

1 **Towards a simple representation of chalk hydrology in land**

2 **surface modelling**

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6 **Abstract**

7 Modelling and monitoring of hydrological processes in the unsaturated zone of chalk, a
8 porous medium with fractures, is important to optimize water resources assessment and
9 management practices in the United Kingdom (UK). However, incorporating the processes
10 governing water movement through chalk unsaturated zone in a numerical model is
11 complicated mainly due to the fractured nature of chalk that creates high-velocity preferential
12 flow paths in the subsurface. In general, flow through chalk unsaturated zone is simulated
13 using dual-porosity concept, which often involves calibration of relatively large number of
14 model parameters, potentially undermining applications to large regions. Therefore, this
15 approach may be not be suitable for large-scale land surface modelling applications. In this
16 study, a simplified parameterization, namely the Bulk Conductivity (BC) model is proposed
17 for simulating hydrology in chalk unsaturated zone. This new parameterization is
18 implemented in the Joint UK Land Environment Simulator (JULES) and applied to a study
19 area encompassing the Kennet catchment in the Southern UK. The simulation results are
20 evaluated using field measurements and satellite remote sensing observations of various
21 fluxes and states of the hydrological cycle (e.g., soil moisture, runoff and latent heat flux) at
22 two distinct spatial scales (i.e., point and catchment). The results demonstrate that the
23 inclusion of the BC model in JULES improves simulated land surface mass and energy fluxes
24 over the chalk-dominated Kennet catchment. Therefore, the simple approach described in this

25 study may be used to incorporate the flow processes through chalk unsaturated zone in large
26 scale land surface modelling applications.

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

28 **1. Introduction**

29 Chalk can be described as a fine-grained porous medium traversed by fractures [*Price et al.*,
30 1993]. Previous studies showed that the unsaturated zone of the chalk aquifers plays an
31 important role on groundwater recharge in the UK [e.g., *Lee et al.*, 2006; *Ireson et al.*, 2009].
32 Therefore, both monitoring [e.g., *Bloomfield*, 1997; *Ireson et al.*, 2006] and modelling [e.g.,
33 *Bakopoulou*, 2015; *Brouyère*, 2006; *Ireson and Butler*, 2011, 2013; *Sorensen et al.*, 2014]
34 strategies have been adapted previously to understand the governing hydrological processes
35 in the chalk unsaturated zone.

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

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

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

62 The above mentioned studies illustrate the importance of representing chalk in land surface
63 modelling. However, including chalk hydrology in large-scale land surface modelling using
64 the contemporary dual-porosity concept can be complicated because this approach generally
65 involves relatively large number of parameters. In this context, we propose a new
66 parameterization, namely the Bulk Conductivity (BC) model as a first step towards a simple
67 chalk representation suitable for land surface modelling. The BC model is included in JULES
68 and evaluated at two distinct spatial scales (i.e., point and catchment). At the point-scale, the
69 BC model is evaluated using observed soil moisture data. The proposed model is then applied
70 to the Kennet catchment in the Southern England and the fluxes and states of the hydrological
71 cycle are simulated for multiple years. The simulation results are evaluated using observed
72 latent heat flux (LE) and runoff to assess the performance of the BC model in simulating land
73 surface processes at the catchment scale.

74 **2. A model of flow through chalk unsaturated zone**

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

$$80 \quad K_{sb} = K_s + K_s f_m \frac{S - S_0}{1 - S_0} \quad \text{if } S > S_0 \quad (1)$$

$$81 \quad \text{with } S = \frac{\theta - \theta_r}{\theta_s - \theta_r}$$

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

85 At the first step of evaluation, the K_s , S_0 and f_m parameters are estimated based on existing
86 literature to assess the performance of the uncalibrated BC model. In this uncalibrated BC
87 model, K_s for chalk matrix is 16 mmd^{-1} according to *Le Vine et al.* [2016] for the catchment
88 investigated in this study (Figure 1). Equation 1 indicates that the onset of water flow through
89 the fracture system of chalk is controlled by the threshold S_0 . According to *Wellings and Bell*
90 [1980], water flow through fractures dominates over matrix flow in chalk when the pressure
91 head in soil becomes higher than $-0.50 \text{ mH}_2\text{O}$. We consider a value of $S_0 = 0.80$ for the
92 uncalibrated BC model, which is based on observed soil moisture-matric potential
93 relationship in the study area (Figure S1).

94 In *Zehe et al.* [2001], f_m was defined as the ratio of the saturated water flow rate in all
95 macropores in a model element to the corresponding value in soil matrix, which can be
96 determined based on the density and length of fractures at small scales. In addition, f_m has

97 also been considered as a calibration parameter previously [e.g., *Blume, 2008; Zehe et al.,*
 98 2013]. In this study, we define f_m as a characteristic soil property reflecting the influence of
 99 fractures on soil water movement [*Zehe and Blöschl, 2004*], and estimate it from the relative
 100 difference of permeability between chalk matrix and fractured chalk system that can be of the
 101 order 10^4 - 10^6 according to *Price et al. [1999]*. Consequently, we consider a macroporosity
 102 factor of $f_m = 10^5$ for the uncalibrated BC model.

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

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

$$114 \quad RMSE = \frac{1}{nd} \sum_1^{nd} \sqrt{\left(\frac{1}{nt-1} \sum_2^{nt} (\Delta\theta_{d,t}^{obs} - \Delta\theta_{d,t}^{sim})^2 \right)} \quad (2)$$

115 where nd is the number of soil layers, nt is the number of soil moisture observations available
 116 for a layer d , $\Delta\theta^{obs}$ is the observed variability of soil moisture and $\Delta\theta^{sim}$ is the simulated
 117 variability of soil moisture. Note that we consider $\Delta\theta$ for this optimization because of its
 118 relevance to the water flux and recharge through chalk unsaturated zone [e.g., *Ireson and*
 119 *Butler, 2011*]. Latin hypercube technique [e.g., *McKay et al., 2016*] is used to generate 2000
 120 random samples for each BC model parameter within the respective range discussed above.

121 We perform simulations using these random samples and calculate model performance
122 (Equation 2) to select the optimum parameter values for the BC model (discussed in section
123 4.1).

124 **3. Methods**

125 **3.1. Study area**

126 The study area encompasses the Kennet catchment located in the Southern England with an
127 area of about 1033 km² (Figure 1a). Generally, Kennet is rural in nature with scattered
128 settlements and has a maximum altitude of approximately 297 m (Above Ordnance Level).
129 The River Kennet discharges into the North Sea through London. The major tributaries of
130 this river are Lambourn, Dun, Enborne, and Foudry Brook. An average annual rainfall of
131 approximately 760 mm was recorded in the catchment over a 40 year period from 1961-1990.

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

139 **3.2. Field measurements and remotely sensed data**

140 Table 1 summarizes the field measurements and remote sensing data used in this study. We
141 use *in-situ* soil moisture and runoff measurements along with remotely sensed LE data to
142 assess model performance in simulating the mass and energy balance components of the
143 hydrological cycle. Point scale soil moisture measurements at two adjacent sites (~20 m
144 apart) at the Warren Farm (Figure 1) were provided by Centre for Ecology and Hydrology

145 (CEH). A Didcot neutron probe was used at these locations to measure fortnightly soil
146 moisture at different depths below land surface (10 cm apart down to 0.8 m, 20 cm apart
147 between 0.8-2.2 m, and 30 cm apart between 2.2-4.0 m) [Hewitt *et al.*, 2010].

148 The National River Flow Archive (NRFA) coordinates discharge measurements from the
149 gauging station networks across UK. These networks are operated by the Environmental
150 Agency (England), Natural Resources Wales, Scottish Environment Protection Agency, and
151 Rivers Agency (Northern Ireland). We use discharge measurement provided by NRFA to
152 calculate the runoff ratio over the Kennet catchment in this study.

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

158 **3.3. Land surface model**

159 In this study, we use the Joint UK Land Environment Simulator (JULES [e.g., *Best et al.*,
160 2011; *Clark et al.*, 2011]) version 4.2. JULES is a flexible modelling platform with a modular
161 structure aligned to various physical processes developed based on the Met Office Surface
162 Exchange Scheme (MOSES [e.g., *Cox et al.*, 1999; *Essery et al.*, 2003]). Meteorological data
163 including precipitation, incoming short- and longwave radiation, temperature, specific
164 humidity, surface pressure, and wind speed are required to drive JULES. Each grid box in
165 JULES can comprise nine surface types (broadleaf trees, needle leaf trees, C3 grass, C4 grass,
166 shrubs, inland water, bare soil, and ice) represented by respective fractional coverage. Each
167 surface type is represented by a tile and a separate energy balance is calculated for each tile.

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

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

182 **3.4. Model configurations and input data**

183 In this study, simulations are performed at two distinct spatial scales, namely point and
184 catchment. At the point scale, JULES is configured to simulate the mass and energy fluxes at
185 the Warren Farm site (Figure 1a). A total subsurface depth of 5 m is considered in the model
186 with a vertical discretization ranging from 10 cm at the land surface to 50 cm at the bottom of
187 the model domain. Note that this discretization is consistent with the soil moisture
188 measurement depths mentioned in section 3.2. The vegetation type is implemented as C3
189 grass using the default parameters in JULES. Point scale simulations were performed over 2
190 consecutive years from 2003-2005 at an hourly time step. Except for precipitation, hourly
191 atmospheric forcing data to drive JULES was obtained from an automatic weather station

192 operated by the CEH at Warren Farm. In order to estimate hourly precipitation data to run
193 JULES, rain gauge measurements from the Met Office [*Met Office*, 2006] were used. Inverse
194 distance interpolation technique [e.g. *Garcia et al.*, 2008; *Ly et al.*, 2013] was applied on
195 rainfall measurements from 13 gauges closest to Warren Farm (distance varies from 25-60
196 km) to obtain hourly precipitation for the point scale simulations.

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

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

217 *Genuchten*, 1980] model with parameter values (Table 2) obtained from *Schaap and Leij*
218 [1998].

219 Table 3 summarizes the hydraulic properties for chalk used in this study. These properties are
220 obtained based on existing literature as a first step when evaluating the uncalibrated BC
221 model. The BC model parameters are subsequently optimized to minimize the differences
222 between observed and simulated $\Delta\theta$.

223 In this study, we consider two different model configurations, namely *default* and *macro*
224 (Figure 2). The *default* configuration corresponds to the standard parameterizations of JULES
225 that does not represent chalk hydrology in the model. In this configuration, each soil column
226 in JULES is considered to be vertically homogeneous with the soil properties defined in
227 Table 2, which is motivated by the Met Office JULES Global Land 4.0 configuration
228 described in *Walters et al.* [2014]. The *macro* configuration, in contrast, explicitly represents
229 chalk by applying the BC model starting at 30 cm below land surface to the bottom of the
230 model domain (i.e. 500 cm). Therefore, the soil column in the *macro* configuration can be
231 divided into topsoil (0-30 cm) and chalk (30-500 cm) in *macro*. Note that except for this
232 inclusion of chalk, *default* and *macro* configurations are identical in terms of model set up
233 and input data.

234 The topsoil depth of 30 cm in the *macro* configuration is defined based on several augured
235 soil samples collected during a field campaign at Warren Farm in 2015 (Figure 2). This depth
236 is corroborated by additional information from the British Geological Survey (BGS) operated
237 borehole records (http://www.ukso.org/pmm/soil_depth_samples_points.html), which show
238 that topsoil depths vary from 10-40 cm over the study area. We therefore apply the *macro*
239 configuration assuming a spatially homogeneous topsoil depth of 30 cm for both point and
240 catchment scale simulations.

241 **4. Results and discussion**

242 **4.1. Point scale simulations**

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

252 The results show that despite the *macro* configuration improves simulated θ , it shows
253 considerable discrepancies with observed $\Delta\theta$, which is consistent throughout the whole chalk
254 profile (results from other model layers are not shown). In order to minimize the differences
255 between observed and modelled $\Delta\theta$ from the *macro* configuration, we optimize the BC model
256 following the methodology described in section 2. The optimization results are summarized
257 in Figure 4. Note that for each combination considered in the optimization, 2000 model runs
258 were performed using randomly sampled parameters as discussed in section 2. Figure 4
259 presents the results from the model runs yielding the lowest RMSE.

260 The RMSE between observed and simulated $\Delta\theta$ for the model configurations considered in
261 the optimization is shown in Figure 4a. This figure illustrates that the RMSE of the *default*
262 configuration is larger than that of *macro*, indicating better model performance in
263 reproducing $\Delta\theta$ for the latter. Therefore, it appears that the uncalibrated BC model (i.e., the
264 *macro* configuration) is better in reproducing soil moisture variability compared to *default*.

265 Figure 4b, c and d presents the BC model parameter values from the model run producing the
266 lowest RMSE for each configuration. Concerning single BC model parameters, Figure 4a
267 shows that optimizing S_0 results in a 16% reduction of RMSE compared to the *macro*
268 configuration. Optimizing K_s marginally improves model performance, which is observed
269 from a slightly lower (4%) RMSE than *macro*. Optimizing both K_s and S_0 simultaneously
270 results in the largest reduction (24%) of RMSE compared to *macro*.

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

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

286 In order to assess the model performance in simulating soil moisture over the entire column,
287 the relative bias ($\Delta\mu$, see Appendix) of simulated θ from the *default* and *macro_{opt}*
288 configurations at Warren Farm for various depth ranges are shown in Figure 6. In the soil

289 layers (0-30 cm), θ from the two configurations are comparable with the *default* showing
290 slightly lower mean relative bias ($\Delta\mu_{\text{mean}}$) of -0.03 than *macro_{opt}* ($\Delta\mu_{\text{mean}} = -0.09$). However,
291 in the chalk layers (30-500 cm), *default* simulates substantially drier conditions,
292 corresponding to $\Delta\mu_{\text{mean}} \leq -0.28$. In contrast, the *macro_{opt}* configuration considerably
293 improves the agreement between the simulated and observed θ in the chalk layers with
294 $\Delta\mu_{\text{mean}} \geq -0.05$. Therefore, the results indicate that the inclusion of the BC model in JULES
295 improves the performance of overall soil moisture simulation (both θ and $\Delta\theta$) at Warren
296 Farm especially in the chalk layers.

297 The drainage flux through the bottom of soil column (d_b) of a land surface model can be
298 considered as the potential recharge flux to groundwater [e.g., *Sorensen et al.*, 2014]. Figure
299 7 compares the daily sum of d_b from the *default* and *macro_{opt}* configurations at the Warren
300 Farm site. The rainfall characteristics over the study period is shown in Figure 7a. In Figure
301 7b, the *macro_{opt}* configuration shows considerable d_b during the colder months, while slow
302 drainage prevails throughout the rest of the year. In contrast, the *default* configuration shows
303 relatively high d_b in summer compared to the colder months. In general, the recharge rate
304 through chalk unsaturated zone during the warmer periods of the year is lower than that in the
305 winter months [*Wellings and Bell*, 1980; *Ireson et al.*, 2009]. Therefore, the *macro_{opt}*
306 configuration appears to be more consistent with the recharge mechanism in chalk compared
307 to *default*.

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

313 4.2. Catchment scale simulations

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

326 Figure 8 shows differences between $LE_{default}$ and LE_{opt} especially for relatively high LE ,
327 indicating discrepancies especially during the warmer months of the year. Figure 9 presents
328 spatially averaged time series of monthly LE_{MOD} , $LE_{default}$ and LE_{opt} . This figure shows that
329 the differences between $LE_{default}$ and LE_{opt} increases substantially in summer compared to the
330 colder months of the year, which is consistent with Figure 8. Consequently, the *default*
331 configuration underestimates LE in summer compared to LE_{MOD} , which is improved in case
332 of the *macro_{opt}* configuration. In contrast, the differences between $LE_{default}$ and LE_{opt} are
333 negligible during the colder months of the year.

334 Table 4 compares observed and simulated daily average runoff from the two model
335 configurations over the Kennet catchment from 2006-2011. The runoff ratio (RR , see
336 Appendix), which is equal to the mean volume of flow divided by the volume of precipitation

337 [e.g., Kelleher et al., 2015], assesses the partitioning of precipitation into runoff over the
338 catchment. The *default* configuration ($RR = 0.82$) shows considerably higher RR compared to
339 observation ($RR = 0.40$), indicating overestimation of runoff by the model. Including chalk
340 hydrology in the model remarkably improves the agreement between observed and simulated
341 mean runoff over the Kennet catchment, which is assessed from a runoff ratio of $RR = 0.37$
342 for the *macro_{opt}* configuration.

343 In Table 4, the relative bias ($\Delta\mu$) of 1.04 between observed and simulated runoff from the
344 *default* configuration again indicates the overestimation by the model. In comparison,
345 *macro_{opt}* shows a relative bias ($\Delta\mu = -0.05$), indicating improvement between observed and
346 simulated mean runoff volume compared to *default*. The relative difference in standard
347 deviation ($\Delta\sigma$, see Appendix) compares the variability of observed and simulated runoff in
348 Table 4. This comparison shows that the *default* configuration overestimates the variability of
349 runoff over the Kennet catchment ($\Delta\sigma = 2.04$), which is improved in case of *macro* ($\Delta\sigma =$
350 0.70).

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

359 In this section, the BC model is evaluated using observed mass and energy fluxes over the
360 Kennet catchment. The *default* configuration showed considerably low LE over the

361 catchment, which was pronounced during the warmer period of the year. The agreement
362 between observed and simulated LE was improved in case of the *macro_{opt}* configuration
363 compared to *default*. It was also observed that the overall runoff prediction was improved by
364 *macro_{opt}* compared to *default*. Given its simplicity, our results indicate that the proposed
365 parameterization is suitable for use in land surface modelling applications.

366 **5. Summary and Conclusions**

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

374 The proposed BC model is a single continuum approach of modelling preferential flow [e.g.,
375 *Beven and Germann, 2013*] that involves only 2 parameters, namely macroporosity factor (f_m)
376 and relative saturation threshold (S_0). Initially, these parameters along with the saturated
377 hydraulic conductivity of the chalk matrix were estimated from existing literature. Finally,
378 the BC model parameters were optimized to minimize the differences between observed and
379 simulated soil moisture variability. Our results indicated that S_0 is the most influential
380 parameter in the model when representing water movement through a soil-chalk column,
381 followed by the saturated hydraulic conductivity of chalk matrix while f_m showed low
382 sensitivity. Hence, the parameterization is further improved by optimizing both saturated
383 hydraulic conductivity of chalk matrix and S_0 to minimize the differences between observed
384 and simulated soil moisture variability.

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

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

400 **Acknowledgements**

401 We gratefully acknowledge the support by the “A Multi-scale Soil moisture
402 Evapotranspiration Dynamics study – AMUSED” project funded by Natural Environment
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404 thank Ned Hewitt and Jonathan Evans from the Centre for Ecology and Hydrology (CEH) for
405 providing the data for the point-scale analyses at the Warren Farm. Finally, we would like to
406 thank Miguel Rico-Ramirez (University of Bristol) for helping preparing the precipitation
407 data from the rain gauge network used for the point-scale simulations, Thorsten Wagener
408 (University of Bristol) for his valuable suggestions on model diagnostics, and Joost Iwema

409 (University of Bristol) for helping with the soil samples collected during the 2015 field work
410 campaign.

411 **Appendix**

412 **Definition of Statistical Metrics**

413 Coefficient of determination (R^2) for observation $y = y_1, \dots, y_n$ and prediction $f = f_1, \dots, f_n$
414 is defined as

$$415 \quad R^2 = 1 - \frac{SS_{res}}{SS_{tot}}$$

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

$$418 \quad SS_{res} = \sum_{i=1}^n (y_i - f_i)^2 \quad \text{and}$$

$$419 \quad SS_{tot} = \sum_{i=1}^n (y_i - \bar{y})^2 \quad \text{with } \bar{y} \text{ being the mean of } y.$$

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

$$422 \quad RR = \frac{\mu_{runoff}}{\mu_{rain}}$$

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

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

$$425 \quad \Delta\mu = \frac{\mu_{mod} - \mu_{obs}}{\mu_{obs}}$$

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

429 Relative difference in standard deviation ($\Delta\sigma$) between observed and simulated time series

430 can be defined as

$$431 \quad \Delta\sigma = \frac{\sigma_{mod} - \sigma_{obs}}{\sigma_{obs}}$$

432 where σ_{obs} and σ_{mod} are the standard deviation of observed and simulated time series,

433 respectively [e.g., *Gudmundsson et al.*, 2012].

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447 **References**

- 448 Bakopoulou, C. (2015), Critical assessment of structure and parameterization of JULES land
449 surface model at different spatial scales in a UK Chalk catchment, PhD thesis, Imperial
450 College London, UK, available at: <https://spiral.imperial.ac.uk:8443/handle/10044/1/28955>.
- 451 Bell, V. A. and R. J. Moore (1998), A grid-based flood forecasting model for use with
452 weather radar data: Part 1. Formulation, *Hydrol. Earth Syst. Sc.*, 2, 265-281.
- 453 Bell, V. A., A. L. Key, R. G. Jones, and R. J. Moore (2007), Development of a high
454 resolution grid-based river flow model for use with regional climate model output, *Hydrol.*
455 *Earth Syst. Sc.*, 11, 532-549.
- 456 Best, M. J., M. Pryor, D. B. Clark, G. G. Rooney, R. I. H. Essery, C. B. Ménard, J. M.
457 Edwards, M. A. Hendry, A. Porson, N. Gedney, L. M. Mercado, S. Sitch, E. Blyth, O.
458 Boucher, P. M. Cox, C. S. B. Grimmond, and R. J. Harding (2011), The Joint UK Land
459 Environment Simulator (JULES), Model Description – Part 1: Energy and Water
460 Fluxes, *Geosci. Model Dev.*, 4, 677-699.
- 461 Beven, K., and P. Germann (2013), Macropores and water flow in soils revisited, *Water*
462 *Resour. Res.*, 49, 3071-3092.
- 463 Bloomfield, J. (1997), The role of diagenesis in the hydrogeological stratification of
464 carbonated aquifers: An example from the chalk at Fair Cross, Berkshire, UK, *Hydrol. Earth*
465 *Syst. Sc.*, 1, 19-33.
- 466 Blume, T. (2008), Hydrological processes in volcanic ash soils: measuring, modelling and
467 understanding runoff generation in an undisturbed catchment, PhD thesis, Institut für

468 Geoökologie, Universität Potsdam, Potsdam, Germany, available at: [https://publishup.uni-](https://publishup.uni-potsdam.de/opus4-ubp/files/1524/blume_diss.pdf)
469 [potsdam.de/opus4-ubp/files/1524/blume_diss.pdf](https://publishup.uni-potsdam.de/opus4-ubp/files/1524/blume_diss.pdf)

470 Brouyère, S. (2006), Modelling the migration of contaminants through variably saturated
471 dual-porosity, dual-permeability chalk, *J. Contam, Hydrol.*, 82, 195-219.

472 Chen, X., and Q. Hu (2004), Groundwater influences on soil moisture and surface
473 evaporation, *J. Hydrol.*, 297, 285-300.

474 Clark, D. B., L. M. Mercado, S. Sitch, C. D. Jones, N. Gedney, M. J. Best, M. Pryor, G. G.
475 Rooney, R. L. H. Essery, E. Blyth, O. Boucher, R. J. Harding, C. Huntingford, and P. M. Cox
476 (2011), The Joint UK Land Environment Simulator (JULES), Model Description – Part 2:
477 Carbon Fluxes and Vegetation Dynamics, *Geosci. Model Dev.* 4, 701-722.

478 Cox, P. M., R. A. Betts, C. B. Bunton, R. L. H. Essery, P. R. Rowntree and J. Smith (1999),
479 The impact of new land surface physics on the GCM simulation of climate and climate
480 sensitivity, *Clim. Dynam.*, 15, 183-203.

481 Dadson, S. J., I. Ashpole, P. Harris, H. N. Davies, D. B. Clark, E. Blyth, and C. M. Taylor
482 (2010), Wetland inundation dynamics in a model of land surface climate: Evaluation in the
483 Niger inland delta region, *J. Geophys. Res.*, 115.

484 Dadson, S. J., V. A. Bell, and R. G. Jones (2011), Evaluation of a grid based river flow model
485 configured for use in a regional climate model, *J. Hydrol.*, 411, 238-250.

486 Dettinger, M. D., and H. F. Diaz (2000), Global characteristics of streamflow seasonality and
487 variability, *J. Hydrometeorol.*, 1, 289-310.

488 Essery, R., M. Best, and P. Cox (2001), MOSES 2.2 technical documentation (Hadley Centre
489 technical note 30), Hadley Centre, Met Office, UK.

490 Garcia, M., C. D. Peters-Lidard, and D. C. Goodrich (2008), Spatial interpolation of
491 precipitation in a dense gauge network for monsoon storm events in the southwestern United
492 States, *Water Resour. Res.*, 44.

493 Gascoin, S., A. Duchare, P. Ribstein, M. Carli, and F. Habtes (2000), Adaptation of a
494 catchment-based land surface model to the hydrological setting of the Somme River basin
495 (France), *J. Hydrol.*, 368, 105-116.

496 Gudmundsson, L., T. Wagener, L. M. Tallaksen, and K. Engeland (2012), Evaluation of nine
497 large-scale hydrological models with respect to the seasonal runoff climatology in Europe,
498 *Water Resour. Res.*, 48.

499 Gupta, H. V., H. Kling, K. K. Yilmaz, and G. F. Martinez (2009), Decomposition of the mean
500 squared error and NSE performance criteria: implications for improving hydrological
501 modelling, *J. Hydrol.*, 377, 80-91.

502 Haria, A. H., M. G. Hodnett, and A. C. Johnson (2003), Mechanisms of groundwater
503 recharge and pesticide penetration to chalk aquifer in southern England, *J. Hydrol.*, 275, 122-
504 137.

505 Hartmann, A., N. Goldscheider, T. Wagener, J. Lange, and M. Weiler (2014), Karst water
506 resources in a changing world: Review of hydrological modeling approaches, *Rev. Geophys.*,
507 52, 218–242, doi:10.1002/2013RG000443.

508 Hewitt, N., M. Robinson, and D. McNeil (2010), Pang and Lambourn hydrometric review
509 2009, Wallingford, NERC/Centre for Ecology and Hydrology, (CEH project number:
510 C04076).

511 Ireson, A. M., S. A. Mathias, H. S. Wheater, A. P. Butler and J. Finch (2009), A model for
512 flow in the chalk unsaturated zone incorporating progressive weathering, *J. Hydrol.*, 365,
513 244-260.

514 Ireson, A. M. and A. P. Butler (2011), Controls on preferential recharge to chalk aquifers, *J.*
515 *Hydrol.*, 398, 109-123.

516 Ireson, A. M. and A. P. Butler (2013), A critical assessment of simple recharge models:
517 application to the UK chalk, *Hydrol. Earth Syst. Sc.*, 17, 2083-2096.

518 Ireson, A. M., H. S. Wheater, A. P. Butler, S. A. Mathias, J. Finch, and J. D. Cooper (2006),
519 Hydrological processes in the chalk unsaturated zone – insight from an intensive field
520 monitoring program, *J. Hydrol.*, 330, 29-43.

521 Ireson, A. M., S. A. Mathias, H. S. Wheater, A. P. Butler, and J. Finch (2009), A model for
522 flow in the chalk unsaturated zone incorporating progressive weathering, *J. Hydrol.*, 365,
523 244-260.

524 Jackson, C. and Spink, A. (2004) User's Manual for the Groundwater Flow Model
525 ZOOMQ3D, IR/04/140, British Geological Survey, Nottingham, UK.

526 Kelleher, C., T. Wagener, and B. McGlynn (2015), Model-based analysis of the influence of
527 catchment properties on hydrologic partitioning across five mountain headwater
528 subcatchments, *Water Resour. Res.*, 51, 4109-4136.

529 Kling, H., M. Fuchs, and M. Paulin (2012), Runoff conditions in the upper Danube basin
530 under an ensemble of climate change scenarios. *Journal of Hydrology*, Volumes 424-425, 6
531 March 2012, 264-277.

532 Lehner, B., K. Verdin, and A. Jarvis (2008), New global hydrography derives from
533 spaceborne elevation data, *EOS, Transactions, AGU*, 89(10), 93-94.

534 Le Vine, N., A. Butler, N. McIntyre, and C. Jackson (2016), Diagnosing hydrological
535 limitations of a land surface model: application of JULES to a deep-groundwater chalk basin,
536 *Hydrol. Earth Syst. Sc.*, 20, 143-159.

537 Lee, L. J. E., D. S. L. Lawrence, and M. Price (2006), Analysis of water-level response to
538 rainfall and implications for recharge pathways in the chalk aquifer, SE England, *J. Hydrol.*,
539 330, 604-620.

540 Ly, S., C. Charles, and A. Degré (2013), Different methods for spatial interpolation of rainfall
541 data for operational hydrology and hydrological modeling at watershed scale. A review,
542 *Biotechnol. Agron. Soc. Environ.* 17, 392-406.

543 Mathias, S. A., A. P. Butler, B. M. Jackson, and H. S. Wheater (2006), Transient simulations
544 of flow and transport in the chalk unsaturated zone, *J. Hydrol.*, 330, 10-28.

545 Met Office (2006), UK hourly rainfall data, Part of the Met Office Integrated Data Archive
546 System (MIDAS), NCAS British Atmospheric Data Centre, 21 March 2016,
547 <http://catalogue.ceda.ac.uk/uuid/bbd6916225e7475514e17fdbf11141c1>.

548 Morton, D., C. Rowland, C. wood, L. Meek, C. Marston, G. Smith, R. Wadsworth, and I. C.
549 Simpson (2011), Final report for LCM2007 – the new UK Land Cover Map (CS technical
550 report no 11/07), Centre for Ecology and Hydrology, UK.

551 Mu, Q., F. A. Heinsch, M. Zhao, and S. W. Running (2007), Development of a global
552 evapotranspiration algorithm based on MODIS and global meteorology data, *Remote Sens.*
553 *Environ.*, 111, 519-536.

554 Price, A., R. A. Downing, and W.M. Edmunds (1993), The chalk as an aquifer. In: Downing,
555 R. A., M. Price, and G. P. Jones *The hydrogeology of the chalk of north-west Europe*. Oxford:
556 Claredon Press. 35-58.

557 Price, M., R. G. Low, and C. McCann (2000), Mechanisms of water storage and flow in the
558 unsaturated zone of chalk aquifer, *J. Hydrol.*, 54-71.

559 Rawls, W. J., D. L. Brankensiek, and K. E. Saxton (1982), Estimation of soil water
560 properties, *Trans. ASAE*, 25(5), 1316–1320.

561 Robinson, E. L., E. Blyth, D. B. Clark, J. Finch, and A. C. Rudd (2015), Climate hydrology
562 and ecology research support system potential evapotranspiration dataset for Great Britain
563 (1961- 2012) [CHESS-PE], NERC-Environmental Information Data Centre.

564 Schär C., D. Lüthi, U. Beyerle, and E. Heise (1999), A soil precipitation feedback: A process
565 study with a regional climate model, *J. Clim.*, 12, 722–741.

566 Schaap, M. G., and F. J. Leij (1998), Database-related accuracy and uncertainty of
567 pedotransfer functions, *Soil Sci.*, 163(10), 765-779.

568 Sorensen, J. P. R., J. W. Finch, A. M. Ireson, and C. R. Jackson (2014), Comparison of varied
569 complexity models simulating recharge at the field scale, *Hydrol. Process.*, 28, 2091-2102.

570 Van den Daele, G. F. A., J. A. Barker, L. D. Connell, T. C. Atkinson, W. G. Darling, and J.
571 D. Cooper (2007), *J. Hydrol.*, 342, 157-172.

572 Van Genuchten, M. Th. (1980), A closed-form equation for predicting the hydraulic
573 conductivity of unsaturated soils, *Soil Sci. Soc. Am. J.*, 44, 892-898.

574 Walters, D. N., K. D. Williams, I. A. Boutle, A. C. Bushell, J. M. Edwards, P. R. Field, A. P.
575 Lock, C. J. Morcrette, R. A. Stratton, J. M. Wilkinson, M. R. Willett, N. Bellouin, A. Bodas-
576 Salcedo, M. E. Brooks, D. Copesey, P. D. Earnshaw, S. C. Hardiman, C. M. Harris, R. C.
577 Levine, C. MacLachlan, J. C. Manners, G. M. Martin, S. F. Milton, M. D. Palmer, M. J.
578 Roberts, J. M. Rodríguez, W. J. Tennant, and P. L. Vidale (2014), The Met Office unified
579 model global atmosphere 4.0 and JULES global land 4.0 configurations, *Geosci. Model Dev.*,
580 7, 361-386.

581 Wellings, S. R., and J. P. Bell (1980), Movement of water and nitrate in the unsaturated zone
582 of upper chalk near Winchester, Hants., England, *J. Hydrol*, 48, 119-136.

583 Williams, K., and D. Clark (2014), Disaggregation of daily data in JULES (Hadley Centre
584 technical note 96), Hadley Centre, Met Office, UK.

585 Zehe, E. and G. Blöschl (2004), Predictability of hydrologic response at the plot and
586 catchment scales: Role of initial conditions, *Water Resour. Res.*, 40.

587 Zehe, E., T. Maurer, J. Ihringer, and E. Plate (2001), Modeling water flow and mass transport
588 in a loess catchment, *Phys. Chem. Earth (B)*, 26, 487-507.

589 Zehe, E., U. Ehret, T. Blume, A. Kleidon, U. Scherer, and M. Westhoff (2013), A
590 thermodynamic approach to link self-organization, preferential flow and rainfall-runoff
591 behaviour, *Hydrol. Earth Syst. Sc.*, 17, 4297-4322.

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595 **Tables**

596 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

597 ^aMeasured at Warren Farm.

598 ^bLocations are shown in Figure 1a.

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

Texture	K_s (ms ⁻¹)	Porosity (-)	α (m ⁻¹)	n (-)
Loam	3.7×10^{-6}	0.463	3.33	1.56
Silt loam	2.0×10^{-6}	0.50	1.2	1.39
Clay	1.7×10^{-7}	0.475	2.12	1.2

602

604 Table 3. Hydraulic properties of chalk

Properties	Unoptimized		Optimized value
	Value	Source	
K_s (md ⁻¹)	16	Le Vine et al., 2016	15
S_0 (-)	0.8	Observations	0.67
f_m (-)	1×10^5	Price et al., 1993	6.1×10^5
α (m ⁻¹)	3.0	Le Vine et al., 2016	-
n (-)	1.4	Le Vine et al., 2016	-

605

606 Table 4. Comparison between observed and simulated daily average runoff from the two
607 configurations over the Kennet catchment.

Metric	Observed	Simulated (<i>default</i>)	Simulated (<i>macro</i>)
RR	0.40	0.82	0.37
$\Delta\mu$	-	1.04	-0.05
$\Delta\sigma$	-	2.04	0.70

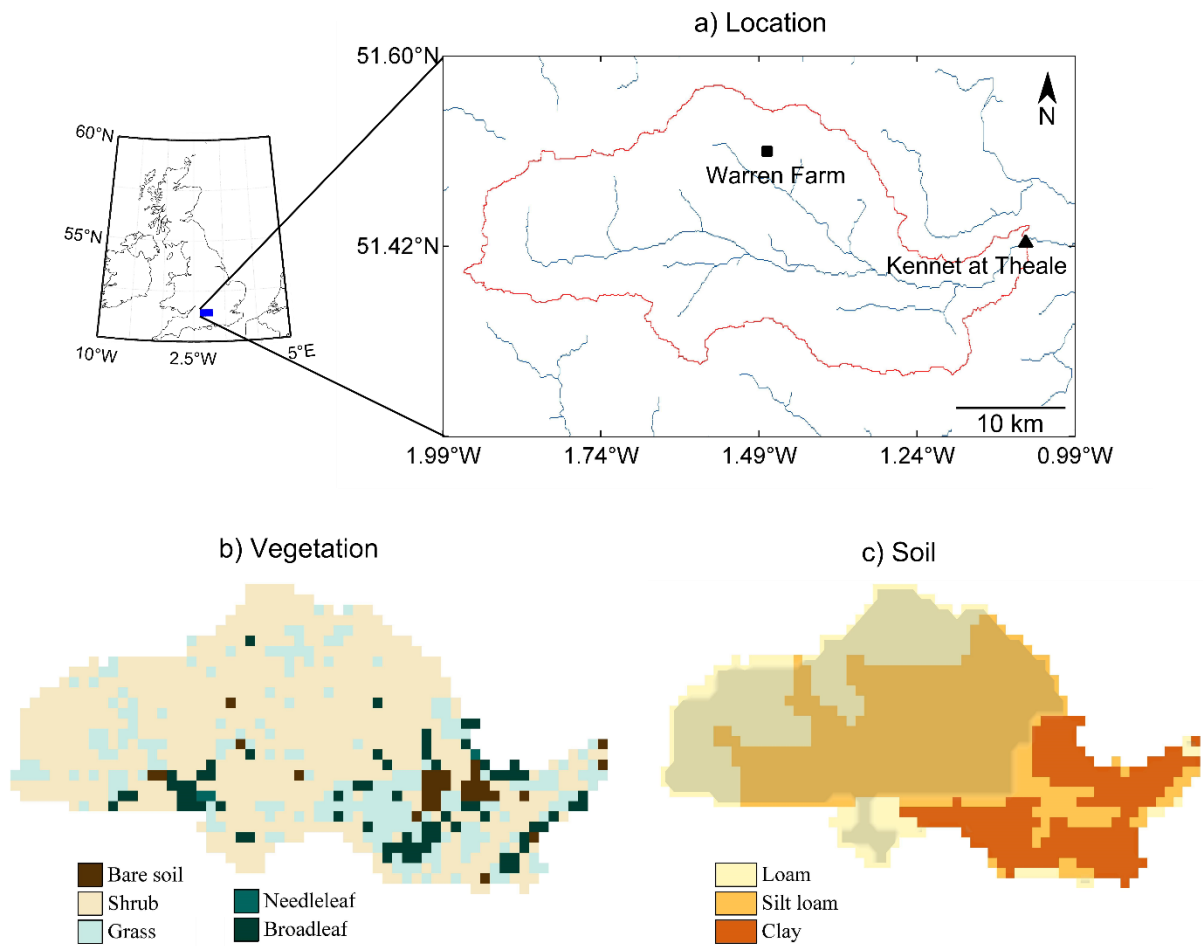
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611 **Figures**

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



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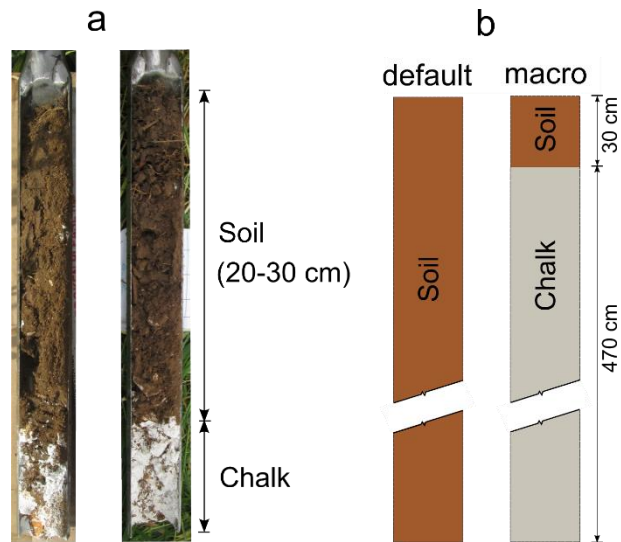
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622 Figure 2. Example of soil profiles collected at Warren Farm during a field campaign in 2015

623 (a), and the two model configurations (b).

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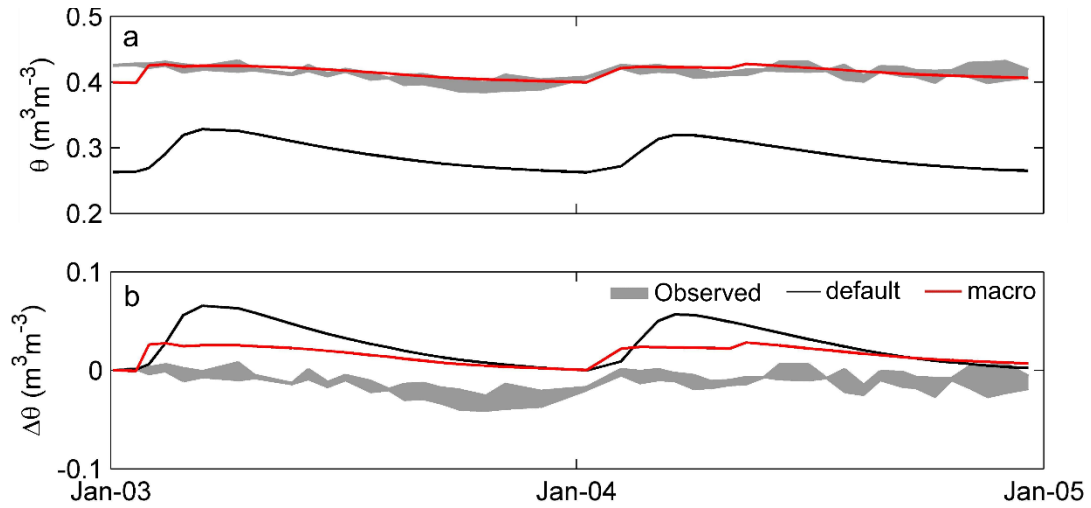
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637 Figure 3. Comparison between observed and simulated (a) soil moisture (θ) and (b) change in
638 soil moisture ($\Delta\theta$) from the *default* and *macro* configurations at a depth of 2m below land
639 surface. The shaded areas constructed from 2 soil moisture probes at the Warren Farm site
640 denote the range of observed data in these plots.



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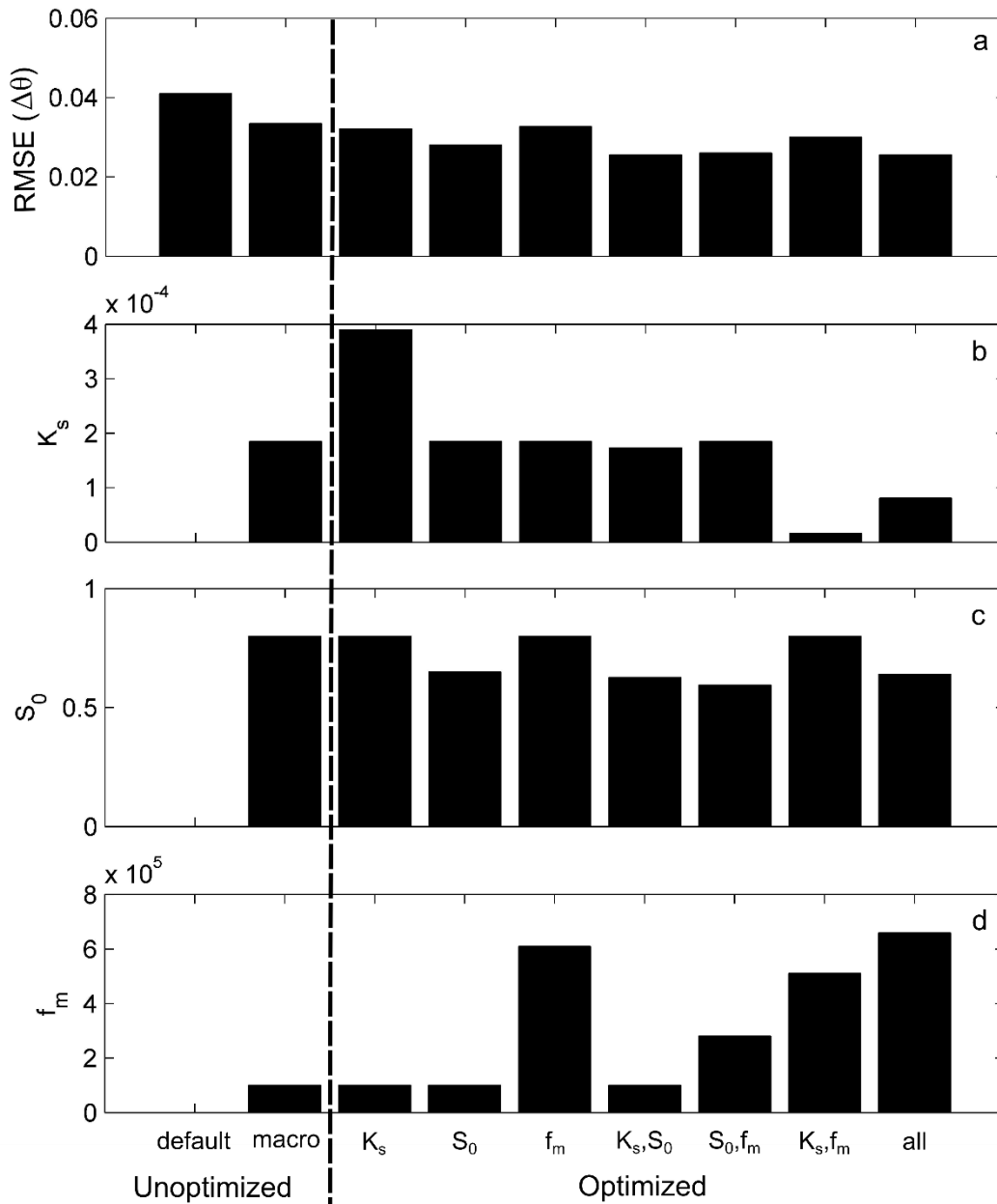
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652 Figure 4. (a) Model performance in reproducing observed and simulated $\Delta\theta$, (b) K_s , (c) S_0 and
 653 (d) f_m for various parameter combinations considered in the optimization. Note that except for
 654 the *default* and *macro*, the simulation yielding the lowest RMSE (out of 2000 model runs) is
 655 presented in this plot.

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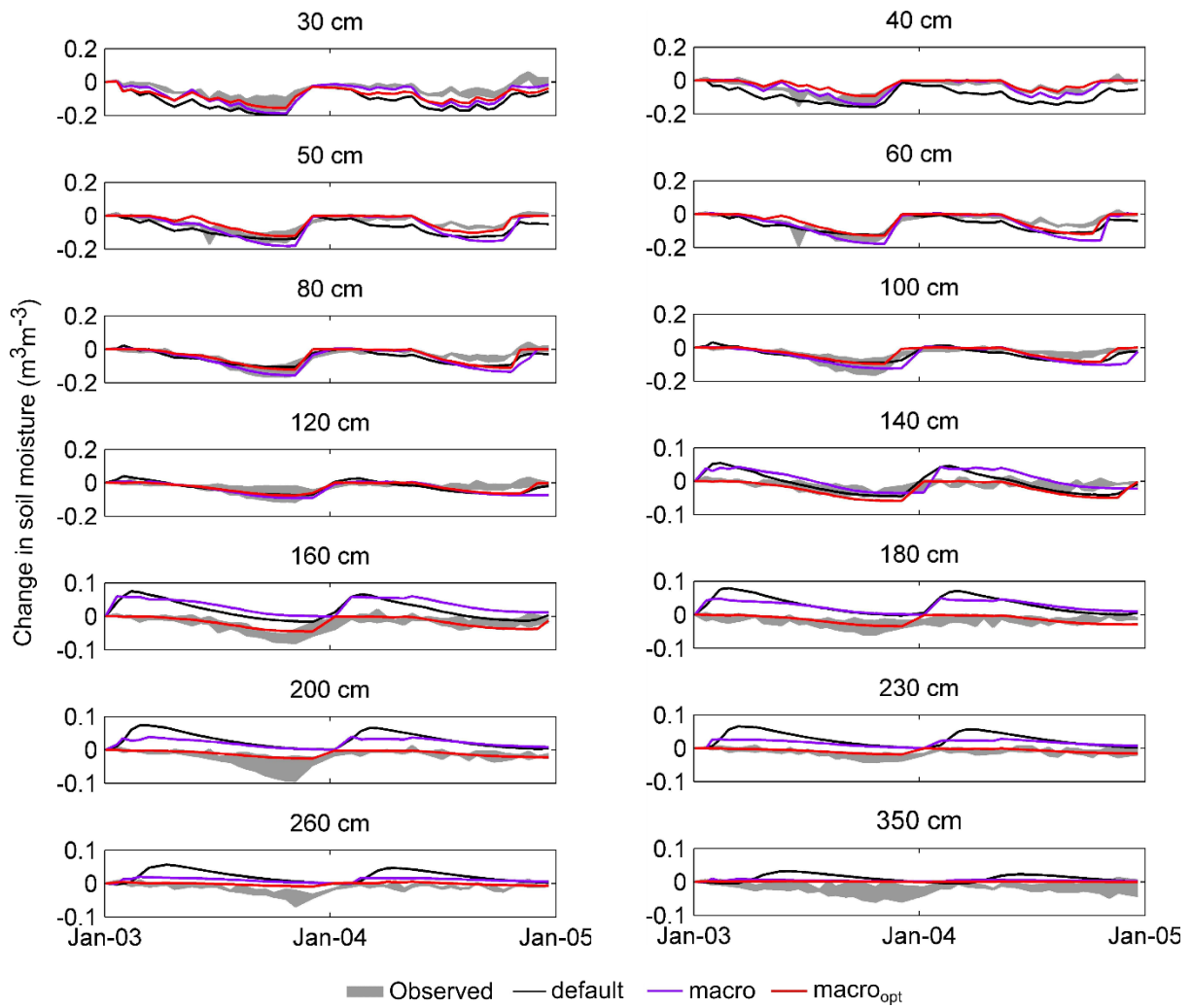


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659 Figure 5. Comparison between observed and simulated $\Delta\theta$ from *default*, *macro* and *macro_{opt}*
 660 configurations at various depths below land surface. The shaded area, which is constructed
 661 from 2 soil moisture probes at the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

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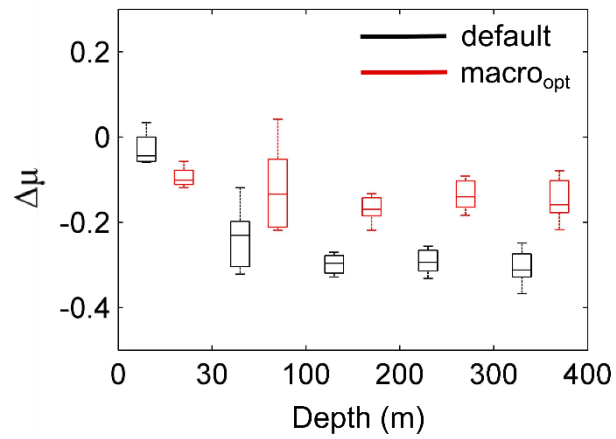
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668 Figure 6. Box plot of relative bias ($\Delta\mu$) of simulated soil moisture from *default* and *macro*
669 configurations at different depth ranges shown in individual intervals (e.g., 0-30 cm, 30-100
670 cm, and so on).

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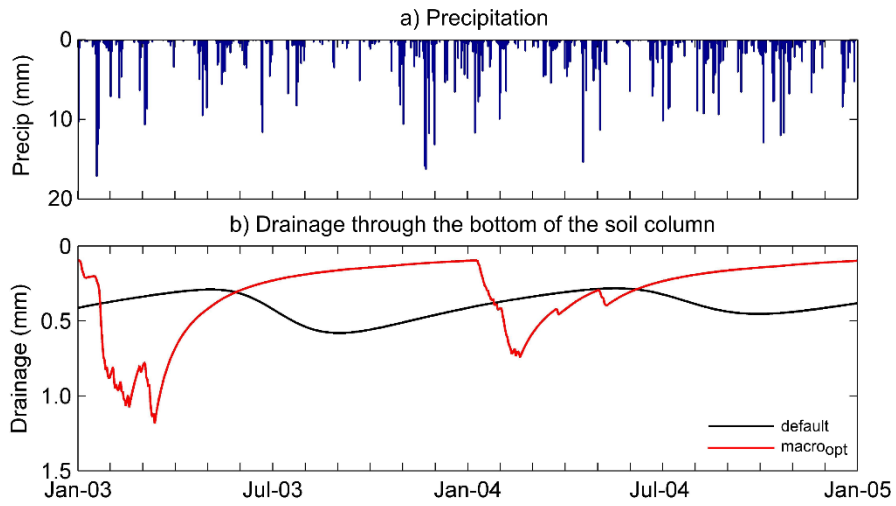
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684 Figure 7. (a) Precipitation and (b) daily sum of drainage through the bottom of the soil
685 column at Warren Farm over the two simulated years (2003-2005).

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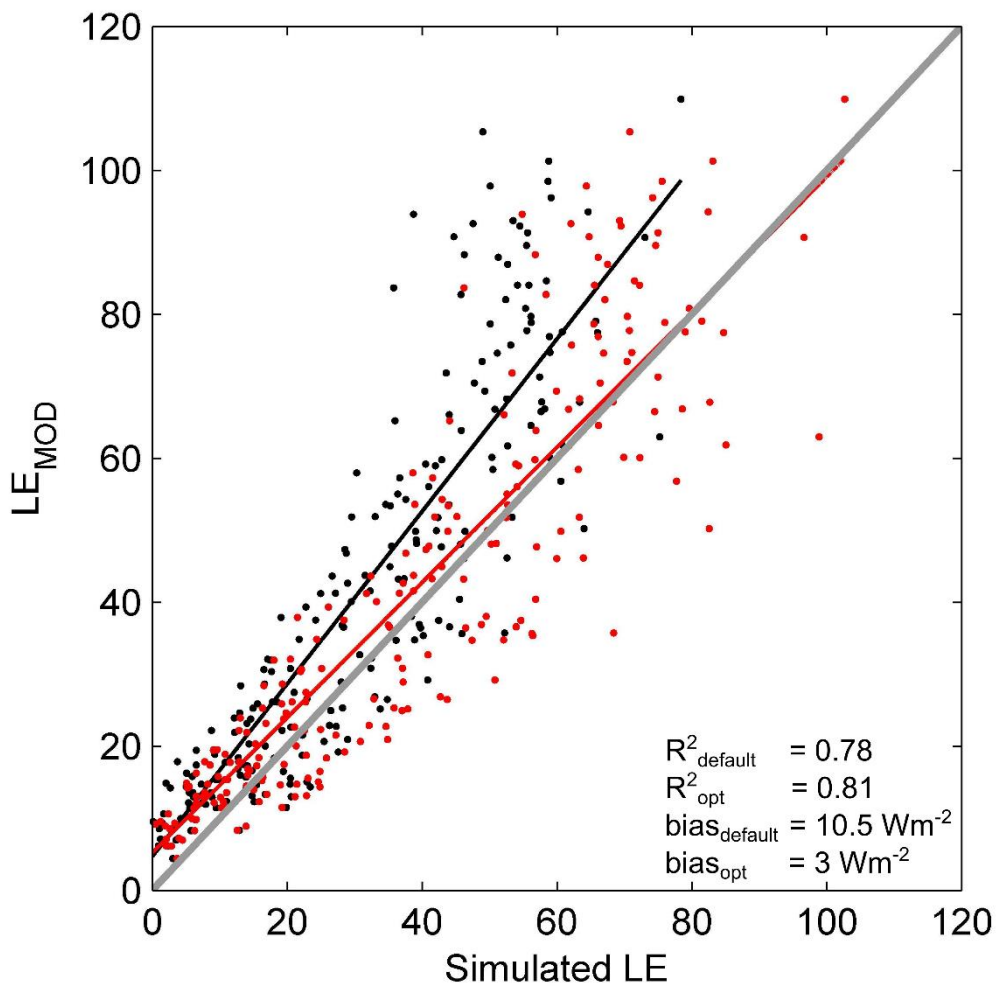
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699 Figure 8. Catchment average 8 day composites of MODIS estimated LE (LE_{MOD}) against
700 simulated LE from *default* and *macro* configurations ($LE_{default}$ and LE_{macro} , respectively) along
701 with the linear models fitted for $LE_{default}$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

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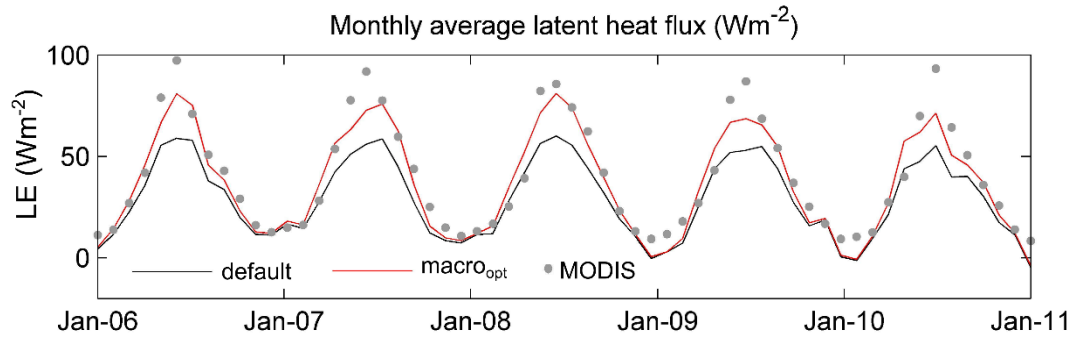
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708 Figure 9. Spatially averaged monthly latent heat flux (LE) from MODIS, *default* and *macro_{opt}*
709 configurations over the Kennet catchment.

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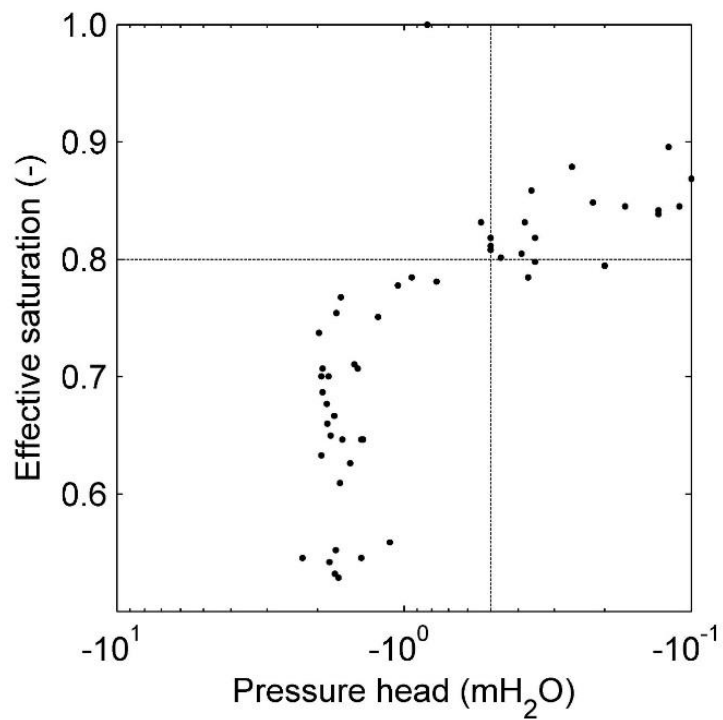
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723 **Supplementary materials**

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

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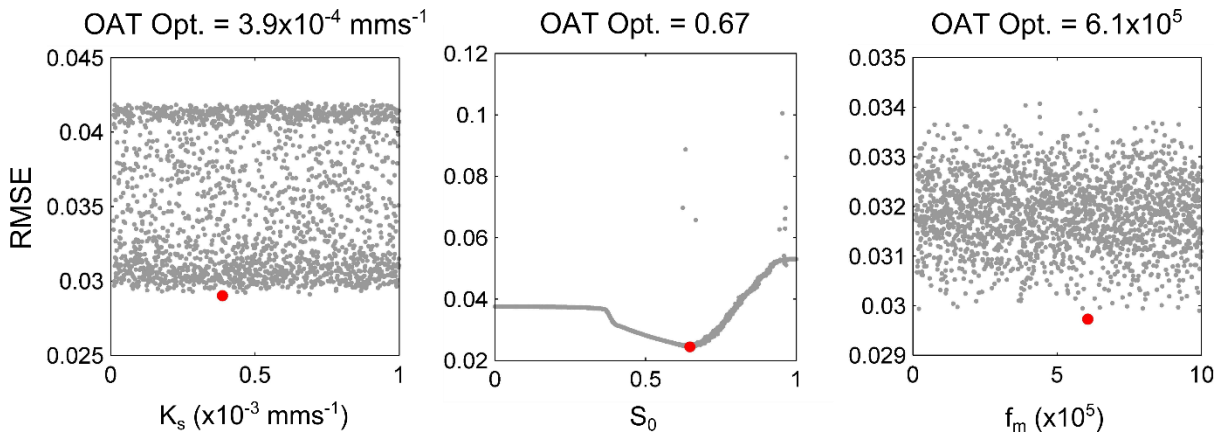
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736 Figure S2. Sensitivity of the BC model parameters on the model performance in simulating
737 $\Delta\theta$. Note that the parameters are considered one-at-a-time (OAT), and the vertical axis have
738 different RMSE ranges.

739



Towards a simple representation of chalk hydrology in land surface modelling

The effect of chalk representation in land surface modelling

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Abstract

Modelling and monitoring of hydrological processes in the unsaturated zone of ~~the~~ chalk, ~~which is~~ 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. However, efficient simulations of water movement through chalk unsaturated zone is difficult mainly due to the fractured nature of chalk, which 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. ~~Complex hydrology in the chalk aquifers may also influence land surface mass and energy fluxes because processes in the hydrological cycle are connected via non-linear feedback mechanisms. In this study, it is hypothesized that explicit representation of chalk hydrology in a land surface model influences land surface processes by affecting water movement through the shallow subsurface. In order to substantiate this hypothesis, In this study, a simplified macroporosity parameterization, namely the Bulk Conductivity (BC)~~

25 ~~model is~~ proposed for simulating hydrology in chalk unsaturated zone. This new
26 ~~parameterization is~~ implemented in the Joint UK Land Environment Simulator (JULES) ~~and,~~
27 ~~which is~~ applied ~~to on~~ a study area encompassing the Kennet catchment in the Southern UK.
28 The simulation results are evaluated using field measurements and satellite remote sensing
29 observations of various fluxes and states ~~of in~~ the hydrological cycle (e.g., soil moisture,
30 runoff, ~~and~~ latent heat flux) at two distinct spatial scales (i.e., point and catchment). The
31 results demonstrate that the inclusion of the BC model in JULES improves simulated land
32 surface mass and energy fluxes over the chalk-dominated Kennet catchment. Therefore, the
33 simple approach described in this study may be used to incorporate the flow processes
34 through chalk unsaturated zone in large scale land surface modelling applications. ~~The results~~
35 ~~reveal the influence of representing chalk hydrology on land surface mass and energy balance~~
36 ~~components such as surface runoff and latent heat flux via subsurface processes (i.e., soil~~
37 ~~moisture dynamics) in JULES, which corroborates the proposed hypothesis.~~
38 **Keywords:** Chalk hydrology, macroporosity, land surface modelling, bulk conductivity
39 model.

40 1. Introduction

41 Chalk can be described as a fine-grained porous medium traversed by fractures [*Price et al.*,
42 1993]. Previous studies showed that ~~T~~the unsaturated zone of the chalk aquifers plays an
43 important role on groundwater recharge ~~various important processes (e.g., recharge) of the~~
44 ~~hydrological cycle~~ in the UK [e.g., *Lee et al.*, 2006; *Ireson et al.*, 2009]. Therefore, both
45 monitoring [e.g., *Bloomfield*, 1997; *Ireson et al.*, 2006] and modelling [e.g., *Bakopoulou*,
46 2015; *Brouyère*, 2006; *Ireson and Butler*, 2011, 2013; *Sorensen et al.*, 2014] strategies have
47 been adapted previously to understand the governing hydrological processes in the chalk
48 unsaturated zone.

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

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

62 ~~The aforementioned studies revealed the importance of representing the matrix fracture flow~~
63 ~~nature in simulating subsurface hydrological processes in chalk dominated aquifers.~~ In recent
64 years, representation of chalk has ~~also~~ gained attention in land surface modelling. *Gascoïn et*
65 *al.* [2009] applied the Catchment Land Surface Model (CLSM) over the Somme River basin
66 in northern France. A linear reservoir was included in the TOPMODEL based runoff
67 formulation of CLSM to account for the contribution of chalk aquifers to river discharge. *Le*
68 *Vine et al.* [2016] applied the Joint UK Land Environment Simulator (JULES [*Best et al.*,
69 2011]) over the Kennet catchment in southern England to evaluate the hydrological
70 limitations of land surface models. In that study, two intersecting Brooks and Corey [curves](#)
71 ~~were curve was~~ proposed, which allowed a dual curve soil moisture retention representation
72 for the two distinct flow domains of chalk (i.e., matrix and fracture) in the model.
73 Considering this dual Brooks and Corey curve, a three-dimensional groundwater flow model

74 (ZOOMQ3D [Jackson and Spink, 2004]) was coupled to JULES to demonstrate the strong
75 influence of representing chalk hydrology and groundwater ~~dynamics flow~~ on simulated soil
76 moisture and runoff.

77 The above mentioned studies ~~illustrate the importance of suggest that the~~ representing ~~ation~~
78 ~~of~~ chalk ~~in~~ affects the hydrological processes simulated by land surface modellings.
79 ~~However, including chalk hydrology in large-scale land surface modelling using the~~
80 ~~contemporary dual-porosity concept can be complicated because this approach generally~~
81 ~~involves relatively large number of parameters. In this context, we propose a new~~
82 ~~parameterization, namely the Bulk Conductivity (BC) model as a first step towards a simple~~
83 ~~chalk representation suitable for land surface modelling. The BC model is included in JULES~~
84 ~~and evaluated at two distinct spatial scales (i.e., point and catchment). Because the processes~~
85 ~~of the hydrological cycle are connected via non-linear feedback mechanisms [e.g., Kollet and~~
86 ~~Maxwell, 2008; Rahman et al., 2014], the representation of water flow through the matrix-~~
87 ~~fracture system of chalk may also influence simulated land surface energy fluxes (e.g., latent~~
88 ~~heat flux), which has not yet been explicitly discussed. In this context, our hypothesis is that a~~
89 ~~consistent representation of water movement through chalk in a land surface model affects~~
90 ~~the exchange of mass and energy fluxes at the surface, which may be important to consider in~~
91 ~~water resources assessment and management practices (e.g., flood and drought prediction~~
92 ~~over chalk dominated areas). In order to substantiate this hypothesis, a macroporosity~~
93 ~~parameterization, namely the Bulk Conductivity (BC) model is implemented in JULES and~~
94 ~~evaluated at two distinct spatial scales (i.e., point and catchment). At the point-scale, the BC~~
95 model is evaluated ~~using against~~ observed soil moisture data. The proposed model is then
96 applied ~~to over~~ the Kennet catchment in the Southern England and the fluxes and states of the
97 hydrological cycle are simulated for multiple years. ~~The simulation results are evaluated~~
98 ~~using observed latent heat flux (LE) and runoff to assess the performance of the BC model in~~

99 [simulating land surface processes at the catchment scale.](#) ~~to demonstrate the importance of~~
100 ~~representing chalk hydrology, which supports the proposed hypothesis.~~

101 **2. A model of flow through chalk unsaturated zone**

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

$$107 \quad K_{sb} = K_s + K_s f_m \frac{S - S_0}{1 - S_0} \quad \text{if } S > S_0 \quad (1)$$

$$108 \quad \text{with } S = \frac{\theta - \theta_r}{\theta_s - \theta_r}$$

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

112 [At the first step of evaluation, the \$K_s\$, \$S_0\$ and \$f_m\$ parameters are estimated based on existing](#)
113 [literature to assess the performance of the uncalibrated BC model. In this uncalibrated BC](#)
114 [model, \$K_s\$ for chalk matrix is \$16 \text{ mmd}^{-1}\$ according to *Le Vine et al.* \[2016\] for the catchment](#)
115 [investigated in this study \(Figure 1\).](#)

116 Equation 1 indicates that the onset of water flow through the fracture system of chalk is
117 controlled by the threshold S_0 . According to *Wellings and Bell* [1980], water flow through
118 fractures dominates over matrix flow in chalk when the pressure head in soil becomes higher
119 than $-0.50 \text{ mH}_2\text{O}$. [We consider a value of \$S_0 = 0.80\$ for the uncalibrated BC](#)
120 [model](#), which is based on observed soil moisture-matric potential relationship in the study
121 area (Figure S1).

122 In Zehe et al. [2001], f_m was defined as the ratio of the saturated water flow rate in all
 123 macropores in a model element to the corresponding value in soil matrix, which can be
 124 determined based on the density and length of fractures at small scales. In addition, f_m has
 125 also been considered as a calibration parameter previously [e.g., Blume, 2008; Zehe et al.,
 126 2013]. In this study, we define f_m as a characteristic soil property reflecting the influence of
 127 fractures on soil water movement [Zehe and Blöschl, 2004], and estimate it from the relative
 128 difference of permeability between chalk matrix and fractured chalk system that can be of the
 129 order 10^4 - 10^6 according to Price et al. [1999]. Consequently, we consider a macroporosity
 130 factor of $f_m = 10^5$ for the uncalibrated BC model.

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

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

$$142 \quad RMSE = \frac{1}{nd} \sum_1^{nd} \sqrt{\left(\frac{1}{nt-1} \sum_2^{nt} (\Delta\theta_{d,t}^{obs} - \Delta\theta_{d,t}^{sim})^2 \right)} \quad (2)$$

143
 144 where nd is the number of soil layers, nt is the number of soil moisture observations available
 145 for a layer d , $\Delta\theta^{obs}$ is the observed variability of soil moisture and $\Delta\theta^{sim}$ is the simulated

146 variability of soil moisture. Note that we consider $\Delta\theta$ for this optimization because of its
147 relevance to the water flux and recharge through chalk unsaturated zone [e.g., Ireson and
148 Butler, 2011]. Latin hypercube technique [e.g., McKay et al., 2016] is used to generate 2000
149 random samples for each BC model parameter within the respective range discussed above.
150 We perform simulations using these random samples and calculate model performance
151 (Equation 2) to select the optimum parameter values for the BC model (discussed in section
152 4.1).

153 ~~In Zehe et al. [2001], f_m was defined as the ratio of the saturated water flow rate in all~~
154 ~~macropores in a model element to the corresponding value in soil matrix, which can be~~
155 ~~determined based on density and length of fractures at small scales. In addition, f_m has also~~
156 ~~been considered as a calibration parameter previously [e.g., Blume, 2008; Zehe et al., 2013].~~
157 ~~In this study, we define f_m as a characteristic soil property reflecting the influence of fractures~~
158 ~~on soil water movement [Zehe and Blöschl, 2004], and estimate it from the relative difference~~
159 ~~of permeability between chalk matrix and fractured chalk system that can be of the order 10^5~~
160 ~~according to Price et al. [1999]. Consequently, we consider a macroporosity factor of $f_m =$~~
161 ~~10^5 in this study.~~

162 **3. Methods**

163 **3.1. Study area**

164 The study area encompasses the Kennet catchment located in the Southern England with an
165 area of about 1033 km² (Figure 1a). Generally, Kennet, ~~in general~~, is rural in nature with
166 scattered settlements and has a maximum altitude of approximately 297 m (Above Ordnance
167 Level). The River Kennet discharges into the North Sea through London. The major Major
168 tributaries of this river are Lambourn, Dun, Enborne, and Foudry Brook. An average annual

169 rainfall of approximately 760 mm was recorded in the catchment over a 40 year period from
170 1961-1990.

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

178 **3.2. Field measurements and remotely sensed data**

179 Table 1 summarizes the field measurements and remote sensing data used in this study. We
180 use *in-situ* soil moisture and runoff measurements along with remotely sensed [LE latent heat](#)
181 [flux \(LE\)](#) data to assess model performance in simulating the mass and energy balance
182 components of the hydrological cycle. Point scale soil moisture measurements at two
183 adjacent sites (~20 m apart) at the Warren Farm (Figure 1) were provided by Centre for
184 Ecology and Hydrology (CEH). A Didcot neutron probe was used at these locations to
185 measure fortnightly soil moisture at different depths below land surface (10 cm apart down to
186 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.*,
187 2010].

188 The National River Flow Archive (NRFA) coordinates discharge measurements from [the](#)
189 gauging station networks across UK. These networks are operated by [the](#) Environmental
190 Agency (England), Natural Resources Wales, ~~the~~ Scottish Environment Protection Agency,
191 and Rivers Agency (Northern Ireland). We use discharge measurement provided by NRFA to
192 calculate the runoff ratio over the Kennet catchment in this study.

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

198 **3.3. Land surface model**

199 In this study, we use the Joint UK Land Environment Simulator (JULES [e.g., *Best et al.*,
200 2011; *Clark et al.*, 2011]) version 4.2. JULES is a flexible modelling platform with a modular
201 structure aligned to various physical processes developed based on the Met Office Surface
202 Exchange Scheme (MOSES [e.g., *Cox et al.*, 1999; *Essery et al.*, 2003]). Meteorological data
203 including precipitation, incoming short- and longwave radiation, temperature, specific
204 humidity, surface pressure, and wind speed are required to drive JULES. Each grid box in
205 JULES can comprise nine surface types (broadleaf trees, needle leaf trees, C3 grass, C4 grass,
206 shrubs, inland water, bare soil, and ice) represented by respective fractional coverage. Each
207 surface type is represented by a tile and a separate energy balance is calculated for each tile.

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

214 Surface runoff is calculated by combining the equations of throughfall and grid box average
215 infiltration in JULES. In order to direct the generated runoff to a channel network, river
216 routing is implemented based on the discrete approximation of one-dimensional kinematic

217 wave equation [e.g., *Bell et al.*, 2007]. In this approach, river network is derived from the
218 digital elevation model (DEM) of the study area and different wave speeds are applied to
219 surface and subsurface runoff components and channel flows [e.g., *Bell and Moore*, 1998]. A
220 return flow term accounts for the transfer of water between subsurface and land surface [e.g.,
221 *Dadson et al.*, 2010, 2011].

222 **3.4. Model configurations and input data**

223 *3.4.1. Point scale*

224 ~~At the point scale, JULES is configured to simulate the mass and energy fluxes at Warren~~
225 ~~Farm (Figure 1). A total subsurface depth of 5 m is considered in the model with a vertical~~
226 ~~discretization ranging from 10 cm at the land surface to 50 cm at the bottom of the model~~
227 ~~domain. Note that this discretization is consistent with the soil moisture measurement depths~~
228 ~~mentioned in section 3.2. The vegetation type is implemented as C3 grass using the default~~
229 ~~parameters in JULES. The soil hydraulic properties are estimated based on texture (Table 2),~~
230 ~~which is predominantly loamy at Warren Farm. The saturation pressure head relationship is~~
231 ~~described using the Van Genuchten [*Van Genuchten*, 1980] model with parameter values~~
232 ~~(Table 2) obtained from *Schaap and Leij* [1998] in the model.~~

233 ~~Point scale simulations were performed over 2 consecutive years from 2003–2005 at an~~
234 ~~hourly time step. Except for precipitation, hourly atmospheric forcing data to drive JULES~~
235 ~~was obtained from an automatic weather station operated by the CEH at Warren Farm. In~~
236 ~~order to estimate hourly precipitation data to run JULES, rain gauge measurements by the~~
237 ~~Met Office [*Met Office*, 2006] were used. Inverse distance interpolation technique [e.g.~~
238 ~~*Garcia et al.*, 2008; *Ly et al.*, 2013] was applied on rainfall measurements from 13 gauges~~
239 ~~closest to Warren Farm (distance varies from 25–60 km) to obtain hourly precipitation for the~~
240 ~~point scale simulations.~~

241 3.4.2. Catchment scale

242 At the catchment scale, JULES is configured over the study area (Figure 1) with a uniform
243 lateral grid resolution of 1 km with 70 x 40 cells in x and y dimensions, respectively. The
244 vertical discretization is identical to that of the point scale simulations described in the
245 previous section. Spatially distributed vegetation type information for the study area (Figure
246 1b) is obtained from the Land Cover Map 2007 (LCM2007) dataset [e.g., Morton *et al.*,
247 2011]. Harmonized World Soil Database (HWSD) from the Food and Agricultural
248 Organization of UNO (FAO) is used to obtain the texture of different soil types in the region
249 (Figure 1c). Van Genuchten model, with parameter values (Table 2) obtained from Schaap
250 and Leij [1998] is used to represent the saturation pressure head relationship for different soil
251 types, which is identical to the point scale simulations.

252 Simulations were performed over 5 consecutive years from 2006–2011 at the catchment scale.
253 Note that the simulation periods of catchment and point scale (2003–2005) does not coincide
254 due to the availability of soil moisture measurements described in section 3.2. Spatially
255 distributed meteorological data from the Climate, Hydrology, and Ecology research Support
256 System (CHESS) was used to obtain the atmospheric forcing to drive JULES. The CHESS
257 data includes 1 km resolution gridded daily meteorological variables [Robinson *et al.*, 2015].
258 This daily data is downscaled using a disaggregation technique described in Williams and
259 Clark [2014] to obtain hourly atmospheric forcing. The flow direction required for river
260 routing is extracted from the USGS HydroSHEDS digital elevation data [Lehner *et al.*, 2008].

261 3.5. Setup of numerical experiments

262 We consider two different model configurations, namely, *default* and *macro* (Figure 2), to
263 explore the influence of chalk hydrology on simulated land surface processes in JULES. The
264 *default* configuration corresponds to the standard parameterizations of JULES that does not

265 represent chalk hydrology in the model. In this configuration, each soil column in JULES is
266 considered to be vertically homogeneous with the soil properties defined in Table 2, which is
267 motivated by the Met Office JULES Global Land 4.0 configuration described in *Walters et*
268 *al.* [2014]. The *macro* configuration, in contrast, explicitly represents chalk hydrology in the
269 model. The *macro* setup modifies the *default* configuration by applying chalk hydraulic
270 properties (Table 3) from 30 cm below land surface to the bottom of the model domain (i.e.
271 500 cm). The BC model is applied in the chalk layers (30–500 cm) to simulate water flow in
272 the *macro* configuration. Therefore, soil columns in the model can be divided into topsoil (0–
273 30 cm) and chalk (30–500 cm) in *macro*. Note that except for this inclusion of chalk, *default*
274 and *macro* configurations are identical in terms of model set up and input data.

275 The topsoil depth of 30 cm is defined based on several augured soil samples collected during
276 a field campaign at Warren Farm in 2015 (Figure 2). This depth is corroborated by additional
277 information from the British Geological Survey (BGS) operated borehole records
278 (http://www.ukso.org/pmm/soil_depth_samples_points.html), which show that topsoil depths
279 vary from 10–40 cm over the study area. We therefore apply the *macro* configuration
280 assuming a spatially homogeneous 30 cm topsoil depth for both point and catchment scale
281 simulations.

282 In this study, simulations are performed at two distinct spatial scales, namely point and
283 catchment. At the point scale, JULES is configured to simulate the mass and energy fluxes at
284 the Warren Farm site (Figure 1a). A total subsurface depth of 5 m is considered in the model
285 with a vertical discretization ranging from 10 cm at the land surface to 50 cm at the bottom of
286 the model domain. Note that this discretization is consistent with the soil moisture
287 measurement depths mentioned in section 3.2. The vegetation type is implemented as C3
288 grass using the default parameters in JULES. Point scale simulations were performed over 2
289 consecutive years from 2003–2005 at an hourly time step. Except for precipitation, hourly

290 atmospheric forcing data to drive JULES was obtained from an automatic weather station
291 operated by the CEH at Warren Farm. In order to estimate hourly precipitation data to run
292 JULES, rain gauge measurements from the Met Office [Met Office, 2006] were used. Inverse
293 distance interpolation technique [e.g. Garcia et al., 2008; Ly et al., 2013] was applied on
294 rainfall measurements from 13 gauges closest to Warren Farm (distance varies from 25-60
295 km) to obtain hourly precipitation for the point scale simulations.

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

311 We estimate the soil hydraulic properties based on texture (Table 2). At the point scale, loam
312 soil is dominant at the Warren Farm site. At the catchment scale, the Harmonized World Soil
313 Database (HWSD) from the Food and Agricultural Organization of UNO (FAO) is used to
314 obtain the texture of different soil types over Kennet (Figure 1c). The saturation-pressure

315 head relationship for different soil types is described using the Van Genuchten [Van
316 Genuchten, 1980] model with parameter values (Table 2) obtained from Schaap and Leij
317 [1998].

318 Table 3 summarizes the hydraulic properties for chalk used in this study. These properties are
319 obtained based on existing literature as a first step when evaluating the uncalibrated BC
320 model. The BC model parameters are subsequently optimized to minimize the differences
321 between observed and simulated $\Delta\theta$.

322 In this study, we consider two different model configurations, namely *default* and *macro*
323 (Figure 2). The *default* configuration corresponds to the standard parameterizations of JULES
324 that does not represent chalk hydrology in the model. In this configuration, each soil column
325 in JULES is considered to be vertically homogeneous with the soil properties defined in
326 Table 2, which is motivated by the Met Office JULES Global Land 4.0 configuration
327 described in Walters *et al.* [2014]. The *macro* configuration, in contrast, explicitly represents
328 chalk by applying the BC model starting at 30 cm below land surface to the bottom of the
329 model domain (i.e. 500 cm). Therefore, the soil column in the *macro* configuration can be
330 divided into topsoil (0-30 cm) and chalk (30-500 cm) in *macro*. Note that except for this
331 inclusion of chalk, *default* and *macro* configurations are identical in terms of model set up
332 and input data.

333 The topsoil depth of 30 cm in the *macro* configuration is defined based on several augured
334 soil samples collected during a field campaign at Warren Farm in 2015 (Figure 2). This depth
335 is corroborated by additional information from the British Geological Survey (BGS) operated
336 borehole records (http://www.ukso.org/pmm/soil_depth_samples_points.html), which show
337 that topsoil depths vary from 10-40 cm over the study area. We therefore apply the *macro*

338 configuration assuming a spatially homogeneous topsoil depth of 30 cm for both point and
339 catchment scale simulations.

340 **4. Results and discussion**

341 **4.1. Point scale simulations**

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

351 The results show that despite the *macro* configuration improves simulated θ , it shows
352 considerable discrepancies with observed $\Delta\theta$, which is consistent throughout the whole chalk
353 profile (results from other model layers are not shown). In order to minimize the differences
354 between observed and modelled $\Delta\theta$ from the *macro* configuration, we optimize the BC model
355 following the methodology described in section 2. The optimization results are summarized
356 in Figure 4. Note that for each combination considered in the optimization, 2000 model runs
357 were performed using randomly sampled parameters as discussed in section 2. Figure 4
358 presents the results from the model runs yielding the lowest RMSE.

359 The RMSE between observed and simulated $\Delta\theta$ for the model configurations considered in
360 the optimization is shown in Figure 4a. This figure illustrates that the RMSE of the *default*
361 configuration is larger than that of *macro*, indicating better model performance in

362 reproducing $\Delta\theta$ for the latter. Therefore, it appears that the uncalibrated BC model (i.e., the
363 *macro* configuration) is better in reproducing soil moisture variability compared to ~~the default~~
364 ~~configuration~~. Figure 4b, c and d presents the BC model parameter values from the model run
365 producing the lowest RMSE for each configuration. Concerning single BC model parameters,
366 Figure 4a shows that optimizing S_0 results in a 16% reduction of RMSE compared to the
367 *macro* configuration. Optimizing K_s marginally improves model performance, which is
368 observed from a slightly lower (4%) RMSE than *macro*. Optimizing both K_s and S_0
369 simultaneously results in the largest reduction (24%) of RMSE compared to *macro*.
370 Additionally, Figure 4 suggests that the sensitivity of S_0 on the model performance in
371 simulating $\Delta\theta$ is substantially higher compared to K_s and f_m , which is corroborated by the
372 sensitivity of the individual model parameters (Figure S2). Figure 4a also reveals the
373 interesting fact that the RMSE from the configuration with optimized K_s and S_0 is identical to
374 that of the one ~~the one with optimized~~ all 3 parameters optimized simultaneously (i.e., K_s , S_0
375 and f_m). Therefore, we select the *macro* configuration with optimized K_s and S_0 (*macro_{opt}*
376 hereafter) to simulate chalk hydrology over the study area.

377 ~~Figure 3 shows observed and simulated volumetric soil moisture from the *default* model~~
378 ~~configuration at Warren Farm from 2003–2005. This figure shows that simulated soil~~
379 ~~moisture at shallow soil layers (up to 50 cm) compares reasonably well with the observed~~
380 ~~data. However, in the deeper layers, the model considerably underestimates soil moisture.~~
381 ~~Figure 4 compares observed and simulated volumetric soil moisture from the *macro*~~
382 ~~configuration at Warren Farm over the simulation period. This figure shows that especially in~~
383 ~~the deeper soil layers, the agreement between observed and simulated soil moisture improves~~
384 ~~remarkably relative to the *default* configuration throughout the simulation period. Notice~~
385 ~~again that the *default* and *macro* configurations are identical in terms of model setup and~~
386 ~~inputs except for the consideration of chalk. Therefore, the differences in soil moisture~~

387 ~~simulations between the two model configurations can be attributed to the representation of~~
388 ~~chalk hydrology in JULES.~~

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

397 In order to assess the model performance in simulating soil moisture over the entire chalk
398 profile column, Figure 5 presents the relative bias ($\Delta\mu$, see Appendix) of simulated soil
399 moisture θ from the *default* and *macro_{opt}* two model configurations at Warren Farm for
400 various depth ranges are shown in Figure 6. In the soil layers (0-30 cm), θ from the two
401 configurations are comparable with both the *default* and *macro* configurations showing
402 slightly lower mean relative bias ($\Delta\mu_{mean}$) of -0.03 reproduces soil moisture reasonably well
403 with the latter showing slightly better than *macro_{opt}* ($\Delta\mu_{mean} = -0.09$). agreement with
404 observations. However, in the chalk layers (30-500 cm), *default* fails to reproduce the soil
405 moisture dynamics efficiently, simulating substantially drier conditions, corresponding
406 to which are observed from the mean relative bias ($\Delta\mu_{mean}$) of $\Delta\mu_{mean} \leq -0.28$ for this
407 configuration. In contrast, the *macro_{opt}* configuration considerably remarkably
408 improves the agreement between the simulated and with the observed θ soil moisture profile
409 in the chalk layers with the largest calculated $\Delta\mu_{mean} \geq -0.05$. Therefore, the results
410 indicate that the inclusion of the BC model in JULES improves the performance of overall
411 soil moisture simulation (both θ and $\Delta\theta$) at Warren Farm especially in the chalk layers.

412 The drainage flux through the bottom of soil column (d_b) of a land surface model can be
413 considered as the potential recharge flux to groundwater [e.g., Sorensen et al., 2014].
414 Therefore, the inclusion of the BC model in JULES appears to improve the performance of
415 overall soil moisture simulation at Warren Farm especially in the chalk layers. Figure 67
416 compares the daily sum of drainage through the bottom of the soil column (d_b) from the
417 default and $macro_{opt}$ configurations at the Warren Farm site. The rainfall characteristics over
418 the study period is shown in Figure 67a. In Figure 67b, the $macro_{opt}$ configuration shows
419 considerable d_b during the colder months, while slow drainage prevails throughout the rest of
420 the year. In contrast, the default configuration shows relatively high d_b in summer compared
421 to the colder months. In general, the recharge rate through chalk unsaturated zone during the
422 warmer periods of the year is lower than that in the winter months [Wellings and Bell, 1980;
423 Ireson et al., 2009]. Therefore, the $macro_{opt}$ configuration appears to be more consistent with
424 the recharge mechanism in chalk compared to default.

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

430 In order to explore the reason of the discrepancies between simulated soil moisture from the
431 two model configurations, Figure 6 shows S and water flux (w_f) profiles along with drainage
432 through the bottom boundary (d_b) of default and macro for the entire simulation period.
433 Figure 6b plots the contours of daily accumulated w_f through chalk (30–500 cm) over daily
434 average S for the macro configuration (S_{macro}). Figure 6c shows S ($S_{default}$) and w_f through the
435 same profile for the default configuration. A comparison between Figure 6b and 6c reveals
436 that default is considerably drier compared to macro ($S_{default} < S_{macro}$) throughout the profile,

437 which is consistent with Figure 5. Figure 6b shows notable flux through the profile following
438 strong precipitation events (Figure 6a), indicating fast water flow through subsurface in the
439 *macro* configuration (especially in winter). The *default* configuration, on the other hand,
440 shows relatively slower movement of water in the subsurface (Figure 6c).

441 According to the BC model, fracture flow in chalk is activated in a soil grid if S exceeds S_0
442 (defined as 0.80), which is achieved predominantly during winter following strong
443 precipitation events because of the prevailing wet conditions. Therefore, the activation of
444 fracture flow explains the fast water movement patterns after strong precipitation events
445 observed in Figure 6b. This result is consistent with Ireson *et al.* [2009], who showed that
446 fracture flow through chalk dominates at Warren Farm during wet periods. Compared to the
447 *macro* configuration, *default* does not show fast water flow to the deeper soil layers because
448 the latter does not represent the matrix fracture flow nature of chalk in JULES.

449 Figure 6d compares daily sum of d_b from the two configurations. The *macro* configuration
450 generally shows lower drainage compared to *default* with an exception in March 2003.
451 Because of the gravity drainage lower boundary condition, water flow through the bottom of
452 the model domain depends on K_s at the deepest soil layer in JULES. In chalk (*macro*
453 configuration), K_s at the deepest soil layer is smaller compared to *default* (loam soil)
454 especially when $S_0 < 0.8$ (Equation 1), which explains the lower drainage flux in case of the
455 *Chalk* configuration. The reason of higher d_b in *macro* compared to *default* in March 2003 is
456 the strong precipitation events (Figure 6a) causing considerable fracture flow and $S > 0.8$ at
457 the bottom of the model domain (Figure 6b).

458 Figure 6 outlines the differences in simulated subsurface processes by the two model
459 configurations. Fracture flow in chalk is activated according to the BC approach during wet
460 periods that allows recharge at deeper soil layers in *macro*, which is absent in case of the

461 *default* configuration. Moreover, the *default* configuration generally shows higher drainage
462 flux through the lower boundary compared to *macro*. The combination of relatively low
463 recharge and high drainage through lower boundary is the reason of the drier conditions
464 simulated by *default*. In contrast, the *macro* configuration is characterized by fast recharge at
465 the deeper soil layers through fractures and slow drainage through the bottom because of
466 considerably lower K_s compared to *default*, which is the reason of relatively higher simulated
467 soil moisture by this configuration that compares well with observations.

468 Several previous studies have discussed the influence of root zone soil moisture on land
469 surface mass and energy balance components [e.g., *Wetzel and Chang, 1987; Chen and Hu,*
470 *2004*]. Therefore, the differences in soil moisture from two configurations discussed above
471 may affect the land surface mass and energy fluxes in the model. In order to investigate this
472 effect, Figure 7 shows the difference between daily average latent heat flux (LE) time series
473 from *default* and *macro* configurations ($LE_{default}$ and LE_{macro} , respectively) at Warren Farm
474 over the simulation period. This figure shows that the *default* configuration generally
475 simulates lower LE compared to *macro* especially in the warmer months of the year.

476 The underestimation of LE in Figure 7 can be attributed to the differences in simulated soil
477 moisture by the two configurations (Figure 3 and 4). In winter, abundant soil moisture is
478 available in both *default* and *macro* to meet the relatively low evapotranspiration (ET)
479 demand due to the prevailing energy limited conditions. Therefore, Figure 7 shows negligible
480 differences between $LE_{default}$ and LE_{macro} in winter. However, in summer, the discrepancies
481 between soil moisture from the two model configurations result in marked differences
482 between $LE_{default}$ and LE_{macro} because of the increased ET demand, which is consistent with
483 previous studies [e.g., *Rahman et al., 2016*].

484 ~~In this section, subsurface and land surface processes simulated by *default* and *macro*~~
485 ~~configurations are discussed at the point scale. The simulation results show notable~~
486 ~~differences in soil moisture and *LE* from the two configurations. Because the only difference~~
487 ~~between *default* and *macro* configurations is the representation of the chalk hydrology, it~~
488 ~~appears that a consistent representation of chalk in JULES affects land surface processes via~~
489 ~~subsurface hydrodynamics supporting our hypothesis. In the next section, we test this~~
490 ~~hypothesis regionally by evaluating the mass and energy fluxes of the hydrological cycle at~~
491 ~~the catchment scale.~~

492 4.2. Catchment scale simulations

493 In the previous section, it was observed that the *default* configuration generally
494 underestimates θ compared to *macro_{opt}*. Previous studies have demonstrated the
495 interconnections between shallow soil moisture and LE [e.g., *Chen and Hu*, 2004]. In order to
496 assess the differences between the LE from the *default* and *macro_{opt}* configurations at the
497 catchment scale, Figure 7-8 plots spatially averaged 8-day composites of LE from MODIS
498 (LE_{MOD}) against ~~the LE from these configurations~~ *default* and *macro_{opt}* configurations
499 (LE_{default} and ~~LE_{macro}~~ LE_{opt}, respectively) over the Kennet catchment. In this figure, ~~the~~ the
500 agreement between simulated LE and LE_{MOD} is evaluated using the coefficient of
501 determination (R^2 , see Appendix) and mean bias. Comparison between LE_{default} and LE_{MOD}
502 shows a coefficient of determination of $R^2_{default} = 0.78$ and a mean bias of $bias_{default} = 10.5$
503 Wm^{-2} . The agreement between simulated LE and LE_{MOD} improves in case of the *macro_{opt}*
504 ~~macro~~ configuration, which is reflected by an increased coefficient of determination of
505 $R^2_{macro} = 0.81$ and a reduced mean bias of $bias_{opt} = 3 Wm^{-2}$.

506 Figure 8-7 shows differences between LE_{default} and ~~LE_{opt}~~ LE_{macro} especially for relatively high
507 LE, indicating discrepancies especially during the warmer months of the year. Figure 9a

508 presents spatially averaged time series of monthly LE_{MOD} , $LE_{default}$ and LE_{opt} ~~LE_{macro}~~ . This
509 figure shows ~~that the negligible differences in LE from the two configurations during the~~
510 ~~colder months of the year, while~~ differences between $LE_{default}$ and LE_{opt} ~~LE_{macro}~~ increases
511 substantially in summer compared to the colder months of the year, which is consistent with
512 Figure 78. Consequently, the *default* configuration underestimates LE ~~especially~~ in summer
513 compared to LE_{MOD} , which is improved ~~when chalk hydrology is explicitly considered in~~
514 ~~JULES~~ in case of the *macro_{opt} macro* configuration. In contrast, the differences between
515 $LE_{default}$ and LE_{opt} between are negligible during the colder months of the year.

516 ~~Figure 9b plots spatially averaged time series of daily $S_{default}$ and S_{macro} over the Kennet~~
517 ~~catchment. Note that average S at the first 8 vertical model layer (0–100 cm below land~~
518 ~~surface) is presented in this figure, which highlights the difference in root zone moisture~~
519 ~~content from the two model configurations. Figure 9b shows relatively lower S simulated by~~
520 ~~the *default* configuration compared to S_{macro} . In JULES, LE depends on surface conductance~~
521 ~~to evaporation, which is controlled by the mean soil moisture in the root zone. Therefore, the~~
522 ~~differences in $S_{default}$ and S_{macro} is consistent with the underestimation of LE by the *macro*~~
523 ~~configuration (Figure 9a). Note that despite the differences in S between the two~~
524 ~~configurations over the entire simulation period, Figure 9a shows significant LE differences~~
525 ~~only in summer. This is due to the prevailing energy limited conditions during the colder~~
526 ~~months over the region, which was discussed in the previous section. Figure 9 suggest that~~
527 ~~representing chalk hydrology in JULES considerably influences simulated LE by modifying~~
528 ~~shallow soil moisture at the catchment scale, also supporting our hypothesis.~~

529 Table 4 compares observed and simulated daily average runoff from the two model
530 configurations over the Kennet catchment from 2006-2011. The runoff ratio (RR , see
531 Appendix), which is equal to the mean volume of flow divided by the volume of precipitation
532 [e.g., Kelleher et al., 2015], assesses the partitioning of precipitation into runoff over the

533 catchment. The *default* configuration ($RR = 0.82$) shows considerably higher RR compared to
534 observation ($RR = 0.40$), indicating overestimation of runoff by the model. Including chalk
535 hydrology in the model remarkably improves the agreement between observed and simulated
536 mean runoff over the Kennet catchment, which is assessed from a runoff ratio of $RR = 0.378$
537 for the *macro_{opt}* configuration.

538 In Table 4, the relative bias ($\Delta\mu$) of 1.04 between observed and simulated runoff from the
539 *default* configuration again indicates the overestimation by the model. In comparison,
540 *macro_{opt}* shows a relative bias ($\Delta\mu = -0.05$), indicating improvement between
541 observed and simulated mean runoff volume compared to *default*. The relative difference in
542 standard deviation ($\Delta\sigma$, see Appendix) compares the *variability magnitude* of observed and
543 simulated runoff in Table 4. This comparison shows that the *default* configuration
544 overestimates the variability of runoff over the Kennet catchment ($\Delta\sigma = 2.04$), which is
545 improved in case of *macro* ($\Delta\sigma = 0.70$).

546
547 It was demonstrated previously that the *default* configuration predicts lower
548 evapotranspiration (ET) compared to *macro_{opt}* over the Kennet catchment due to the
549 differences in simulated θ . In JULES, moisture from soil and canopy is depleted to meet the
550 evapotranspiration (ET) demand. Additionally, surface runoff generation depends on canopy
551 water storage in the model [Best et al., 2011]. Because of this connection between ET and
552 surface runoff generation via canopy water storage, the differences in runoff demonstrated in
553 Table 4 can be attributed to the disagreements between $LE_{default}$ and LE_{macro} (demonstrated in
554 Figure 8) due to the relatively drier conditions simulated by *default*.

555 ~~In JULES, moisture from soil and canopy water storage is depleted to meet the ET demand.~~
556 ~~Additionally, surface runoff generation depends on canopy water storage in the model [Best~~

557 *et al.*, 2011]. Because of this connection between ET and surface runoff generation via
558 canopy water storage, the differences in runoff demonstrated in Table 4 can be attributed to
559 the disagreement between $LE_{default}$ and LE_{macro} demonstrated in Figure 9a. Therefore, it
560 appears that LE in JULES is affected by the inclusion of chalk hydrology, which
561 consequently influences surface runoff generation corroborating our hypothesis.

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

569 **5. Summary and Conclusions**

570 In this study, we proposed a simple parameterization~~we hypothesized that a consistent~~
571 ~~representation of chalk hydrology affects land surface mass and energy balance components~~
572 ~~via subsurface hydrodynamics simulated by a land surface model. In order to support this~~
573 ~~hypothesis, namely the~~ Bulk Conductivity (BC) model ~~that to~~ simulates water flow
574 through the matrix-fracture system of chalk in large scale land surface modelling
575 applications. This parameterization was implemented in the Joint UK Land Environment
576 Simulator (JULES) and. ~~This model was~~ applied to ~~on~~ the Kennet catchment located in the
577 southern UK to simulate the mass and energy fluxes of the hydrological cycle for multiple
578 years. Two model configurations, ~~namely~~ namely *default* and *macro* were considered with
579 the latter representing using the BC model to simulate chalk hydrology ~~in JULES using the~~
580 BC model.

581 The proposed BC model is a single continuum approach of modelling preferential flow [e.g.,
582 *Beven and Germann, 2013*] that involves only 2 parameters, namely macroporosity factor (f_m)
583 and relative saturation threshold (S_0). Initially, these parameters along with the saturated
584 hydraulic conductivity of the chalk matrix were estimated from existing literature. Finally,
585 the BC model parameters were optimized to minimize the differences between observed and
586 simulated soil moisture variability. Our results indicated that S_0 is the most influential
587 parameter in the model when representing water movement through a soil-chalk column,
588 followed by the saturated hydraulic conductivity of chalk matrix while f_m showed low
589 sensitivity. Hence, the parameterization is further improved by optimizing both saturated
590 hydraulic conductivity of chalk matrix and S_0 to minimize the differences between observed
591 and simulated soil moisture variability.

592 The simulation results were evaluated using observed mass and energy fluxes both at point
593 and catchment scales. The results demonstrated that the inclusion of the BC model in JULES
594 improves simulated soil moisture variability at the point scale compared to a model
595 configuration that does not represent chalk in the subsurface (i.e., the *default* configuration).
596 At the catchment scale, it was illustrated that the proposed parameterization improves
597 simulated latent heat flux and overall runoff compared to the *default* configuration. The
598 discrepancies between the measured and simulated fluxes and states can be improved by a
599 comprehensive model calibration, which is out of the scope of this study and should be the
600 subject of future research.

601 Note that the complexity of the BC model for simulating water flow through chalk
602 unsaturated zone is substantially lower compared to more commonly used models for this
603 purpose (e.g., dual-porosity models). Despite its simplicity, it appears that the proposed
604 parameterization improves mass and energy fluxes simulated by JULES over the Kennet
605 catchment. As mentioned previously, representing chalk hydrology in land surface models

606 using the dual-porosity concept is complicated mainly due to the relatively large number of
607 parameters involved in such approach. Therefore, the simplified parameterization proposed in
608 this study may be useful for large-scale land surface modelling applications over chalk-
609 dominated areas.

610 ~~The results showed that JULES generally underestimates root zone soil moisture without a~~
611 ~~consistent representation of chalk hydrology. Consequently, *LE* is underestimated by the~~
612 ~~model without chalk representation. The effect of chalk hydrology was also observed on~~
613 ~~runoff, which was attributed to the interconnection between *LE* and runoff generation in the~~
614 ~~model. Therefore, representing the matrix fracture flow nature of chalk in a land surface~~
615 ~~model affects land surface processes via shallow soil moisture dynamics, which supports the~~
616 ~~proposed hypothesis.~~

617 ~~*Habtes et al.* [2010] argued that flood flow in chalky catchments is influenced by the~~
618 ~~hydrological processes in the unsaturated zone. Implementing the BC model in JULES, this~~
619 ~~study showed that representing chalk hydrology significantly affects subsurface and land~~
620 ~~surface mass and energy fluxes. Therefore, the matrix fracture flow nature of the aquifer may~~
621 ~~be important to consider in flood forecasting in chalk dominated catchments.~~

622 ~~*Leeper et al.* [2011] discussed the influence of shallow soil moisture on simulated~~
623 ~~atmospheric processes over karst landscapes because of the subsurface land surface~~
624 ~~connection in the terrestrial system. In this study, we demonstrated that considering chalk~~
625 ~~hydrology considerably affects land surface mass and energy fluxes via subsurface~~
626 ~~hydrodynamics. This effect may be important to consider in numerical weather prediction~~
627 ~~models over the regions dominated by chalk because of the karst behaviour of chalk aquifers~~
628 ~~[e.g., *MacDonald et al.*, 1998; *Hartmann et al.*, 2014].~~

629 ~~*Le Vine et al.* [2016] argued that the deep groundwater system in a chalk dominated~~
630 ~~catchment may influence the mass and energy balance components of the hydrological cycle,~~
631 ~~which is not considered in this study. The reason for that is JULES simulates water flow at~~
632 ~~shallow subsurface considering free drainage lower boundary condition and does not allow~~
633 ~~lateral movement of water between the soil columns. The effect of groundwater dynamics can~~
634 ~~be represented in JULES by coupling a three dimensional groundwater flow model [e.g., *Le*~~
635 ~~*Vine et al.*, 2016; *Maxwell and Miller*, 2005], which will be addressed in future.~~

636

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648

649 **Appendix**

650 **Definition of Statistical Metrics**

651 Coefficient of determination (R^2) for observation $y = y_1, \dots, y_n$ and prediction $f = f_1, \dots, f_n$
652 is defined as

$$653 \quad R^2 = 1 - \frac{SS_{res}}{SS_{tot}}$$

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

$$656 \quad SS_{res} = \sum_{i=1}^n (y_i - f_i)^2 \quad \text{and}$$

$$657 \quad SS_{tot} = \sum_{i=1}^n (y_i - \bar{y})^2 \quad \text{with } \bar{y} \text{ being the mean of } y.$$

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

$$660 \quad RR = \frac{\mu_{runoff}}{\mu_{rain}}$$

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

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

$$663 \quad \Delta\mu = \frac{\mu_{mod} - \mu_{obs}}{\mu_{obs}}$$

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

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

$$669 \quad \Delta\sigma = \frac{\sigma_{mod} - \sigma_{obs}}{\sigma_{obs}}$$

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

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References

[Bakopoulou, C. \(2015\), Critical assessment of structure and parameterization of JULES land surface model at different spatial scales in a UK Chalk catchment, PhD thesis, Imperial College London, UK, available at: <https://spiral.imperial.ac.uk:8443/handle/10044/1/28955>.](https://spiral.imperial.ac.uk:8443/handle/10044/1/28955)

Bell, V. A. and R. J. Moore (1998), A grid-based flood forecasting model for use with weather radar data: Part 1. Formulation, *Hydrol. Earth Syst. Sc.*, 2, 265-281.

Bell, V. A., A. L. Key, R. G. Jones, and R. J. Moore (2007), Development of a high resolution grid-based river flow model for use with regional climate model output, *Hydrol. Earth Syst. Sc.*, 11, 532-549.

Best, M. J., M. Pryor, D. B. Clark, G. G. Rooney, R. I. H. Essery, C. B. Ménard, J. M. Edwards, M. A. Hendry, A. Porson, N. Gedney, L. M. Mercado, S. Sitch, E. Blyth, O. Boucher, P. M. Cox, C. S. B. Grimmond, and R. J. Harding (2011), The Joint UK Land Environment Simulator (JULES), Model Description – Part 1: Energy and Water Fluxes, *Geosci. Model Dev.*, 4, 677-699.

Beven, K., and P. Germann (2013), Macropores and water flow in soils revisited, *Water Resour. Res.*, 49, 3071-3092.

709 Bloomfield, J. (1997), The role of diagenesis in the hydrogeological stratification of
710 carbonated aquifers: An example from the chalk at Fair Cross, Berkshire, UK, *Hydrol. Earth*
711 *Syst. Sc.*, 1, 19-33.

712 Blume, T. (2008), Hydrological processes in volcanic ash soils: measuring, modelling and
713 understanding runoff generation in an undisturbed catchment, PhD thesis, Institut für
714 Geoökologie, Universität Potsdam, Potsdam, Germany, available at: [https://publishup.uni-](https://publishup.uni-potsdam.de/opus4-ubp/files/1524/blume_diss.pdf)
715 [potsdam.de/opus4-ubp/files/1524/blume_diss.pdf](https://publishup.uni-potsdam.de/opus4-ubp/files/1524/blume_diss.pdf)

716 Brouyère, S. (2006), Modelling the migration of contaminants through variably saturated
717 dual-porosity, dual-permeability chalk, *J. Contam. Hydrol.*, 82, 195-219.

718 Chen, X., and Q. Hu (2004), Groundwater influences on soil moisture and surface
719 evaporation, *J. Hydrol.*, 297, 285-300.

720 Clark, D. B., L. M. Mercado, S. Sitch, C. D. Jones, N. Gedney, M. J. Best, M. Pryor, G. G.
721 Rooney, R. L. H. Essery, E. Blyth, O. Boucher, R. J. Harding, C. Huntingford, and P. M. Cox
722 (2011), The Joint UK Land Environment Simulator (JULES), Model Description – Part 2:
723 Carbon Fluxes and Vegetation Dynamics, *Geosci. Model Dev.* 4, 701-722.

724 Cox, P. M., R. A. Betts, C. B. Bunton, R. L. H. Essery, P. R. Rowntree and J. Smith (1999),
725 The impact of new land surface physics on the GCM simulation of climate and climate
726 sensitivity, *Clim. Dynam.*, 15, 183-203.

727 Dadson, S. J., I. Ashpole, P. Harris, H. N. Davies, D. B. Clark, E. Blyth, and C. M. Taylor
728 (2010), Wetland inundation dynamics in a model of land surface climate: Evaluation in the
729 Niger inland delta region, *J. Geophys. Res.*, 115.

730 Dadson, S. J., V. A. Bell, and R. G. Jones (2011), Evaluation of a grid based river flow model
731 configured for use in a regional climate model, *J. Hydrol.*, 411, 238-250.

732 Dettinger, M. D., and H. F. Diaz (2000), Global characteristics of streamflow seasonality and
733 variability, *J. Hydrometeorol.*, 1, 289-310.

734 Essery, R., M. Best, and P. Cox (2001), MOSES 2.2 technical documentation (Hadley Centre
735 technical note 30), Hadley Centre, Met Office, UK.

736 Garcia, M., C. D. Peters-Lidard, and D. C. Goodrich (2008), Spatial interpolation of
737 precipitation in a dense gauge network for monsoon storm events in the southwestern United
738 States, *Water Resour. Res.*, 44.

739 Gascoin, S., A. Duchare, P. Ribstein, M. Carli, and F. Habtes (2000), Adaptation of a
740 catchment-based land surface model to the hydrological setting of the Somme River basin
741 (France), *J. Hydrol.*, 368, 105-116.

742 Gudmundsson, L., T. Wagener, L. M. Tallaksen, and K. Engeland (2012), Evaluation of nine
743 large-scale hydrological models with respect to the seasonal runoff climatology in Europe,
744 *Water Resour. Res.*, 48.

745 Gupta, H. V., H. Kling, K. K. Yilmaz, and G. F. Martinez (2009), Decomposition of the mean
746 squared error and NSE performance criteria: implications for improving hydrological
747 modelling, *J. Hydrol.*, 377, 80-91.

748 [Habtes, F., S. Gascoin, S. Korkmaz, D. Thiéry, M. Zribi, N. Amraoui, M. Carli, A. Ducharne,](#)
749 [E. Leblois, E. Ledoux, E. Martin, J. Noilhan, C. Ottlé, and P. Viennot \(2010\), Multi-model](#)
750 [comparison of a major flood in the groundwater-fed basin of the Somme River \(France\),](#)
751 [Hydrol. Earth Syst. Sc., 14, 99-117.](#)

752 Haria, A. H., M. G. Hodnett, and A. C. Johnson (2003), Mechanisms of groundwater
753 recharge and pesticide penetration to chalk aquifer in southern England, *J. Hydrol.*, 275, 122-
754 137.

755 Hartmann, A., N. Goldscheider, T. Wagener, J. Lange, and M. Weiler (2014), Karst water
756 resources in a changing world: Review of hydrological modeling approaches, *Rev. Geophys.*,
757 52, 218–242, doi:10.1002/2013RG000443.

758 Hewitt, N., M. Robinson, and D. McNeil (2010), Pang and Lambourn hydrometric review
759 2009, Wallingford, NERC/Centre for Ecology and Hydrology, (CEH project number:
760 C04076).

761 [Ireson, A. M., S. A. Mathias, H. S. Wheater, A. P. Butler and J. Finch \(2009\), A model for](#)
762 [flow in the chalk unsaturated zone incorporating progressive weathering, *J. Hydrol.*, 365,](#)
763 [244-260.](#)

764 Ireson, A. M. and A. P. Butler (2011), Controls on preferential recharge to chalk aquifers, *J.*
765 *Hydrol.*, 398, 109-123.

766 Ireson, A. M. and A. P. Butler (2013), A critical assessment of simple recharge models:
767 application to the UK chalk, *Hydrol. Earth Syst. Sc.*, 17, 2083-2096.

768 Ireson, A. M., H. S. Wheater, A. P. Butler, S. A. Mathias, J. Finch, and J. D. Cooper (2006),
769 Hydrological processes in the chalk unsaturated zone – insight from an intensive field
770 monitoring program, *J. Hydrol.*, 330, 29-43.

771 Ireson, A. M., S. A. Mathias, H. S. Wheater, A. P. Butler, and J. Finch (2009), A model for
772 flow in the chalk unsaturated zone incorporating progressive weathering, *J. Hydrol.*, 365,
773 244-260.

774 Jackson, C. and Spink, A. (2004) User's Manual for the Groundwater Flow Model
775 ZOOMQ3D, IR/04/140, British Geological Survey, Nottingham, UK.

776 Kelleher, C., T. Wagener, and B. McGlynn (2015), Model-based analysis of the influence of
777 catchment properties on hydrologic partitioning across five mountain headwater
778 subcatchments, *Water Resour. Res.*, 51, 4109-4136.

779 Kling, H., M. Fuchs, and M. Paulin (2012), Runoff conditions in the upper Danube basin
780 under an ensemble of climate change scenarios. *Journal of Hydrology*, Volumes 424-425, 6
781 March 2012, 264-277.

782 ~~Kollet, S. J., and R. M. Maxwell (2008), Capturing the influence of groundwater dynamics on~~
783 ~~land surface processes using an integrated, distributed watershed model, *Water Resour. Res.*,~~
784 ~~44.~~

785 Lehner, B., K. Verdin, and A. Jarvis (2008), New global hydrography derives from
786 spaceborne elevation data, *EOS, Transactions, AGU*, 89(10), 93-94.

787 Le Vine, N., A. Butler, N. McIntyre, and C. Jackson (2016), Diagnosing hydrological
788 limitations of a land surface model: application of JULES to a deep-groundwater chalk basin,
789 *Hydrol. Earth Syst. Sc.*, 20, 143-159.

790 Lee, L. J. E., D. S. L. Lawrence, and M. Price (2006), Analysis of water-level response to
791 rainfall and implications for recharge pathways in the chalk aquifer, SE England, *J. Hydrol.*,
792 330, 604-620.

793 ~~Leeper, R., R. Mahmood, and R. I. Quintanar (2011), Influence of karst landscape on~~
794 ~~planetary boundary layer atmosphere: A Weather Research Forecasting (WRF) model-based~~
795 ~~investigation, *J. Hydrometeorol.*, 12, 1512-1529.~~

796 Ly, S., C. Charles, and A. Degré (2013), Different methods for spatial interpolation of rainfall
797 data for operational hydrology and hydrological modeling at watershed scale. A review,
798 *Biotechnol. Agron. Soc. Environ.* 17, 392-406.

799 ~~MacDonald, A. M., L. J. Brewerton, and D. J. Allen (1998), Evidence of rapid groundwater
800 flow and karst type behaviour in the chalk of Southern England, In: Robins, N. S.
801 (ed.) *Groundwater pollution, aquifer recharge and vulnerability*, Geological Society,
802 London, Special publications, 130, 95-106.~~

803 Mathias, S. A., A. P. Butler, B. M. Jackson, and H. S. Wheater (2006), Transient simulations
804 of flow and transport in the chalk unsaturated zone, *J. Hydrol.*, 330, 10-28.

805 ~~Maxwell, R.M. and N.L. Miller (2005), Development of a coupled land surface and
806 groundwater model, *J. Hydrometeorol.*, 6(3), 233-247.~~

807 ~~Maxwell, R. M., F. K. Chow, S. J. Kollet (2007), The groundwater-land-surface-atmosphere
808 connection: Soil moisture effects on the atmospheric boundary layer in fully-coupled
809 simulations, *Adv. Water Resour.*, 30, 2447-2466.~~

810 Met Office (2006), UK hourly rainfall data, Part of the Met Office Integrated Data Archive
811 System (MIDAS), NCAS British Atmospheric Data Centre, 21 March 2016,
812 <http://catalogue.ceda.ac.uk/uuid/bbd6916225e7475514e17fdbf11141c1>.

813 Morton, D., C. Rowland, C. wood, L. Meek, C. Marston, G. Smith, R. Wadsworth, and I. C.
814 Simpson (2011), Final report for LCM2007 – the new UK Land Cover Map (CS technical
815 report no 11/07), Centre for Ecology and Hydrology, UK.

816 Mu, Q., F. A. Heinsch, M. Zhao, and S. W. Running (2007), Development of a global
817 evapotranspiration algorithm based on MODIS and global meteorology data, *Remote Sens.*
818 *Environ.*, 111, 519-536.

819 Price, A., R. A. Downing, and W.M. Edmunds (1993), The chalk as an aquifer. In: Downing,
820 R. A., M. Price, and G. P. Jones *The hydrogeology of the chalk of north-west Europe*. Oxford:
821 Claredon Press. 35-58.

822 Price, M., R. G. Low, and C. McCann (2000), Mechanisms of water storage and flow in the
823 unsaturated zone of chalk aquifer, *J. Hydrol.*, 54-71.

824 ~~Rahman, M., M. Sulis, and S. J. Kollet (2014), The concept of dual boundary forcing in land~~
825 ~~surface-subsurface interactions of the terrestrial hydrologic and energy cycles, *Water Resour.*~~
826 ~~*Res.*, 50, 8531-8548.~~

827 ~~Rahman, M., M. Sulis, and S. J. Kollet (2016), Evaluating the dual boundary forcing concept~~
828 ~~in subsurface-land surface interactions of the hydrological cycle, *Hydrol. Process.*~~

829 Rawls, W. J., D. L. Brankensiek, and K. E. Saxton (1982), Estimation of soil water
830 properties, *Trans. ASAE*, 25(5), 1316-1320.

831 Robinson, E. L., E. Blyth, D. B. Clark, J. Finch, and A. C. Rudd (2015), Climate hydrology
832 and ecology research support system potential evapotranspiration dataset for Great Britain
833 (1961- 2012) [CHESS-PE], NERC-Environmental Information Data Centre.

834 Schär C., D. Lüthi, U. Beyerle, and E. Heise (1999), A soil precipitation feedback: A process
835 study with a regional climate model, *J. Clim.*, 12, 722-741.

836 Schaap, M. G., and F. J. Leij (1998), Database-related accuracy and uncertainty of
837 pedotransfer functions, *Soil Sci.*, 163(10), 765-779.

838 Sorensen, J. P. R., J. W. Finch, A. M. Ireson, and C. R. Jackson (2014), Comparison of varied
839 complexity models simulating recharge at the field scale, *Hydrol. Process.*, 28, 2091-2102.

840 Van den Daele, G. F. A., J. A. Barker, L. D. Connell, T. C. Atkinson, W. G. Darling, and J.
841 D. Cooper (2007), *J. Hydrol.*, 342, 157-172.

842 Van Genuchten, M. Th. (1980), A closed-form equation for predicting the hydraulic
843 conductivity of unsaturated soils, *Soil Sci. Soc. Am. J.*, 44, 892-898.

844 Walters, D. N., K. D. Williams, I. A. Boutle, A. C. Bushell, J. M. Edwards, P. R. Field, A. P.
845 Lock, C. J. Morcrette, R. A. Stratton, J. M. Wilkinson, M. R. Willett, N. Bellouin, A. Bodas-
846 Salcedo, M. E. Brooks, D. Copesey, P. D. Earnshaw, S. C. Hardiman, C. M. Harris, R. C.
847 Levine, C. MacLachlan, J. C. Manners, G. M. Martin, S. F. Milton, M. D. Palmer, M. J.
848 Roberts, J. M. Rodríguez, W. J. Tennant, and P. L. Vidale (2014), The Met Office unified
849 model global atmosphere 4.0 and JULES global land 4.0 configurations, *Geosci. Model Dev.*,
850 7, 361-386.

851 Wellings, S. R., and J. P. Bell (1980), Movement of water and nitrate in the unsaturated zone
852 of upper chalk near Winchester, Hants., England, *J. Hydrol*, 48, 119-136.

853 [Wetzel P. J., and J. T. Chang \(1987\), Concerning the relationship between evapotranspiration](#)
854 [and soil moisture. *J. Clim. Appl. Meteorol.*, 26, 18-27.](#)

855 Williams, K., and D. Clark (2014), Disaggregation of daily data in JULES (Hadley Centre
856 technical note 96), Hadley Centre, Met Office, UK.

857 Zehe, E. and G. Blöschl (2004), Predictability of hydrologic response at the plot and
858 catchment scales: Role of initial conditions, *Water Resour. Res.*, 40.

859 Zehe, E., T. Maurer, J. Ihringer, and E. Plate (2001), Modeling water flow and mass transport
860 in a loess catchment, *Phys. Chem. Earth (B)*, 26, 487-507.

861 Zehe, E., U. Ehret, T. Blume, A. Kleidon, U. Scherer, and M. Westhoff (2013), A
862 thermodynamic approach to link self-organization, preferential flow and rainfall-runoff
863 behaviour, *Hydrol. Earth Syst. Sc.*, 17, 4297-4322.

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871 **Tables**

872 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

873 ^aMeasured at Warren Farm.

874 ^bLocations are shown in Figure 1a.

875

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

Texture	K_s (ms^{-1})	Porosity (-)	α (m^{-1})	n (-)
Loam	3.7×10^{-6}	0.463	3.33	1.56
Silt loam	2.0×10^{-6}	0.50	1.2	1.39
Clay	1.7×10^{-7}	0.475	2.12	1.2

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881 [Table 3. Hydraulic properties of chalk.](#)

Properties	Value	Source
K_s (ms^{-1})	1.85×10^{-7}	Price et al., 1993
Porosity (-)	0.40	Price et al., 1993
α (m^{-1})	3.4	Le Vine et al., 2016
n (-)	1.4	Le Vine et al., 2016

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883 [Table 3. Hydraulic properties of chalk](#)

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Properties	Unoptimized		Optimized value
	Value	Source	
K_s (md^{-1})	16	Le Vine et al., 2016	15
S_0 (-)	0.8	Observations	0.67
f_m (-)	1×10^5	Price et al., 1993	6.1×10^5
α (m^{-1})	3.0	Le Vine et al., 2016	-
n (-)	1.4	Le Vine et al., 2016	-

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886 Table 4. Comparison between observed and simulated daily average runoff from the two
 887 configurations over the Kennet catchment.

Metric	Observed	Simulated (<i>default</i>)	Simulated (<i>macro</i>)
RR	0.40	0.82	0.378
$\Delta\mu$	-	1.04	-0.05-0.07
$\Delta\sigma$	-	2.04	0.700-56

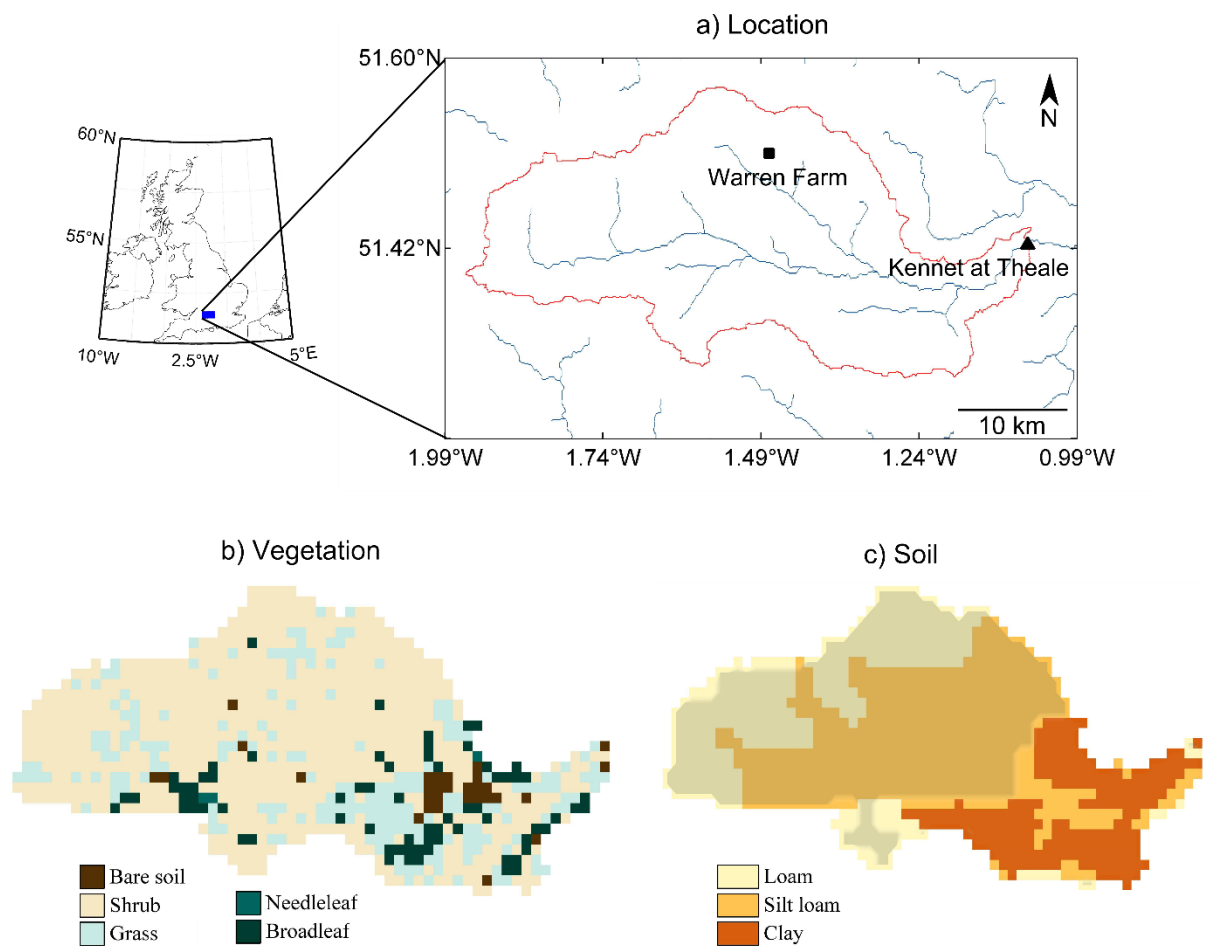
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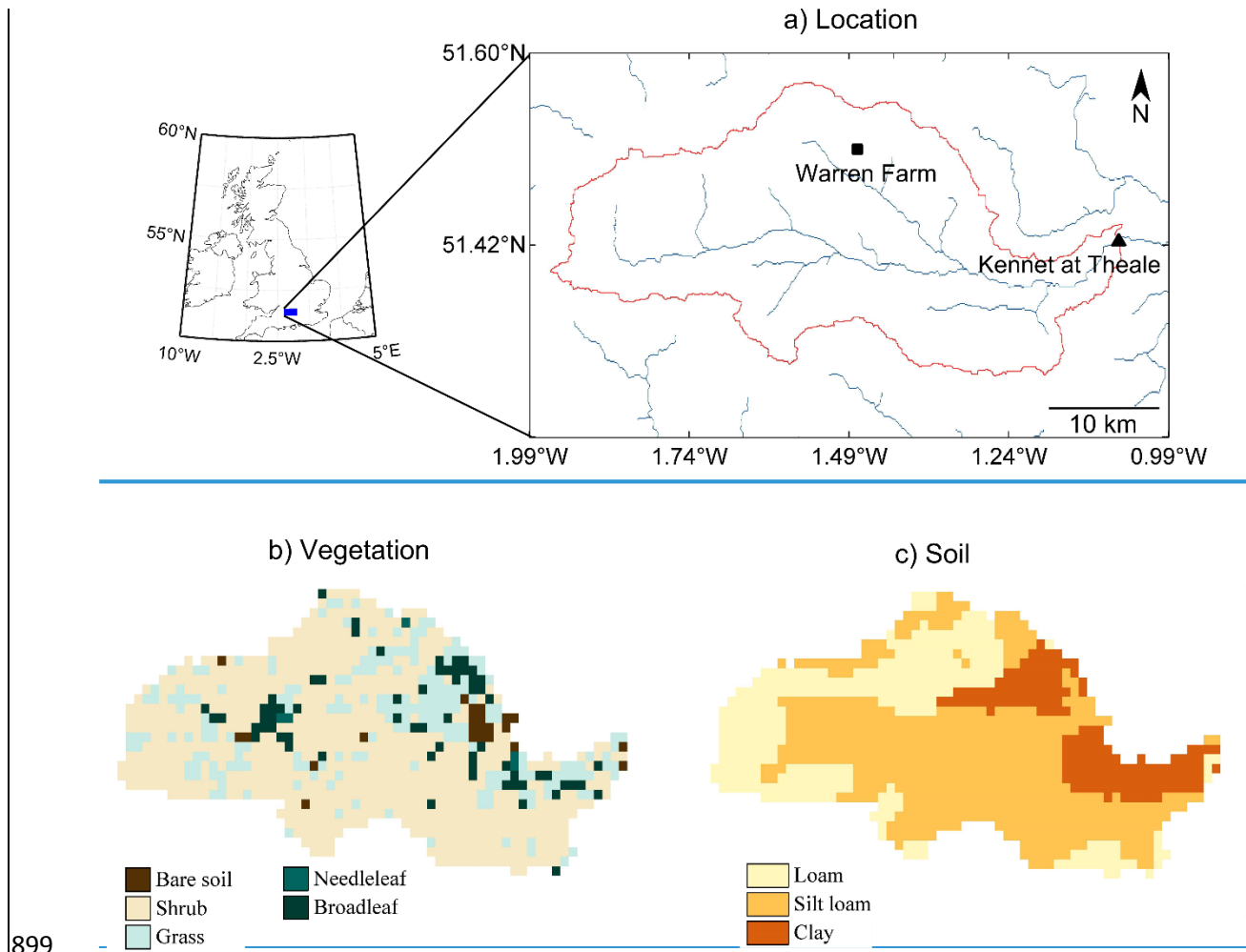
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891 **Figures**

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



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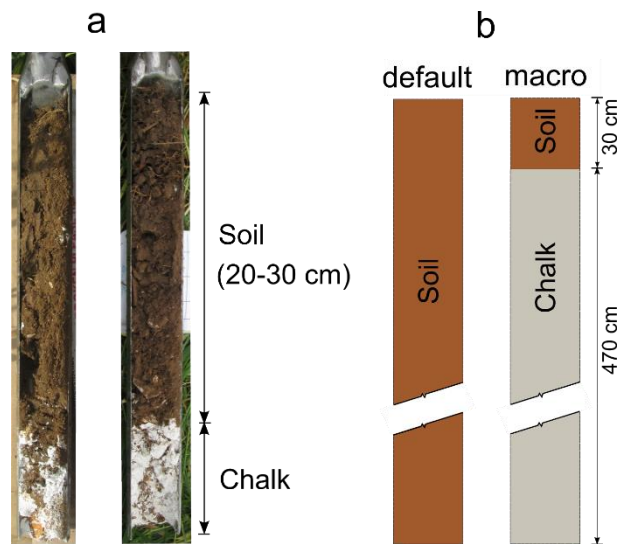
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904 Figure 2. Example of soil profiles collected at Warren Farm during a field campaign in 2015

905 (a), and the two model configurations (b).

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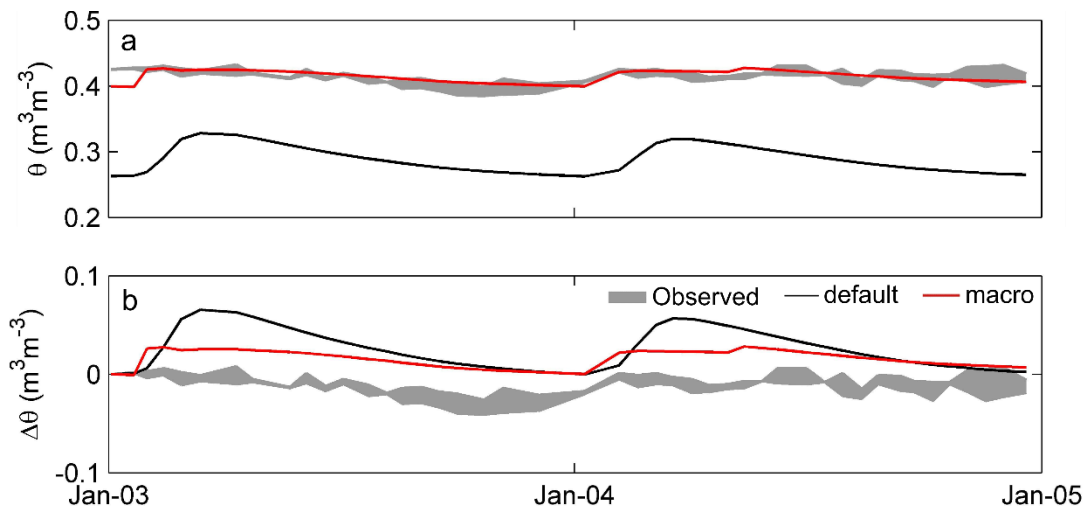
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919 [Figure 3. Comparison between observed and simulated \(a\) soil moisture \(\$\theta\$ \) and \(b\) change in](#)
 920 [soil moisture \(\$\Delta\theta\$ \) from the *default* and *macro* configurations at a depth of 2m below land](#)

921 [surface. The shaded areas constructed from 2 soil moisture probes at the Warren Farm site](#)
922 [denote the range of observed data in these plots.](#)



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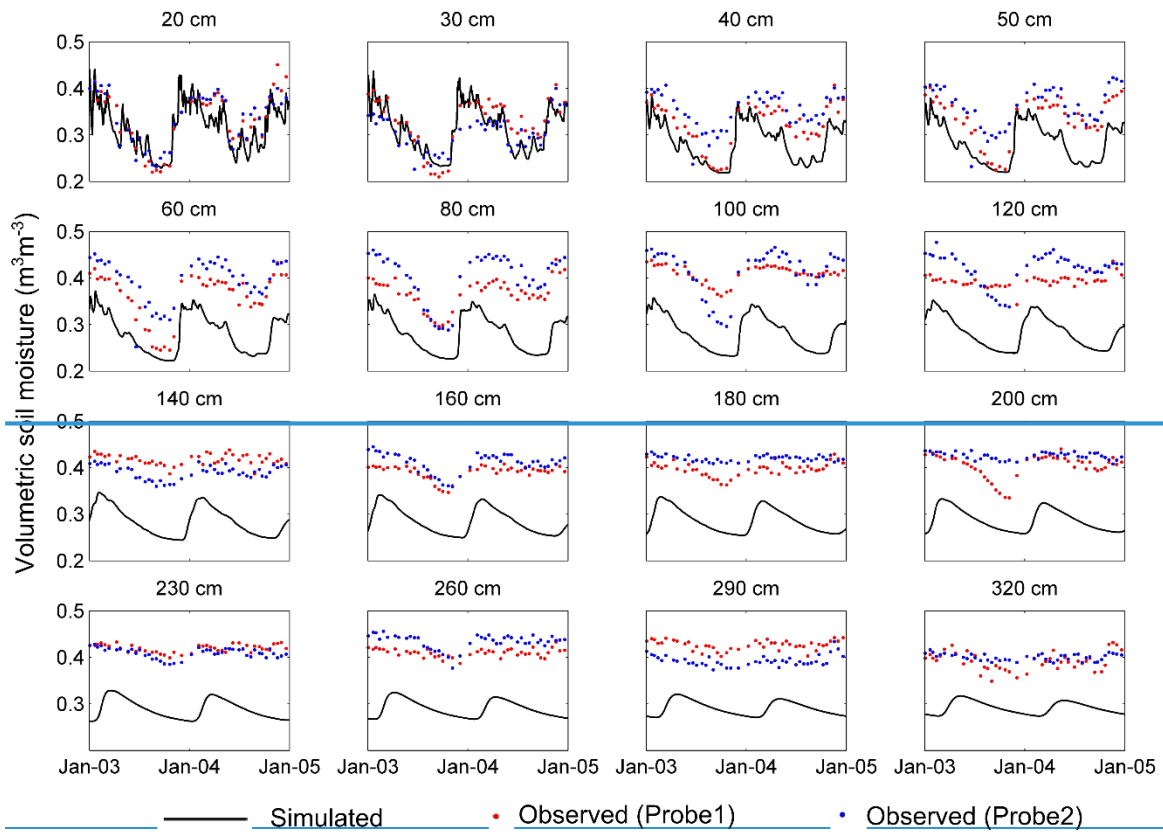
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934 [Figure 3. Observed and simulated \(*default configuration*\) volumetric soil moisture from](#)

935 [Warren Farm.](#)



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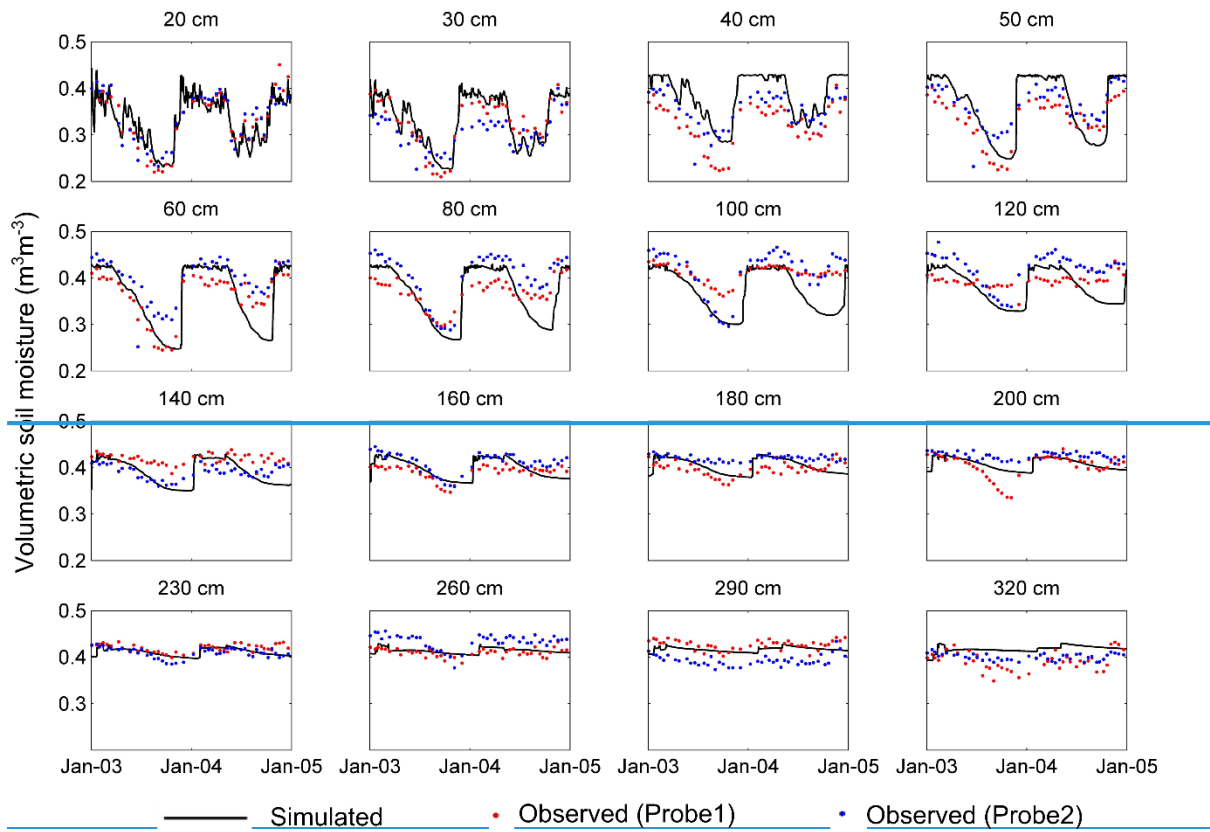
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945 **Figure 4. Observed and simulated (*macro* configuration) volumetric soil moisture from**

946 **Warren Farm.**



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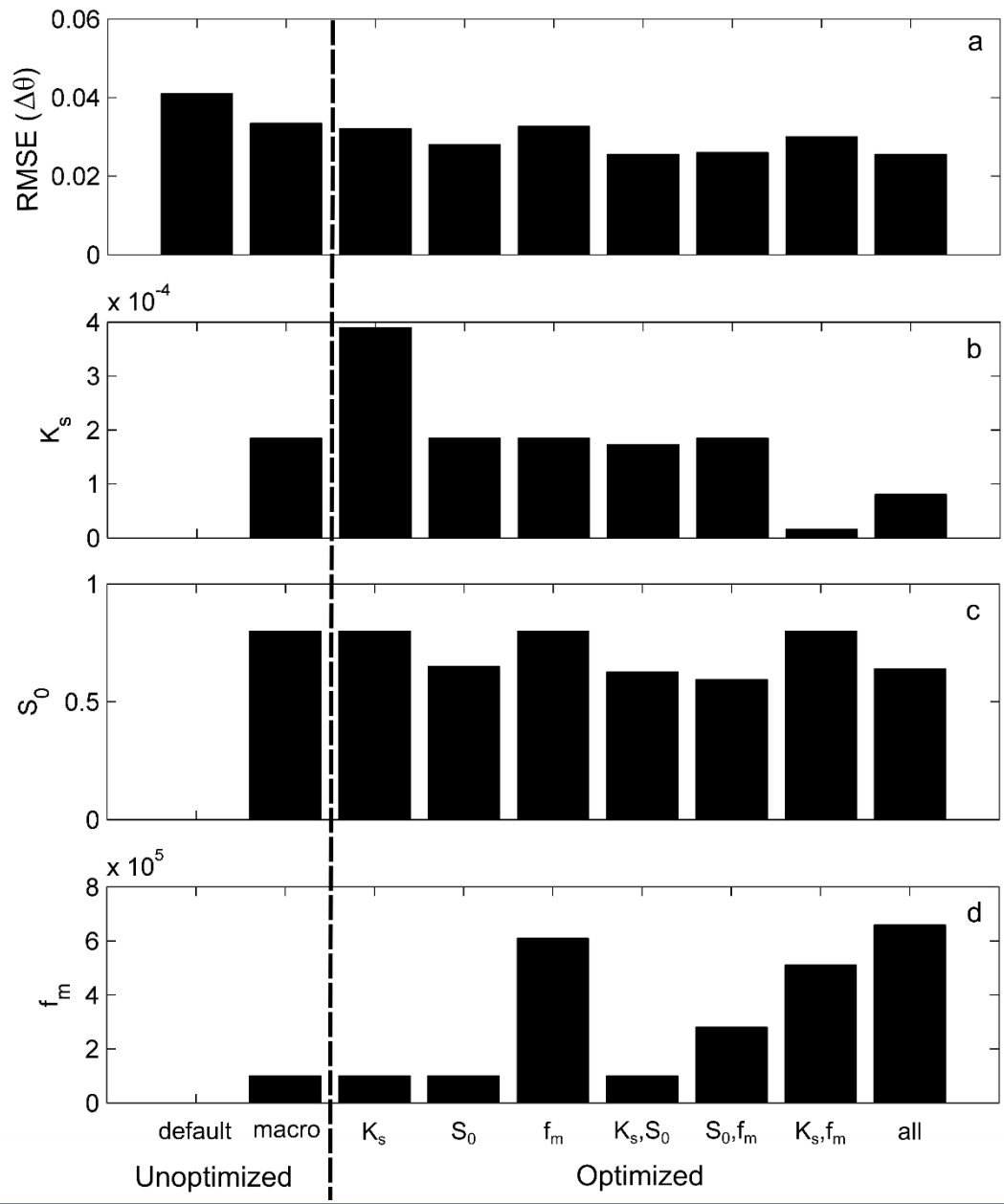
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951 [Figure 4. \(a\) Model performance in reproducing observed and simulated \$\Delta\theta\$, \(b\) \$K_s\$, \(c\) \$S_0\$ and](#)
 952 [\(d\) \$f_m\$ for various parameter combinations considered in the optimization. Note that except for](#)
 953 [the *default* and *macro*, the simulation yielding the lowest RMSE \(out of 2000 model runs\) is](#)
 954 [presented in this plot.](#)

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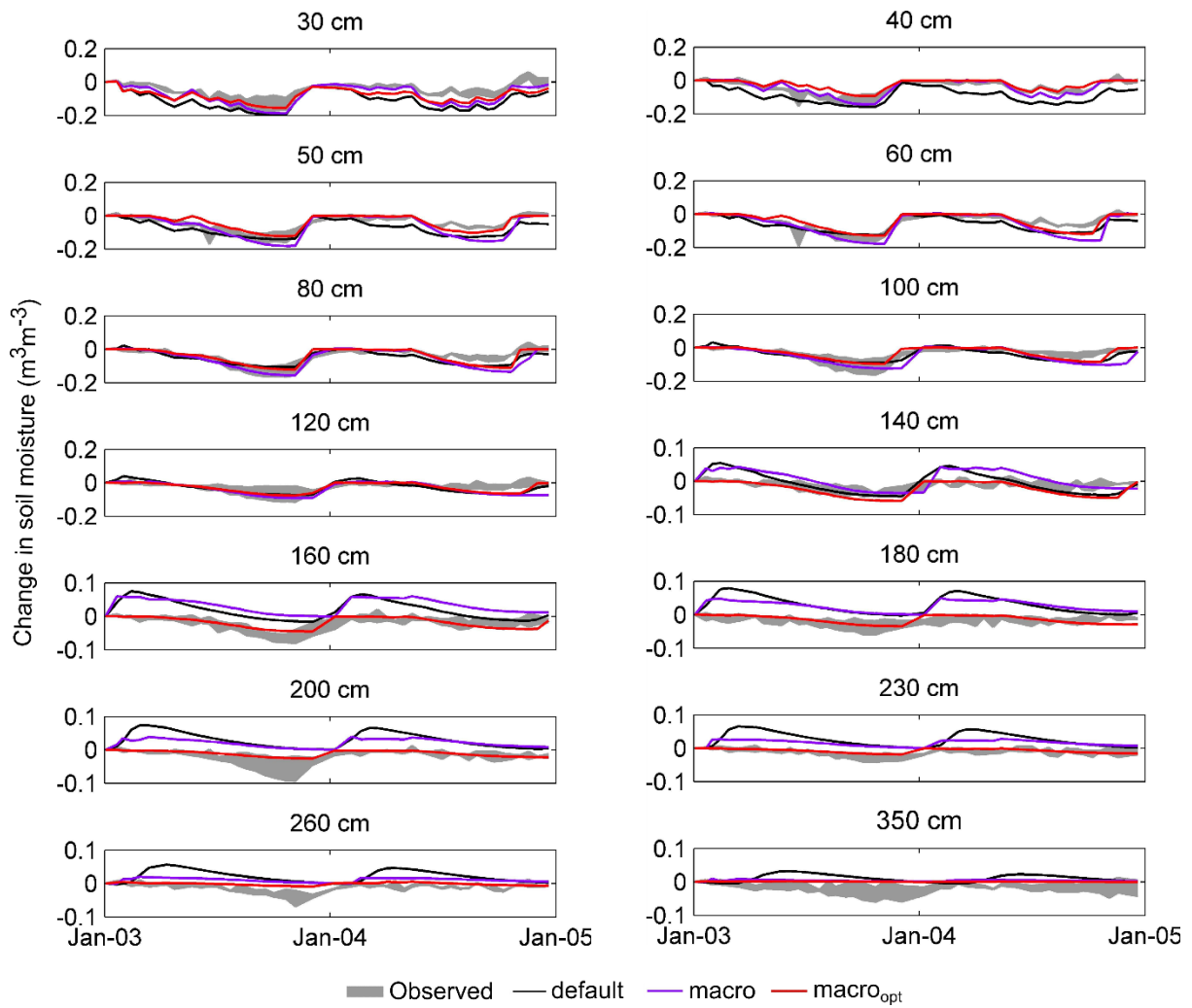
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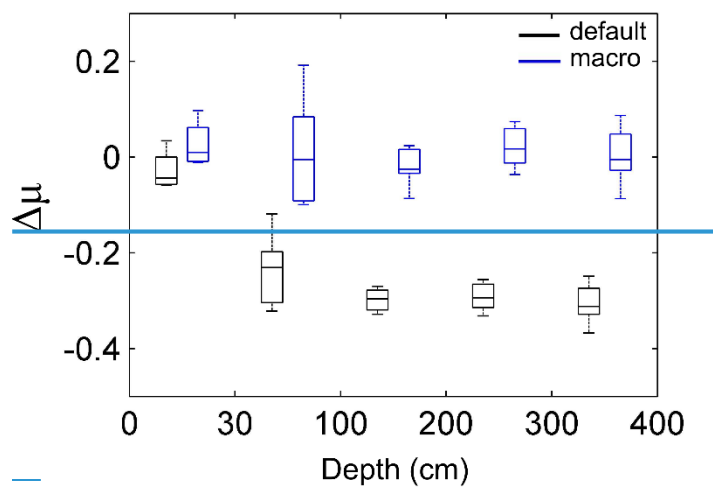
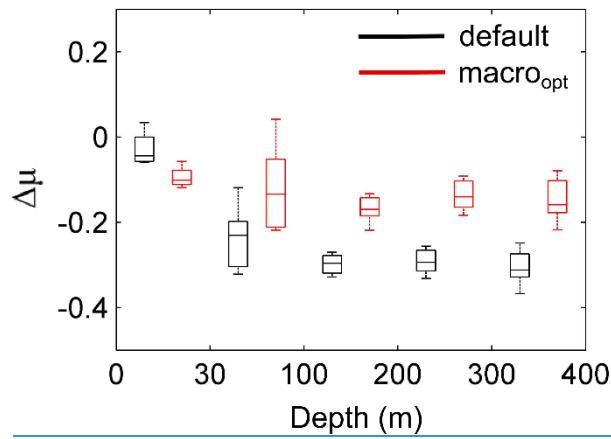
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963 [Figure 5. Comparison between observed and simulated \$\Delta\theta\$ from *default*, *macro* and *macro_{opt}*](#)
 964 [configurations at various depths below land surface. The shaded area, which is constructed](#)
 965 [from 2 soil moisture probes at the Warren Farm site, denotes the range of \$\Delta\theta\$.](#)



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973 Figure 65. Box plot of relative bias ($\Delta\mu$) of simulated soil moisture from *default* and *macro*
974 configurations at different depth ranges shown in individual intervals (e.g., 0-30 cm, 30-100
975 cm, and so on).



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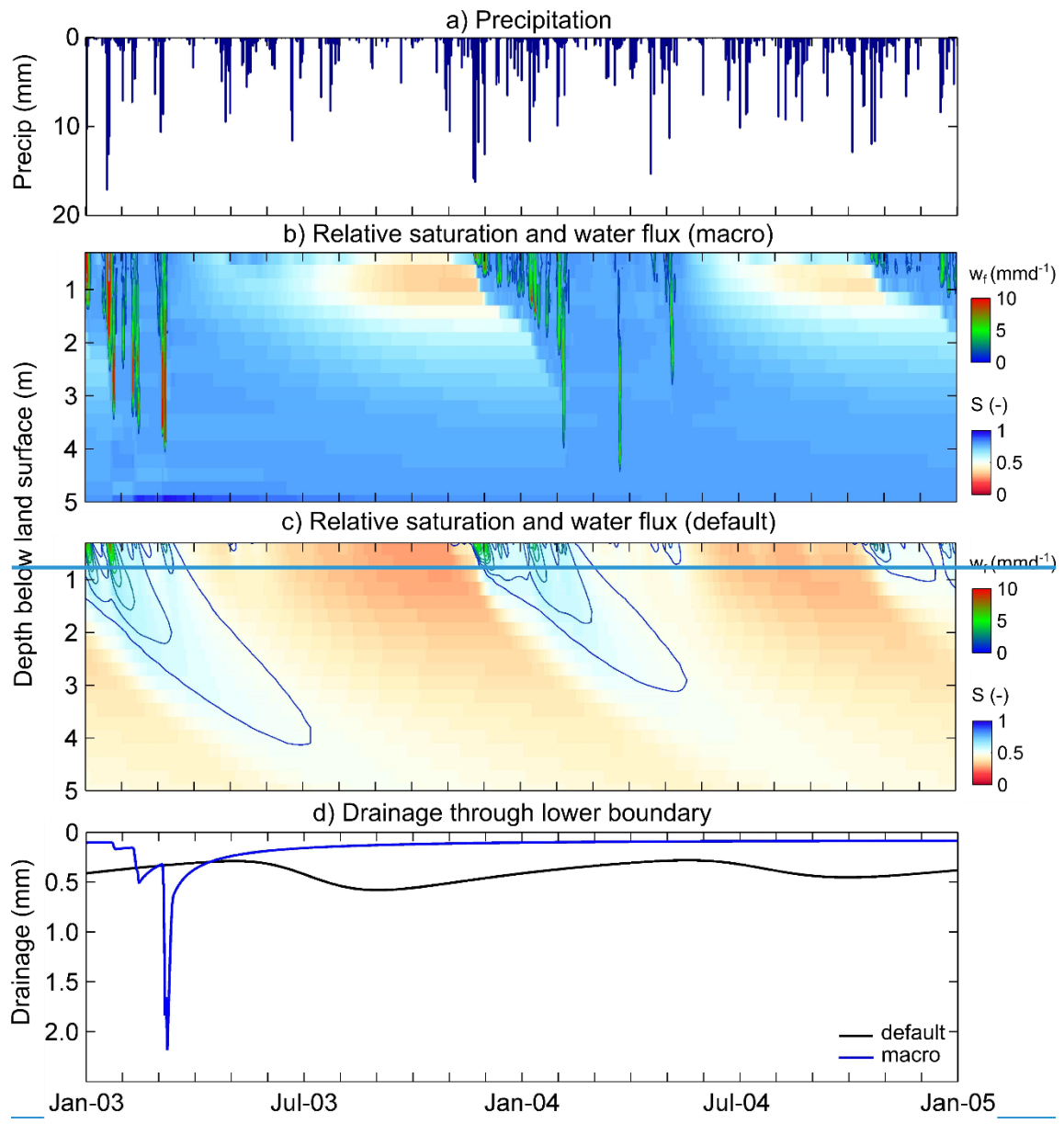
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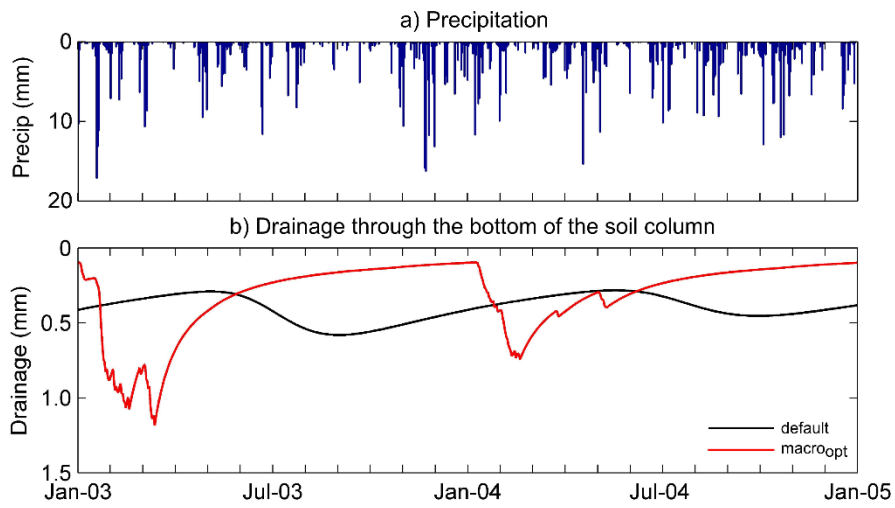
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990 ~~Figure 6. Precipitation (a), daily accumulated downward water flux (w_d , contour lines) plotted~~
991 ~~over relative saturation (S , coloured shading) for *macro* (b), daily accumulated downward~~
992 ~~water flux plotted over relative saturation for *default* (c), and daily accumulated drainage flux~~
993 ~~through the bottom boundary simulated by the two model configurations (d) at Warren Farm~~
994 ~~over the two simulated years (2003–2005).~~



996 [Figure 7. \(a\) Precipitation and \(b\) daily sum of drainage through the bottom of the soil](#)
 997 [column at Warren Farm over the two simulated years \(2003-2005\).](#)

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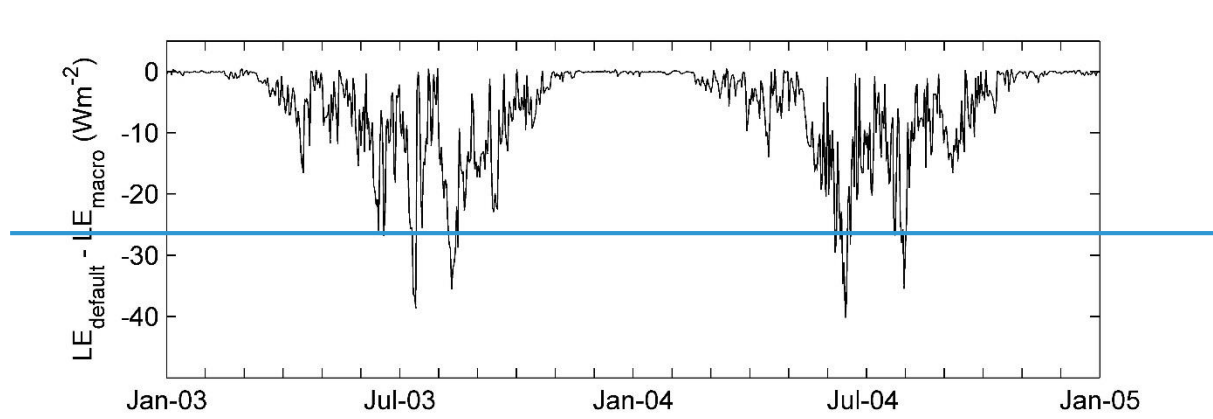
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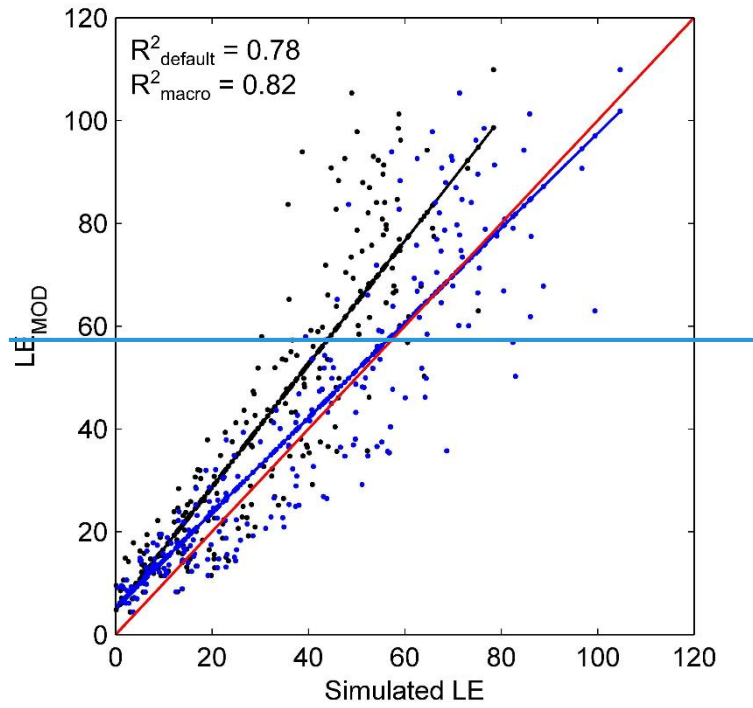
Figure 7. Differences between daily average latent heat flux time series simulated by *default* and *macro* configurations ($LE_{default}$ and LE_{macro} , respectively) at Warren Farm.



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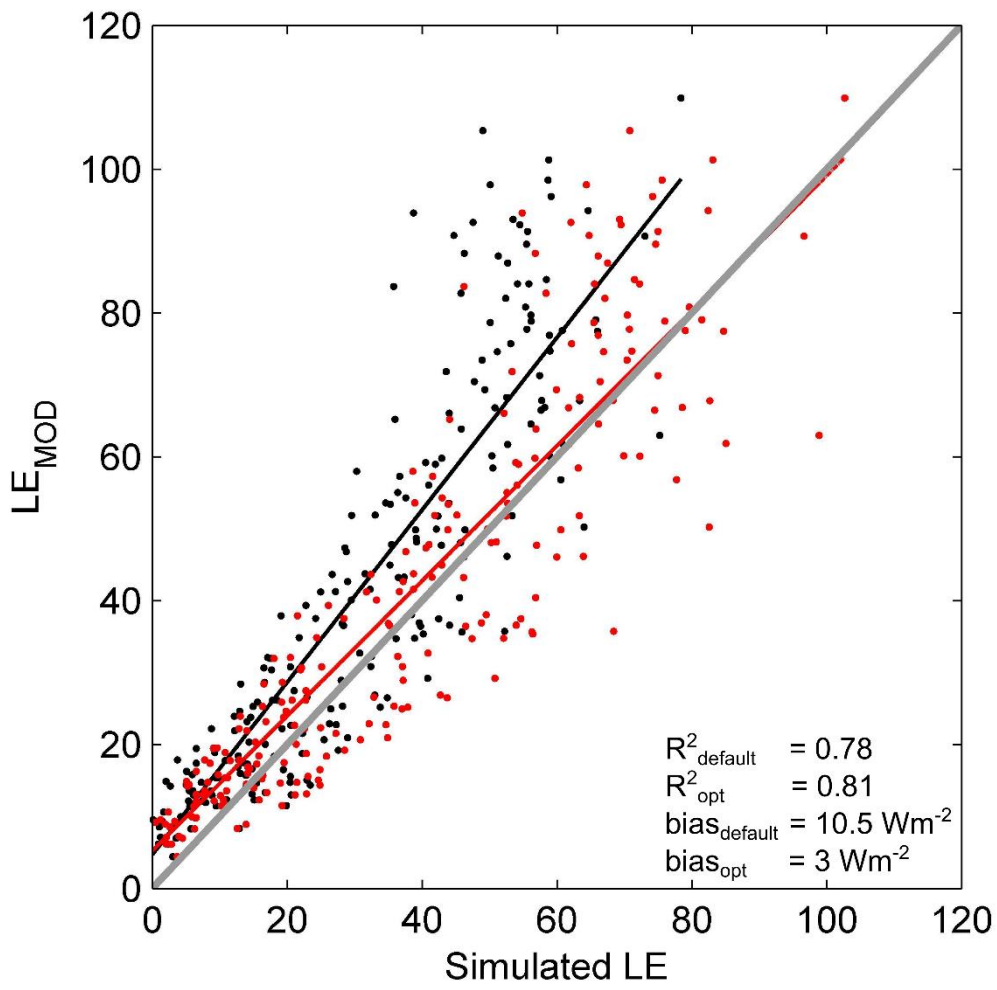
1027 Figure 8. Catchment average 8 day composites of MODIS estimated LE (LE_{MOD}) against
1028 simulated LE from *default* and *macro* configurations (LE_{default} and LE_{macro} , respectively) along

1029 with the linear models fitted for $LE_{default}$ (black line) and LE_{macro} (blue-red line). The 1:1 line
1030 is shown in grey-red, which represents the perfect fit between LE_{MOD} and simulated LE .



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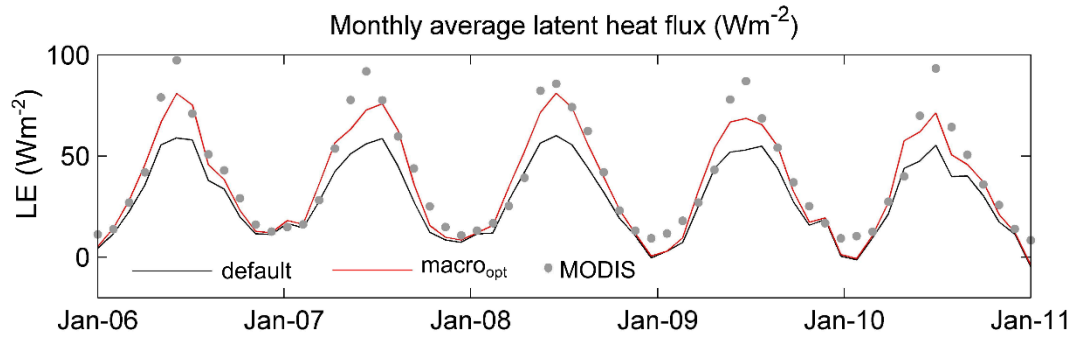
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1038 [Figure 9. Spatially averaged monthly latent heat flux \(*LE*\) from MODIS, *default* and *macro_{opt}*](#)

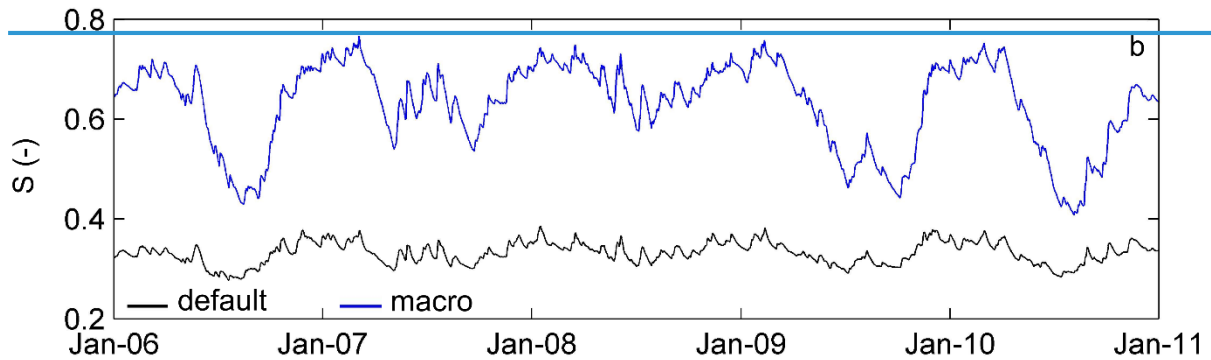
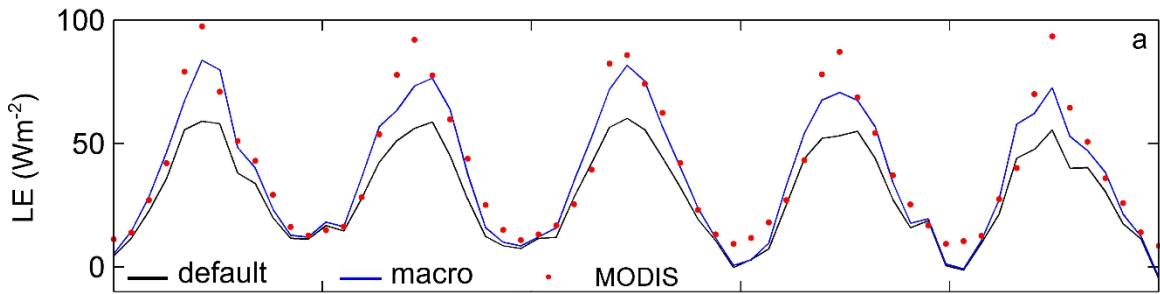
1039 [configurations over the Kennet catchment.](#)

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1042 **Figure 9. Spatially averaged monthly latent heat flux (LE) from MODIS, *default*, and *macro***
 1043 ***configurations* (a), and average (0–100 cm below land surface) daily relative saturation (S)**
 1044 **from *default* and *macro* configurations (b) over the Kennet catchment.**



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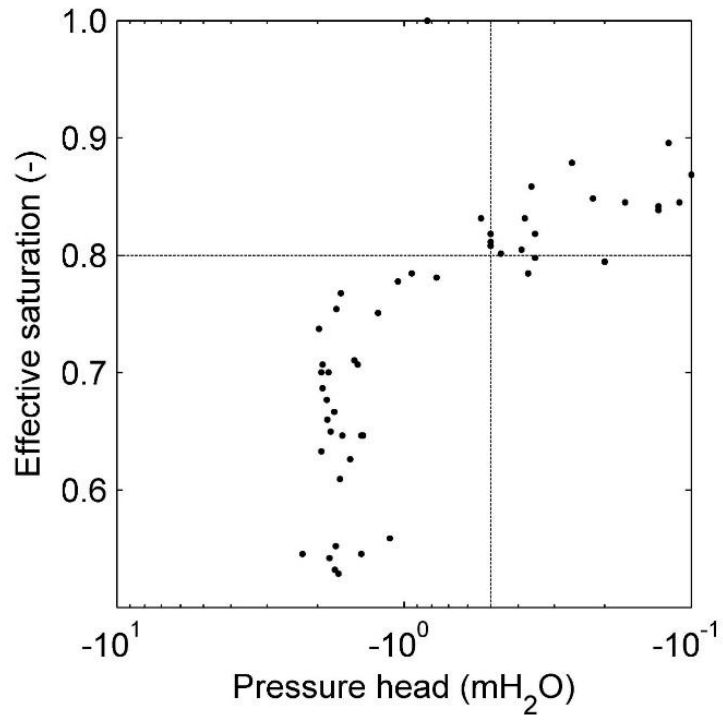
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1057 **Supplementary materials**

1058 Figure S1. Saturation-pressure head relationship (May 2003 - December 2005) at Warren

1059 Farm measured fortnightly at 40 cm below land surface. (Source: Ned Hewett, CEH, personal
1060 communication).

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1070 [Figure S2. Sensitivity of the BC model parameters on the model performance in simulating](#)

1071 [\$\Delta\theta\$. Note that the parameters are considered one-at-a-time \(OAT\), and the vertical axis have](#)

1072 [different RMSE ranges.](#)

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