**Assessing the performance of a physically-based hydrological model using a proxy-catchment approach in an agricultural environment**

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**Abstract**

Physically-based models are useful frameworks for testing intervention strategies designed to reduce elevated sediment loads in agricultural catchments. Evaluating the success of these strategies depends on model accuracy, generally established by a calibration and evaluation process. In this contribution, the physically-based SHETRAN model was assessed in two similar UK agricultural catchments. The model was calibrated on the Blackwater catchment (18 km2) and evaluated in the adjacent Kit Brook catchment (22 km2) using 4-years of 15-minute discharge and suspended sediment flux data. Model sensitivity to changes in single and multiple combinations of parameters as well as sensitivity to changes in Digital Elevation Model (DEM) resolution were assessed. Model flow performance was reasonably accurate; with a Nash-Sutcliffe efficiency coefficient (NSE) of 0.78 in Blackwater and 0.60 in Kit Brook. In terms of event prediction, the mean of the absolute percentage of difference (μAbsdiff) between measured and simulated flow volume (Qv), peak discharge (Qp), sediment yield (Sy) and peak sediment flux (Sp) showed larger values in Kit Brook (48% [Qv], 66% [Qp], 298% [Sy], 438% [Sp]) compared to the Blackwater catchment (30% [Qv], 41% [Qp], 106% [Sy], 86% [Sp]). Results indicate that SHETRAN can produce reasonable flow prediction but performs less well in estimation of sediment flux, despite reasonably similar hydro-sedimentary behaviour between catchments. The sensitivity index showed flow volume sensitive to saturated hydraulic conductivity and peak discharge to the Strickler coefficient; sediment yield was sensitive to the overland flow erodibility coefficient and peak sediment flux to raindrop/leaf soil erodibility coefficient. The multi-parameter sensitivity analysis showed that different combinations of parameters produced similar model responses. Model sensitivity to grid resolution presented similar flow volumes for different DEM resolutions, whereas event peak and duration (for both flow and sediment flux) were highly sensitive to changes in grid size.

Keywords: catchment modelling, model sensitivity, proxy-catchment, sediment yield, SHETRAN

**1. Introduction**

Surface flow and soil erosion are natural processes affected by changes in agricultural land use and management in catchments. Increases in surface runoff, event peak flows, and suspended sediment loads have been related to altered agricultural practices and management interventions (Deasy, Brazier, Heathwaite, & Hodgkinson, 2009; Deasy, Titman, & Quinton, 2014; Smith et al., 2018). Hydrological models provide useful frameworks for testing, understanding and predicting catchment behaviour under different agricultural change scenarios and in response to mitigation measures designed to reduce surface runoff, erosion and suspended sediment loads.

Physically-based spatially-distributed (PBSD) hydrological models represent processes using fundamental physical equations (Merritt, Letcher, & Jakeman, 2003) usually simulating the hydrological cycle and sediment generation processes (Daniel et al., 2011). These type of models are generally classified according to their spatial scale, temporal distribution, variables and process descriptions (Aksoy & Kavvas, 2005). PBSD models have the advantage, over empirical or conceptual models, in their ability to better represent the effect of changes in catchment conditions as their parameters relate to physical properties (Bathurst, 2011). However, a frequent problem with PBSD models is the large number of parameters required; some of which may be unavailable or inaccessible, particularly in data scarce regions (Tarawneh, Bridge, & Macdonald, 2016). This data uncertainty can be reduced by a model calibration approach, followed by an evaluation procedure, providing increased confidence in model outputs for further application.

Klemeš, (1986) described several approaches for model calibration and evaluation. For example, the split-sample test uses measured data, divided into two periods of similar length, one for calibration and the other for evaluation; or the proxy-catchment test which comprises model calibration in one catchment and evaluation in a nearby catchment. The proxy-catchment approach is recommended as a framework for testing model performance (Pechlivanidis, Jackson, McIntyre, & Wheater, 2011; Xu & Singh, 2004) but is less commonly applied as it requires more resources than the split-sample test. Comparatively few studies use the proxy-catchment approach for model evaluation (Arsenault, Brissette, & Martel, 2018; Gumindoga, Rwasoka, Nhapi, & Dube, 2017; Yang, Herath, & Musiake, 2002) with limited applications using PBSD models (Refsgaard, Storm, & Refsgaard, 1995). Moreover, studies that adopt this model testing approach in combination with high-resolution measurements of discharge and sediment flux were not found in the available literature.

Another common criticism of PBSD model is grid size applications (Beven, 1991; Brazier et al., 2011), as parameter values applied to a catchment grid are usually an average of a physical property (measured or calibrated). This generalization fails to capture natural variability in a given property and may affect hydrological process representation (Thomas et al., 2016). Thompson, Bell, and Butler, (2001) found that decreasing the DEM resolution tends to produce a smoother topography, as larger grids average the elevation of the covered area, losing important landscape detail. The loss of the topographic features can also lead to changes in overland flow pathways affecting sediment transport and deposition processes (Thomas et al., 2017). Moreover, the change in spatial resolution may affect model representation of tributaries (Daniel et al., 2011). Errors can be minimized by using the finest possible grid resolution. However, this requires more computing capacity and increases model run times (e.g. De Figueiredo & Bathurst, 2007). Despite the scale resolution problem being addressed in several studies (Lesschen, Schoorl, & Cammeraat, 2009; Valeo & Moin, 2000; Zhang & Montgomery, 1994), there is a lack of information on the effects of changes in DEM resolution on flow and sediment fluxes at an event scale with comparison against measured data. Furthermore, understanding PBSD model sensitivity to DEM resolution may be important for assessing predictions of the effectiveness of management interventions to reduce agricultural impacts, particularly when accurate representation of an intervention (e.g. minimum width of field buffer strips) is dependent on grid size. The selection of one PBSD model over another often depends on the available information and accessibility. The SHETRAN model was selected in the present study for its capability to simulate flow and sediment flux on an event- and continuous-basis, at any given resolution (with a maximum limit of 300 x 300 grids [windows version v4.4.5x64]). Moreover, event-based sediment prediction on a continuous-basis can reduce errors related to initial conditions (Bussi et al., 2014). The SHETRAN model has been designed to simulate a wide range of land uses (e. g. agricultural, forest or urban) and has been used globally, with a limited number of applications in the UK (Bathurst, Ewen, Parkin, O’Connell, & Cooper, 2004; Birkinshaw, 2008; Janes, Holman, Birkinshaw, O’Donnell, & Kilsby, 2017).

This study represents the first application of SHETRAN using a proxy-catchment approach with a semi-coarse spatial resolution (50 x 50 m) at a high temporal resolution (15-minutes). Continuous flow and suspended sediment data from two nearby agricultural catchments in the UK were used for model calibration and evaluation, with the assessment of model efficiency focusing on flow volume, peak discharge, sediment yield, peak sediment flux, and event duration (flow and sediment) for a range of DEM grid sizes.

**2. Materials and methods**

2.1 The SHETRAN model

SHETRAN uses deterministic equations and finite-difference solutions to simulate water flow, sediment transport and contaminant transport processes (Ewen, Parkin, & O’Connel, 2000). It has a distributed response at a catchment scale limited by 300 x 300 grids, each one containing soil and vegetation information. Soil profiles represented by columns of stacked grids (up to 6 layers) allow lateral and vertical flow transport for a three-dimensional subsurface flow simulation. The river network is modelled as channel links along the edges of grids (Birkinshaw, 2010).

Water flow comprises the sub-processes of: evapotranspiration/interception, overland/channel, and variably saturated subsurface. The first uses climatological data of rainfall and potential evapotranspiration (PE). The PE can be introduced by the user, or calculated by the model using the Penman-Monteith equation (Monteith, 1965; Penman, 1948). The interception process which calculates the amount of rainfall stored by the canopy is based on the canopy surface storage capacity (Rutter, Morton, & Robins, 1975). Evaporation from soil occurs at a rate determined by the proportion of bare ground. This soil moisture control is assessed by the state of the unsaturated flow limits, the losses on the soil are calculated by a simple linear relation between the soil moisture tension (ᴪ) and the actual and potential evapotranspiration ratio (AE/PE), specified in the model as a table of AE/PE values against ᴪ. SHETRAN simulates soil erosion by raindrop/leaf drip impact and overland flow, overland and channel transport of eroded sediment, and deposition (Lukey et al., 1995a).

In SHETRAN, the reported parameters to which the model is most sensitive on the water flow component are: potential-actual evapotranspiration ratio (AE/PE), saturated hydraulic conductivity (Ksat), and overland Strickler coefficient (Stk) (Anderton, Latron, & Gallart, 2002; Bathurst, 1986; Op de Hipt et al., 2017). The actual-potential evapotranspiration ratio (AE/PE) influences water balance; the saturated hydraulic conductivity (Ksat) affects the surface-subsurface infiltration and storage; and the overland Strickler coefficient (Stk) has an effect on the surface flow velocity (Ewen et al., 2000). It is suggested by SHETRAN developers that AE/PE and soil depth are calibrated in the first instance; afterwards, if necessary, Ksat and Stk (Birkinshaw, n.d.). In the sediment transport component, the reported parameters to which model is most sensitive are raindrop soil erodibility coefficient (Kr) and overland flow erodibility coefficient (Kf) (Adams & Elliott, 2006; Op de Hipt et al., 2017) with the parameters’ values associated to catchment soil conditions and vegetation characteristics. For example, Verhaegen, (1987) established a relationship between Kr and soil texture. However, relationships between soil texture and Kfare not commonly reported, hence calibration of this coefficient is often used.

Performance of the SHETRAN water flow component has been reported in a number of studies using the Nash-Sutcliffe efficiency coefficient (NSE). The term ranges from one, for a perfect match, to negative infinity. The reported NSE values for SHETRAN are between 0.6 to 0.8 (Adams, Western, & Seed, 2012; Janes et al., 2017; Mourato, Moreira, & Corte-Real, 2015). Inaccurate peak discharge prediction has been addressed in previous SHETRAN applications where better estimation of base flow and poorer prediction of discharge peaks has been reported (Zhang, Santos, Moreira, Freire, & Corte-Real, 2013). Under-estimation of event peak discharge was also found by comparing simulated flow with data from eight gauging stations within a 2,400 km2 catchment in the UK (Janes et al., 2017). Conversely, successful double-peak discharge predictions were obtained in a UK catchment (Birkinshaw, 2008). However, in this study, estimation of phreatic level against two measured sites was not accurate. This phreatic surface level is related to base flow. To assess model uncertainty, the ‘blind validation’ method (Ewen & Parkin, 1996) was developed, which consists of establishing parameter bounds for the prediction of certain hydrological variables (e.g. hydrographs, phreatic surface level, peak discharge, soil water potential, runoff) and calculating the degree (perceptual value established by the user) to which a measured variable lies within the predicted range. Using this method, a successful prediction of phreatic level (90%) but poorer prediction of peak discharge (81% [outlet] and 55% [channel]) was obtained for a UK catchment (Bathurst et al., 2004).

The sediment transport component efficiency has also been assessed. However, as continuous measurements of sediment flux are more difficult to obtain, evaluation has largely focused on individual events with different coefficients. For example, in a small catchment in New Zealand, the difference between observed and predicted sediment loads (kg) for seven events varied between -3.3 (-97%) and 55 (134%) depending on the event (Adams & Elliott, 2006). Similarly, a single event in four nearby catchments in New Zealand (Elliott, Oehler, Schmidt, & Ekanayake, 2012) showed sediment yield error of 1, 3, 13 and 110% and NSE values of 0.61, 0.70, 0.86 and 0.65, respectively for each catchment. Additionally, the coefficient of determination (R2) between simulated and measured daily sediment yield on two subcatchments of the Brazilian Sumé catchment showed values of 0.35 and 0.28 (De Figueiredo & Bathurst, 2007). Furthermore, using the ‘blind validation’, errors associated with 5-year sediment yields were reported with values ranging from 1% to 198% in a catchment in France (Lukey, Sheffield, Bathurst, Hiley, & Mathys, 2000).

The parameters to which SHETRAN is most sensitive varied according to catchment characteristics (location, topography, vegetation, etc.). Nonetheless, SHETRAN studies showed similar Stk values for land cover with the highest values for urban areas, followed by cropland, grassland and woodland as the lowest (Bathurst, Moretti, El-Hames, Beguería, & García-Ruiz, 2007; Bathurst, Moretti, El-Hames, Moaven-Hashemi, & Burton, 2005; Birkinshaw, 2008; Elliott et al., 2012; Wicks & Bathurst, 1996). Moreover, on-site studies also indicated a similar Stk trend for land covers (Engman & ASCE, 1986; Kværnø & Stolte, 2012; Rahimy, 2011; Schob, Schmidt, & Tenholtern, 2006). In SHETRAN, hillslope surface runoff is simulated as a sheet flow (fine, extensive and surficial) rather than confined flow (e.g. rills or gullies). The flow depth and velocity is an average value in each grid; therefore a coarse spatial resolution will generate a wider sheet flow (equal to the size of the grid). The dependence of overland flow erosion by surface flow, makes the Kf coefficient an important parameter to be considered in the calibration process, with the empirical value representing a combined sheet and rill flow effect (Wicks & Bathurst, 1996). Nonetheless, different erodibility coefficient values were calculated in plot scale studies with different agricultural land uses (Wicks, Bathurst, & Johnson, 1992). Wicks et al. (1992) showed that erodibility coefficient variation depends on the land use (tilled, clipped grass, grazed, ungrazed). However, there is high variation of soil erodibility coefficients in SHETRAN applications, with Kr ranges from 0.05 to 70 (J-1), and Kf between 5 x 10-7 to 2 x 10-5 (kg m-2 s-1) (Bathurst, 2011). Most of the reported SHETRAN studies employ single values for the erodibility coefficients (Kf and Kr). Moreover, the values varied with the spatial resolution of model applications (Bathurst et al., 2005; Bathurst, Burton, Clarke, & Gallart, 2006; Janes et al., 2017; Lukey et al., 2000).

2.2 Study area

The Blackwater (18 km2) and Kit Brook (22 km2) catchments are part of the River Axe hydrological network in south-west England (Figure 1). Catchment digital elevation models (DEMs) derived from Ordnance Survey (OS) data were obtained through EDINA Digimap with a 5 m resolution. The elevation of the Blackwater catchment ranges from 49 m at the outlet up to 250 m on the crest (southeast) and slopes range from 0 - 36° across the catchment. The Kit Brook catchment elevation rises from 42 m at the outlet to 251 m in the upper northeast reaches, with slope angles ranging between 0 - 36°.

The nearest rainfall station with 15 minute data available for the period overlapping hydrological measurements was at Raymond’s Hill (Met Office, 2018, [50°46'0.84"N 2°57'46.08"W, 85 m]), approximately 5 km south of the catchments. Mean daily temperature data was obtained from Seavington station (ID 9092 [50°56'26.9"N 2°51'35.6"W, 85m]) approximately 16 km north of the catchments, which was used to estimate daily potential evapotranspiration (PE, mm) using a PET formula (Oudin, Michel, & Anctil, 2005). Climatological data range from 1 October 2009 to 30 September 2014.

Measurements of pressure and turbidity were obtained with a 15 minute time step. Troll 9500 probes were installed at the outlet of each catchment in September 2010 and measurements continued until December 2014. Pressure data was converted to flow (m3 s-1) based on the stage-discharge rating curve using available measurements collected for each catchment. An extrapolation method was used based on four types of regression equation; linear, quadratic and power. Mean and base flow values were also obtained from similar size catchments in the region (CEH, 2018) and compared to estimated flow. The quadratic equation gave values closest to other gauged flow and the highest regression coefficients (R2=0.9 [Blackwater], 0.9 [Kit Brook]). Flow duration curves were calculated and show similar flow responses between the catchments (Figure 2). In Kit Brook, the fraction of daily discharge over annual mean flow was slightly higher than in Blackwater 90% of the time, whereas Blackwater exceeded Kit Brook only during periods of high flow; suggesting a higher permeability in Kit Brook than Blackwater. Turbidity data were converted to suspended sediment concentration (mg l-1) based on the regression equation, y = 1.1049 x - 15.005 (R2 = 0.9) (Little, 2012), and suspended sediment flux (kg s-1) was computed from sediment concentration and flow. Issues with turbidity data quality arose during some periods; therefore, it was necessary to exclude some events from further analysis.

The most recent land cover for each catchment was characterised by a 2010 ground-based field survey of the Blackwater catchment from the Westcountry Rivers Trust and by digitising 2010 imagery from Google Earth for Kit Brook. The 2010 survey map was classified into four land covers; (1) urban, (2) deciduous woodland, (3) arable crops and (4) grass. In Blackwater the land cover was grass (60%), arable crops (27%), deciduous woodland (12%) and urban (1%) with comparable land cover proportions observed in the Kit Brook catchment: 57%, 29% 13% and 1%, respectively. In the south west region of England, winter cereals are the most common crop type (DEFRA, 2015); hence, winter barley was used as the simulated arable crop for both catchments. Soil data was acquired from the National Soil Resources Institute (NSRI) of Cranfield University (Cranfield University, 2018). Five soil types were identified in the Blackwater catchment; the one with the largest extent (40%), namely WICKHAM (Eutric Luvic Planosols) had a soil texture of 21% sand, 41% silt and 30% clay. Each soil is characterised by five depth layers between 0 and 1.5 m; and the properties for each soil type and layer vary depending on the land use (Hollis et al., 2015). Six soil classifications with five depth layers (0 – 1.5 m) were identified in the Kit Brook catchment; BATCOMBE (18% sand, 58% silt and 24% clay) and CHARITY (16% sand, 58% silt and 26% clay) soils cover the 37% and 31% of the catchment, respectively. The NSRI soils database provides the international standard soil classification (IUSS, 2007) related to the soil classification of England and Wales, in which WICKHAM corresponds to Eutric Luvic Planosols, BATCOMBE to Profundic Chromic Endostagnic Luvisols and CHARITY to Chromic Luvisols. The QUORND soil which covers 20% of the Kit Brook catchment was substituted for HENCE soil (60% sand, 25% silt and 15% clay) due to the lack of information available in the NSRI.

2.3 Event selection

Individual flow events were selected in both catchments to enable event-based analysis of suspended sediment flux for model calibration and testing. Issues with turbidity data quality arose during some periods; for example sensor fouling or burial, leading to periods of persistent high turbidity values until cleaning or on occasion large rapid variations in measured turbidity occurred that were unrelated to any change in flow. Therefore, it was necessary to exclude some events from further analysis due to these data quality issues. Discharge event analysis focused on selecting a subsets of events in each catchment that were determined to have ‘good quality’ flow and turbidity data. The start of a flow event was defined by when flow exceeded the base flow and where sediment flux increased above the prior baseline data. The end of an event was determined when flow fell to the pre-event level or to a new temporary base level which exceeded the flow prior to the event (Robson & Reed, 2008). Total flow volume (m3) (Equation 1), maximum flow peak (m3 s-1), sediment yield (t ha-1) (Equation 2) and maximum sediment flux peak (kg s-1) of each event were obtained. The reference date for each event was stipulated as the day in which the maximum flow peak was found. Based on this event selection, 53 events were identified in Blackwater and 46 in Kit Brook. For most selected events, a clockwise suspended sediment concentration-discharge (C-Q) hysteresis behaviour (Williams, 1989) was observed in both catchments (i.e., sediment peak arrives before the discharge at the outlet and/or presenting sediment exhaustion).

Qv = Ʃ [(Qi) (900)] Equation 1

Sy = {Ʃ [(Sedi) (900)] (0.0011)}/ {(ha)} Equation 2

Where, Q = Flow (m s-1), Sed = Sediment flux (kg s-1), and i = number of time steps (15 min) in an event.

2.4 Model setup

The use of a 25 x 25 m grid size for Blackwater produced a grid number of 239 x 170, fitting with the model grid limit (300 x 300), but this limit was exceeded for Kit Brook (180 x 355). Furthermore, a run time of 15 days was observed for this resolution over the complete simulation period. Therefore, the 50 x 50 m grid size was selected to produce a reasonable running time (24 hrs for 5-year); and this grid was converted from the 5 x 5 m DEM in both catchments

Vegetation and sediment parameter values (Appendix A) were selected from a literature review (Birkinshaw, 2008; Lukey et al., 2000; Wicks et al., 1992). NSRI data was used in the model with a soil depth up to 1.5 m; parameter values (e.g. Ksat, θres, θsat) varied according to each soil layer and land cover (Appendix B). Rainfall data with a 15 minute time-step and calculated daily potential evapotranspiration were used for an initial simulation from October 2010 to September 2014 with a ‘spin up’ hydrological year (October 2009 - September 2010) to obtain phreatic surface level equilibrium.

2.5 Calibration and evaluation processes

Calibration aims to improve model performance by changing values of selected parameters, either through manual or automated methods. A ‘manual’ process is commonly applied, in which parameters are changed ‘one-at-a-time’ (OAT) (Rabitz, 1989). This necessitates determination of which parameters require calibration and consideration of the relationship between parameters. It also requires a choice of the model output to be calibrated (e.g. runoff, phreatic level, sediment concentration, discharge peaks, sediment flux peaks, etc.). Furthermore, multiple different combinations of parameter values might give a good fit (Beven & Binley, 1992; Jetten & Maneta, 2011). The decision on parameters to be calibrated depends on information about previous applications (i.e., sensitivity analysis) and/or user experience.

The calibration process was performed in the Blackwater catchment. The first simulation used five soil layers (0 - 1.5 m), although for an accurate base flow, subsequent simulations required the addition of a layer (6th [1.5 – 20 m]) to represent soil from subsoil to bedrock (Birkinshaw, n.d.). The water flow component was calibrated by comparing the measured 4-year discharge record to the model simulation and by quantitative comparison of the selected discharge events. Afterward, the sediment transport component was calibrated using the selected events. Using the proxy-catchment approach, model evaluation was undertaken in the Kit Brook catchment for the same ‘spin up’ and run period using parameter values from the final Blackwater calibration.

The Nash-Sutcliffe efficiency (NSE) (Equation 3) was used to assess model fit with the continuous discharge record. For assessing event-based performance, the coefficient of determination (R2) between measured and simulated data was calculated for flow (R2Q) and sediment flux (R2Sed), respectively. Coefficient values (NSE and R2) higher than 0.5 are considered as good-fit (Moriasi, Arnold, Van Liew, Harmel, & Veith, 2007).

NSE = 1 – {[Ʃ((Si - Oi)2)]/[Ʃ((Oi - µO)2)]} Equation 3

Where, Oi = observe measurement at the time i (i = 1…m), Si = model simulation at the time i (i = 1…m), and µO = mean of observe measurements (1… m)

Measured and simulated flow volume (Qv [m3]), maximum flow discharge (Qp [m3 s-1]), sediment yield (Sy [t ha-1]) and maximum sediment flux (Sp [kg s-1]) were obtained for each selected event. The absolute percentage difference between measured and simulated data (Qv, Qp, Sy, and Sp) for each event (Absdiff) was calculated. The mean of the Absdiff was used to quantify event model performance (Equation 4).

µAbsdiff = (1/n) {Ʃ [│(Oj - Sj)/(Oj)│] 100} Equation 4

Where, n = number of events, O = Measured: Qv, Qp, Sy and Sp, S = Simulated: Qv, Qp, Sy and Sp, and j = event (1…n).

Simulations were run by changing parameters values using the OAT method with the objective of reaching the highest possible NSE and the minimum µAbsdiff. Model accuracy in flow and sediment flux prediction was assessed for the final calibration (Blackwater) and for the evaluated simulation (Kit Brook) using the previous coefficients; and additionally by comparing measured against simulated data using: a) monthly mean runoff; b) a monthly window of the coefficient of determination (R2) for discharge and sediment flux (i.e., R2Q and R2Sed) for the selected events; and c) R2 for Qv, Qp, Sy and Sp.

2.6 Sensitivity analysis

The parameters reported as the most sensitive in other studies of SHETRAN sensitivity (Bathurst, 1986; Bathurst et al., 2004; Op de Hipt et al., 2017; Parkin et al., 1996; Wicks & Bathurst, 1996; Wicks et al., 1992; Wicks, Bathurst, Johnson, & Ward, 1988) include: actual-potential evaporation ratio (AE/PE), Strickler coefficient (Stk), saturated hydraulic conductivity (Ksat), raindrop soil erodibility coefficient (Kr) and overland flow erodibility coefficient (Kf). In the present study, the sensitivity analysis consisted of varying values of selected parameters upward and downward, relative to the base run (final calibration), by factors of 10 (F10), 0.1 (F0.1) and 0.01 (F0.01) with the OAT method. The factorial changes were applied to the parameters’ value for each of the four land cover types, and the maximum possible value was used when a parameter value exceeded the physical limit.

An adaptation of the sensitivity index (SI) (Sheikh, van Loon, Hessel, & Jetten, 2010) was implemented using model outputs of the sensitivity simulations (F10 and F0.01) and the base run (F1). The SI was calculated for each assessed parameter according to equation 5. Model outputs analysed included 4-year cumulative flow volume (Qv) and the mean of flow peaks (µQp) for the parameters in the water flow component (AE/PE, Stk and Ksat); and 4-year sediment yield (Sy) and mean of sediment flux peaks (µSp) for the parameters in the sediment transport component (Kr and Kf)

SI = (F10out – F0.01out)/F1out Equation 5

Where, F10out = model output by factor change of 10 on the corresponding parameter, F0.01out = model output by the factor change of 0.01 on the corresponding parameter, and F1out = model output for the base run on the corresponding parameter.

The multi-parameter approach to sensitivity analysis consisted of running simulations with a combination of parameter changes for the water flow (AE/PE, Stk and Ksat) and sediment transport components (Kr and Kf). Factorial change of parameters from F0.1 to F10 on the water flow component produced 27 simulations and 9 simulations on the sediment transport component (Figure 6). The percentage of difference (Pctdiff) for each model output relative to the base run was calculated by equation 6. The base run simulation (Soutbr)for the parameters on the water flow and sediment transport components correspond to simulation number 14 and 5, respectively (Figure 6).

Model sensitivity to grid resolution was examined by running simulations of the Blackwater catchment with grid sizes of: a) 25 x 25 m, b) 50 x 50 m, c) 100 x 100 m and d) 200 x 200 m. Considering the longer model run time associated with the finest resolution (15 days), the climate records were restricted to three years (Oct 2009 - Sep 2010 [‘spin up’], Oct 2010 – Sep 2012). Model sensitivity to changes in grid resolution was assessed by comparing outputs of the base run (50 x 50 m, final calibration) against each resolution (Equation 6). The model output considered were: 4-years flow volume (Qv), mean of discharge peaks (μQp), mean of event flow duration (μQw), 4-years sediment yield (Sy), mean of sediment flux peaks (μSp) and mean of event sediment duration (μSw). The width of the fluxes (flow [Qw] and sediment [Sw]) was measured as the distance between the intercept points to the left and right of the one-half peak height (Robson & Reed, 2008).

Pctdiff = ([Soutbr – Souti]/Sout1) 100 Equation 6

Where, Soutbr = model output of base run simulation, and Souti = model output of simulation i (i= 1...m), m = 27 for the multi-parameter analysis on the water flow component, 9 on the sediment transport component; and 4 for the simulation on model sensitivity to grid resolution.

The catchment representation of grid size resolution (25 x 25 m, 50 x 50 m, 100 x 100 m and 200 x 200 m) was assessed using probability density plots of the distribution of topographic slope and percentage of land cover represented. Model comparison with measured flow and sediment flux were undertaken for each of the grid size simulations using the same coefficients as in the model calibration and evaluation processes (NSE, µAbsdiff [Qv, Qp, Sy, and Sp]).

**3. Results**

3.1 Model calibration in Blackwater catchment

The water flow component was calibrated by changing four parameters. The parameter value and NSE for continuous discharge and the µAbsdiff (Qv and Qp) of the best fit simulation are presented in Table 1. The sequence in the table follows the order in which parameters were calibrated. After obtaining the best-fit discharge, four parameters were calibrated for the sediment transport component in which the µAbsdiff (Sy and Sp) were calculated for each simulation. The second baseline simulation appearing in Table 1 corresponds to the last calibration for the water flow component and set-up values in the sediment transport component. The Kf value required an escalation of the plot measurements reported for tillage and clipped grass (Wicks et al., 1992). An over prediction for the majority of events was observed with the Kf value of 59 x 10-10 (kg m-2 s-1) and an under prediction with 6.9 x 10-10 (kg m-2 s-1). The highest Kf was chosen for cropland and the lowest for grass and woodland. A similar procedure was performed for Kr parameter using plot values reported in Wicks et al. (1992).

Monthly mean runoff (Figure 3a) showed the lowest differences between simulated and measured data during autumn (2 mm) and winter period (-6 mm), whereas simulated runoff during spring and summer exceeded measured by 23 mm and 17 mm, respectively. The simulated annual runoff showed an over estimation of 5%.

Model performance on event-scale showed that 83% of the discharge events and 64% of the sediment flux events has R2values higher than 0.5 (Figure 4a-b). This indicates an accurate representation of event timing by the model. Moreover, model presented better prediction of flow volume (Qv [R2 = 0.8]) than flow peak (Qp [R2 = 0.6]) (Figure 4c-d). Correspondingly, the absolute percentage of difference between the measured and simulated data [µAbsdiff] showed lower values for Qv (30%) than Qp (41%). A high variability was observed in the representation of sediment export compared with measured data; better prediction of sediment yield (Sy [R2 = 0.4]) than sediment flux peaks (Sp [R2 = 0.2]) were observed using the coefficient of determination (Figure 4e-f). In contrast, the µAbsdiff was higher for Sy (106%) than Sp (86%; Table 2).

3.2 Model evaluation in Kit Brook catchment

Model simulation of flow and sediment flux in Kit Brook showed a lower NSE, larger µAbsdiff (Qv, Qp, Sy and Sp) and similar R2 compared to the calibrated results for the Blackwater catchment (Table 2). Model runs in Kit Brook used the final calibrated parameter values obtained from the Blackwater simulation. The measured mean monthly runoff (mm) was higher than simulated, especially for winter months. In contrast to Blackwater, simulated mean annual runoff in Kit Brook was 10% under predicted (Figure 3b).

The model showed poorer performance when comparing Kit Brook with Blackwater on an event basis. Events with R2 higher than 0.5, represent the 80% of the total discharge events (Figure 5a) and 41% of the sediment flux events (Figure 5b). The 46 measured events in Kit Brook presented a higher model predictive performance for Qv (R2 = 0.8) than Qp (R2 = 0.6) (Figure 5c-d), which correspond to µAbsdiff values for Qv and Qp of 48 and 66%, respectively. Lower performance was observed for sediment prediction (R2 = 0.6 [Sy] and R2 = 0.3 [Sp]) (Figure 5e-f); corresponding to µAbsdiff valuesfor Sy and Sp of 298% and 438%, respectively.

The higher observed permeability in Kit Brook, based on comparison of the flow duration curves (Figure 2), supported adjustment of the Ksat for the 6th soil layer in this catchment. Increasing the Ksat value in this layer showed a difference of 7% between simulated and measured annual runoff. Furthermore, better NSE and μAbsdiff coefficients (Table 2) were observed with this Ksat adjustment. However, the coefficient of determination for the event analysis (R2Q and R2Sed) did not vary significantly compared with the non-adjusted Kit Brook simulation (Appendix C).

3.3 Model sensitivity

The sensitivity index (Table 3) showed that variations of Ksat affected flow volume (Qv) the most and Stk affected the mean of discharge peaks (μQp). Variations in AE/PE had little effect on both flow volume and mean of flow peaks. For the sediment transport component, sediment yield (Sy) was most sensitive to the Kf parameter, whereas the mean of sediment flux peaks (μSp) was more sensitive to Kr. Nonetheless, SI differences between the erodibility coefficients (Kr and Kf) were relatively small for both model responses (Sy and μSp).

The multi-parameter approach to sensitivity analysis on the water flow component showed how different combinations of the parameters, especially Stk and Ksat, can produce similar percentage of differences (Pctdiff) with respect to the base run (Figure 6a). For example, simulations S8 and S16 reduced flow volume (Qv) by 15%. Likewise, similar Pctdiff in mean of flow peaks (μQp) were observed in simulations with different combination of Ksat and Stk values. For example, the simulations S8 and S15 presented μQp changes of -66%; and S2 and S21 produced changes of approximately 53%. An equifinality problem, in terms of flow volume and peaks, appears when increases in Ksat occur in combination with decreases in Stk, and vice versa. Although, the shape of hydrographs vary between simulations. Specifically, S8 presented more prolonged events with lower flow peaks compared with S16, resulting in similar Qv changes. Whereas, S15 presented higher base flow during the 4-year period than S8, as consequence the mean of flow peaks showed similar μQp reductions when compared with the base simulation (S14).

The multi-parameter analysis of parameters on the sediment transport component (Figure 6b) showed that minor changes in Kr combined with high Kf values produced similar sediment yield with respect to the base run (Pctdiff [Sy = 100%]); for example, simulations S3 (Kr [F0.1], Kf [F10]) and S6 (Kr [F1], Kf [F10]). Likewise, on the mean of sediment flux peaks (μSp) large changes in Kr combined with small changes in Kf (e.g. S7 and S8) presented similar differences compared to the base run (Pctdiff [μSp = 100%]).

In terms of sensitivity to DEM resolution, the probability density distribution of slopes for each DEM resolution shows that decreasing grid size leads to increasing variance in the distribution of slope angles (Figure 7a). The change in grid size produced only a very minor effect on land cover proportions represented in simulations (Figure 7b). The largest difference between grid resolutions was in channel network lengths (Figure 7c-f).

The DEM resolution simulations show that increasing grid size from 25 to 200 m leads to increases in Qw and decreases in Qp and Qv (Figure 8a). Only small differences (Qv, Qp and Qw) were observed between grid sizes simulations of 25 m and 50 m. In terms of sediment exports, increasing grid size (25 m - 200 m) produced a decrease in Sp and increase in Sw. In contrast, Sy exhibited a much smaller but more varied response (Figure 8b).

In general, a better estimation (NSE, µAbsdiff and R2) was obtained for the 50 m grid size when comparing simulations of each resolution with measured data. (Table 4). The coefficients showed a better fit to measured data with decreasing grid size, except R2. Moreover, the two finest resolutions simulations (25 and 50 m) presented only slight differences between coefficients, especially NSE and µAbsdiff.

**4. Discussion**

SHETRAN predicted streamflow well in both catchments (Figure 3). The addition of a deep, low conductivity and homogenous soil-rock layer (1.5 – 20 m depth) below the upper soil profile (parameterised using NSRI soil hydraulic data) enabled more accurate simulation of base flow (Table 2), which decreased gradually during extended dry periods. Moreover, the hydraulic conductivity of bedrock (2.7 to 20 m) in previous SHETRAN applications (Birkinshaw, 2008; Birkinshaw & Ewen, 2000) was similar to the present study.

Flow measurements derived from the stage-discharge rating curve may contribute to event-scale model uncertainty. Nevertheless, under-estimation of discharge peaks and accurate base flow was obtained in both catchments. By contrast, accurate peak discharge estimation and under prediction of phreatic level (base flow) in SHETRAN have previously been reported, and vice versa (Adams, Parkin, Rutherford, Ibbitt, & Elliott, 2005; Bathurst et al., 2004; Birkinshaw, 2008; Ewen & Parkin, 1996; Janes et al., 2017; Zhang et al., 2013). Furthermore, similar behaviour have been observed with other hydrological models (Croke, Merritt, & Jakeman, 2004; De Roo & Jetten, 1999; Marsik & Waylen, 2006).

The proxy-catchment test in this study showed better performance in the calibrated catchment (Blackwater) than the evaluated catchment (Kit Brook) probably due a higher soil permeability in Kit Brook than Blackwater (Figure 2). Nonetheless, SHETRAN showed reasonably accurate flow prediction in both catchments, which are similar in terms of area, relief and land cover characteristics. The prediction errors (e.g. Qv and Sy) may be attributed more to the parametrization and DEM resolution rather than lack of model process representation. An important factor to consider for model predictions is that soil (NSRI) under grass represents physical and hydraulic properties of permanent grass land cover, whereas the land cover may include permanent and temporary grass. Soils under temporary grass could have different properties (water retention curve, bulk density and soil porosity) than under permanent grass. Moreover, temporary grass may be located in rotation fields, where soil physical properties can vary depending on time since last cultivation, and take between 2 to 9 years to recover (Thorud & Frissell, 1976; Tuzzin de Moraes et al., 2016) and up to 20 years in loamy soils (Froehlich, Miles, & Robbins, 1985).

In general, simulated discharge in both catchments compared well with measured discharge in terms of event timing, and reproduced discharge peaks well during wet periods (Figure 4a-5a).However, the under-estimation of peak discharge by SHETRAN could also be attributed to local infiltration variability, in terms of sub-field scale runoff and run-on patches not represented in the model, as well as the absence of representation of impervious and hydrologically-smooth roads and paths. These features could act as efficient flow pathways connecting runoff-generating areas to the stream network (Croke, Mockler, Fogarty, & Takken, 2005; Jordán-López, Martínez-Zavala, & Bellinfante, 2009), and have been implemented in other models (Elliot, 2004; Tiemeyer, Moussa, Lennartz, & Voltz, 2007) but not identified in any SHETRAN application.

The best-fit calibration for the Blackwater catchment resulted in lower mean errors at the event-scale (i.e., µAbsdiff [Sy and Sp]) than Kit Brook (Table 2). The lower model performance in Kit Brook (i.e., µAbsdiff) may be attributed to higher soil permeability in the catchment compared with its neighbour (Figure 2). A Ksat adjustment in the 6th soil layer produced an improvement in model performance (Table 2). Nonetheless, coefficients of the adjusted simulation presented lower values when compared with the best-fit calibration in Blackwater. This could be related to the necessary substitution of the HENSE soil type (covering 20% of the catchment) with the QUORND, based on their similar soil description as a result of the absence of soil parameters in the NSRI dataset (Cranfield University, 2018). Moreover, the lack of a land cover map produced by field-scale survey for Kit Brook (in contrast to Blackwater) could limit distinction between fields with permanent versus temporary grass cover. It is also possible that NSRI soil parameters in Kit Brook are less accurate (i.e., data extrapolation for arable soil) as cultivated soils in this catchment have been reported to be more degraded than soils in Blackwater catchment (Palmer, 2007).

Model sediment yield (i.e., µAbsdiff) showed lower estimation errors in the calibration process (Blackwater) and higher errors in the evaluation process (Kit Brook) compared with other studies (Adams & Elliott, 2006; Elliott et al., 2012; Lukey et al., 2000). In relation to sediment flux peaks, considerable uncertainty has been described in other SHETRAN applications (Elliott et al., 2012; Lukey et al., 1995a; Wicks & Bathurst, 1996) and is a common problem in PBSD models (e.g. Phomcha, Wirojanagud, Vangpaisal, & Thaveevouthti, 2011; Rankinen et al., 2010). Adams and Elliott, (2006) explain this lack of prediction performance in SHETRAN is a consequence of variation in soil cohesive strength, where increases in soil moisture can reduce soil cohesion and increase erodibility. The SHETRAN model does not represent spatial-temporal variability in soil erodibility within overland flow erosion. Seasonal changes in erosion are represented via variability in rainfall intensity in the raindrop/leaf drip impact equation and by temporal changes in the proportion of ground shielded by vegetation canopy (Lukey, Bathurst, Hiley, & Ewen, 1995b).

Suspended sediment concentration (C) - discharge (Q) hysteresis behaviour was present in the majority of measured events and could influence SHETRAN sediment load predictions as the model predicts arrival of both fluxes at the same time (Adams et al., 2012; Elliott et al., 2012; Sheikh et al., 2010), which might be expected based on the sediment routing equation. It is possible that if major runoff sources occur in a more distant location from the channel network than sediment sources, then some hysteresis effects could be observed between simulated flow and sediments. This difference in runoff and sediment source locations could in part be related to crop rotation, which was not represented in the calibration, as the 2010 land cover map was used for the 5 years of simulation (2009-2014). Moreover, urban areas (e.g. village and roads) can act as sources of flow and sediment transport (Jones, Swanson, Wemple, & Snyder, 2000), and parameters representing the hydraulic properties of these urban areas are not captured in the NSRI dataset. Furthermore, it was not possible to represent roads at the catchment scale due to the model-limited minimum grid size (>25 m). The above factors could explain some C-Q hysteresis behaviour that was observed in the measured data, but not reproduced by SHETRAN.

The parameters to which the model is most sensitive on the water flow component were saturated hydraulic conductivity (Ksat) and the Strickler coefficient (Stk) (Table 3). These finding were consistent with other studies (Bathurst, 1986; Bathurst et al., 2006). The sediment transport component showed similar sensitivity index values between the erodibility coefficients (Kf and Kr). This similarity in sensitivity means that increases in either erodibility coefficient affect sediment output and sediment peaks to a similar extent. It is important to note that SHETRAN simulated a sheet surface flow as wide as the grid size (i.e., 50 x 50 m). Therefore, calibration of Kf was prioritised over Kr. This is consistent with the reported increase in Kf values (kg m-2 s-1) with decreasing grid size. (Bathurst et al., 2007, 2005; Janes et al., 2017; Lukey et al., 2000). The studies also showed increases in raindrop/leaf erodibility coefficient (Kr) values with decreases in grid size but with a lower ratio of change.

The multi-parameter sensitivity analysis of the SHETRAN water flow component (Figure 6a) showed that different parameter combinations, particularly those including Stk and Ksat, can produce similar changes in flow volume and discharge peaks. Anderton et al. (2002) followed a comparable approach, although parameters were limited to the infiltration module on the water flow component (i.e., Ksat and Van Genuchten α and n). The authors found similar modelled flow response to some combinations of Ksat and soil depth (0 - 0.2 m and 0.2 - 3.3 m). Furthermore, an automatic calibration procedure in Zhang et al. (2013) showed an equifinality problem with the adjustment of Stk, Ksat and soil depth. Likewise, combinations of erodibility coefficients (Kr and Kf) produced similar changes in sediment yield and sediment peaks (Figure 6b). The method did not consider feedback from the water flow component to the sediment transport component as this required an excessively large number of simulations (i.e., 243). However, this interaction may represent an important effect in the prediction of overland flow erosion with surface runoff.

The results of the multi-parameter sensitivity analysis demonstrate how different combinations of Stk-Ksat can produce similar changes in simulated water yield and event flow peaks. This occurred with some parameters having very high values compared with calibrated values (e.g. F10 Ksat = 0.5 m day-1). Nonetheless, comparable measured values (i.e., 0.3 m day-1) have been reported at field-scale (Chappell & Franks, 1996) in the nearby Slapton Wood catchment. Similarly, Kr-Kf combinations can provide comparable changes in sediment yield and in the mean of sediment flux peaks without necessarily selecting the appropriate parameter value.

Testing sensitivity to grid resolution showed that decreasing grid size increases the variance in the slope angle distribution (Figure 7a) leading to increases in simulated event peaks (μQp and μSp) and a decrease in event duration (μQw and μSw) with only slight variations in flow volume (Qv) (Figure 8a). More complex behaviour was observed for Sy (Figure 8b) which could be explained by differences in the channel network produced by the contrasting DEM grid resolutions (Figure 7c-f). The differences between base run (50 x 50 m) coefficients in Table 2 and Table 4 relates to the use of the first two years (2010 – 2012) only for DEM simulations. The model performed better in wet than dry periods and during the first year, rainfall (694 mm) was 68% of the annual average total during the complete measurement period (1,021 mm). Compared to measured data (2010 - 2012), the simulation with the best performance was the 50 x 50 m (Table 4); this was expected as it was calibrated. Nonetheless, similar model evaluation coefficients were observed between the 25 x 25 m and 50 x 50 m simulations. It is possible that a better event prediction could be obtained by using the 25 x 25 m resolution for the calibration process, but this represents an important compromise between model run times versus grid size.

**5. Conclusion**

SHETRAN showed reasonable performance in Blackwater and Kit Brook catchments by producing an accurate flow prediction for the 4-year period. Moreover, SHETRAN simulations of discharge and sediment flux performed well in terms of event timing in both catchments. Larger errors in event-scale estimation for both discharge and sediment yield were observed in Kit Brook than Blackwater. Adjustment of Ksat for the lowermost subsoil-bedrock layer improved model event-scale accuracy in Kit Brook. Nonetheless, prediction of sediment yield and sediment flux peaks remained overestimated. The proxy-catchment test demonstrated that SHETRAN can predict event-scale flow with reasonable accuracy, but requires catchment-specific calibration for sediment flux prediction.

The sensitivity index showed flow volume (Qv) was most sensitive to saturated hydraulic conductivity (Ksat), and flow peaks (μQp) to the Strickler coefficient (Stk); whereas sediment yield (Sy) was slightly more sensitive to the overland flow erodibility coefficient (Kf), and sediment flux peaks (Sp) to the raindrop/leaf soil erodibility coefficient (Kr). The multi-parameter sensitivity analysis showed potential equifinality behaviour occurring with Ksat increases in combination with Stk decreases, and vice versa. Similar effects were observed for combinations of Kr and Kf.

The model showed better performance for the base run (50 x 50 m) than the other grid size simulations (range 25 - 200 m grid size) with small differences between the base run and the finest resolution (25 x 25 m). The DEM grid size variations showed the largest effects in event peaks and duration for both flow and sediment flux, with least variability in predicted event sediment yields.

**6. Data Availability Statement**

The data that support the findings of this study are available on request from the corresponding author. The data are not publicly available due to privacy or ethical restrictions.

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