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1 **The effect of chalk representation in land surface modelling**

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5 **Abstract**

6 Modelling and monitoring of hydrological processes in the unsaturated zone of the chalk,
7 which is a porous medium with fractures, is important to optimize water resources assessment
8 and management practices in the United Kingdom (UK). However, efficient simulations of
9 water movement through chalk unsaturated zone is difficult mainly due to the fractured
10 nature of chalk, which creates high-velocity preferential flow paths in the subsurface.
11 Complex hydrology in the chalk aquifers may also influence land surface mass and energy
12 fluxes because processes in the hydrological cycle are connected via non-linear feedback
13 mechanisms. In this study, it is hypothesized that explicit representation of chalk hydrology
14 in a land surface model influences land surface processes by affecting water movement
15 through the shallow subsurface. In order to substantiate this hypothesis, a macroporosity
16 parameterization is implemented in the Joint UK Land Environment Simulator (JULES),
17 which is applied on a study area encompassing the Kennet catchment in the Southern UK.
18 The simulation results are evaluated using field measurements and satellite remote sensing
19 observations of various fluxes and states in the hydrological cycle (e.g., soil moisture, runoff,
20 latent heat flux) at two distinct spatial scales (i.e., point and catchment). The results reveal the
21 influence of representing chalk hydrology on land surface mass and energy balance
22 components such as surface runoff and latent heat flux via subsurface processes (i.e., soil
23 moisture dynamics) in JULES, which corroborates the proposed hypothesis.

24 **Keywords:** Chalk hydrology, macroporosity, land surface modelling, bulk conductivity
25 model.



26 **1. Introduction**

27 Chalk can be described as a fine-grained porous medium traversed by fractures [*Price et al.*,
28 1993]. The unsaturated zone of chalk aquifers play an important role on various important
29 processes (e.g., recharge) of the hydrological cycle in the UK [e.g., *Lee et al.*, 2006; *Ireson et*
30 *al.*, 2009]. Therefore, both monitoring [e.g., *Bloomfield*, 1997; *Ireson et al.*, 2006] and
31 modelling [e.g., *Brouyère*, 2006; *Ireson and Butler*, 2011, 2013; *Sorensen et al.*, 2014]
32 strategies have been adapted previously to understand the governing hydrological processes
33 in the chalk unsaturated zone.

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

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

47 The aforementioned studies revealed the importance of representing the matrix-fracture flow
48 nature in simulating subsurface hydrological processes in chalk-dominated aquifers. In recent
49 years, representation of chalk has also gained attention in land surface modelling. *Gascoin et*



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

61 The above mentioned studies suggest that the representation of chalk affects the hydrological
62 processes simulated by land surface models. Because the processes of the hydrological cycle
63 are connected via non-linear feedback mechanisms [e.g., *Kollet and Maxwell*, 2008; *Rahman*
64 *et al.*, 2014], the representation of water flow through the matrix-fracture system of chalk
65 may also influence simulated land surface energy fluxes (e.g., latent heat flux), which has not
66 yet been explicitly discussed. In this context, our hypothesis is that a consistent representation
67 of water movement through chalk in a land surface model affects the exchange of mass and
68 energy fluxes at the surface, which may be important to consider in water resources
69 assessment and management practices (e.g., flood and drought prediction over chalk-
70 dominated areas). In order to substantiate this hypothesis, a macroporosity parameterization,
71 namely the *Bulk Conductivity* (BC) model is implemented in JULES and evaluated at two
72 distinct spatial scales (i.e., point and catchment). At the point-scale, the BC model is
73 evaluated against observed soil moisture data. The proposed model is then applied over the
74 Kennet catchment in the Southern England and the fluxes and states of the hydrological cycle



75 are simulated for multiple years to demonstrate the importance of representing chalk

76 hydrology, which supports the proposed hypothesis.

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

78 In this study, the *Bulk Conductivity* (BC) model based on the work by *Zehe et al.* [2001] is

79 incorporated to represent the flow of water through the fractured chalk unsaturated zone.

80 According to this approach, if the relative saturation (S) exceeds a certain threshold (S_0) at a

81 soil grid, the saturated hydraulic conductivity (K_s) is increased to a bulk saturated hydraulic

82 conductivity (K_{sb}) as follows

$$83 \quad K_{sb} = K_s + K_s f_m \frac{S - S_0}{1 - S_0} \quad \text{if } S > S_0 \quad (1)$$

$$84 \quad \text{with } S = \frac{\theta - \theta_r}{\theta_s - \theta_r}$$

85 where f_m is a macroporosity factor (-), θ is soil moisture (m^3m^{-3}), θ_s is soil moisture at

86 saturation (m^3m^{-3}), and θ_r is the residual soil moisture (m^3m^{-3}). Note that S ranges from zero

87 in case of completely dry soils to one for fully wet soils.

88 Equation 1 indicates that the onset of water flow through the fracture system of chalk is

89 controlled by the threshold S_0 . According to *Wellings and Bell* [1980], water flow through

90 fractures dominates over matrix flow in chalk when the pressure head in soil becomes higher

91 than -0.50 mH_2O . In this study, $S_0 = 0.80$, which is based on observed soil moisture-matrix

92 potential relationship in the study area (Figure S1).

93 In *Zehe et al.* [2001], f_m was defined as the ratio of the saturated water flow rate in all

94 macropores in a model element to the corresponding value in soil matrix, which can be

95 determined based on density and length of fractures at small scales. In addition, f_m has also

96 been considered as a calibration parameter previously [e.g., *Blume, 2008; Zehe et al., 2013*].

97 In this study, we define f_m as a characteristic soil property reflecting the influence of fractures



98 on soil water movement [Zehe and Blöschl, 2004], and estimate it from the relative difference
99 of permeability between chalk matrix and fractured chalk system that can be of the order 10^5
100 according to Price *et al.* [1999]. Consequently, we consider a macroporosity factor of $f_m =$
101 10^5 in this study.

102 **3. Methods**

103 **3.1. Study area**

104 The study area encompasses the Kennet catchment located in the Southern England with an
105 area of about 1033 km² (Figure 1a). Kennet, in general, is rural in nature with scattered
106 settlements and has a maximum altitude of approximately 297 m (Above Ordnance Level).
107 River Kennet discharges into the North Sea through London. Major tributaries of this river
108 are Lambourn, Dun, Enborne, and Foudry Brook. An average annual rainfall of
109 approximately 760 mm was recorded in the catchment over a 40 year period from 1961-1990.
110 Solid geology of the Kennet catchment is dominated by chalk, which is overlain by thin soil
111 layer. While lower chalk outcrops along the northern catchment boundary, progressively
112 younger rocks are found in the southern part. In general, surface runoff production is very
113 limited over the regions of the catchment where chalk outcrops. The flow regime shows a
114 distinct characteristics of slow response to groundwater held within the chalk aquifer [Le
115 Vine *et al.*, 2016]. According to Ireson and Butler [2013], the unsaturated zone of chalk
116 shows slow drainage over summer and bypass flow during wet periods in this catchment.

117 **3.2. Field measurements and remotely sensed data**

118 Table 1 summarizes the field measurements and remote sensing data used in this study. We
119 use in-situ soil moisture and runoff measurements along with remotely sensed latent heat flux
120 (*LE*) data to assess model performance in simulating the mass and energy balance
121 components of the hydrological cycle. Point scale soil moisture measurements at two



122 adjacent sites (~20 m apart) at the Warren Farm (Figure 1) were provided by Centre for
123 Ecology and Hydrology (CEH). A Didcot neutron probe was used at these locations to
124 measure fortnightly soil moisture at different depths below land surface (10 cm apart down to
125 0.8 m, 20 cm apart between 0.8-2.2 m, and 30 cm apart between 2.2-4 m) [Hewitt *et al.*,
126 2010].

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

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

137 **3.3. Land surface model**

138 In this study, we use the Joint UK Land Environment Simulator (JULES [e.g., *Best et al.*,
139 2011; *Clark et al.*, 2011]) version 4.2. JULES is a flexible modelling platform with a modular
140 structure aligned to various physical processes developed based on the Met Office Surface
141 Exchange Scheme (MOSES [e.g., *Cox et al.*, 1999; *Essery et al.*, 2003]). Meteorological data
142 including precipitation, incoming short- and longwave radiation, temperature, specific
143 humidity, surface pressure, and wind speed are required to drive JULES. Each grid box in
144 JULES can comprise nine surface types (broadleaf trees, needle leaf trees, C3 grass, C4 grass,



145 shrubs, inland water, bare soil, and ice) represented by respective fractional coverage. Each
146 surface type is represented by a tile and a separate energy balance is calculated for each tile.
147 Subsurface heat and water transport equations are solved based on finite-difference
148 approximation in JULES as described in *Cox et al.* [1999]. Moisture transport in the
149 subsurface is described by the finite difference form of Richards' equation. The vertical soil
150 moisture flux is calculated using the Darcy's law. While the top boundary condition to solve
151 Richards' equation is infiltration at soil surface, the bottom boundary condition in JULES is
152 free drainage that contributes to subsurface runoff.
153 Surface runoff is calculated by combining the equations of throughfall and grid box average
154 infiltration in JULES. In order to direct the generated runoff to a channel network, river
155 routing is implemented based on the discrete approximation of one-dimensional kinematic
156 wave equation [e.g., *Bell et al.*, 2007]. In this approach, river network is derived from the
157 digital elevation model (DEM) of the study area and different wave speeds are applied to
158 surface and subsurface runoff components and channel flows [e.g., *Bell and Moore*, 1998]. A
159 return flow term accounts for the transfer of water between subsurface and land surface [e.g.,
160 *Dadson et al.*, 2010, 2011].

161 **3.4. Model configurations and input data**

162 *3.4.1. Point scale*

163 At the point scale, JULES is configured to simulate the mass and energy fluxes at Warren
164 Farm (Figure 1). A total subsurface depth of 5 m is considered in the model with a vertical
165 discretization ranging from 10 cm at the land surface to 50 cm at the bottom of the model
166 domain. Note that this discretization is consistent with the soil moisture measurement depths
167 mentioned in section 3.2. The vegetation type is implemented as C3 grass using the default
168 parameters in JULES. The soil hydraulic properties are estimated based on texture (Table 2),



169 which is predominantly loamy at Warren Farm. The saturation-pressure head relationship is
170 described using the Van Genuchten [*Van Genuchten*, 1980] model with parameter values
171 (Table 2) obtained from *Schaap and Leij* [1998] in the model.

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

180 3.4.2. Catchment scale

181 At the catchment scale, JULES is configured over the study area (Figure 1) with a uniform
182 lateral grid resolution of 1 km with 70 x 40 cells in x and y dimensions, respectively. The
183 vertical discretization is identical to that of the point scale simulations described in the
184 previous section. Spatially distributed vegetation type information for the study area (Figure
185 1b) is obtained from the Land Cover Map 2007 (LCM2007) dataset [e.g., *Morton et al.*,
186 2011]. Harmonized World Soil Database (HWSD) from the Food and Agricultural
187 Organization of UNO (FAO) is used to obtain the texture of different soil types in the region
188 (Figure 1c). Van Genuchten model, with parameter values (Table 2) obtained from *Schaap*
189 *and Leij* [1998] is used to represent the saturation-pressure head relationship for different soil
190 types, which is identical to the point scale simulations.

191 Simulations were performed over 5 consecutive years from 2006-2011 at the catchment scale.

192 Note that the simulation periods of catchment and point scale (2003-2005) does not coincide



193 due to the availability of soil moisture measurements described in section 3.2. Spatially
194 distributed meteorological data from the Climate, Hydrology, and Ecology research Support
195 System (CHESS) was used to obtain the atmospheric forcing to drive JULES. The CHESS
196 data includes 1 km resolution gridded daily meteorological variables [Robinson *et al.*, 2015].
197 This daily data is downscaled using a disaggregation technique described in Williams and
198 Clark [2014] to obtain hourly atmospheric forcing. The flow direction required for river
199 routing is extracted from the USGS HydroSHEDS digital elevation data [Lehner *et al.*, 2008].

200 **3.5. Setup of numerical experiments**

201 We consider two different model configurations, namely, *default* and *macro* (Figure 2), to
202 explore the influence of chalk hydrology on simulated land surface processes in JULES. The
203 *default* configuration corresponds to the standard parameterizations of JULES that does not
204 represent chalk hydrology in the model. In this configuration, each soil column in JULES is
205 considered to be vertically homogeneous with the soil properties defined in Table 2, which is
206 motivated by the Met Office JULES Global Land 4.0 configuration described in Walters *et*
207 *al.* [2014]. The *macro* configuration, in contrast, explicitly represents chalk hydrology in the
208 model. The *macro* setup modifies the *default* configuration by applying chalk hydraulic
209 properties (Table 3) from 30 cm below land surface to the bottom of the model domain (i.e.
210 500 cm). The BC model is applied in the chalk layers (30-500 cm) to simulate water flow in
211 the *macro* configuration. Therefore, soil columns in the model can be divided into topsoil (0-
212 30 cm) and chalk (30-500 cm) in *macro*. Note that except for this inclusion of chalk, *default*
213 and *macro* configurations are identical in terms of model set up and input data.

214 The topsoil depth of 30 cm is defined based on several augured soil samples collected during
215 a field campaign at Warren Farm in 2015 (Figure 2). This depth is corroborated by additional
216 information from the British Geological Survey (BGS) operated borehole records



217 (http://www.ukso.org/pmm/soil_depth_samples_points.html), which show that topsoil depths
218 vary from 10-40 cm over the study area. We therefore apply the *macro* configuration
219 assuming a spatially homogeneous 30 cm topsoil depth for both point and catchment scale
220 simulations.

221 **4. Results and discussion**

222 **4.1. Point scale simulations**

223 Figure 3 shows observed and simulated volumetric soil moisture from the *default* model
224 configuration at Warren Farm from 2003-2005. This figure shows that simulated soil
225 moisture at shallow soil layers (up to 50 cm) compares reasonably well with the observed
226 data. However, in the deeper layers, the model considerably underestimates soil moisture.
227 Figure 4 compares observed and simulated volumetric soil moisture from the *macro*
228 configuration at Warren Farm over the simulation period. This figure shows that especially in
229 the deeper soil layers, the agreement between observed and simulated soil moisture improves
230 remarkably relative to the *default* configuration throughout the simulation period. Notice
231 again that the *default* and *macro* configurations are identical in terms of model setup and
232 inputs except for the consideration of chalk. Therefore, the differences in soil moisture
233 simulations between the two model configurations can be attributed to the representation of
234 chalk hydrology in JULES.

235 Figure 5 presents the relative bias ($\Delta\mu$, see Appendix) of simulated soil moisture from the
236 two model configurations at Warren Farm for various depth ranges. In the soil layers (0-30
237 cm), both *default* and *macro* configurations reproduces soil moisture reasonably well with the
238 latter showing slightly better agreement with observations. However, in the chalk layers (30-
239 500 cm), *default* fails to reproduce the soil moisture dynamics efficiently, simulating
240 substantially dry conditions, which are observed from the mean relative bias ($\Delta\mu_{\text{mean}}$) of



241 $\Delta\mu_{\text{mean}} > 0.28$ for this configuration. In contrast, the *macro* configuration remarkably
242 improves the agreement with the observed soil moisture profile in the chalk layers with the
243 largest calculated $\Delta\mu_{\text{mean}} = -0.02$. Therefore, the inclusion of the BC model in JULES appears
244 to improve the performance of overall soil moisture simulation at Warren Farm especially in
245 the chalk layers.

246 In order to explore the reason of the discrepancies between simulated soil moisture from the
247 two model configurations, Figure 6 shows S and water flux (w_f) profiles along with drainage
248 through the bottom boundary (d_b) of *default* and *macro* for the entire simulation period.

249 Figure 6b plots the contours of daily accumulated w_f through chalk (30-500 cm) over daily
250 average S for the *macro* configuration (S_{macro}). Figure 6c shows S (S_{default}) and w_f through the
251 same profile for the *default* configuration. A comparison between Figure 6b and 6c reveals
252 that *default* is considerably drier compared to *macro* ($S_{\text{default}} < S_{\text{macro}}$) throughout the profile,
253 which is consistent with Figure 5. Figure 6b shows notable flux through the profile following
254 strong precipitation events (Figure 6a), indicating fast water flow through subsurface in the
255 *macro* configuration (especially in winter). The *default* configuration, on the other hand,
256 shows relatively slower movement of water in the subsurface (Figure 6c).

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



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

274 Figure 6 outlines the differences in simulated subsurface processes by the two model
275 configurations. Fracture flow in chalk is activated according to the BC approach during wet
276 periods that allows recharge at deeper soil layers in *macro*, which is absent in case of the
277 *default* configuration. Moreover, the *default* configuration generally shows higher drainage
278 flux through the lower boundary compared to *macro*. The combination of relatively low
279 recharge and high drainage through lower boundary is the reason of the drier conditions
280 simulated by *default*. In contrast, the *macro* configuration is characterized by fast recharge at
281 the deeper soil layers through fractures and slow drainage through the bottom because of
282 considerably lower K_s compared to *default*, which is the reason of relatively higher simulated
283 soil moisture by this configuration that compares well with observations.

284 Several previous studies have discussed the influence of root zone soil moisture on land
285 surface mass and energy balance components [e.g., *Wetzel and Chang, 1987; Chen and Hu,*
286 *2004*]. Therefore, the differences in soil moisture from two configurations discussed above
287 may affect the land surface mass and energy fluxes in the model. In order to investigate this
288 effect, Figure 7 shows the difference between daily average latent heat flux (LE) time series
289 from *default* and *macro* configurations ($LE_{default}$ and LE_{macro} , respectively) at Warren Farm



290 over the simulation period. This figure shows that the *default* configuration generally
291 simulates lower *LE* compared to *macro* especially in the warmer months of the year.

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

300 In this section, subsurface and land surface processes simulated by *default* and *macro*
301 configurations are discussed at the point scale. The simulation results show notable
302 differences in soil moisture and *LE* from the two configurations. Because the only difference
303 between *default* and *macro* configurations is the representation of the chalk hydrology, it
304 appears that a consistent representation of chalk in JULES affects land surface processes via
305 subsurface hydrodynamics supporting our hypothesis. In the next section, we test this
306 hypothesis regionally by evaluating the mass and energy fluxes of the hydrological cycle at
307 the catchment scale.

308 4.2. Catchment scale simulations

309 Figure 8 plots spatially averaged 8-day composites of *LE* from MODIS (LE_{MOD}) against
310 $LE_{default}$ and LE_{macro} over the Kennet catchment. In this figure, the agreement between
311 simulated *LE* and LE_{MOD} is evaluated using the coefficient of determination (R^2 , see
312 Appendix) that outlines the differences between *LE* simulated by the two model
313 configurations. Comparison between $LE_{default}$ and LE_{MOD} shows a coefficient of determination



314 of $R^2_{default} = 0.78$. The agreement between simulated LE and LE_{MOD} improves in case of
315 *macro* configuration, which is reflected by an increased coefficient of determination of R^2_{macro}
316 $= 0.82$.

317 Figure 8 shows differences between $LE_{default}$ and LE_{macro} especially for relatively high LE ,
318 indicating discrepancies especially during the warmer months of the year. Figure 9a presents
319 spatially averaged time series of monthly LE_{MOD} , $LE_{default}$ and LE_{macro} . This figure shows
320 negligible differences in LE from the two configurations during the colder months of the
321 year, while differences between $LE_{default}$ and LE_{macro} increases substantially in summer.
322 Consequently, the *default* configuration underestimates LE especially in summer compared to
323 LE_{MOD} , which is improved when chalk hydrology is explicitly considered in JULES in the
324 *macro* configuration.

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



338 Table 4 compares observed and simulated daily average runoff from the two model
339 configurations over the Kennet catchment from 2006-2011. The runoff ratio (RR , see
340 Appendix), which is equal to the mean volume of flow divided by the volume of precipitation
341 [e.g., Kelleher *et al.*, 2015], assesses the partitioning of precipitation into runoff over the
342 catchment. The *default* configuration ($RR = 0.82$) shows considerably higher RR compared to
343 observation ($RR = 0.40$), indicating overestimation of runoff by the model. Including chalk
344 hydrology in the model remarkably improves the agreement between observed and simulated
345 mean runoff over the Kennet catchment, which is assessed from a runoff ratio of $RR = 0.38$
346 for the *macro* configuration.

347 In Table 4, the relative bias ($\Delta\mu$) of 1.04 between observed and simulated runoff from the
348 *default* configuration again indicates the overestimation by the model. In comparison, *macro*
349 shows a relative bias ($\Delta\mu = -0.07$), indicating improvement between observed and simulated
350 mean runoff volume compared to *default*. The relative difference in standard deviation ($\Delta\sigma$,
351 see Appendix) compares the magnitude of observed and simulated runoff in Table 3. This
352 comparison shows that the *default* configuration overestimates the variability of runoff over
353 the Kennet catchment ($\Delta\sigma = 2.04$), which is improved in case of *macro* ($\Delta\sigma = 0.56$).

354 In JULES, moisture from soil and canopy water storage is depleted to meet the ET demand.
355 Additionally, surface runoff generation depends on canopy water storage in the model [Best
356 *et al.*, 2011]. Because of this connection between ET and surface runoff generation via
357 canopy water storage, the differences in runoff demonstrated in Table 4 can be attributed to
358 the disagreement between $LE_{default}$ and LE_{macro} demonstrated in Figure 9a. Therefore, it
359 appears that LE in JULES is affected by the inclusion of chalk hydrology, which
360 consequently influences surface runoff generation corroborating our hypothesis.

361 5. Summary and Conclusions



362 In this study, we hypothesized that a consistent representation of chalk hydrology affects land
363 surface mass and energy balance components via subsurface hydrodynamics simulated by a
364 land surface model. In order to support this hypothesis, the *Bulk Conductivity* (BC) model
365 that simulates water flow through the matrix-fracture system of chalk was implemented in the
366 Joint UK Land Environment Simulator (JULES). This model was applied on the Kennet
367 catchment located in the southern UK to simulate the mass and energy fluxes of the
368 hydrological cycle for multiple years. Two model configurations, namely *default* and *macro*
369 were considered with the latter representing chalk hydrology in JULES using the BC model.

370 The proposed BC model is a single continuum approach of modelling preferential flow [e.g.,
371 *Beven and Germann, 2013*] that involves only 2 parameters, namely macroporosity factor (f_m)
372 and relative saturation threshold (S_0). In addition, these parameters can be estimated from the
373 physical properties of chalk in this study. Despite its simplicity, the BC model was able to
374 reproduce the hydrological processes in chalk without model calibration, which was assessed
375 by comparing the model results with observations. The discrepancies between the measured
376 and simulated fluxes and states can be improved by a comprehensive model calibration,
377 which is out of the scope of this study and should be the subject of future research.

378 The results showed that JULES generally underestimates root zone soil moisture without a
379 consistent representation of chalk hydrology. Consequently, LE is underestimated by the
380 model without chalk representation. The effect of chalk hydrology was also observed on
381 runoff, which was attributed to the interconnection between LE and runoff generation in the
382 model. Therefore, representing the matrix-fracture flow nature of chalk in a land surface
383 model affects land surface processes via shallow soil moisture dynamics, which supports the
384 proposed hypothesis.



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

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

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

404

405 **Acknowledgements**

406 We gratefully acknowledge the support by the “A Multi-scale Soil moisture
407 Evapotranspiration Dynamics study – AMUSED” project funded by Natural Environment
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 410 providing the data for the point-scale analyses at the Warren Farm. Finally, we would like to
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 413 (University of Bristol) for his valuable suggestions on model diagnostics, and Joost Iwema
 414 (University of Bristol) for helping with the soil samples collected during the 2015 field work
 415 campaign.

416

417 **Appendix**

418 **Definition of Statistical Metrics**

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

$$421 \quad R^2 = 1 - \frac{SS_{res}}{SS_{tot}}$$

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

$$424 \quad SS_{res} = \sum_{i=1}^n (y_i - f_i)^2 \quad \text{and}$$

$$425 \quad SS_{tot} = \sum_{i=1}^n (y_i - \bar{y})^2 \quad \text{with } \bar{y} \text{ being the mean of } y.$$

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

$$428 \quad RR = \frac{\mu_{runoff}}{\mu_{rain}}$$

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



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

$$431 \quad \Delta\mu = \frac{\mu_{mod} - \mu_{obs}}{\mu_{obs}}$$

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

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

$$437 \quad \Delta\sigma = \frac{\sigma_{mod} - \sigma_{obs}}{\sigma_{obs}}$$

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

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620 **Tables**

621 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

622 ^aMeasured at Warren Farm.

623 ^bLocations are shown in Figure 1a.

624

625 Table 2. Hydraulic properties for different soil types (refer to Figure 1c). Saturated hydraulic
 626 conductivity (K_s) and porosity data are obtained from *Rawls et al.* [1982]. The Van Genuchten
 627 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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630 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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633 Table 4. Comparison between observed and simulated daily average runoff from the two
 634 configurations over the Kennet catchment.

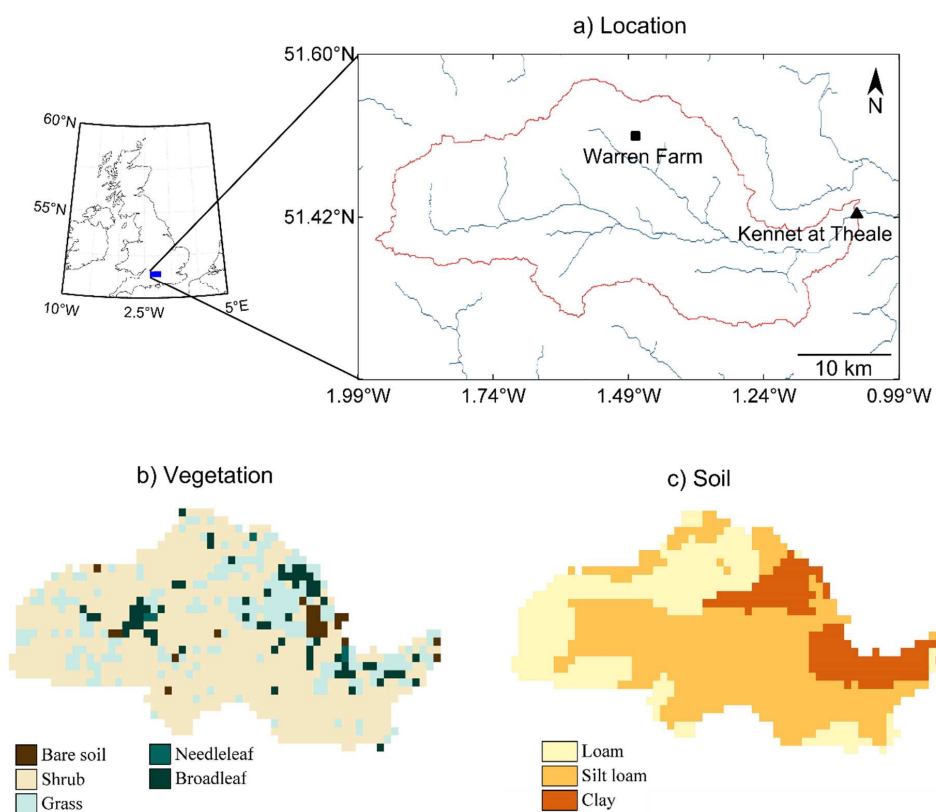
Metric	Observed	Simulated (<i>default</i>)	Simulated (<i>macro</i>)
RR	0.40	0.82	0.38
$\Delta\mu$	-	1.04	-0.07
$\Delta\sigma$	-	2.04	0.56

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636 **Figures**

637 Figure 1. Location (a), vegetation cover (b), and soil texture (c) over the study area. The red
638 line in (a) outlines the Kennet catchment boundary, while the river network is shown in blue.
639 The black triangle in (a) shows the location of the discharge gauging station at the catchment
640 outlet.



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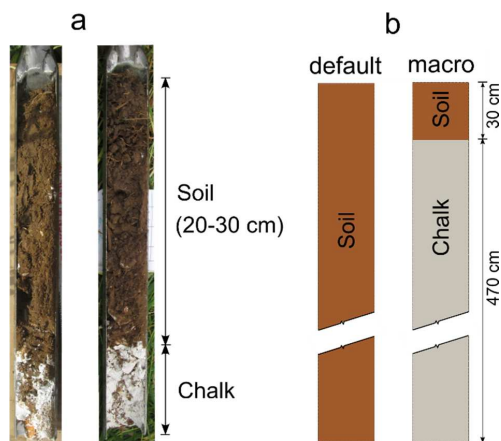
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646 Figure 2. Example of soil profiles collected at Warren Farm during a field campaign in 2015
647 (a), and the two model configurations (b).



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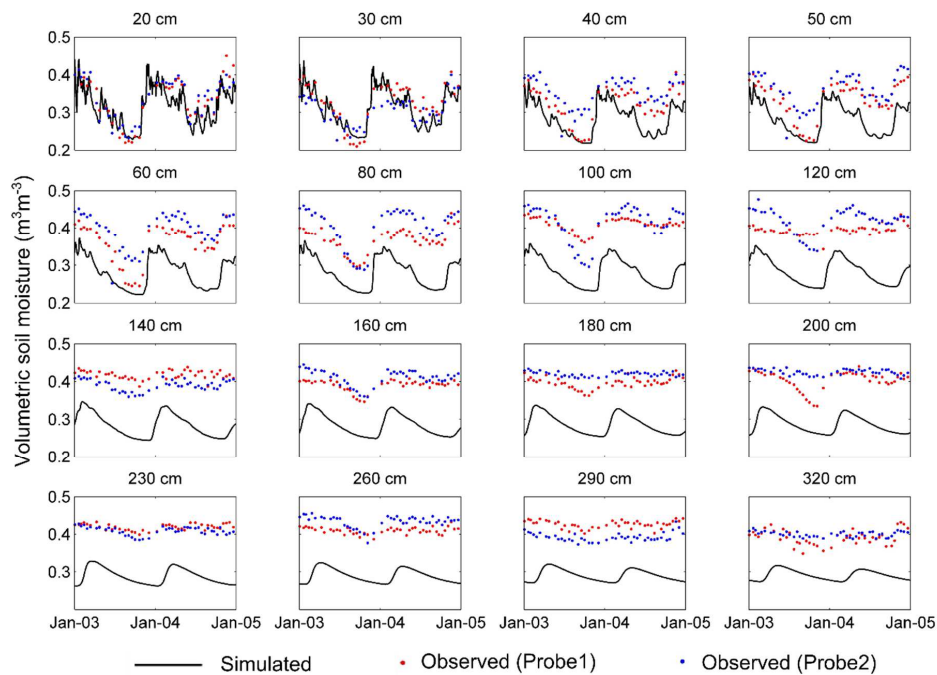
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660 Figure 3. Observed and simulated (*default configuration*) volumetric soil moisture from
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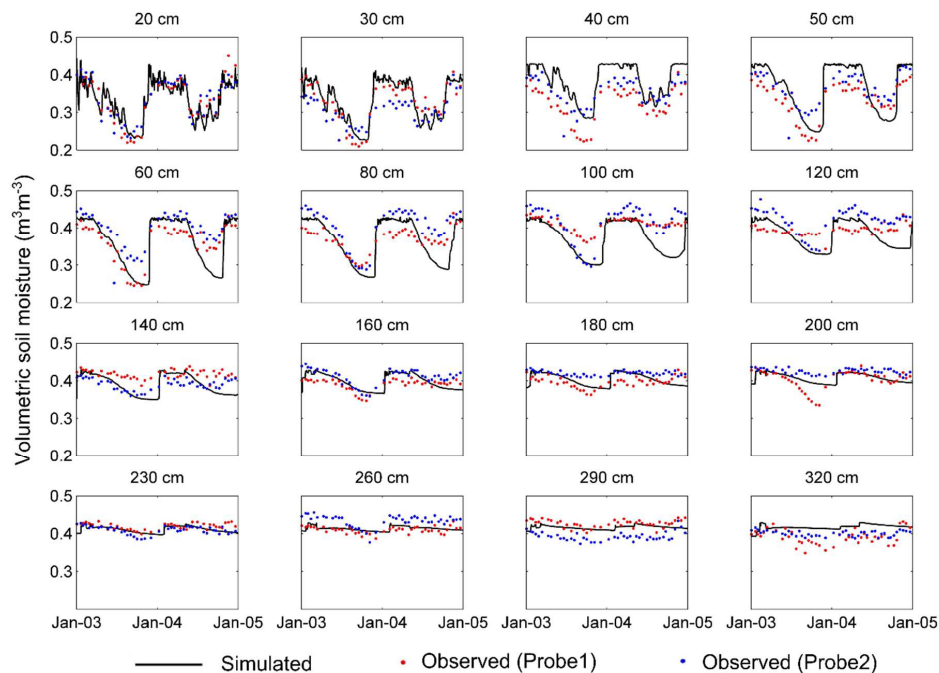
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671 Figure 4. Observed and simulated (*macro configuration*) volumetric soil moisture from
672 Warren Farm.



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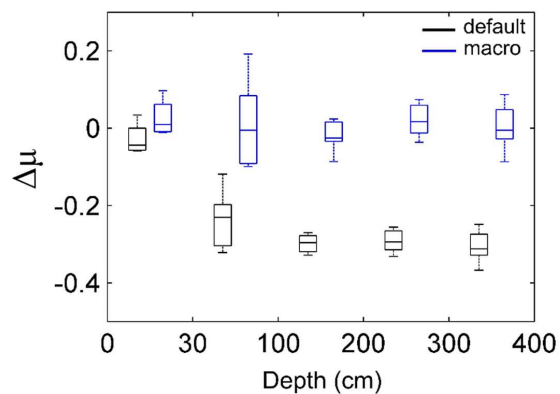
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683 Figure 5. Box plot of relative bias ($\Delta\mu$) of simulated soil moisture from *default* and *macro*
684 configurations at different depth ranges shown in individual intervals (e.g., 0-30 cm, 30-100
685 cm, and so on).



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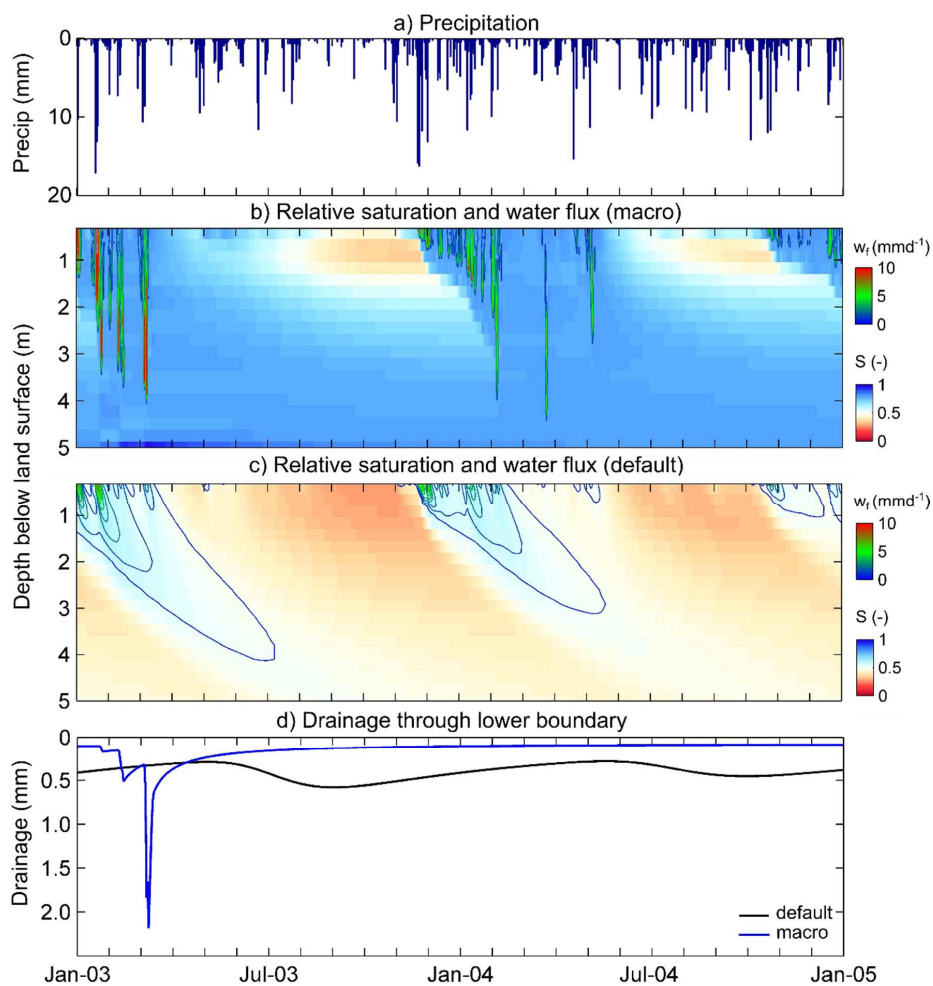
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698 Figure 6. Precipitation (a), daily accumulated downward water flux (w_f , contour lines) plotted
699 over relative saturation (S , coloured shading) for *macro* (b), daily accumulated downward
700 water flux plotted over relative saturation for *default* (c), and daily accumulated drainage flux
701 through the bottom boundary simulated by the two model configurations (d) at Warren Farm
702 over the two simulated years (2003-2005).

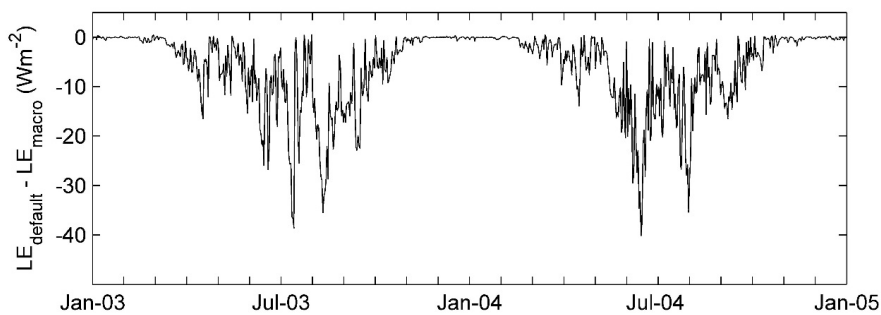


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705 Figure 7. Differences between daily average latent heat flux time series simulated by *default*
706 and *macro* configurations ($LE_{default}$ and LE_{macro} , respectively) at Warren Farm.



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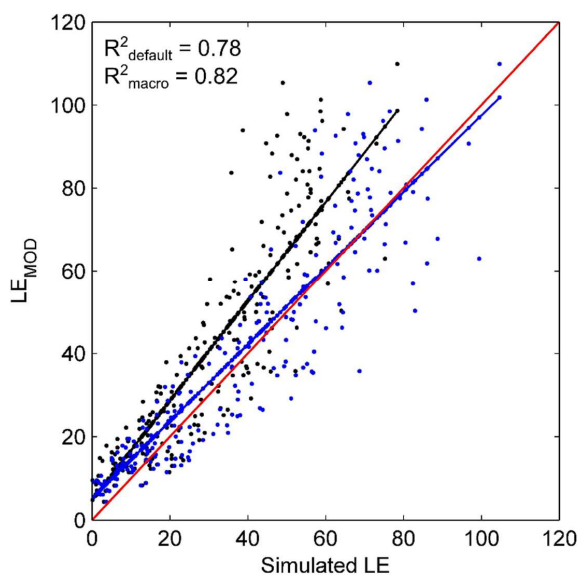
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720 Figure 8. Catchment average 8 day composites of MODIS estimated LE (LE_{MOD}) against
721 simulated LE from *default* and *macro* configurations ($LE_{default}$ and LE_{macro} , respectively) along
722 with the linear models fitted for $LE_{default}$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



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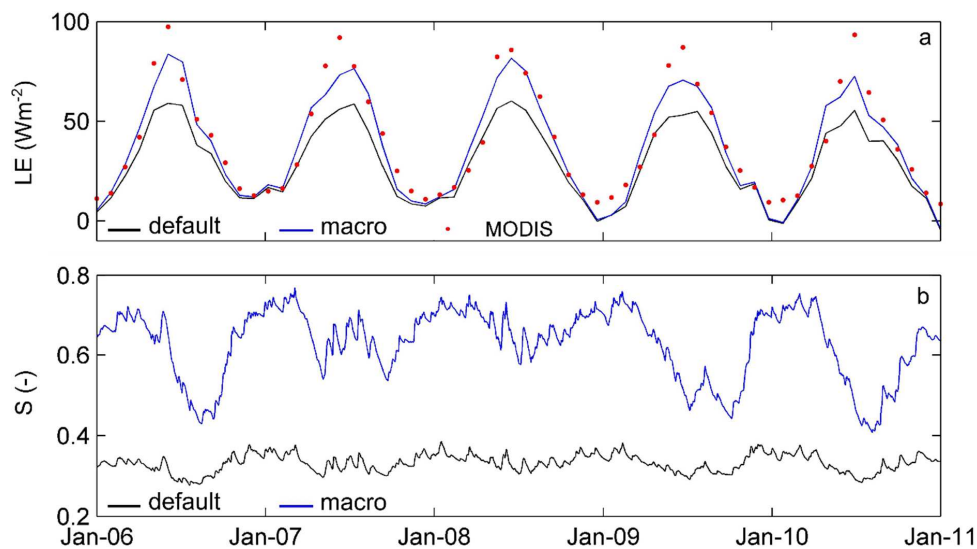
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731 Figure 9. Spatially averaged monthly latent heat flux (LE) from MODIS, *default*, and *macro*
732 configurations (a), and average (0-100 cm below land surface) daily relative saturation (S)
733 from *default* and *macro* configurations (b) over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



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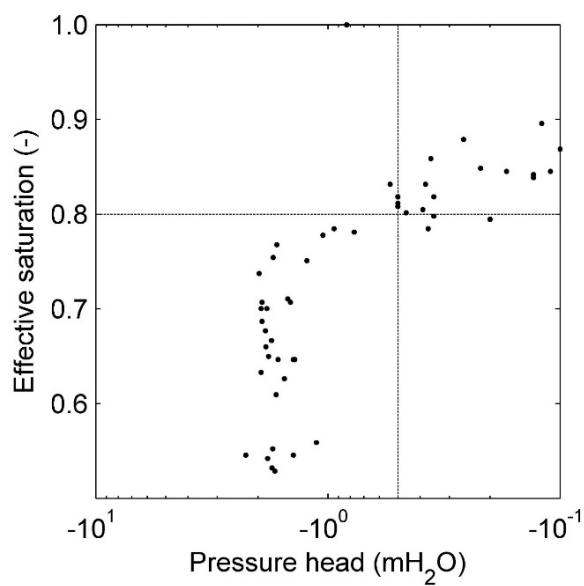


743 **Supplementary materials**

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

745 Farm measured fortnightly at 40 cm below land surface. (Source: Ned Hewett, CEH, personal

746 communication).



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