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## **Environmental Modelling & Software**

journal homepage: www.elsevier.com/locate/envsoft



# Development of a system for automated setup of a physically-based, spatially-distributed hydrological model for catchments in Great Britain



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ARTICLE INFO	A B S T R A C T
<i>Keywords:</i> SHETRAN	The use of physically-based spatially-distributed models to solve problems in hydrology has been limited by their intensive data and setup time requirements. We have therefore created a system that enables the automatic setup.
Physically based Hydrological model	of a robust, physically-based spatially-distributed SHETRAN model for any catchment, gauged or ungauged, in Great Britain. National-scale datasets for topography, soil, landuse, geology and climate have been collated,

change, either for individual or multiple catchments.

1. Introduction

Data

GUI

Robust numerical models are an essential tool for research in hydrological processes and for informing flood and water management around the world. These models can be classified differently, depending on whether they represent processes in conceptual or physically-based ways (e.g. O'Connell, 1991; Wheater et al., 1993; Singh, 1995; Refsgaard, 1996). Conceptual models use a series of connected stores or reservoirs to emulate catchment responses. These models parameterise key hydrological processes and often require calibration of parameters with limited physical meaning (Pechlivanidis et al., 2011). This forms a potential issue in applying conceptual models to particular types of problem, such as prediction outside of calibration limits and under changing conditions (Beven, 2012). As more complex, physically-based models are potentially useful for investigating a number of prominent hydrological problems, such as predictions under non-stationary land use or climate, it is logical to take advantage of recent advances in computing power and data availability to facilitate their wider use. This helps to overcome the common criticism that physically-based models require prohibitively large data, time and computational resource requirements (Beven, 2012). As such, this study has the purpose of creating, for the first time, a physically-based hydrological modelling system for Great Britain using the SHETRAN model (Abbott et al., 1986; Ewen et al., 2000) and national datasets that are freely available for

academic research.

processed and stored to allow rapid retrieval and configuration of catchment models with minimal user-inter-

vention. These maps can be easily replaced by national datasets of other countries or global datasets, ensuring the system's international transferability. A graphical user interface has been developed to facilitate the model setup process. The resultant system, SHETRAN-GB, has the potential to significantly aid the deployment of SHETRAN for addressing important issues relating to water resources, hydrological extremes and climate

SHETRAN is a physically-based, spatially-distributed hydrological model, which has its origins in the Système Hydrologique Europeén (SHE) model developed by the British Institute of Hydrology, the Danish Hydraulic Institute and the French company SOGREAH (Abbott et al., 1986; Ewen et al., 2000). The foundations of SHE were strongly influenced by Freeze and Harlan (1969) who proposed a blueprint for a physically-based hydrological model, with these principles taken further and additional processes incorporated during the development of SHETRAN. The model is based on the solution of finite difference approximations to equations describing fully three-dimensional coupled surface/subsurface water flow and transport of sediments and reactive solutes, as described in Ewen et al. (2000). Since its inception, SHE-TRAN has been used in a wide variety of applications, including assessment of the impacts of groundwater abstraction impacts on streamflows (Parkin et al., 2007), examination of deforestation impacts on peak flows and sediment yields (Birkinshaw et al., 2011) and nitrate transport (Koo and O'Connell, 2006) to name but a few. A graphical user interface (GUI) was previously developed to improve the usability of SHETRAN (Birkinshaw et al., 2010), but it did not provide data or a standard parameter set to aid model setup.

As Bierkens (2015) notes, national, continental and global scale simulations of hydrology have been carried out previously with land surface models (LSMs), macroscale hydrological models (MHMs) and

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https://doi.org/10.1016/j.envsoft.2018.07.006

Received 4 January 2017; Received in revised form 8 June 2018; Accepted 16 July 2018 Available online 23 July 2018 1364-8152/ © 2018 The Authors. Published by Elsevier Ltd. This is an open access article under the CC BY license

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#### Table 1

Summary table of source datasets used and their associated information.

Data Type	Source	Description	Reference
Catchment boundaries	National River Flow Archive (2012)	Shapefiles of 1170 UK catchment boundaries	Morris et al. (1990)
Meridian 2 Lakes	Ordnance Survey (2012)	Shapefiles of lakes.	Ordnance Survey (2013b)
UKCP09 daily maximum temperature	The Met. Office (2012)	5 km ASCII files, one per day. Used to calculate PET and snowmelt.	Perry et al. (2009)
UKCP09 daily minimum temperature	The Met. Office (2012)	5 km ASCII files, one per day. Used to calculate PET and snowmelt.	(Perry et al., 2009)
UKCP09 monthly relative humidity	The Met. Office (2012)	5 km ASCII files, one per month. Used to calculate PET.	Perry and Hollis (2005)
UKCP09 monthly wind speed	The Met. Office (2012)	5 km ASCII files, one per month. Used to calculate PET.	Perry and Hollis (2005)
UKCP09 monthly sunshine hours	The Met. Office (2012)	5 km ASCII files, one per month. Used to calculate PET.	Perry and Hollis (2005)
UKCP09 daily rainfall	The Met. Office	5 km ASCII files, one per day	Perry et al. (2009)
Land Cover Map 2007	Centre for Ecology and Hydrology (2012)	1 km raster	Morton et al. (2011b)
Soil map created from the European Soil Database layers	European Commission and Joint Research Centre (2012)	Four 1 km rasters	Liedekerke et al. (2006)
Hydrogeology map	British Geological Survey (2012)	Shapefile	British Geological Survey (2014)
Land-form PANORAMA Digital Elevation Model	Ordnance Survey (2012)	50 m raster	Ordnance Survey (2013a)
Flow data	National River Flow Archive (2012)	Individual.csv files	National River Flow Archive (2014a)

increasingly with physically-based hydrological models solving the partial differential equations representing coupled surface/subsurface flows. A recent example of the latter approach is high resolution (1 km) modelling of the continental US with ParFlow (Maxwell et al., 2015). This follows on from other national-scale modelling efforts with process-oriented models of differing origins and complexities. For example, Henriksen et al. (2003a) describe the application of the physicallybased model MIKE SHE for integrated groundwater-surface water simulations across Denmark. Habets et al. (2008) use the land surface scheme (ISBA) coupled with the meteorological analysis system (SA-FRAN) and a groundwater model (MODCOU) to produce a national hydrological modelling system for France. However, there have not been any large-scale applications of SHETRAN to date, or indeed any nationwide physically-based modelling studies for GB. Rather, the current standard national hydrological model for GB is the conceptual 1 km Grid to Grid model (G2G) (Bell et al., 2009), which is in turn based on the Probability Distributed Model (PDM) (Moore, 2007).

In order to facilitate their application at large scales, a number of studies have developed ways of improving the setup and management of data-intensive hydrological models. Some studies have articulated or developed data models using geodatabase structures to support many types of hydrological modelling. For example, Maidment (2002) developed the widely used and flexible ArcHydro system, while Goodall and Maidment (2009) proposed an alternative spatiotemporal data model that is conceptualised around control volumes, fluxes and flux couplers. Olivera et al. (2006) drew on elements from ArcHydro but added additional elements to integrate the ArcGIS geographical information system (GIS) with the Soil and Water Assessment Tool (SWAT) model. More recently, Bhatt et al. (2014) developed an integrated user interface with an underpinning shared geodata model to couple the open source GIS software Quantum GIS with the Penn State Integrated Hydrological Model (PIHM) and demonstrated its power and effectiveness throughout the modelling chain.

Other important advances that have taken place are in enabling rapid access to very large datasets and transforming data in line with the requirements of modelling. Leonard and Duffy (2013, 2014) developed the Essential Terrestrial Variable (ETV) web services and datamodel workflows to transform ETV data ready for use in hydrological models anywhere in the continental US, with particular reference to examples using PIHM. Acknowledging the challenges in centralising and standardising data sources, Billah et al. (2016) use the Variable Infiltration Capacity (VIC) model to demonstrate that data preparation pipelines based on a rule-oriented data management system can be used to provide views on underlying data suitable for modelling. Yet while there are now some advanced solutions for efficiently collating and transforming the information needed for physically-based hydrological models, solutions are not currently available for many regions, including Great Britain (GB). This paper attempts to help address this issue by providing an interface to set up the SHETRAN model for any catchment in GB with national and international datasets prepared and transformed for physically-based hydrological modelling (SHETRAN-GB). The integrated system achieves the automated application, without calibration, of a physically-based (rather than lumped, calibrated) hydrological modelling system using standard, freely available data. The system has been designed so that the datasets for GB could be easily substituted for national datasets of other countries or global datasets. SHETRAN has been shown to work well in a variety of climates including semi-arid basins in Iberia (Guerreiro et al., 2017), tropical basins in west Africa (Op de Hipt et al., 2017), monsoonal climates in India (Naseela et al., 2015) and mountainous catchments influenced by snowmelt (Bathurst et al., 2011) amongst others, giving us confidence that an internatonal version of SHETRAN-GB would be a useful tool for physically based hydrological modellers.

The paper is structured as follows. The input data required for the modelling system are discussed in Section 2, followed by a description of the modifications made to SHETRAN in Section 3. Section 4 outlines the software and user interface and Section 5 describes in more detail the software design and implementation. An example simulation from SHETRAN-GB is given in Section 6. The work is discussed in Section 7 and summarised in the conclusion.

#### 2. Input data

Physically-based hydrological models are very data intensive. SHETRAN requires: a digital elevation model (DEM); a map describing the subsurface properties of a catchment; a land cover map; a time series of rainfall; a time series of potential evapotranspiration (PET) and a mask delineating the watershed of the catchment. These inputs are typically gridded at a resolution between 50 m and 5km and time series data is supplied at a daily or hourly time step.

The datasets chosen for input to the modelling system (see Tables 1 and 2) each cover the whole of Great Britain, which means that the information supplied for each catchment is consistent. This has the advantage that interpreting variations in model performance will not be

### Table 2

Summary	/ table	of the	SHETRAN	input	layers	created	from	the	source	data.
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Layer	Description	Associated parameters	Source dataset
Minimum DEM	DEM based on the minimum elevation value in each resampled grid square	Elevation (m)	OS Land-form PANORAMA DEM
Average DEM	DEM based on the mean elevation value in each resampled grid square	Elevation (m)	OS Land-form PANORAMA DEM
Soil and geology	represents the sub-surface for each grid cell as a column containing multiple layers of soil or rock	Depth, Saturated Water Content, Residual Water Content, Saturated Conductivity (m/day), vanGenuchten- alpha (cm-1), vanGenuchten-n	ESDB, BGS Hydrogeology map
Land cover	represents the vegetation for each grid cell	Canopy storage capacity (mm), Leaf area index, Maximum rooting depth(m), AE/PE at field capacity	CEH LCM 2007
Lakes	Indicates the presence of a lake in a grid square	Strickler coefficient	OS Meridian 2 Lake layer
Rainfall	daily rainfall	Rainfall (mm/day)	UKCP09 daily rainfall
PET	daily PET calculated from FAO Penman- Monteith method	PET (mm/day)	UKCP09 daily maximum temperature, daily minimum temperature, monthly relative humidity, monthly wind speed, monthly sunshine hours
Catchment mask	Delineates the watershed of a catchment	NA	NRFA catchment boundaries

additionally complicated by the confounding effects of using multiple datasets for different catchments. With the exception of the UKCP09 rainfall inputs, which can be substituted by the CEH-GEAR rainfall inputs (see below), the datasets are all also freely available to download under an academic licence, making the models suitable for use by any research group. It has been presumed that the quality control processes undertaken in the construction of each dataset make them sufficient for direct application in the modelling system without any further quality review or refinement.

The fully distributed nature of SHETRAN means that model structure and properties need to be specified for each grid cell. All maps required as part of this were resampled to a 100 m, 500 m and 1 km resolution and aligned with the British National Grid (BNG) for consistency and ease-of-use. Maps at these three resolutions can be selected from the GUI. For small catchments ( $< 10 \text{ km}^2$ ) it is expected that users will select a 100 or 500 m resolution and for medium-large catchments use a 1 km resolution. Indeed, the 1 km resolution maps form the standard SHETRAN-GB setup. This standard 1 km resolution is partly dictated by the scales of the available soil and land cover datasets, but it could be argued that higher spatial resolution models are desirable, in order to more realistically capture the significant heterogeneity that can occur at sub-kilometre scales in catchments (Paniconi and Putti, 2015). For example, with respect to the representation of soils, it is recognised that effective parameters are required at this comparatively coarse resolution to implicitly account for the many soil types and complex variations in structure and properties that could be present within a single grid square. Some authors, such as Beven (2006), argue that this compensation by effective parameterisation could undermine the physical basis of the model to some degree. However, the extent to which this issue represents a problem can be evaluated with respect to model performance. If the dynamics of catchment models appear to be conceptually plausible and consistent with available evaluation data, the selected spatial resolution can be effectively justified for the purpose of national-scale modelling of water resources, climate change impacts and land-use change impacts.

The 1 km spatial resolution therefore represents a balance between the information content of available data and pragmatic considerations with respect to computing resources and run-times in particular (for example a 1 km resolution SHETRAN model for a 500 km<sup>2</sup> catchment over 10 years takes approximately 35 min to run on a desktop computer), as well as perceived priorities for investigation and evaluation. This was also guided by the recent work of Zhang (2012), who investigated the influence of spatial and temporal resolution in SHE-TRAN. Zhang (2012) found that simulations can be significantly improved by increasing the temporal resolution of forcing inputs particularly rainfall - from daily to hourly intervals. In contrast, improvements due to increasing spatial resolution were found to be more varied and to depend upon the level of catchment homogeneity. This highlights the general importance of improving the temporal resolution of inputs relative to the spatial resolution, although this will vary depending on specific model use. Furthermore, the 1 km resolution is consistent with other large-scale, national modelling studies, such as the UK Grid-To-Grid model (Bell et al., 2007) and the national MIKE SHE model for Denmark (Henriksen et al., 2003b), which also use a 1 km grid resolution. Recent versions of the national MIKE SHE model for Denmark have moved to a 500 m grid resolution (Højberg et al. (2013), Olsen et al. (2013)).

The digital elevation model (DEM) used in this study was based on the 50 m Ordnance Survey (OS) Land-Form Panorama data (Ordnance Survey, 2013a). This raster was then resampled to a 1 km resolution using bilinear resampling to determine the average elevation for each grid square. One of the applications of the DEM in SHETRAN is in generation of the location of river channels for routing within the model. These are referred to in SHETRAN as river links. Tests suggested that these links more closely follow actual river paths when the minimum elevations in each grid square - taken from the original resolution of the Panorama DEM - are accounted for. A DEM based on the minimum elevation values in each 1 km grid square was therefore created with which the river locations were then calculated.

SHETRAN represents the catchment sub-surface for each grid cell as a column containing multiple layers of soil or rock. The European Soil Database (ESDB) v2.0 (Liedekerke et al., 2006) was identified as the most suitable dataset for meeting the requirements of this modelling system. It is a Europe-wide, 1 km resolution database in which hydraulic properties were assigned by a collaboration of 12 European countries. Liedekerke et al. (2006) standardized both the particle size and the hydraulic data across Europe by fitting the Mualem-van Genuchten model parameters (Van Genuchten, 1980) to the individual hydraulic properties stored in the ESDB. The ESDB layers containing the information that SHETRAN uses (dominant topsoil texture, depth to textural change, dominant subsoil texture and depth to rock) were selected and combined into one raster file of unique soil classes for SHETRAN. Bedrock depths were not available as a national dataset, therefore, as an initial representation of geology, a 20 m thick bedrock layer was added to the bottom of each soil column. The data for this were taken from the British Geological Survey (BGS) 1:625 000 scale digital hydrogeological map (British Geological Survey, 2014). 236 unique subsurface column types were identified on this basis and coded for use in SHETRAN.

The Centre for Ecology and Hydrology (CEH) land cover map (LCM) 2007 (Morton et al., 2011a) is derived from satellite images and digital cartography, using land cover classifications based on the UK Biodiversity Action Plan Broad Habitats that lead to the definition of 23 land cover types. The map was simplified into the 7 basic land cover types

typically used with SHETRAN: arable, bare ground, grass, deciduous forest, evergreen forest, shrub and urban (Birkinshaw, 2011).

Most previous work with SHETRAN has used point rainfall data (Bathurst et al., 2011; Elliott et al., 2012; Birkinshaw et al., 2014). This approach is adequate for modelling individual catchments under certain conditions, but a more coherent dataset is necessary for setting up a nationwide system so that a collective approach to catchment modelling may be followed, minimising errors from non-standardisation or bias. SHETRAN was therefore updated to take gridded rainfall as input and the UKCP09 5 km gridded precipitation dataset was initially selected as the fundamental rainfall input for the modelling system (Perry et al., 2009). This dataset, created by the Met Office, is based on a large amount of data from the UK's comparatively dense gauge network and provides full coverage of the UK at a daily resolution for 1958-2007. In addition, CEH have recently developed a new 1 km gridded daily rainfall product, CEH-GEAR (Gridded Estimates of daily and monthly Areal Rainfall for the United Kingdom (1890-2012)) (Tanguy et al., 2014). Unlike the UKCP09 5 km gridded dataset, which uses inversedistance weighting to interpolate station data into a gridded format, CEH-GEAR uses natural neighbour interpolation. The gridded daily values are also adjusted by a monthly correction factor to ensure that they are consistent with gridded monthly rainfall totals calculated from a denser station network. Unlike the UKCP09 dataset, the CEH-GEAR rainfall is freely available. Either dataset can be used for model setup and can be selected in the python code rather than through the GUI.

The Met Office Rainfall and Evaporation Calculation System (MORECS) is often used as an evaporation data source for hydrological modelling in the UK (Hough and Jones, 1997), for example by the Environment Agency regional groundwater models (Shepley et al., 2012). It provides nationwide, real-time assessments of rainfall, potential evapotranspiration (PET) and soil moisture (Hough and Jones, 1997), but the data are not freely available. Other distributed estimates of PET are very limited, such that the approach taken in this work was to calculate PET directly from the gridded variables available within the UKCP09 dataset using the FAO Penman-Monteith method (Allen et al., 1998) to produce a UK wide 5 km  $\times$  5 km grid of time-varying PET. This method also allows the SHETRAN-GB system to be more directly compatible with UKCP09 weather generator outputs, which calculates PET in the same way (Kilsby et al., 2007).

Daily maximum and minimum temperature data are used to provide input to the snowmelt module of SHETRAN. There are options for both temperature-index and energy balance approaches to modelling snowpacks within SHETRAN, but the former, simpler method is used here as it has lower input data requirements. Given the climatology of the UK, this modelling decision is likely to have most bearing on upland and mountainous regions, for which estimation of all the inputs required for energy balance is particularly complicated due to topographic complexity.

SHETRAN was modified to allow for input of a map showing the position of lakes in a catchment, in order to improve their representation in catchment simulations. The data layer used as input is the OS Meridian 2 lakes layer (Ordnance Survey, 2013b). This dataset is available as a vector file, which was converted to a 1 km raster.

#### 3. Existing functionality of SHETRAN and new modifications

Currently, the subsurface in SHETRAN is treated as a variably saturated heterogeneous porous medium, and fully 3D flow and transport can be simulated for combinations of confined, unconfined, and perched systems. The 'unsaturated zone' is modelled as an integral part of the subsurface. Overland flow is produced as a result of both infiltration excess and saturation excess and is simulated using the diffusion approximation of the Saint-Venant equations. A network of 1D channels flows around the edge of the grid squares and the flow in these is also modelled using the diffusion approximation of the Saint-Venant equations. The surface and subsurface are fully coupled. There is no explicit modelling of pipes as these are not provided in any national dataset. Lakes are not explicitly modelled but occur as a result of the physical characteristics of the catchment. The catchments are assumed to have no flow boundary conditions apart from the outlet where there is assumed to be a weir. The catchments are set to be saturated initially but the results from the first two years of simulation (a 2 year spin-up period) are not used in the analysis.

SHETRAN has been modified in several ways in order to improve its performance using national datasets. The modifications include the following:

- SHETRAN now accommodates spatially varying rainfall and potential evapotranspiration data, as opposed to only point rainfall data as used in most prior work. This allows for use of recently developed gridded products and provides more realistic representation of important variability within catchments. Each model grid square is assigned a code in an ASCII map that corresponds to a time series in a separate input file.
- There is now also a better process within SHETRAN for removing sinks in the DEM - i.e. grid squares at a lower elevation than all neighbouring grid squares - to prevent unrealistic levels of ponding and surface storage, which would act to reduce flows in an unrealistic way. This is achieved in an iterative process. The elevation of all the grid squares where there is a sink is gradually increased until it is no longer at a lower elevation than its neighbours. This is then repeated until there are no sinks throughout the catchment.
- A minimum DEM (describing the minimum elevation in a grid square) is now used in combination with an average DEM (describing the average elevation in a grid square) to more accurately route the river links calculated within SHETRAN. The position of the river links is calculated from the minimum DEM by analysing the number of upstream grid squares that flow into a particular grid square. When these reach a certain number (the default is 20) a river channel is produced (Birkinshaw, 2010). The channel elevations are based on the 2 adjacent grid squares. The elevations are then modified so that there is always a downward flow path. The average DEM is used for all other processes
- SHETRAN has been modified to accept a map of lake locations so that they can be accurately represented within catchments. If a lake grid cell intersects a river link, it is treated as an open water body by reducing the default Strickler coefficient controlling surface roughness from 20 to 3. The Strickler coefficient is the inverse of Mannings roughness coefficient (Gauckler (1867), Manning (1891)). This acts to effectively slow flow and increase storage of water in the channel. All river channels have an individual Stickler parameter associated with them, SHETRAN now adjusts this parameter so that it corresponds with the lake value. As a results of these physical characteristics and the low Strickler coefficient in the channel, when there is heavy rain and large river inflows the water level in these channels increase and overflow into the nearby grid squares occurs. This surface water (which corresponds to lake water storage) gradually builds up and then reduces once the rain stops.
- Changes have also been made so that it is possible to assign Strickler coefficients as a function of land cover, rather than applying one parameter value for the whole catchment, as has generally been the case in the past. The option was always available within SHETRAN although not normally used. This allows roughness to vary with vegetation as would be expected (e.g. concrete surfaces have a low roughness and thus high Strickler coefficient, whereas vegetated surfaces are rougher giving them a lower Strickler coefficient).

#### 4. Automatic set up of shetran

In order to develop a national modelling system based on SHETRAN, a large array of data for the whole of Great Britain and the period 1960–2006 as described above, was integrated into a framework

catchment? By:	Gauge locations []
Station Number	Lockerbie Langhole
Station Number Please enter the gauge number of your catchment	ti 72004
Develution	72004 NAME Lune at Caton ABOUT Headwaters rise from Fell and the Pennines. Mixed geology with Carboniferous
Resolution Please bear in mind that finer resolution	Limestone; Silurian shales; Millstone Grit and Coal Measur
models will take longer to run.	Substantial Drift cover, Agriculture in valleys; grassland with
1km	moss in highest areas.
	5
Simulation run time	
Records are available from	Kebdal (
01/01/1960 to 31/12/2006	Ulverston
Start Date	in European Manual Andrea
GC/WW/AAAA	Morecaure + C
End Date	Lanciste, Skie
31/01/1999 ★★▼	Google Maps Engine Poulton-le-Fylde
	Blac Map data @2013 Google For non-commercial use Terms

Fig. 1. A screenshot of the user interface of SHETRAN-GB. Users are able to select catchments by browsing the map, entering the station number or uploading their own catchment boundary. The resolution, start and end date of the simulation are also selected by the user.

that features a new, user-friendly graphical interface, which extracts and prepares the data required for a SHETRAN simulation of any catchment in Great Britain. Previously, models would be set up manually. This involved finding and downloading the appropriate datasets, importing them into GIS to fill sinks, delineate catchment boundaries and extract the relevant area from each data layer, then convert these to SHETRAN input files and assign the parameters individually. This new GUI has vastly reduced the time it takes to set up and run a model from months (Birkinshaw, 2010) to seconds. The resultant model is an uncalibrated model based on the fixed set of parameters from national datasets. The system represents substantial progress in the ability to deploy SHETRAN for individual or very large numbers of catchments.

The Python scripts underlying the system take input from a user interface (scripted in HTML and Javascript) to automatically set up a model for a catchment (see Fig. 1). Users define the catchment, resolution and start and end date of the simulation. For gauged catchments, an existing catchment boundary can be selected from a map, while for ungauged catchments a shapefile or ASCII map of the catchment boundary can be uploaded to extract an appropriate model. The gauged catchment boundaries used in this work were determined on the basis of the records for all of the gauged catchments in the UK held by the National River Flow Archive (NRFA) (National River Flow Archive, 2014b). The algorithm underpinning catchment setup takes a boundary shapefile or gauge number as input to delineate the catchment along with the start and end date of the simulation as input. It then creates a project directory, creates or selects the catchment mask and uses that to extract the other data and write it in the appropriate format for input to SHETRAN. The SHETRAN data pre-processor is run, generating the input files for SHETRAN.

The automated setup of SHETRAN-GB catchments is based on a single standard 'conceptual model' derived from the available datasets. The sub-surface can have 2–3 layers defined by the soil and geology datasets. These are further broken down by SHETRAN into a total of 35 computational layers. Other key 'universal' parameters are set to fixed values. This standard 'conceptual model' cannot be changed in an automated way through the GUI but could be changed easily by the underlying model set up code. Individual models can also be altered by hand after set up with the GUI.

#### 5. Software design and implementation

The software is designed for those wishing to use a physically-based hydrological model but do not have access to detailed datasets for their catchment of interest. New users of SHETRAN often wish to begin modelling with a default set of parameters and subsequently refine the model when they become comfortable with the program. The GUI makes it much easier for someone to start using SHETRAN from scratch, but it is of little benefit to those with a full set of detailed data about their catchment, as this will surpass the information provided by national datasets. Experienced users of SHETRAN will also benefit from the software as they will be able to easily set up a catchment quickly.

The software requires a regular desktop computer with Windows and Python 2.7 with 'osgeo', 'Image', 'Imagedraw' and 'Tornado' modules and their dependencies. SHETRAN-GB is 245.1 GB as a bundle of Python scripts. exe files and an ASCII data archive. No preprocessing is required before use. The GUI only takes a few seconds to produce an average catchment model. It takes 170 s to extract the full time series of data for the largest gauged catchment in Great Britain (9948 km<sup>2</sup>).

The software has been designed so that the underlying code can be run with or without the GUI. The GUI is a clean and simple tool for setting up one catchment model at a time, but the underpinning Python code can be run in parallel to set up many catchments at once. The Python model setup code interacts with the JavaScript interface through the 'Tornado' module, receiving information about the required start and end dates of the simulation, and the catchment boundary. If the catchment exists in the boundary catalogue, the existing catchment ASCII files are retrieved. If the catchment does not exist (i.e. a shapefile has been uploaded instead), an additional module is called that converts the uploaded shapefile into an ASCII mask using the 'osgeo' module.

Once the ASCII mask has been generated, it is used to extract the other spatial information required from national maps. The national maps are not read into memory; rather, the lines of the files are skipped over until the required point is reached. The relevant lines are read into memory and then the file is closed. This is to make the system adaptable to much higher resolution national maps when they become available. All maps are stored using the British National Grid coordinate system which provides the regular array required for SHETRAN. The values in the extracted maps are used to retrieve the corresponding time series data.

Parameters are preassigned based on extensive experience from previous studies, although parameter values can be adjusted later. The automated setup of SHETRAN models means that common errors can be avoided. The SHETRAN input files are very detailed and it is easy to make a typing error or assign the wrong value to a parameter. The automated set up ensures that every map is the same size, resolution and location and that each parameter is assigned correctly. This adds a level of credibility and reduces the probability of errors in the model, especially for large heterogeneous catchments.

#### 6. Example simulation

The Eden catchment was simulated to demonstrate the suitability of the datasets for use in a national, physically-based modelling system. The Eden is a commonly studied area in the UK and so we are able to compare an uncalibrated version of SHETRAN set up by the system described in this paper to a calibrated version set up for another study. Janes et al. (2018) calibrate SHETRAN to river flows for the Eden at Kirkby Stephen (70 km<sup>2</sup> in area) and at Temple Sowerby (616 km<sup>2</sup>) over the period 1991-2001. The two catchments achieve Nash-Sutcliffe Efficiencies (NSE, Nash and Sutcliffe (1970)) of 0.85 and 0.86 respectively, R<sup>2</sup> (Moriasi et al., 2007) of 0.88 and 0.7 and PBIAS (Moriasi et al., 2007) of 14 and 8 for the validation period 2001-2007. Uncalibrated SHETRAN-GB simulations produce NSE values of 0.78 and 0.80 (see Fig. 2), R<sup>2</sup> of 0.79 and 0.81, and percentage bias in the water balance (PBIAS) of -8.6 and -1.0 for the same catchments for the period 1992-2002. This shows that the data used for the automated setup of SHETRAN-GB is appropriate but that model performance can be improved with calibration.

To provide an indication of the robustness of the system, some key potential uncertainties for the Eden catchment are now explored. Fig. 3 compares the river channel network automatically derived in SHETRAN from the digital elevation model at 1 km and 500 m resolution to the existing river network map (Ordnance Survey, 2018). The derived river network at both resolutions corresponds well to the main river channel through the catchment. At 500 m resolution, the secondary river channels are also well represented with only a few errors. This illustrates the importance of resolution (rather than the underlying data) in the uncertainty associated with the DEM. Rainfall data has many uncertainties associated with it including mechanical errors, recording errors, evaporation from partly-filled buckets, wind-induced undercatch, and snow-effects that can reduce rainfall totals by over 40% (McMillan et al., 2012; Pollock et al., 2018). Uncertainty is also introduced by gridding gauge data due to the interpolation method used. The UKCP09 and CEH-GEAR daily rainfall datasets use different interpolation methods, but are still highly correlated. Indeed, when the 24 h accumulation for each CEH-GEAR 1 km time series is compared with its corresponding 5 km grid square, the Spearman's rank and Pearson correlation coefficients range from 0.9 to 1. PET is another very uncertain variable as it can be calculated in approximately 50 ways (Lu et al., 2007) and cannot be directly measured. Lu et al. (2007) test six of these methods, including Penman-Monteith, and find that PET can vary by up to 500 mm/year in their study area of the southeastern United States depending on the PET method used. Other uncertainties in the land cover, soil and geological data are very difficult to quantify without collecting field data from the catchment itself but there are undoubtedly large uncertainties associated with the significant heterogeneity that can occur at sub-kilometre scales in catchments. More extensive analysis of the system's performance for a large number of catchments, including the uncertainties associated with the input datasets will follow in subsequent work. Such analyses are facilitated by the flexibility of SHETRAN-GB, which enables substitution of alternative datasets to assess their impacts on simulations.

#### 7. Discussion

This paper outlines the automated set up of a physically-based model for catchments in GB. The aim of this was to increase the usability of SHETRAN and to provide a uniform framework for exploring the possibility of a national, uncalibrated model based on parameters from established datasets so that ungauged catchments can be effectively modelled with some certainty. Additional experiments will test this theory, whereas this paper focuses on describing the modelling framework itself.

There are many positives to using such a framework. The time taken to set up a model has been vastly reduced, allowing the modeller to focus on other aspects of the modelling process (calibration, uncertainty analysis, exploration of a wider range of model outputs). The data used are currently the best available and they can easily be replaced by new or improved data sets when they become available. The models are based on a standard set of parameters, which provides consistency between models. The automated process reduces errors and uncertainties by removing the possibility of errors when manually setting up the complex model input files. However, such a strict framework does restrict the modeller from developing their own conceptual model of the catchment and does nothing to help incorporate other, more detailed local datasets. There is also the danger that these models will be used without due consideration of catchment processes. Whilst increased automation (of both model setup and automatic calibration) can improve efficiency and reliability in hydrological modelling, it is important not to overlook the role of detailed local knowledge of an area and the role of a modeller's expertise.

The GUI has been designed to be simple and easy to use whilst the underlying code has been designed to be flexible. There is much scope to use the code for other purposes, for example, building different conceptual models (e.g. altering the boundary conditions, the universal parameters etc.), generating input files for models other than SHETRAN or even applying the framework to other countries. Many countries already have national datasets which could easily replace those presented here. Indeed, as a starting point for any country, a series of global datasets could be used including the Shuttle Radar Topography Mission (SRTM) DEM (Jarvis et al., 2008), the FAO harmonised world soil database (Nachtergaele and Batjes, 2012), the NASAUSGS Global Land Survey (GLS) datasets (Gutman et al., 2013) and a global, 50-yr, 3hourly, 1.0° dataset of meteorological forcings (Sheffield et al., 2006). The global maps would need to be projected onto an equal area grid and have SHETRAN compatible properties assigned to them, as described here, before being incorporated into the system. As discussed in the introduction, SHETRAN has been used to model catchments across the



Fig. 2. An example simulation of the Eden at Temple Sowerby using the automated, uncalibrated set up of SHETRAN. NSE = 0.8.

world and it is likely that the main limiting factor for international modelling would be the quality of the input datasets used, not the physical processes being represented in SHETRAN itself. The most difficult data to obtain would be a parameterized hydrogeological dataset and this would be a major limitation when trying to model groundwater dominated catchments.

### 8. Conclusion

This paper has detailed the datasets, processing and software development involved in setting up a national SHETRAN modelling system for Great Britain. Freely available data were collated and processed into 1 km rasters aligned with the British National Grid. The datasets together describe the country's physical, hydrological and climatic characteristics. Modifications were made to SHETRAN itself to permit more realistic input data, such as by allowing distributed precipitation inputs, as well as to enhance representation of some hydrological processes. For example, channel delineation was improved by using a minimum DEM, with modifications also made to handle DEM sinks and improve the treatment of lakes in SHETRAN. A graphical user-interface was developed so that modellers can rapidly set up a SHETRAN catchment model. The system could be straightforwardly transferred to other regions of the world using global or national datasets. Forthcoming publications will examine the robustness of the system, assess the performance of simulations and outline ways in which it could be used for impact case studies. Whilst the datasets have been set up and used in SHETRAN, it would be very simple to use exactly the same data in any other model code. The xml file, precipitation data and ASCII grids produced could be easily adapted to be used by any other distributed hydrological model.

#### 9. Software availability

SHETRAN-GB was developed by Elizabeth Lewis and Stephen Birkinshaw. The software is available from Elizabeth Lewis (elizabeth. lewis2@ncl.ac.uk) Cassie Building, Newcastle University, Newcastle upon Tyne, NE1 7RU, UK. Software first available from January 2016 for free under academic licence. Software requires a regular desktop



Fig. 3. The river network generated by SHETRAN for the Eden at Temple Sowerby using the automated, uncalibrated set up of SHETRAN compared to the actual river network at 1 km resolution (left) and 500 m resolution (right).

computer with Windows and Python 2.7 with 'osgeo', 'Image', 'Imagedraw' and 'tornado' modules SHETRAN-GB is 245.1 GB as a bundle of python scripts. exe files and an ASCII data archive. Technical documentation is embedded directly in the code through comments. User documentation is provided separately which provides a worked example of how to use the software.

#### Acknowledgements

Funding: this work was supported by the Natural Environment Research Council [NE/J500239/1]. Hayley J Fowler is funded by the Wolfson Foundation and the Royal Society as a Royal Society Wolfson Research Merit Award (WM140025) holder. Contains data from the UK National River Flow Archive, hosted by the Centre for Ecology & Hydrology and operated in partnership with UK hydrometric measuring authorities. ©Crown Copyright 2009. The UK Climate Projections data have been made available by the Department of the Environment, Food and Rural Affairs (Defra) and Department of Energy and Climate Change (DECC) under licence from the Met Office, Newcastle University, University of East Anglia and Proudman Oceanographic Laboratory. These organisations accept no responsibility for any inaccuracies or omissions in the data, nor for any loss or damage directly or indirectly caused to any person or body by reason of, or arising out of, any use of this data. LCM 2007 ©and database right NERC (CEH) 2011. All rights reserved. Contains Ordnance Survey data ©Crown copyright and database right 2007.

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