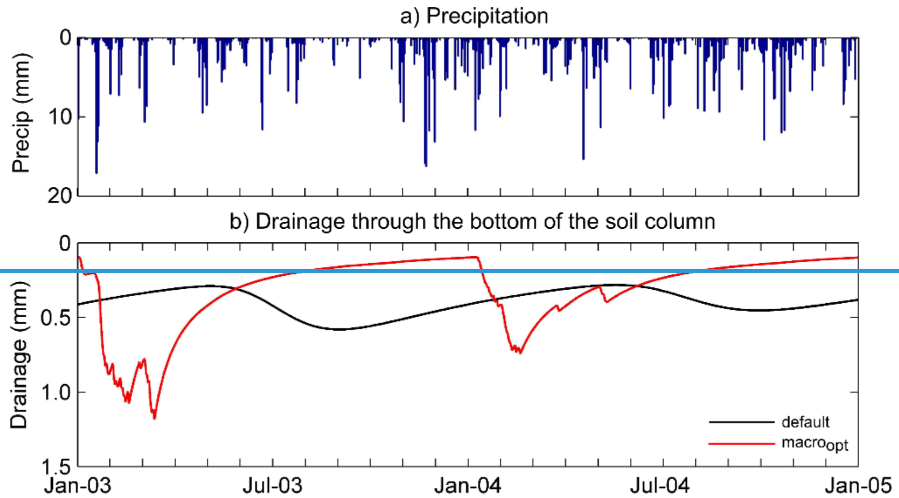


Figure ~~7~~6. (a) Daily p~~P~~recipitation and (b) daily ~~sum of~~ drainage through the bottom of the soil column at Warren Farm over the two simulated years (2003-2005).


a) Precipitation
Precip (mm)
0
10
20
b) Drainage through the bottom of the soil column
Drainage (mm)
0
0.5
1.0
1.5
default
macro$_{opt}$
Jan-03
Jul-03
Jan-04
Jul-04
Jan-05

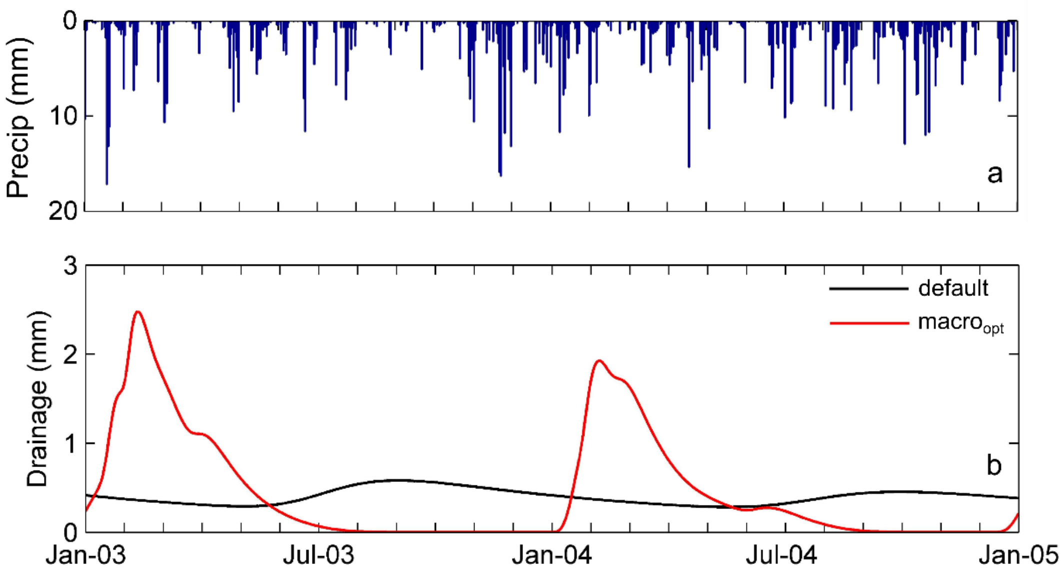
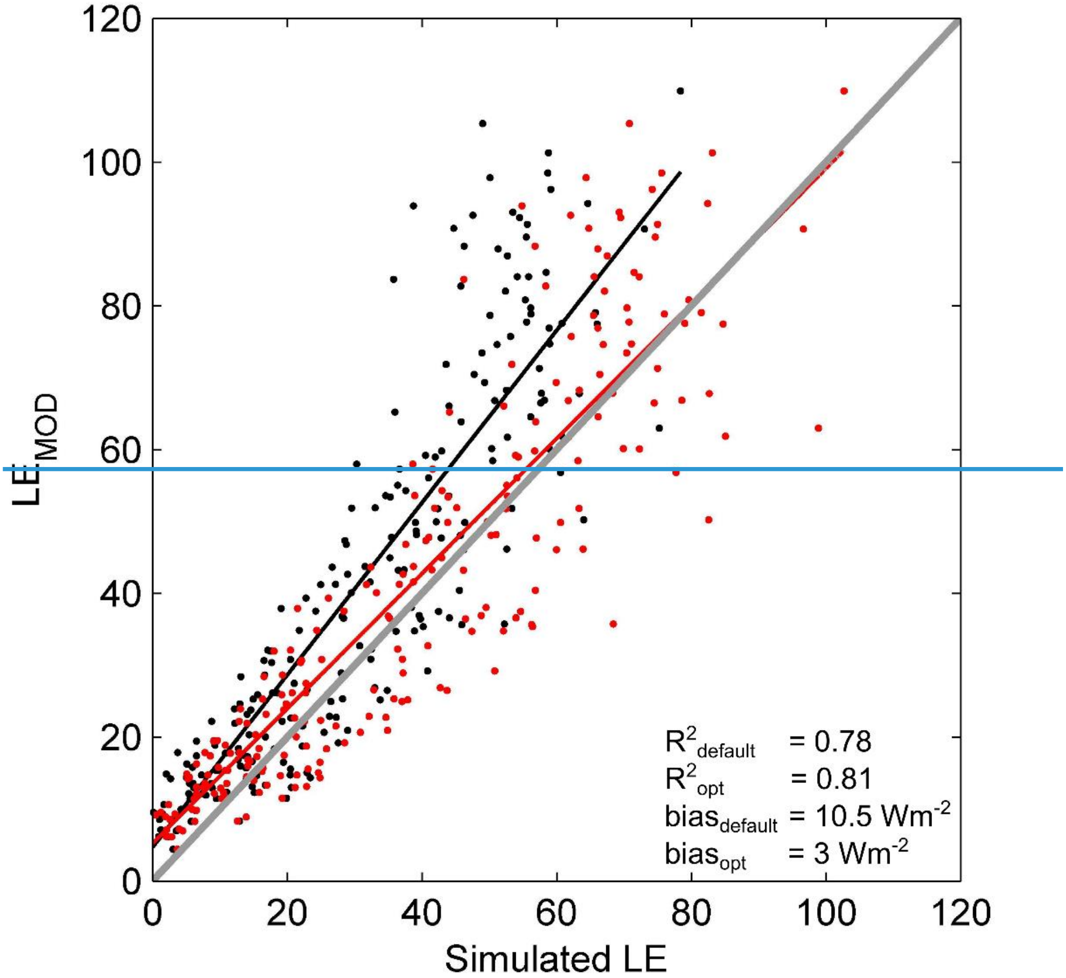

Precip (mm)
0
10
20
a
Drainage (mm)
3
2
1
0
default
macro$_{opt}$
b
Jan-03
Jul-03
Jan-04
Jul-04
Jan-05

Figure ~~8~~7. Catchment average 8 day composites of MODIS estimated *LE* (LE_{MOD}) against simulated *LE* from *default* and *macro* configurations ($LE_{default}$ and LE_{macro}, respectively) along with the linear models fitted for $LE_{default}$ (black line) and LE_{macro} (red line). The 1:1 line is shown in grey, which represents the perfect fit between LE_{MOD} and simulated *LE*.



120
100
80
60
40
20
0
LE_MOD
0
20
40
60
80
100
120
Simulated LE
R²default = 0.78
R²opt = 0.81
biasdefault = 10.5 Wm-2
biasopt = 3 Wm-2

814

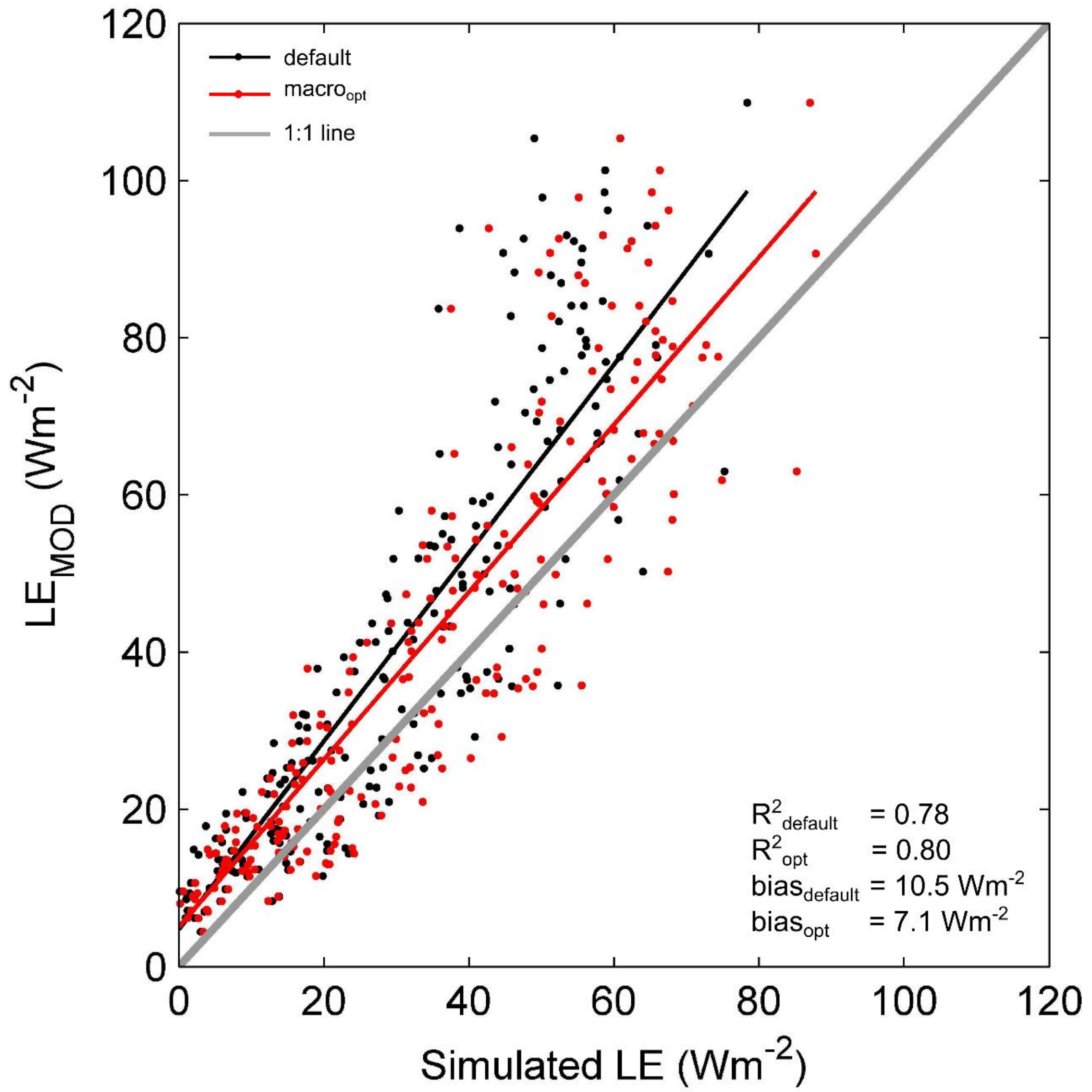
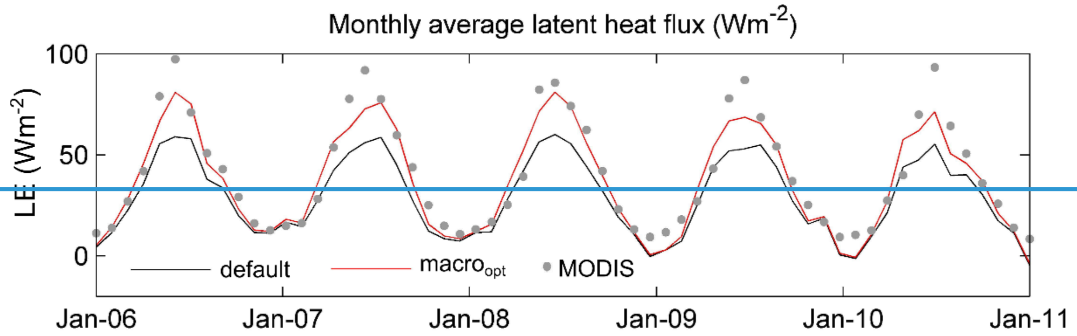
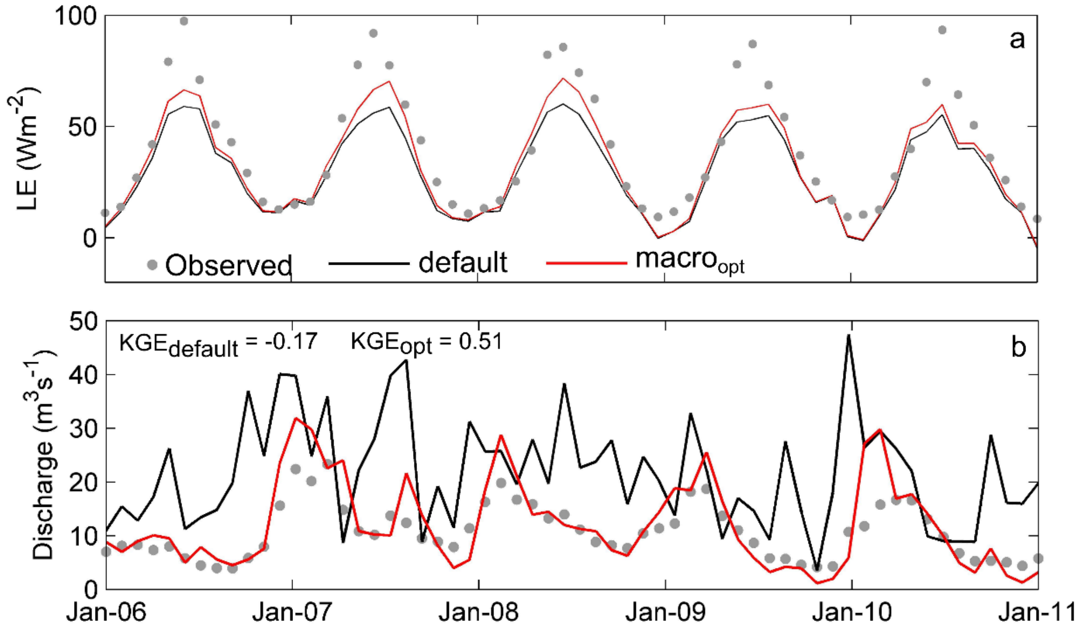


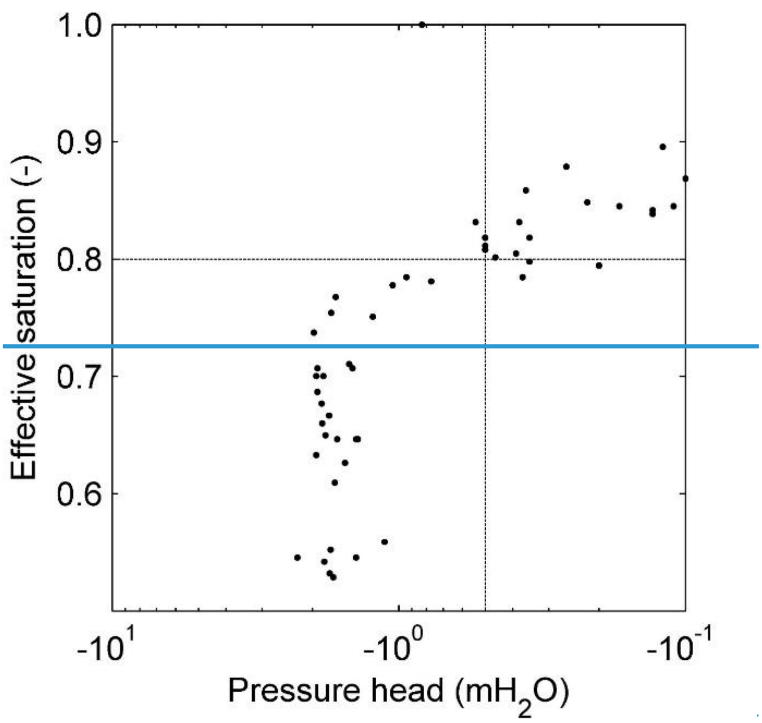
Figure ~~9~~8. (a) Spatially averaged monthly latent heat flux (*LE*) from MODIS, *default* and *macro$_{opt}$* configurations over the Kennet catchment and (b) monthly average observed and simulated discharge from the *default* and *macro$_{opt}$* configurations at the "Kennet at Theale" gauging station.


Monthly average latent heat flux (Wm-2)
LE (Wm-2)
100
50
0
default
macroopt
MODIS
Jan-06
Jan-07
Jan-08
Jan-09
Jan-10
Jan-11


a
LE (Wm-2)
100
50
0
Observed
default
macroopt
b
KGEdefault = -0.17
KGEopt = 0.51
Discharge (m3s-1)
50
40
30
20
10
0
Jan-06
Jan-07
Jan-08
Jan-09
Jan-10
Jan-11

~~Supplementary materials~~

~~Figure S1. Saturation-pressure head relationship (May 2003 – December 2005) at Warren Farm measured fortnightly at 40 cm below land surface. (Source: Ned Hewett, CEH, personal communication).~~



~~Figure S2. Sensitivity of the BC model parameters on the model performance in simulating~~ ~~$\Delta\theta$. Note that the parameters are considered one-at-a-time (OAT), and the vertical axis have different RMSE ranges.~~