# Using observed river flow data to improve the hydrological functioning of the JULES land surface model (vn4.3) used for regional coupled modelling in Great Britain (UKC2)

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Abstract. Land surface models (LSMs) represent terrestrial hydrology in weather and climate modelling operational systems and research studies. We aim to improve hydrological performance in the Joint UK Land Environment Simulator (JULES) LSM that is used for distributed hydrological modelling within the new land-atmosphere-ocean coupled prediction system UKC2 (UK regional Coupled environmental prediction system 2). Using river flow observations from gauge stations, we study the capability of JULES to simulate river flow at 1 km<sup>2</sup> spatial resolution within 13 catchments in Great Britain that exhibit a variety of climatic and topographic characteristics. Tests designed to identify where the model results are sensitive to the scheme and parameters chosen

- 15 for runoff production, indicate that different catchments require different parameters and even different runoff schemes for optimal results. We introduce a new parameterization of topographic variation that produces the best daily river flow results (in terms of Nash-Sutcliffe efficiency and mean bias) for all 13 catchments. The new parameterization introduces a dependency on terrain slope, constraining surface runoff production to wet soil conditions over flatter regions, whereas over steeper regions the model produces surface runoff for every rainfall event regardless of the soil wetness state. This new parametrization improves the model performance
- 20 across Great Britain. As an example, in the Thames catchment, that has extensive areas of flat terrain, the Nash-Sutcliffe efficiency exceeds 0.8 using the new parameterization. We use cross-spectral analysis to evaluate the amplitude and phase of the modelled versus observed river flows over time scales of two days to ten years. This demonstrates that model performance is modified by changing the parameterization by different amounts over annual, weekly-to-monthly and multi-day time scales in different catchments, providing insights into model deficiencies at particular time scales, but reinforces the newly developed
- 25 parameterization.

#### **1** Introduction

The land surface provides a two-way link between terrestrial hydrology and meteorology. Improving the representation of runoff generation in models of the land surface which are coupled to the atmosphere and oceans, could potentially improve meteorological forecasts as well as hydrological predictions. For the UK, a fully coupled (land, atmosphere, ocean) environmental prediction system

is being built at 1.5 km<sup>2</sup> spatial resolution (UKC2; Lewis et al., 2018). The land surface component of this coupled system is the Joint UK Land Environment Simulator (JULES) model. In this paper, we focus on the runoff generation process. Conceivably improved runoff to the sea surrounding the UK influencing sea surface salinity could influence meteorological forecasts in the UK.

Different stages of the development of the JULES capability for this process have been published (Best et al., 2011; Blyth, 2002;
Clark and Gedney, 2008), and analysis of runoff outputs has been carried out at the site level (Blyth, 2002; Blyth et al., 2011; Weedon et al., 2015), for a set of Rhône subcatchments treated as single grid cells (Clark and Gedney, 2008) and at the global scale with JULES simulations at 0.5° or 1° (Blyth et al., 2011; Gudmundsson et al., 2012; Papadimitriou et al., 2016; 2017). However, a regional scale analysis of the process at ~1 km<sup>2</sup> spatial resolution was needed in order to implement an appropriate JULES hydrological parameterization for the coupled system within UKC2.

- 10 Runoff in Land Surface Models (LSMs) is typically represented as the sum of surface runoff and baseflow. Most current LSMs (JULES included) simulate surface runoff as saturation excess, infiltration excess, or a combination of both components (Clark et al., 2015; Schellekens et al., 2017). JULES uses the soil hydraulic characteristics to determine the infiltration excess component (Best et al., 2011) and a parameterization of the saturated fraction of the soil representing the subgrid variability of soil moisture to determine the saturation excess component (Blyth, 2002; Clark and Gedney, 2008). The sub-surface runoff is simulated in many
- 15 LSMs as the free drainage of water through the bottom of the soil column as represented in the model (e.g. Balsamo et al., 2009; Campoy et al., 2013; Oleson et al., 2010; Walko et al., 2000). JULES provides two options to calculate the baseflow: a) as subsurface runoff, assuming a simple free drainage approach; or b) as the lateral sub-surface flow within the soil column, adopting a parameterization in terms of the spatial distribution of topography (Beven and Kirkby, 1979; Clark and Gedney, 2008).

The island of Great Britain represents an ideal platform to study the runoff generation in LSMs since it has a range of climatic and

- 20 topographic characteristics plus has a comprehensive set of river flow gauge stations with data stored at the National River Flow Archive (NRFA, UK). The differences in precipitation are high and show a clear west-east and north-south contrast, with yearly means above 10 mm d<sup>-1</sup> in western Scotland and below 2 mm d<sup>-1</sup> in the southeast of England (CEH-GEAR dataset; Keller et al., 2015; Tanguy et al., 2014). Furthermore, regional precipitation regimes in the island range between 3 and 5 mm d<sup>-1</sup> in Scotland and Wales, whereas in the English lowlands (Southeast) the mean monthly precipitation varies between 1.5 and 2.5 mm d<sup>-1</sup> (Robinson
- et al., 2017b). In addition to this precipitation variability, topographic differences and varied soil types (e.g. the high permeability of chalky soils in the Thames catchment and other eastern regions; Farrant and Cooper, 2008) result in a wide range of percentage runoff and baseflow index (BFI) responses, reported for the UK by Boorman et al. (1995) in the Hydrology of Soil Types (e.g. BFI = 0.86 for the Avon catchment at Knapp Mill in Southwest England and BFI = 0.33 for the Ribble catchment at Samlesbury in Northwest England). Hydrological models typically overcome the problem of these regional heterogeneous characteristics as they
- 30 solve runoff for individual catchments and use parameters calibrated to observed river flow (Bastola et al., 2011; Prudhomme et al., 2010). Nevertheless, there have been significant efforts in the hydrological community to generalise the catchment parameterization for regional scales (Crooks et al., 2014; Wagener and Wheater, 2006) and to estimate parameters over data poor or ungauged regions

using catchment similarity concepts (Beck et al., 2016; Mizukami et al., 2017). However, a widely used LSM in the research community like JULES requires physically-based parameters that produce sensible results at the regional and global scale, independently of the region studied (i.e. avoiding local calibration).

- In this work we perform, firstly, a sensitivity study of alternative runoff production schemes and parameters to identify the best representation of observed daily river flow at a range of selected catchments in Great Britain. Then, based on those catchment results, we present a novel model development that introduces a topography dependency in the parameter that determines the soil wetness at which a grid cell starts generating saturation excess runoff in relation to the subgrid saturation fraction. The development optimizes the generation of daily river flow compared to observations and avoids catchment calibration. Finally, as the ambition of UKC2 is to work towards a coupled prediction system for longer timescales (Lewis et al., 2018), the implications of the new approach are investigated further using cross-spectral analysis to assess the performance against observations over scales ranging
- from days to multiple years.

# 2 Methods and data

### 2.1 The JULES LSM

The JULES LSM is a widely used community land surface model. It works coupled to the atmosphere in the Unified Model (UM of the UK Met Office) both for operational weather forecasting and for climate applications as the land surface component of the Hadley Centre family of climate models (HadGEM3 and UKESM1), participants in CMIP (<u>https://www.wcrp-climate.org/wgcmcmip</u>). Additionally, JULES can be run uncoupled as a standalone tool to assess water resources (e.g. Schellekens et al., 2017; Blyth et al., 2018) and to study land-atmosphere interactions and impacts (Betts, 2007; Harrison et al., 2008; Van den Hoof et al., 2013). Details of the structure and processes represented in JULES are described by Best et al., (2011; energy and water fluxes) and Clark

20 et al., (2011; carbon fluxes and vegetation dynamics).

JULES divides the land into grid boxes and resolves sub-daily water and energy fluxes at the land surface and through vertical soil layers (typically 4 layers of 0.1, 0.25, 0.65 and 2.0 m thickness, down to 3.0 m). A detailed description of the model hydrological methods is given in Best et al. (2011), and a thorough description of the hydrological processes in JULES from the water reaching the land surface as precipitation is given in Blyth et al. (2018). Here, we focus on the runoff production process and its parameter variability.

25 variability.

#### 2.1.1 Runoff generation and river routing schemes in JULES

From the precipitated water that arrives at the surface after vegetation interception at each model time step, JULES first determines the infiltration excess component of surface runoff from the soil hydraulic characteristics (Best et al., 2011; Blyth et al., 2018). Then, for saturation excess surface and sub-surface runoff, two scheme options representing subgrid variability can be used. These

approaches are thoroughly described by Clark and Gedney (2008); one based on the Probability Distributed Model (PDM; Moore, 1985; 2007, first included in JULES by Blyth, 2002) and the other one based on TOPMODEL (Beven and Kirkby, 1979).

The PDM approach in JULES calculates the fraction of each model gridbox that is saturated as water infiltrates into the soil and the soil storage is filled. This fraction is given by:

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$$f_{sat} = 1 - \left[1 - \frac{\max(0, S - S_0)}{S_{max} - S_0}\right]^{\frac{b}{b-1}}$$

flow:

where *S* is the areal fraction of gridbox soil water storage,  $S_0$  is the minimum storage at and below which there is no surface saturation (note that  $f_{sat} = 0$  for  $S \le S_0$ ),  $S_{max}$  is the maximum gridbox storage:  $S_{max} = \theta_{sat} z_{pdm}$ , where  $\theta_{sat}$  is the volumetric soil water content at saturation and  $z_{pdm}$  the depth of the soil column considered by the scheme, and *b* is a shape parameter. Any water from precipitation arriving over the saturated fraction of the grid generates surface runoff. The sub-surface runoff,  $R_b$ , is

10 obtained as free drainage at the bottom of the soil column, at a rate determined by the soil hydraulic conductivity at the bottom soil layer  $K_N$  (i.e.  $R_b = K_N$ ; Cox et al., 1999). Therefore, the two parameters that can be used for calibration of PDM within JULES are *b* and  $S_0$ .

The TOPMODEL approach also uses a saturated fraction for each model gridbox and estimates the saturation excess runoff at the surface as  $R_s = f_{sat}W_0$ , where  $W_0$  is the precipitated water that reaches the top soil layer. However, within TOPMODEL  $f_{sat}$  is calculated in terms of the gridbox distribution of the topographic index  $\lambda$  that is obtained from subgrid topographic data, as the proportion of the grid cell where the topographic index is higher than a critical value at which the local water table is found at the surface (Best et al., 2011; Gedney and Cox, 2003). The sub-surface runoff or baseflow,  $R_b$ , is obtained as the lateral sub-surface

$$R_b = \frac{\alpha K_{s0}}{f} e^{-\Lambda} e^{-fz_w}$$

20 A is the gridbox mean of the topographic index,  $K_{s0}$  is the saturated conductivity at the surface,  $\alpha$  is the anisotropy factor that accounts for differences in the saturation conductivity between the vertical and horizontal directions, f is a decay parameter (also used to implement an exponential decay of the hydraulic conductivity through the soil vertical layers from  $K_{s0}$  at the surface in the calculation of water vertical transport), and  $z_w$  is the mean gridbox water table depth calculated as a diagnostic from the gridbox soil moisture profile. Since  $f_{sat}$  is constrained by topographic data within TOPMODEL, only f and  $\alpha$  parameters can be used for calibration exercises.

Once JULES has calculated the gridbox runoff following either of the approaches described above, the River Flow Model (RFM; Bell et al., 2007) is used to route surface and sub-surface runoff from inland grid cells across the river network and out to sea at

each model time step (i.e. sub-daily, not at daily steps). RFM is a kinematic wave equation scheme that incorporates scale dependent parameters and has been recently introduced into JULES (Lewis et al., 2018).

# 2.2 Selected catchments in Great Britain and experimental setup

We select 13 catchments in Great Britain (Fig. 1, Table 1). The spatial resolution used for Fig. 1 and all JULES catchment runs for
this paper is 1 km × 1 km. These 13 catchments are used in the development of a national hydrological modelling framework (Crooks et al., 2014), and represent a range of soil types, precipitation regimes and geographical locations that characterize the island of Great Britain. We acknowledge the availability of river flow data for a larger number of catchments in the NRFA archive, however we focus on catchments large enough for the JULES distributed model to integrate hydrological processes at the km-scale.

### 2.2.1 Ancillary and driving data

- 10 For surface exchanges, JULES divides each land grid cell into a series of tiles that can differ in morphological, physiological and hydrological characteristics according to the land cover. For this work we use the Land Cover Map 2000 (Fuller et al., 2002) produced by CEH (Centre for Ecology and Hydrology, UK), converted to 8 different fractional land cover types at the 1 km<sup>2</sup> horizontal resolution: broadleaf trees, needleleaf trees, grasses, crops, shrubs, water, bare soil and urban cover. The soil hydraulic characteristics are assumed to be spatially uniform for each grid cell, and have been calculated for the model domain from the
- 15 Harmonized World Soil Database (HWSD; FAO/IIASA/ISRIC/ISS-CAS/JRC, 2012). The topographic index λ has been calculated for Great Britain at 50 m<sup>2</sup> resolution from the CEH-IHDTM database (Morris and Flavin, 1990; 1994), following the methodology in Marthews et al. (2015), and then its mean and standard deviation at the 1 km<sup>2</sup> model grid are used as input data for the TOPMODEL approach.

The RFM routing scheme uses values of single flow direction and flow accumulation (number of grid cells flowing to each cell in

20 a river catchment). These river network parameters for the catchments used here were drawn from Davies and Bell (2009), originally calculated from the CEH-IHDTM database (Morris and Flavin, 1990; 1994) following the COTAT algorithm methodology (Paz et al., 2006).

The meteorological driving data used to run the model is CHESS-met (Robinson et al., 2017a). This database provides all the required surface variables to run JULES (precipitation, input longwave and shortwave radiation, air temperature, specific humidity,

25 wind speed and pressure) at 1 km<sup>2</sup> spatial resolution for Great Britain and daily time resolution. The precipitation data in CHESSmet are gridded estimates of daily rainfall from gauge stations (CEH-GEAR; Keller et al., 2015; Tanguy et al., 2014), whereas the rest of the variables are interpolated from the observation-based coarser resolution MORECS dataset (Hough and Jones, 1997; Thompson et al., 1981), taking into account topographic information to disaggregate to the finer scale (Robinson et al., 2017b).

## 2.2.2 Set of experiments and metrics

A series of test runs are conducted for each catchment in Fig. 1, exploring parameter variability, in order to analyse the model performance and find the best hydrological configuration for the simulation of river flow in JULES.

5 0.55, 0.6, 0.65, 0.7, 0.75, 0.8, 0.85, 0.9, 0.95, 1.0, 1.2, 1.4, 1.6, 1.8, 2.0), controlling the saturation fraction calculation once  $S_0$  has been reached. Lower values of *b* result in lower saturation fraction and therefore less surface runoff during precipitation events. We also add a set of tests where *b* is spatially varying as a function of the terrain slope as developed by the Verifications, Impacts and Post-Processing Research group in the UK Met Office (unpublished):

$$b = \min\left(b_{max}, b_{min} + \frac{s/s_{max}}{1 - s/s_{max}}\right)$$

10 where *s* is the gridbox terrain slope,  $s_{max} = 21^\circ$ ,  $b_{min} = 0$  and  $b_{max} = 0.8$ . The terrain slope was calculated from the CEH-IHDTM database (Morris and Flavin, 1990; 1994).

We choose four possible values for the  $S_0$  parameter within the 0-1 range that it can take in the form of fraction of saturation  $(S_0/S_{max} = 0.0, 0.25, 0.5, 0.75)$ , controlling the soil moisture state required to start producing saturation excess surface runoff, i.e., every rainfall event will produce saturation excess runoff when  $S_0/S_{max} = 0.0$  even when the soil is dry (reasonable over steep areas where some saturation fraction is always expected), whereas no surface runoff is produced until the saturated area is 25, 50 or 75 % of the grid cell area in the other 3 tests (since over flatter terrain a precipitation event might be absorbed entirely by the soil and therefore produce no surface runoff). The combined parameter variability tested in the PDM scheme has a strong effect on the surface saturated fraction of the soil, with *b* increasing this fraction at higher values, and  $S_0$  acting as a constraint of the scheme to start producing saturated fractions and also reducing the impact of *b* variability as its value gets closer to  $S_{max}$  (Fig. 2).

- 20 Tests using the TOPMODEL scheme include 8 variations of the *f* decay parameter (f = 1.5, 2.0, 2.5, 3.0, 3.5, 4.0, 4.5, 5.0), controlling the decay of hydraulic conductivity with depth and the baseflow production. This range for *f* is consistent with findings in other JULES studies (Clark and Gedney, 2008; Finney et al., 2012). The anisotropy factor  $\alpha$  is related to the soil stratification, and different authors have adopted different values: Chen and Kumar (2001) calibrated it to a value of 2000 for North America; Niu and Yang (2003) used a range of 10-20; Fan et al. (2007) made it dependent on the soil clay content (values between 2 for sand and
- 48 for clay); and Clark and Gedney (2008) found the value of 100 to best reproduce streamflow with JULES for three Rhône subcatchments. Here, we test four values of the anisotropy factor ( $\alpha = 1, 10, 100, 1000$ ).

Apart from the runoff production at the surface and sub-surface, a key configuration for any LSM to simulate the water cycle is the choice of hydraulic model that computes the water movement through the soil profile (Marthews et al., 2014). JULES provides the

option of using either the Brooks and Corey (1964) approach (BC), or the Van Genuchten (1980) approach (VG), to represent the hydraulic relationships between soil water content, suction and hydraulic conductivity (Best et al., 2011). BC and VG differ in the way they approach the curves relating the soil water content and the water suction for each soil type; while BC curves tried to best represent available measurements using an exponential fit, VG curves are smoothed down to represent an S-shaped relationship

- 5 suggested by the observations. The differences and potential misrepresentations of both approaches are often found at the dry and wet ends of the curves. The VG asymptotic behaviour can cause non-physical results at the dry end, whereas the BC formulation presents abrupt transition to low water suctions at the wet end; potentially causing model instability (Marthews et al., 2014). For every catchment the PDM and TOPMODEL experiments were run using both the BC and VG approaches, driven by input soil hydraulic properties calculated from the HWSD using the corresponding pedotransfer functions: Cosby et al. (1984) for BC and
- 10 Wösten et al. (1999) for VG.

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Given the range of configuration and parameter combinations, a total of 272 simulations were a carried out for each catchment. The simulations cover a total of 10 years (1991-2000) following a 5 year model spin up (using data from 1986-1990). Since the driving CHESS-met dataset is given at the daily time steps, a daily disaggregation scheme (Williams and Clark, 2014) allowed JULES to be run at half-hourly time steps. In terms of precipitation, events start at a random time during the day and last for 2 hours in the case of convective precipitation and for 6 hours in the case of large-scale precipitation.

Although JULES is run at half-hourly time steps including routing between grid boxes using RFM, the model performance is analysed by comparing the simulations with observed daily river flow data at the catchment outlet stations (Table 1) provided by the NRFA. The Thames at Kingston has a naturalised flow record available (to compensate for flow controls at locks and abstraction), but in all the other catchments the modelled flow is compared directly with the gauged flow.

20 The Nash-Sutcliffe efficiency (NS; Nash and Sutcliffe, 1970) is used as our baseline metric,

$$NS = 1 - \frac{\sum_{t=1}^{T} (Q_{obs,t} - Q_{mod,t})^2}{\sum_{t=1}^{T} (Q_{obs,t} - \overline{Q}_{obs})^2}$$

where  $Q_{obs,t}$  and  $Q_{mod,t}$  are the observed and modelled river flows at a particular time t, respectively, T is the total number of observed days, and  $\overline{Q_{obs}}$  is the average observed river flow over the period analysed. NS is widely used in hydrological studies, it measures the accuracy of the model to represent river flow at the given daily time scale and is sensitive to timing differences in peak

flows. A value of 1 for *NS* represents a perfect model, whereas a value of 0 represents no predictive skill (i.e. at NS = 0.0 a model performs no better than using the mean river flow). Calculating the average modelled river flow ( $\overline{Q_{mod}}$ ), we also use the mean *bias* that indicates the model performance in the long-term balance P - ET (precipitation minus evapotranspiration), calculated as

$$bias = 100 \left( \frac{\overline{Q_{mod}}}{\overline{Q_{obs}}} - 1 \right).$$

We acknowledge that river flow simulation model performances using LSMs are influenced by physical processes represented in the model and imposed by the meteorological driving data at multiple time scales. In order to further assess the model performance at time scales longer than daily and relevant for the studied catchments, and to complement findings using *NS* at the daily time scale and mean *bias*, we use a cross-spectral analysis (Weedon et al., 2015) that provides measures on how the average amplitude and

phase of modelled river flow differ from observed river flow.

#### **3 Results**

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#### 3.1 Soil hydraulics

The main difference between the VG and the BC soil hydraulics formulations is that the VG curve of the soil water suction at soil water contents varies more smoothly close to saturation (Dharssi et al., 2009; Marthews et al., 2014), hence we expect wet soils like those of the catchments in Great Britain used here to be better resolved by the VG approach. Hence we expect the generally wet soils of the catchments in Great Britain used here to be better resolved by the VG approach.

*NS* and mean *bias* (as its absolute value) metrics from all the catchment tests are shown as scatter plots that compare results obtained using the BC (y axis) and VG (x axis) approaches (Fig. 3). The VG tests perform better in all catchments as most of the points fall

15 within the VG zone (i.e. below the 1:1 line) in the NS plot (Fig. 3, left), particularly for higher values that indicate better performance. The exception to this result occurs with the Severn1 catchment where the best NS values of around 0.7 are found using the BC formulation. The BC results show consistently higher absolute *bias* (i.e. worse performance) than the VG results (Fig. 3, right). Consequently, we will show only results from VG tests in the following plots.

The origin of the pedotransfer functions used to derive soil hydraulic properties further explain the difference in performance showed

20 in Fig. 3 and support our choice of the VG approach when using JULES for hydrological assessments in Great Britain. For the VG approach the functions were developed from data provided by 20 institutions from 12 European countries, England and Scotland included (Wösten et al., 1999), whereas for the BC approach the original data were taken from 23 localities in the United States (Cosby et al., 1984).

#### 3.2 Sensitivity of runoff generation schemes

25 The first order control of variability in runoff generation within JULES is determined by the choice of hydrological scheme: PDM or TOPMODEL. Fig. 4 shows the performance metrics obtained for each catchment in all tests.

The mean *bias* (Fig. 4, right) tends to be negative in most tests, indicating the underestimation of river flow by the model. The TOPMODEL scheme shows low or no range in *NS* and *bias* within each catchment whereas the PDM tests show higher variability within catchments. PDM results range from a high negative *bias* similar to that of the TOPMODEL results to improved *bias* (towards zero) across the various tests. The low range in metric values in the TOPMODEL tests was expected, because the *f* and  $\alpha$  parameters

5 tested affect the sub-surface runoff production, and therefore the timing of the baseflow discharge, but not directly the surface runoff production through variation of the saturated fraction. As indicated before, the saturated fraction in TOPMODEL is derived from observed topographic characteristics, and cannot be calibrated or changed.

The *NS* metric (Fig. 4, left) shows a larger range according to the parameters used in the PDM tests and, overall, reach higher values (closer to 1), indicating the potential for a better performance. Only for the baseflow dominated catchments (BFI  $\ge$  0.6; Tay,

10 Derwent, Thames and Avon) do the TOPMODEL results approach the better PDM *NS* results. This might be because baseflow in TOPMODEL is more sensitive to the parameters that are tested. The TOPMODEL river flow production gets poor *NS* metric values (below 0.4) on other catchments towards the north with higher total precipitation and lower BFI (i.e. for the Dee, Ribble and Clyde).

The constraint introduced by the  $S_0$  parameter in the PDM scheme seen in Fig. 2 results in an added degree of variability to the PDM tests. The *bias* becomes more negative as  $S_0$  increases, indicating less river flow at the catchment outlets and a poorer

- 15 representation of the P E balance. However, at baseflow dominated catchments like the Thames, Derwent, Avon or the Severn2, the *NS* metric clearly improves for higher  $S_0$  (Fig. 5). Considering the *b* parameter variability, there is a general overall improvement of performance for higher values of *b* (increasing *NS* as the marker size increases in Fig. 5). This is not clear for all catchments; the two Severn catchments and also the northern Tay catchment reach the best performance (*NS*) at *b* values of around 0.5-0.6 for the  $S_0 = 0$  tests (red markers). Over other catchments with discharge heavily influenced by baseflow (Thames, Avon and Derwent) the
- 20 lowest values of *b* produce the higher *NS* metrics when  $S_0$  is low. Conversely high values *b* produce the best *NS* metrics for these catchments as  $S_0$  increases.

#### 3.3 Optimizing the PDM parameters

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Results in Section 3.2 suggested that the PDM approach can produce better results than the TOPMODEL approach in terms of river flow simulation for the selected catchments. However, the best possible PDM parameters vary for each catchment. In this section, we describe how we developed a universal method for optimizing parameter estimation based on topographic data.

In Fig. 6, we relate the best performing PDM parameters to the physical parameter that shows the dominant correlation with the performance results: the mean terrain slope of the particular catchments. The terrain slope was calculated depending on elevations in a  $3 \times 3$  grid cell neighbourhood (Horn, 1981), using the elevation data at 50 m<sup>2</sup> resolution from the CEH-IHDTM database (Morris and Flavin, 1990; 1994), and then calculating the mean angle at the working resolution of 1 km<sup>2</sup>. Plots on the left in Fig. 6 (a-d)

30 illustrate how the mean catchment slope can help determine the optimum PDM parameters: 1) the Thames is the flattest catchment

(mean slope of 2.3°) and the only one where the highest  $S_0$  produces the best result, 2) there are a series of catchments with mean slope in the range 3.5-5° where  $S_0/S_{max} = 0.5$  produces the best performance, and 3) the catchments with mean slope above 5° produce the best results with  $S_0/S_{max} = 0.0$ .

- Focusing on the *b* parameter value represented on the x axis of Fig. 6, the best performance for each catchment (markers highlighted with an outer circle) is consistently found towards the high end of the parameter range, with the exception of the Tay, Derwent and Avon catchments. Hence, we propose a new criterion to simulate river flow for Great British catchments (Fig. 6e) based on the mean catchment slope (*mcs* hereafter), with a fixed b = 2.0 and a simple choice of  $S_0/S_{max} = 0.75$  for catchment slopes below  $3.5^\circ$ ,  $S_0/S_{max} = 0.5$  for catchment slopes between  $3.5^\circ$  and  $5^\circ$ , and  $S_0/S_{max} = 0.0$  for catchment slopes above  $5^\circ$ . Applying this new *mcs* criterion (daily river flow time series and evaluation metrics shown in Fig. 7), JULES performance in most of the 13 catchments is as good as the using the PDM parameters that produce the best performance (shown by highlighted markers in Fig. 6e). A clear exception is the Avon catchment, where the *NS* metric is reduced from 0.68 to 0.60 when changing from the best found performance to *mcs*. The other catchments where *mcs* does not match exactly the best performance tests are the Tay, Ure and Derwent. On the other hand in these catchments, *NS* does not change when switching to use of the *mcs* criterion (Ure, *NS* = 0.74; Derwent, *NS* = 0.57) or is only slightly reduced (Tay, from 0.66 to 0.63).
- 15 Applying the *mcs* criterion we are able to introduce catchment variability in the JULES performance related to different topography characteristics reaching high *NS* values in flat catchments such as the Thames with baseflow dominated runoff, and in steeper catchments such as the Ouse and Ribble with fast surface runoff production during rainfall events and low BFI.

## 3.4 Applying the new criterion mcs at the grid resolution

- A key driver for this work in the context of developing a UK regional coupled environmental prediction system (UKC2; Lewis et al., 2018) is to develop the best possible representation of the hydrology in JULES for the whole Great Britain domain and at a resolution close to the coupled model resolution (approximately 1.5 km<sup>2</sup> at mid-latitudes). It is therefore necessary to be able to apply the new criterion on 1 km<sup>2</sup> grid cells rather than in particular catchments (note that *mcs* is based on catchment-wide PDM parameters for each test). To develop spatially varying parameter sets, a  $S_0/S_{max}$  parameter dependency on terrain slope at the model grid cell resolution is considered. We adopt a simple approach using a linear dependency of  $S_0/S_{max}$  on slope for values
- 25 below a given threshold, representing the PDM parameters in the *mcs* criterion presented in Section 3.3 at the model grid cell resolution, as follows:

$$\begin{cases} b = 2.0\\ S_0/S_{max} = \max\left(1 - \frac{s}{s_{max}}, 0.0\right) \end{cases}$$

where *s* is the grid cell slope and  $s_{max}$  is the maximum slope that results in  $S_0/S_{max}$  higher than zero ( $s_{max} = 6^\circ$  obtained the best results in the case of JULES standalone simulations using the 1 km<sup>2</sup> slope data described in Section 3.3). Effectively, the inclusion

of this slope dependency limits the saturation excess runoff production within flatter regions in wet situations, and it enhances runoff production within steeper regions due to a high b parameter with no limitation by soil water content.

We introduce this linear function for a grid cell slope dependency in the  $S_0/S_{max}$  parameter in the JULES model and integrate a new simulation for each catchment, obtaining the river flow performance metrics reported in Table 2. We stress at this point that the results do not have skill at the Avon and Ock catchments. The Avon is the main outlier in this study due to an unsaturated chalk zone which has known fast flow in the sub-surface and might require a different soil hydrology modelling altogether (Rahman and Rosolem, 2017; Blyth et al., 2018). The Ock is the smallest catchment of the selection (234 km<sup>2</sup>), located upstream within the Thames basin (mean observed river flow of 0.6 m<sup>3</sup> s<sup>-1</sup>), and its results indicate that for upstream small catchments the slope dependency alone does not necessarily solve the parameterization problem (the Ock does not possess as low a mean slope as the 0 Thames as a whole, see Fig. 6). However, for the whole Thames catchment our new parameterization achieves the best result of all

10 Thames as a whole, see Fig. 6). However, for the whole Thames catchment our new parameterization achieves the best result of all selected catchments (NS = 0.82).

# 3.5 Performance comparisons using a Great Britain hydrological model as Benchmark

We show the performance metrics for daily river flow simulations using grid cell slope dependency for the parameter  $S_0/S_{max}$  over the 13 catchments studied (Fig. 8) and illustrate the daily river flow time series for the 3 larger catchments over 2 years (Fig. 9). We

- 15 define in Fig. 8 three performance categories following Crooks et al. (2014): category 1 (*NS* above 0.8, mean *bias* below ±10 %), category 2 (*NS* between 0.6 and 0.8, mean *bias* between 10 % and 20 % in absolute value) and category 3 (*NS* below 0.6, mean *bias* above ±20 %). River flow outputs from the CLASSIC-GB model are used as a benchmarking dataset (green markers), drawn from Crooks et al. (2014). CLASSIC-GB is a grid-based rainfall-runoff model developed for the domain of Great Britain that uses the same 1 km<sup>2</sup> resolution CEH-GEAR precipitation input used here and higher resolution parameters derived from the Hydrology of
- 20 Soil Types (Boorman et al., 1995). It has shown very high performance for catchments in Great Britain (Crooks et al., 2014).

We have additionally carried out simulations where both hydrology schemes PDM and TOPMODEL are switched off (*no hyd* runs, red markers in Fig. 8), where surface runoff can only be generated by infiltration excess (Hortonian runoff). The metrics for this *no hyd* simulations are very low (mostly under category 3) due to a low surface runoff generation and little accuracy in the timing of the baseflow discharge (sub-surface runoff through the simple free drainage approach comes in late; Fig. 9). The infiltration excess

25 surface runoff is rarely invoked in JULES as the rate of water reaching the surface at each time step does not reach the maximum infiltration rate, which is defined as the saturation conductivity at the upper soil layer enhanced by a land cover factor (Best et al., 2011; Clark et al., 2011). This issue has been reported before for the JULES model (Clark and Gedney, 2008) and other LSMs (Balsamo et al., 2009; Boone et al., 2004).

The TOPMODEL tests results using the parameters that best fitted the observations out of all tests detailed in Section 2.2.2 ( $\alpha = 1$ , 30 f = 5.0) are also represented in Fig. 8 (orange markers). Although the *bias* shows very little improvement from the *no hyd* runs due to a low estimation of surface runoff, the *NS* metric shows an improvement in all catchments, as the surface runoff production by saturation excess is active and the rainfall peaks do produce river flow peaks. The baseflow production during dry periods is not as delayed as it is in the *no hyd* runs (Fig. 9). However, only the Thames and the Avon reach category 2 in terms of *NS* performance when using TOPMODEL.

- 5 The markers in different shades of blue in Fig. 8 represent JULES simulations using the PDM scheme. As a representation of the state-of-the-art parameterization for UK hydrology using JULES at the Met Office, we include in this comparison the PDM tests using a grid cell slope dependent *b* parameter as defined in Section 2.2.2 (slate blue markers) and the tests using b = 0.4 and  $S_0/S_{max} = 0.0$  (dark blue), which are the PDM parameters from the Met Office operational weather forecast UK science configuration (UKV; e.g. Tang et al., 2013). These two sets of tests reach a very similar performance skill for all catchments,
- 10 improving the mean *bias* of the TOPMODEL tests as higher surface runoff is generated during rainfall events, and also consistently improving the *NS* metric and reaching the category 2 performance for most catchments. However, over the baseflow-dominated catchments Thames, Derwent and Avon, these PDM parameterizations are still in category 3 in terms of *NS* performance and outperformed by the TOPMODEL tests. This is mostly due to exceedingly "flashy" daily time series of river flow during rainfall events and consequently low baseflow due to drainage through the bottom of the soil column during drier periods, as the soil did
- 15 not get wet enough during the previous wet episodes. The inclusion of the mean catchment terrain slope dependency on the  $S_0/S_{max}$ parameter using the *mcs* criterion (light blue markers) clearly improves the performance from the rest of the tests (except in the Avon catchment), showing how we now include an appropriate characterization not only for flashy catchments on steeper terrain (Dee, Ribble, Severn1-2, Tay; see Fig. 9), but also for flatter catchments where PDM is typically outperformed by TOPMODEL (Thames, Derwent). This improvement on flatter catchments is due to a constraint in the surface runoff production during rainfall
- spells introduced by the  $S_0/S_{max}$  parameter; improving the timing of the baseflow production during dry periods since the soil keeps memory from wet periods when not every rainfall event could produce surface runoff. Finally, the simulations using a linear dependency on grid cell slope for the  $S_0/S_{max}$  parameter as detailed in Section 3.4 (blue markers) lose some of the skill in the *mcs* tests, but improve overall the rest of tests, reaching the category 1 *NS* performance for the Thames catchment (Fig. 9) and category 2 for most of the rest.

#### 25 **3.6 Performance at non-daily time scales**

Simulated river flows using LSMs will result from physical processes represented in the model and the imposed meteorological driving data. Both these factors affect the simulations at a range of different time scales. We have used cross spectral analysis to investigate the implications of the final parameterization using grid slope dependency for  $S_0/S_{max}$  beyond the evaluations using the mean *bias* error and Nash-Sutcliffe efficiency assessed at the daily time scale. In particular, this allows assessment of the average

30 amplitude of discharge at different time scales and separately the average phase difference (lead or lag) of the modelled compared to the observed discharge (Weedon et al., 2015). The time scales investigated cross spectrally range from 2 days to the length of the time series or 10 years. Ideal model performance at a particular frequency leads to an amplitude ratio of exactly 1.0 or a result with 95% confidence intervals (CIs) that overlap 1.0. For clarity in Figs. 10 and 11 we illustrate amplitude ratios, rather than decibels used in engineering. In terms of phase difference an ideal result at a particular frequency would be variations "in phase" (phase difference of exactly  $0.0^{\circ}$  or value with 95% CIs overlapping  $0^{\circ}$ ). Here positive phase differences mean that the model variations lag the observations and negative values indicate the model leading the observations.

- 5 Cross-spectral analysis of the JULES performance at different time scales has been carried out for the final parameterization using grid slope dependency for  $S_0/S_{max}$  for 3 catchments representative of different topographical characteristics (Dee, Severn2 and Thames). Note that JULES discharge performance against observations was assessed with cross spectral analysis by Weedon et al. (2015) but the model was run at daily time steps which caused numerical artefacts in discharge variability (excessive high-frequency attenuation). Here RFM routing was applied sub-daily thereby avoiding the artefacts. The time scales at which amplitude ratios and
- 10 phase differences have been assessed are: annual, slow response scale (SR) and quick response scale (QR). The upper limits of the SR and QR time scales are determined for each catchment as the time that river flow takes to flow from the upper most point of the catchment to the outlet, using the wave speeds that RFM uses in JULES for sub-surface and surface flow, respectively. The lower limits of the time scales are defined as one third of the upper limits. The SR and QR time scales for the 3 catchments analysed are shown in Table 3. Results of the cross-spectral analysis of the daily river flow (power spectra, amplitude ratio spectrum and phase
- 15 difference or phase spectrum) are shown in Fig. 10. If a time series is compared to itself, but offset by a few time steps, there is a resulting trend in the high frequency part of the phase difference spectrum (equation A10 in Weedon et al., 2015). The modelled phase difference trends that approximate the results are shown using black dashed lines in Fig. 10. Note that phase differences distinguishable from zero degrees can result from both simple offsets in the timing of model output compared to observations (causing phase difference trends) and from incorrect modelling of the response times of hydrological stores (Weedon et al., 2015).
- A further comparison between amplitude and phase differences with observations using different parameterizations and at different time scales helps to clarify the implications of our final parameterization and model development (Fig. 11). The annual scale spectral peak is very marked in the wet northern Dee catchment, and all flavours of JULES represented catch it accurately (amplitude ratios are close to 1.0 allowing for the 95% CIs). However, in the Severn2 and Thames catchments we start to see compromised performance at the annual scale, the best TOPMODEL tests outperform the rest for both catchments, even though the final parameterization (slope dependent  $S_0/S_{max}$ ) presents good results in terms of amplitude ratio (0.60 ± 0.04 and 0.76 ± 0.07,

At the SR scale the results agree with the findings using *NS* metric for the three catchments; the new parameterization results are close to  $0^{\circ}$  for phase difference allowing for their 95 % CIs, and close to 1.0 for amplitude ratio with the exception of the Thames catchment, where the amplitude ratio of 1.57 (95% CI: 1.23 to 2.01) is only outperformed by the parameterization using the *mcs* 

respectively) and phase difference  $(10.7^{\circ} \pm 5.75^{\circ} \text{ and } -4.4^{\circ} \pm 7.7^{\circ})$ .

30 criterion. At the QR scale we expected results to resemble the *NS* metric analysis, and we find that over the three catchments the new parameterization results are the best or as good as the *mcs* criterion results as seen in Sections 3.4 and 3.5, with the exception of lead in discharge for the Thames catchment that is apparently higher than that of the rest of the PDM tests.

The cross spectral results illustrated in Figs. 10 and 11 demonstrate that despite the marked improvement in model performance when utilizing the new parameterization judged using *NS* and *bias*, there remains scope for further improvements at multi-day to annual time scales.

#### 4. Discussion

- 5 To our knowledge, this is the first study that analyses river flow model outputs from a LSM over a wide enough area (the 13 selected catchments) driven by the CHESS-met dataset (Robinson et al., 2017a; Robinson et al., 2017b). The availability of this dataset opens new possibilities to study land surface hydrology and interactions with the atmosphere using LSMs (that typically require gridded forcing datasets) at the km-scale driven by gridded rainfall derived from gauge stations. A recent study (Blyth et al., 2018) investigates evapotranspiration trends and components in Great Britain over the last 55 years using CHESS-met and the JULES
- 10 runoff development described in this paper. These authors find that, when compared to flux tower data, the model overestimates evapotranspiration rates. Excesses of evaporation by JULES have also been reported at the global scale (Schellekens et al., 2017) and using eddy covariance flux measurements in temperate Europe (Van den Hoof et al., 2013). The sources of this evaporation bias are beyond the scope of this work and other studies in the model community are investigating the issue (e.g. Blyth et al., 2018). However, the new runoff development reduces the negative runoff bias as shown here, mostly from increased surface runoff during
- 15 the rainy season over mountainous regions. Hence, the evapotranspiration rates in the Blyth et al. (2018) study have been impacted in the right direction. Whether this reduction of evapotranspiration in Great Britain by lower soil moisture availability is consistent with soil moisture observations remains a challenge. We anticipate that this could be approached using a UK network of appropriate data for area-integrated soil moisture currently being developed (COSMOS-UK: <u>https://cosmos.ceh.ac.uk</u>).

We acknowledge that topographic variability at the grid scale is not new to JULES or other LSMs, as it is considered by the

- 20 TOPMODEL scheme. However, we have found that for Great Britain regional integrations the surface runoff production by PDM allows for a better characterization of the topographical variability through the  $S_0$  parameter. This finding within the JULES model and the Great Britain region framework can have significant impacts over other regions and applied to other models that need to account for subgrid variability in the runoff generation process, using a widely available parameter (from digital elevation model datasets) like the grid cell mean slope as the only input, whereas other physical characteristics might be more difficult to obtain or
- are simply unavailable.

The poor performance at the Avon catchment by the PDM scheme has not been solved by our new parameterization, pointing to geological rather than topographical characteristics driving the sub-surface water flow (Rahman and Rosolem, 2017). We argue that a combination of PDM scheme for surface runoff generation and TOPMODEL, or other scheme that incorporates the representation of groundwater dynamics and persistence at the sub-surface (e.g. Fan et al., 2007; Miguez-Macho et al., 2007), should be the way

30 forward for JULES development.

We stress that the issue of the infiltration excess surface runoff rarely being invoked in JULES needs to be further investigated (e.g. Mueller et al., 2016; Largeron et al., 2018). This occurs because the maximum infiltration rate, theoretically invoked by sudden and intense rainfall events, is difficult to reach in LSMs currently driven by precipitation datasets that lack the temporal and spatial resolution to correctly represent intense rainfall events (Balsamo et al., 2009; Boone et al., 2004; Clark and Gedney, 2008). The

5 saturation excess surface runoff is overwhelmingly dominant in this study and might be compensating infiltration excess underestimations.

The performance skill loss when using grid slope dependency instead of mean catchment slope dependency is a compromise that we accept since our development and recommended configuration needs to be applicable for the whole of Great Britain and even for other regions and space scales where particular catchment information might not be available.

- 10 The JULES model does not incorporate anthropogenic effects on river flow in its current state. We acknowledge that human activities (groundwater abstractions, dams, reservoirs) affect the observed river flow in Great Britain and therefore JULES outputs of natural river flow are not expected to reproduce exactly the observed NRFA records. As mentioned in Section 2.2.2, we included the naturalised flow records for the Thames catchment as it is the only catchment with natural flow availability for the studied period. However, the human activities effects on the river flow are difficult to quantify given the lack of data and heterogeneity of
- 15 activities in the studied catchments. A recent study over Great Britain, for instance, showed increase of drought duration in catchments affected by groundwater abstractions and varying effects on drought occurrence depending on the activities (Tijdeman et al., 2018).

The model development described here at the km-scale and over the Great Britain domain is based on the inclusion of a terrain slope dependency in the soil wetness parameter that switches on the saturation excess runoff scheme. Even though the parameter values

20 need to be re-examined for other regions/resolutions, this physical dependency should also be valid at the global scale and its implications in the performance of the JULES model global simulations at 0.25 and 0.5 degrees of spatial resolution are being evaluated in the eartH2Observe project described in Schellekens et al. (2017).

## 5. Conclusions

- Motivated by the search of the best representation of hydrological processes over the land in the context of a coupled UK land-25 ocean-atmosphere model (UKC2; Lewis et al., 2018), we find that the JULES LSM has the potential to simulate daily river flow accurately over selected catchments in Great Britain when driven by the 1 km<sup>2</sup> resolution CHESS-met database, obtaining results comparable to those of a Great Britain rainfall-runoff model (CLASSIC-GB, Crooks et al., 2014). Previous studies using JULES (e.g. Best et al., 2015; Schellekens et al., 2017; Ukkola et al., 2016) use a fixed  $S_0$  parameter within the PDM scheme. In this study we vary the values of  $S_0$  and are able to improve performance (% *bias* and *NS*) as a result. The parameter  $S_0$  controls the soil water
- 30 content necessary to start producing surface runoff.

The parameterization that produces the best results for each catchment uses the mean catchment slope. When applied on a gridded model, a new linear function of slope at the model resolution scale can produce performance metrics comparable to those using the mean catchment slope. The new parameterization constrains surface runoff production to wet soil conditions over flatter regions, whereas over steeper regions the model produces surface runoff for every rainfall event, regardless of the soil wetness conditions.

- 5 Hence, a simple terrain slope dependency has improved greatly the JULES river flow results for different catchments in Great Britain. We stress that this finding should be tested for other regions/scales on JULES and other LSMs, as topography datasets are available at very fine resolution (e.g. <u>https://www.hydrosheds.org/</u>). The capability of an LSM to reproduce the water balance at regional scales with performance (in terms of river flow generation) comparable to hydrological models can potentially impact weather forecast and climate predictions using regional coupled modelling systems such as UKC2.
- 10 We have also shown that cross spectral analysis for evaluating model performance against observations quantifies the mismatches in variability, and separately mismatches in phase, at different time scales that are not otherwise apparent from metrics such as *NS* and RMSE. Potentially the recognition of a specific time scale where a model is performing poorly could help identification of the incorrect behaviour in terms of water transport and/or sub-surface storage. The cross-spectral analysis comparing the modelled river flow with observations has reinforced the choice of the new parameterization for surface runoff production.

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*Model development.* The work presented here has led to a JULES code development that introduces the capability of using  $S_0/S_{max}$  as a model parameter, either as a fixed value or as a grid cell slope dependent value, as well as the capability to read in the model grid topographic slope as an ancillary dataset. The new version of the model with the new parameterization recommended here has been used to study Great Britain evaporation and water budgets during the last 55 years by Blyth et al. (2018), producing outputs publicly available as the CEH CHESS-land dataset (Martínez-de la Torre et al., 2018), and also incorporated in the UKC2 system (Lewis et al., 2018). The new code development is described in ticket #262 of the JULES FCM repository

*Code availability*. This study uses JULES revision 1709, which is between the 4.3 and 4.4 releases. The code can be downloaded from the JULES FCM repository at <u>https://code.metoffice.gov.uk/trac/jules/</u> (registration required).

(https://code.metoffice.gov.uk/trac/jules/), and has become part of the JULES trunk since version 4.9 release.

*Data availability.* JULES LSM output data for this work are available from the corresponding author upon request. The river flow observations at gauging stations used here were facilitated by NRFA and are publicly available (<u>http://nrfa.ceh.ac.uk/</u>). The CHESS-met driving data and the rest of ancillary datasets used here are publicly available through references given in Section 2.2.1.

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River	Station	Catchment area (km <sup>2</sup> )	CEH-GEAR rainfall (mm y <sup>-1</sup> )	BFI
Dee	12002 (Park)	1844	1150	0.53
Tay	15006 (Ballathie)	4587	1575	0.64
Ouse	27009 (Skelton)	3315	939	0.39
Ure	27034 (Kilgram)	510	1411	0.32
Derwent	27041 (Buttercrambe)	1586	771	0.69
Thames	39001 (Kingston)	9948	750	0.63
Ock	39081 (Abingdon)	234	663	0.64
Avon	43021 (Knapp Mill)	1706	889	0.86
Tamar	47001 (Gunnislake)	917	1318	0.46
Severn1	54001 (Bewdley)	4325	984	0.53
Severn2	54057 (Haw Bridge)	9895	850	0.56
Ribble	71001 (Samlesbury)	1145	1347	0.33
Clyde	84013 (Daldowie)	1903	1257	0.46

Table 1. Information about the Great Britain selected catchments in Fig. 1. The outlet stations are identified by their National River Flow Archive (NRFA) station number and their name. The annual rainfall from CEH-GEAR database refer to the studied period (1991-2000). The baseflow index (BFI) data were reported by Boorman et al. (1995).

Catchment	NRFA observed mean river flow (m <sup>3</sup> s <sup>-1</sup> )	Mean bias (%)	NS
Dee	39.5	-20	0.51
Tay	158.2	-15	0.64
Ouse	41.4	-18	0.69
Ure	13.6	-19	0.75
Derwent	11.5	-27	0.49
Thames	71.2	-11	0.82
Ock	0.6	-63	-0.21
Avon	17.0	-20	-0.07
Tamar	19.2	-18	0.63
Severn1	58.0	-7	0.61
Severn2	97.0	-14	0.72
Ribble	27.2	-18	0.74
Clyde	41.7	-24	0.82

Table 2. Mean observed river flow at the 13 selected catchments in Great Britain and performance metrics for the JULES using the PDM parameters detailed in Section 3.4 (fixed b = 2.0 and grid cell slope dependent  $S_0/S_{max}$ ).

Catchment	SR	QR
Dee	9-27 days	2-3 days
Thames	17-51 days	2-5 days
Severn2	18-54 days	2-5 days

Table 3. SR (slow response) and QR (quick response) timescales for the cross-spectral analysis conducted at 3 catchment in Section 3.6.

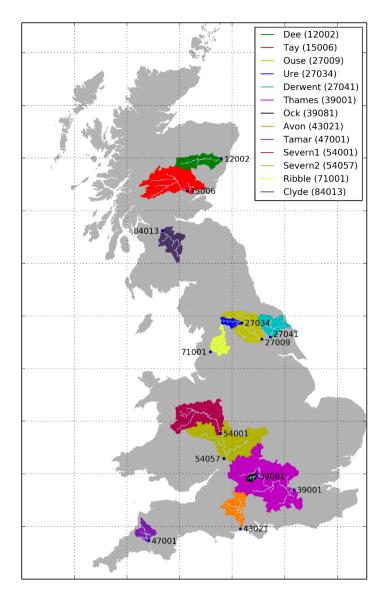


Figure 1. 13 Great Britain selected catchments and their main flow pathways. The outlet stations are represented by a dark blue dot and identified by their National River Flow Archive (NRFA) station number. Note that the catchments Ure, Severn1 and Ock are subcatchments within the larger catchments Ouse, Severn2 and Thames, respectively.

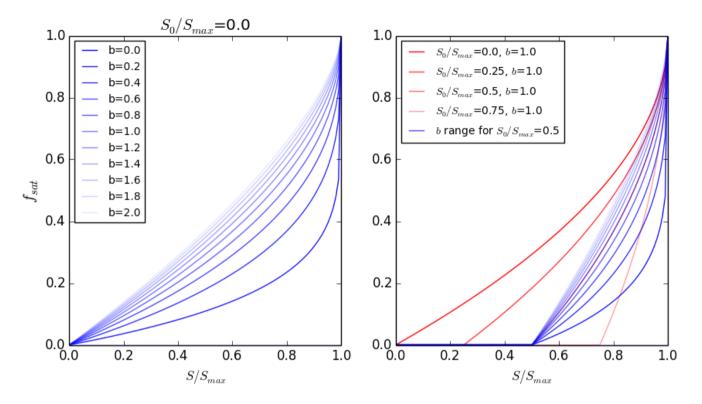


Figure 2. Left: variability of the soil moisture saturation fraction introduced by the *b* parameter in the PDM scheme, for  $S_0/S_{max} = 0.0$ . Right: variability of the soil moisture saturation fraction introduced by the  $S_0/S_{max}$  parameter in the PDM scheme, for b = 1.0 (red lines), and variability introduced by the *b* parameter for  $S_0/S_{max} = 0.5$  (blue lines).

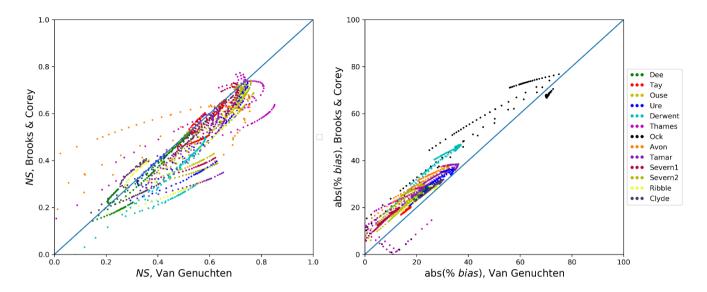


Figure 3. River flow performance metrics (*NS* on the left and absolute value of mean *bias* on the right) for all tests conducted, and for all 13 catchments (colour code in legend). For any given parameter variability test (single dots), metrics obtained using the BC approach for soil hydraulics formulation are indicated on the y axis and metrics using the VG approach are indicated on the x axis.

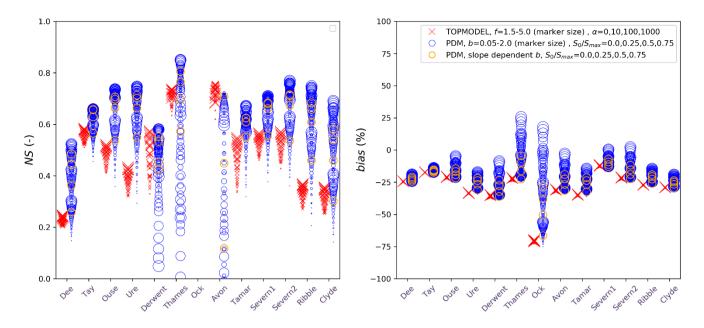


Figure 4. River flow performance metrics for catchment tests detailed in Section 2.2.2 (red crosses for TOPMODEL tests, blue circles for PDM tests with fixed parameters and orange circles for PDM tests with slope dependent b). Left: *NS* efficiency. Right: mean *bias*. The x axis represents the 13 selected catchments (Fig. 1). The marker size represent the parameter correspondent to a given tests (and larger crosses for larger f values

5 in the TOPMODEL tests and larger circles for larger b values in the PDM tests). No distinction is showed here indicating the  $S_0/S_{max}$  or  $\alpha$  parameters. Only results from those tests using the VG approach for soil formulation are showed. Tests at the Ock catchment are not visible since they obtained negative NS.

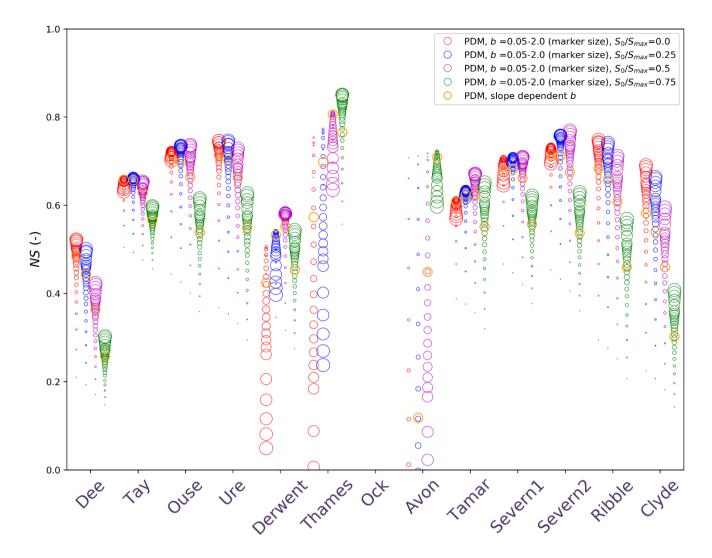


Figure 5. River flow NS efficiency performance metric for the PDM catchment tests detailed in Section 2.2.2. The x axis represents the 13 selected catchments (Fig. 1). The marker colour represent the  $S_0/S_{max}$  value (red, blue, purple and green for values of 0.0, 0.25, 0.50 and 0.75, respectively) and the marker size represent the *b* parameter (larger circles for larger *b* values). The slope dependent *b* tests are represented by orange markers. Only results from those tests using the VG approach for soil formulation are showed. Tests at the Ock catchment are not visible since they obtained

5 Only results from those tests using the VG approach for soil formulation are showed. Tests at the Ock catchment are not visible since they obtained negative *NS*.

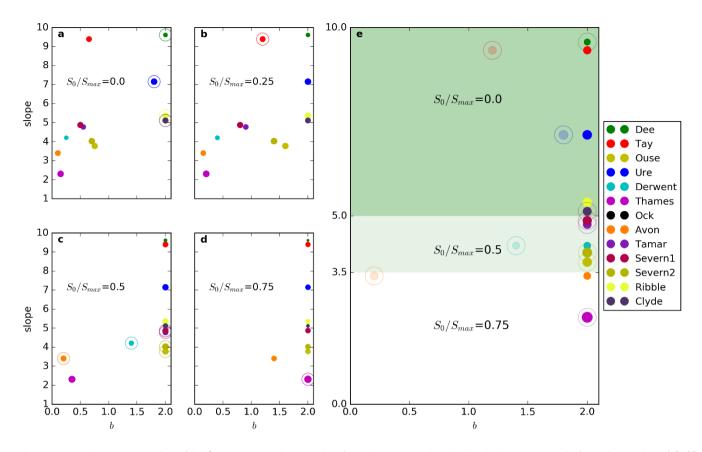


Figure 6. (a to d): Representation of the *b* parameter value (x axis) of catchment tests that obtained a better *NS* metric for a given value of  $S_0/S_{max}$  (stated inside each plot), against the mean catchment slope on the y axis. The marker size represent the *NS* values (larger circles for higher *NS* values). Tests highlighted with an outer circle indicate the best performance of all tests for a given catchment (so the panel where they are indicates  $S_0/S_{max}$  and the x value indicates *b*). Tests where the mean *bias* is higher than 30% are not considered due to poor performance. (e): Best PDM parameter tests selected for each catchment following the criterion *mcs* of fixed b = 2 and slope dependent value of  $S_0/S_{max}$  as follows: 0.0 for mean catchment slopes higher than 5.0° (green background), 0.5 for mean catchment slopes between 3.5° and 5.0° (light green background), and 0.75 for mean catchment slopes lower than 3.5° (white background). For those catchment where *mcs* does not select the test of best *NS* metric (Tay, Ure, Derwent, Avon), the best performance tests are also represented with a degree of transparency.

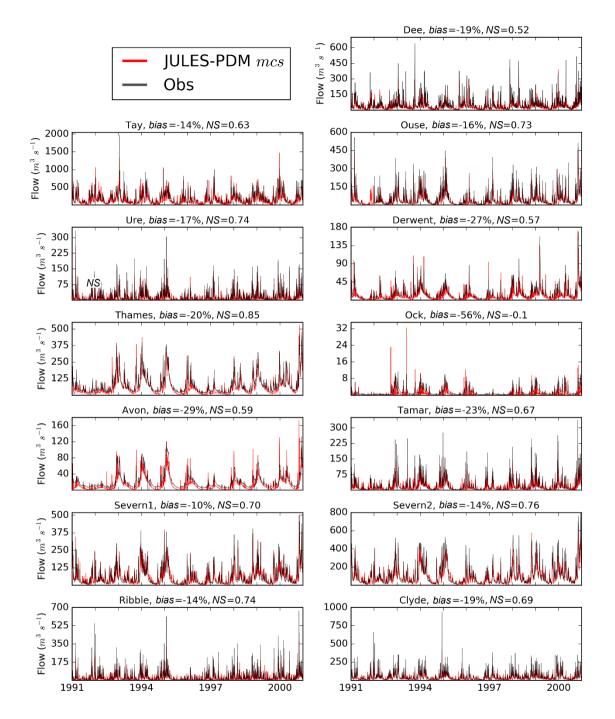


Figure 7. Daily river flow (1991-2000) for the 13 catchments studied (Fig. 1). Observations at the NRFA gauge station (Table 1) in black and simulations at the outlet grid by JULES using the criterion *mcs* in red. On top of each plot the name of the catchment and the performance metrics (mean *bias* and the NS) are given.

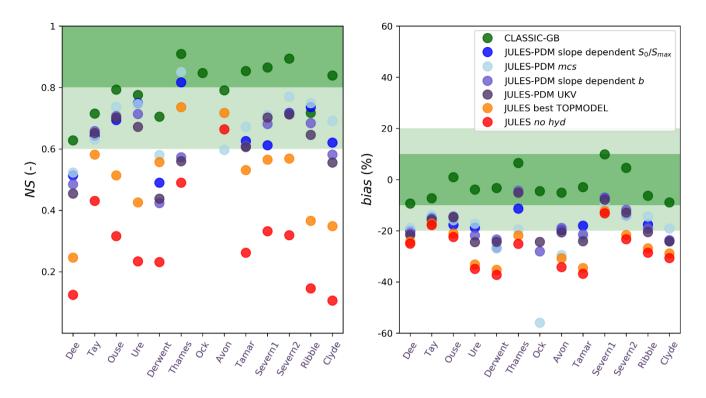


Figure 8. River flow performance metrics for catchment tests: green) CLASSIC-GB model (Crooks et al., 2014); blue) JULES using the PDM parameters detailed in Section 3.4 (fixed b = 2.0 and grid cell slope dependent  $S_0/S_{max}$ ); light blue) JULES using PDM parameters following *mcs* criterion in Section 3.3 (fixed b = 2.0 and mean catchment slope dependent  $S_0/S_{max}$ ); slate blue) JULES using PDM parameters of grid cell slope dependent *b* (Section 2.2.2) and fixed  $S_0/S_{max} = 0.0$ ; dark blue) JULES using PDM parameters defined in the UKV configuration (b = 0.4,  $S_0/S_{max} = 0.0$ ); orange) JULES using TOPMODEL scheme with the parameters that best performance results obtained ( $\alpha = 1$ , f = 5.0); red) JULES using no saturation excess scheme to produce runoff (*no hyd*). Left: *NS* efficiency. Right: mean *bias*. Background plot colours indicate the performance category: green) category 1; light green) category 2; white) category 3.

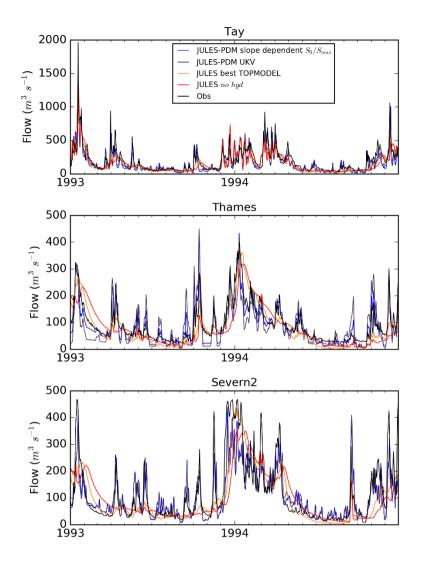


Figure 9. Daily river flow (1993-1994) for the 3 larger catchments studied: Tay, Thames and Severn2 (Fig. 1). Observations at the NRFA gauge station (Table 1) in black. Simulations at the outlet grid by JULES are showed; using the PDM parameters detailed in Section 3.4 (fixed b = 2.0 and grid cell slope dependent  $S_0/S_{max}$ ) in blue, using PDM parameters defined in the UKV configuration (b = 0.4,  $S_0/S_{max} = 0.0$ ) in dark blue, using TOPMODEL scheme with the parameters that best performance results obtained ( $\alpha = 1$ , f = 5.0) in orange, and using no saturation excess

scheme to produce runoff (no hyd) in red.

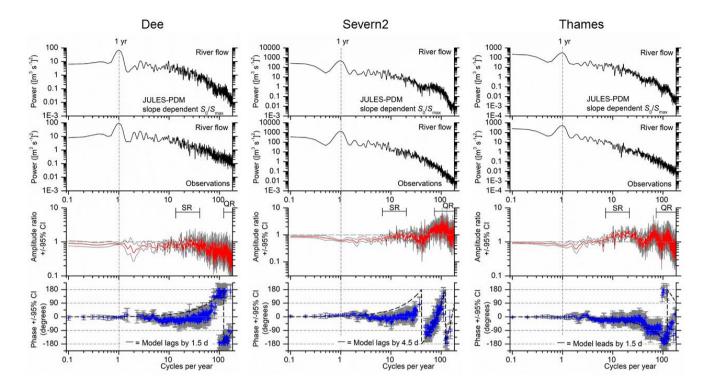


Figure 10. Cross spectral analysis of river flow from JULES-PDM using slope dependent  $S_0/S_{max}$  for three catchments: Dee (left), Severn2 (middle) and Thames (right). In each case the variability and relative timing of daily JULES output river flow is assessed against the daily observed river flow for a range of frequencies (spanning 10 years on the left to 2 days on the right of the spectra). For each catchment the top two panels show the power- or variance-spectra. In the form of spectral analysis applied here the power directly indicates the mean squared amplitude at each frequency (rather than the area under the plot; Weedon et al., 2015). Ideal model performance results in amplitude ratios (third row) indistinguishable from 1.0 and phase differences (bottom row) indistinguishable from 0.0. Theoretical phase difference trends are shown with black dashed lines (bottom row). The amplitude ratio is shown as a red line with the grey lines above and below showing the 95% confidence

10 interval. Phase differences are shown as blue crosses, but only at frequencies where the coherency between series exceeds the 95% confidence level (Weedon et al., 2015). The 95% confidence intervals associated with the phase differences are indicated using vertical grey bars.

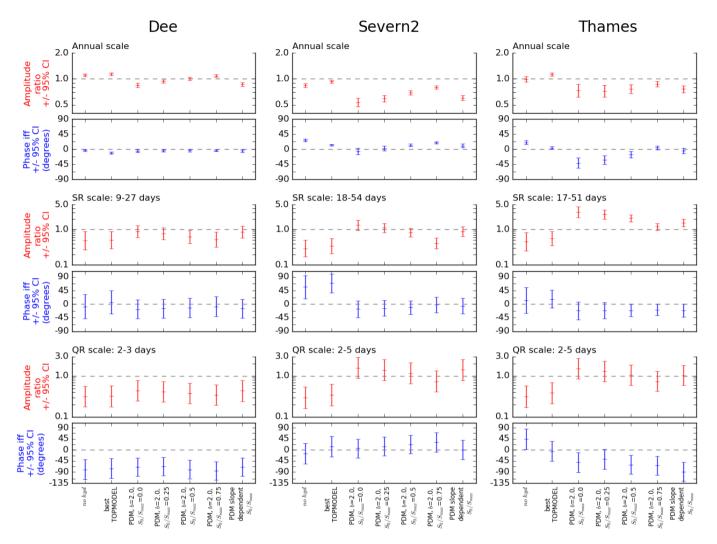


Figure 11. Cross spectral analysis of river flow from JULES using a range of parameterizations from the tests described in Section 2.2.2, for three catchments: Dee (left), Severn2 (middle) and Thames (right). From left to right on x axis of every plot: *no hyd* (as in Figs. 8-9), best TOPMODEL (as in Figs. 8-9), PDM with b = 2.0 and  $S_0/S_{max} = 0.0$ , PDM with b = 2.0 and  $S_0/S_{max} = 0.25$ , PDM with b = 2.0 and  $S_0/S_{max} = 0.5$ , PDM with b = 2.0 and  $S_0/S_{max} = 0.75$ , and PDM with b = 2.0 and grid cell slope dependent  $S_0/S_{max}$  (as in Figs. 8-9). For each catchment, amplitude ratios (red) and phase differences (blue) are shown at the annual scale (top two rows), SR scale (middle two rows) and QR scale (bottom two rows).