Regional water resources assessments using hydrological models: making the methods more transparent and available to a broader community of users.

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Highlights:

- A detailed overview of the Pitman rainfall-runoff model and an associated uncertainty framework are presented.
- A 2-stage uncertainty version of the model that is based on constraining model output ensembles using indices of sub-basin hydrological response.
- The model, uncertainty approach and software implementation are designed to be flexible, relatively easy to understand and applicable for scientific studies or practical water resources assessments.

Abstract: There are many hydrological models available worldwide, and almost as many methods for applying them in regional water resources assessments. However, there has been recent criticism of the way in they are presented in the literature; some leveled at the lack of transparency and the need to spend much time grasping the concepts and accessing models for use. An overview of the Pitman rainfall-runoff model and how it is applied in an uncertainty framework is presented. The paper attempts to clarify some frequently asked questions about the model, the uncertainty approach and the software interface used to apply the model. Some of the paper contains 'user manual' type information, but the remainder presents an argument for the adopted uncertainty approach that is based on constraining model output ensembles using hydrological response indices, a topic of major interest in the hydrological sciences over the last decade or more.

Key words: model accessibility; uncertainty; basin response characteristics; hydrological indices.

1. INTRODUCTION

There are many different models available throughout the world that can be used to simulate the hydrological response of river basins to climate inputs and the volume of the scientific literature on the application of models for either scientific investigations, or practical use, is huge (Pechlivanidis, 2011; Todini, 2011; Bourdin, 2012; Hughes, 2013; Fatichi et al., 2016). The majority of modelling publications supply a basic description of the model (or a linked reference to where the description can be obtained), a summary of the physical characteristics of the area, the objective of the modelling study, a summary of the methods used and a summary of the model results. All of this information is useful to understand the nature of the model and of the study, but is rarely sufficient for another potential user to repeat the experiment or apply the same experiment to their own regions. Typically, the reason for this would be the limited space available in a traditional scientific publication to cover all of the ground necessary for someone else to apply the model in the same way. Many models (and modelling frameworks) are available as open source software, but not all are accompanied by user manuals that are comprehensive enough to repeat the science behind a specific model application. The user manuals that are available (including those that accompany commercial modelling software) typically explain the software utilities, but rarely do they explain the best scientific practice to be followed when using the model. In contrast, there have been frequent calls in recent years for a great deal more openness (Easterbrook, 2014), transparency and community sharing of data, models and methods within the scientific community. Yu et al. (2016) provide a comprehensive discussion of the issues associated with practicing open science as well as a large number of references to other published papers and websites covering the same or similar material. This topic was also referred to in a recent joint editorial published by several hydrological sciences journals (Koutsoyiannis et al., 2016).

Some of the issues raised refer to the transparency and reproducibility of modelling studies and there is a growing trend for the data used in modelling studies to be made more widely available. However, Yu et al. (2016) focus on the fact that 'few resources have been made accessible to the potentially large group of earth science and engineering users' and that 'New users have to invest an extraordinary effort to study the models'. One their conclusions is that 'open science practice in publications would promote the utility of open source software' and 'promote the utility of journal papers'. These issues are arguably of particular relevance to the community of young research hydrologists in developing countries who generally have poor access to experienced hydrological modellers to provide the necessary guidance and mentorship to get them started on their own research projects (Hughes et al., 2014) and to apply similar methods that they have read about in the scientific literature.

The Institute for Water research (IWR) of Rhodes University, South Africa have published a number of modelling studies in the last few years based on the monthly time step Pitman (Pitman, 1973) rainfall-runoff model (Hughes, 2013). The model has been widely used for both research and water resources assessment practice in the southern Africa region, and many of the published studies have been about developing and testing uncertainty approaches for the application of the model (Hughes, 2016). While the IWR has to accept that it is equally guilty of an unintentional lack of complete transparency in the format and content of these publications, part of the reason is that the uncertainty approaches to running the model have been under continual development and refinement. However, we believe that they have now been sufficiently tested and can be applied elsewhere and by others within the hydrological modelling community. Aligned with the principles expressed by Yu et al. (2016) about open science, it seems appropriate to disseminate the ideas more broadly.

The IWR version (Hughes, 2004) of the original Pitman (1973) model is implemented through a generic modelling framework called SPATSIM (SPatial And Time Series Information Management; Hughes and Forsyth, 2006) that facilitates the storage and management of the types of data used in environmental modelling and provides direct links to a range of models and data analysis procedures. In disseminating information about how to use the Pitman model it is therefore also necessary to refer to the way in which the model (and associated data inputs and outputs) is set up within the SPATSIM framework. To avoid a large number of figures in the main body of this paper, reference is made to the existing SPATSIM help system as well as to the pages (SP1 to SP41) of a supplementary powerpoint file accompanying this submission, which includes annotated screen shots of the software. This paper is designed to present not only the details of how to set up an application of the Pitman model within SPATSIM (the 'user manual' component), but also the scientific and conceptual background to setting up an application (the 'hydrological science' component). Many of the citations in this paper provide links to other studies where the model has been applied, while others give credit to the international literature that provided the key ideas behind the approaches used in the application of the model and particularly the methods for incorporating uncertainty.

2. THE BASICS OF SPATSIM

SPATSIM is available for download from the website of the Institute for Water Research at Rhodes University (http://iwr.ru.ac.za/iwr/software/spatsimupdate.php). SP1 illustrates the main SPATSIM screen and the basic concept of the framework is a relational database linking the spatial elements (polygons or points) of a shape file (feature) with data associated with a range of different attribute types. These include single values, text, tables or arrays, time series and even graphical or photo data (SP2). The general principle for accessing any data (either for simple display purposes or for use with a model or data analysis procedure) is the link between the shape file spatial record and the data record in a series of related database tables (see SPATSIM HELP – Database). They key design principle is to keep all of the data that might be relevant to a specific modelling project in one place and accessible through a common software platform. While the SPATSIM help system provides quite detailed guidelines for using the various menu options, a brief summary of some of the more important components from a hydrological modelling perspective is provided in the following sub-sections.

2.1 Importing data to SPATSIM database attributes

The menu items (SP1) include options for importing attribute data from text files in various formats. Most of the attribute data (not time series data) can be entered manually simply by highlighting the attribute name, selecting the one of the display data icons and then clicking on the spatial element of interest (SP3). More commonly, a user will wish to import data for more than one spatial element and bulk import facilities are available to do this based on the contents of the 'Desc.' field of the shape file, which is also used to label the spatial elements on the displayed map. SP4 to SP7 provide some illustrations of how to import data from text files to different attribute types. The design principle has been to make the import of information contained in different original formats as efficient as possible. The 'Attribute' – 'Export Attributes' menu option can be used to create similar text files and exchange data between SPATSIM applications.

2.2 Internal SPATSIM data analysis procedures

A distinction is made in SPATSIM between data analysis procedures that are thought to be common to many hydrological studies and a range of specific models (such as the Pitman model) that use SPATSIM data as input (or generate new data that are stored in SPATSIM). The former are included as internal analysis procedures, while the latter are external model executable files that are linked to SPATSIM (see next sub-section). SP8 illustrates that there are a range of internal procedures and summarises some of the ones that are frequently applied, including a comprehensive summary of time series data (including baseflow analysis; Hughes et al., 2003) and a suite of methods to perform regional rainfall drought assessments (Smakhtin and Hughes, 2007). Many of these procedures generate new information that is saved back to the SPATSIM data for later use with other analysis methods or models.

2.3 External linked data analysis methods and models

The first option under this heading refers to a generic time series display and analysis program (Tsoft) that was developed prior to SPATSIM and then retro-fitted to link with SPATSIM databases (SP 9 and SP10). Full details are not provided here, but Tsoft allows for a very wide range of graphical display options for almost any type of time series data including zooming and panning, visual comparison of different time series, scatterplot and statistical comparisons, monthly distributions, flow duration curves, etc.

One of the key design principles of SPATSIM is to provide a common data repository and application framework for a number of different kinds of water resources assessment models, some of which may share data inputs or outputs. Over the years, this has proved to be very successful and the IWR have developed a wide range of different models including several versions of the Pitman model (Hughes, 2013), a variable time interval rainfall-runoff model (Hughes and Sami, 1994), several models to support environmental flow assessments (Hughes, 2006; Hughes et al., 2014) and many others. The advantage of SPATSIM from a developer's perspective is that all of the input/output procedures are common and code development can focus on the model algorithms. The advantage from a user perspective is that the models are all accessible from a common platform and access a common database. The use of binary large objects for storing time series data also reduces data storage space, although that is not as important an issue now as it used to be. Setting up a model will be discussed in more detail later with reference to the Pitman model, but a short summary is provided here and in SP11 to SP13 of the supplementary file.

When the ‘Application’ – ‘Run Process’ – ‘Select Items’ option is chosen, three spatial element selection icons are activated. The ‘Select Spatial Element’ is used for models that work with single spatial units, while the ‘Select Upstream Elements’ is used for semi-distributed sub-basin models such as the Pitman model. In the latter case it is necessary to have a text attribute highlighted that is populated with the names of the next downstream spatial element in the sequence of sub-basins. A click on the most downstream element will then allow SPATSIM to identify all the spatial elements to be included in the model run, as well as identifying their upstream - downstream connections (SP 11). The next step is to select the model to be applied from the list (top right of SP 11) and begin the process of linking model data requirements (or outputs) to the available SPATSIM attributes (SP 12 to SP 14). The list of models displayed in SP 11 is taken from the first text line of all the *.req files found in the SPATSIM/text_data folder of the current SPATSIM application (see SP 12 for an example). The body of the *.req files lists the type of data used as model inputs or outputs (SP 12) and SP 13 illustrates the process for linking these to existing data stored in a SPATSM database, while SP 14 illustrates how model applications are stored for later running or editing.

2.4 Summary

Some users of SPATSIM, whose sole focus is on a single model, have criticised the approaches to data storage and setting up a model as excessively complicated. However, these criticisms miss the point that SPATSIM was created as a generic framework for storing different types of data and running several models. It is inevitable that there will be an overhead in terms of extra steps in a setup process when trying to cater for a wide range of possibilities. More experienced users of the framework, and especially those who need to run several associated models to achieve their objectives, recognize the advantages of a common data platform and common methods for setting up models and analyzing the results.

3. USING THE PITMAN MODEL IN SPATSIM

This section provides further guidelines for the application of the current IWR version of the Pitman model and the focus is on the use of the software and the hydrological science concepts that users should be familiar with to get the most effective results in the most efficient way. The full details of the model algorithms are not included in this paper but have been presented elsewhere including the original Pitman (1973) report and Hughes (2004) for the more recently added groundwater functions. Arguably, one of the best (and most accessible) sources for a full explanation of the model structure is Kapangaziwiri (2008) because this also includes a detailed exploration of the likely physical meaning of the parameters and model structure. The focus in this paper is on the basic structure of the model (Figure 1), the effects on model outputs of changing the parameter values and the likely range of values in different types of basins. These are considered to be the most important issues when applying the model in either an uncertainty framework, or using simple manual calibration methods. The following explanations and guidelines also refer to the key equifinalities (Beven, 2006) between parameters within the model. The model is semi-distributed and all of the parameter values and climate inputs must be quantified for each sub-basin in the system.

3.1 Parameters for natural hydrological sub-basin responses

The *Rain distribution factor (RDF)* was added as a parameter when the model was applied to tropical areas of southern Africa, while originally a fixed value of 1.28 was used. While the rainfall inputs are monthly depths, most of the model algorithms operate over 4 iterations to avoid large changes in some state variables during high rainfalls and to overcome some of the problems related to the order in which model components are calculated during such times. A smaller RDF value implies more evenly spaced rainfall over the 4 iteration steps, while the default value of 1.28 assumes most of the rain falls within the 2 middle steps. A smaller value of RDF therefore tends to generate less surface runoff as the maximum rainfall depth within any of the iterations will be lower. Values of 0.6 to 0.8 have been used for tropical climates where daily rainfalls within a wet season month tend to be more evenly distributed than in temperate or semi-arid climates (Mwelwa, 2006).

The *Proportion of impervious area (AI)* parameter is rarely used, although could be important for basins with urban areas directly connect to rivers, and refers to the fraction of the area that generates direct runoff from rainfall and the volume of surface runoff is very sensitive to its value.

The IWR version of the model allows for seasonal variations of *Interception capacity (PI1s, PI1w, PI2S, PI2w)* for two different vegetation types. The seasonality between the 'summer (s)' and 'winter (w)' values is controlled by the first column of 'Mean Monthly Distribution Data' input to the model (SP 13 and see also ZMINs and ZMINw). Values of less than 1.5 to about 4.0 mm are appropriate for land covers varying from grassland to forest. The model results using PI values of ~4.0 for plantation forests are consistent with field data provided by Roberts et al. (2015). The *% Area of Veg2 (AFOR)* is used in association with PI2s and PI2w to define that part of the sub-basin where different interception (i.e. PI2) and evaporation rates (FF) are considered to apply. It is typically used when simulating the impacts of commercial afforestation. Similarly, the *Veg2/Veg1 Pot. Evap Ratio (FF)* is used to scale the evaporation demand for vegetation type 2 relative to type 1 and allows for increased evapotranspiration losses from the AFOR part of the sub-basin. Based on experience, a value of 1.4 appears to be appropriate for high water demand commercial forest plantations in South Africa. While *Annual Pan Evaporation (PEVAP mm)* is not strictly a parameter, one advantage of including it in the parameter list is that it can assume uncertain values (see later). The model uses a fixed monthly distribution of potential evapotranspiration (the annual value is distributed using the monthly percentages contained within the 'mean monthly evaporation' input to the model: SP 13). The *Evaporation storage coefficient (R)* has values between 0 and 1 and determines the reduction in evapotranspiration with reductions in relative moisture storage. A value of 1 implies lower rates at low moisture states (shallow rooted vegetation), while a value of 0 generates higher evapotranspiration rates (deep rooted vegetation).

The *Surface runoff parameters (ZMINs, ZMINw, ZAVE and ZMAX mm month^{-1})* define the shape of an asymmetric triangular distribution that quantifies the surface runoff response to rainfall (Figure 2a). Clearly, lower values of ZMIN equate to more frequent surface runoff, while low values of ZMAX can lead to very high volumes of runoff at high rainfall rates. Typical values of ZMIN are from 0 mm (for semi-arid catchments with thin soils) to over 100 mm for areas with deep soils and low slopes. ZMAX values similarly range from as low as 200 mm to over 1 200 mm in tropical areas experiencing very little surface runoff. It is not always easy to decide on the asymmetry of the triangular distribution and it is frequently set to be symmetric (ZAVE = (ZMAX – ZMIN)/2).

The *Maximum moisture storage (ST mm)* represents the maximum storage depth of the unsaturated zone and all rainfall not intercepted or diverted to surface runoff will be added to this storage, while evapotranspiration, drainage and groundwater recharge are outputs. If the maximum value is exceeded in any model time step the balance becomes surface runoff. Typical values range from 100 mm (or even less) in arid areas with thin soils to over 1 000 mm in catchments with deep soils or deep weathered rock material.

The *Interflow parameters (FT in mm month^{-1} and POW)* define the non-linear relationship between interflow runoff and relative moisture storage. FT defines the maximum runoff at ST, while POW represents the power of the function (Figure 2b). FT should always be zero in naturally ephemeral rivers, while values of over 100 mm have been used in areas with very high baseflows. POW tends to vary between 1.8 and 3.5. Similarly, the *Groundwater recharge parameters (GW in mm month^{-1}, GPOW and SL)* define the non-linear relationship between groundwater recharge and relative moisture storage using the same type of function as for interflow, but with an additional parameter defining the moisture content below which recharge ceases (SL).

The *Sub-area routing coefficient (TL in months)* attenuates all of the runoff generated within a single sub-basin and typically has a value of 0.25 months, but could be greater for very large sub-basins (> 1 000 km^2) or less for small sub-basins (< 20 km^2). The *Channel routing coefficient (CL in months)* attenuates the upstream inflow passing through a sub-basin and is only used in sub-basins with large channels (Hughes et al. (2006) used values of 0.1 to 0.25 for downstream sub-basins of the Okavango River) where monthly time-scale attenuations might be expected.

Groundwater storage and outflow parameters (Hughes, 2004): The *drainage density* parameter determines the geometry of the sub-surface groundwater storage zone including the width of outflow to a downstream sub-basin. Both *storativity* (typically between 0.001 and 0.01) and *transmissivity* (typically between 10 and 30 m^2 d^{-1}) affect the rate of groundwater outflow (to the river and to a downstream sub-basin) for a given depth of recharge. The *groundwater slope* (fraction) influences the rate of groundwater outflow to a downstream sub-basin, while *rest water level* (m below surface) is only important in catchments where groundwater levels are generally below the river level. The *riparian strip factor* represents the % of the sub-basin area where groundwater losses to evapotranspiration (from shallow groundwater adjacent to channels) are assumed to occur. The *channel loss parameter* (TLGMax in mm) is used to calculate transmission losses at times when the groundwater level is below the channel and only applies to semi-arid and arid basins. No clear guidelines are available for quantifying this parameter.

3.2 Key equifinalities within the parameter set

The Pitman model has often been criticized for being over-parameterised and subject to high levels of equifinality (similar model outputs for quite different parameter sets). While this cannot be denied, Hughes (2010) argued that equifinality exists in the real world and, from a basin and water management perspective, we often need to explicitly quantify the different sources of total runoff. One source of equifinality is the fact that the low flows can be generated by both an interflow and a groundwater function. Which of these dominates is frequently difficult to determine, unless reliable estimates of groundwater recharge are available. Further equifinality exists within the approaches to simulating the high flows and whether these should be dominated by saturation excess (exceedance of maximum moisture storage), infiltration excess (using ZMIN and ZMAX parameters) or a combination of both.

While resolving equifinalities in any model is best achieved with a 'real world' knowledge of the dominant runoff generation processes (Winsemius et al., 2009; Burt and McDonnell, 2015), obtaining such knowledge is not always practical in large basins and in data scarce and inaccessible regions. In the absence of field-based evidence of the different components of flow, the issues of equifinality can at least be assessed using the single run version of the model (i.e. no uncertainty: see section 3.4 and SP 16) and explore the time series of the various components of the detailed model output for different model parameter combinations. SP 15 lists the model state variables that are output to a binary file as complete time series during a single model run, and these binary files can be included in a Tsoft data profile (SP 10) for plotting and further analysis. It is thus possible, for example, to examine the effects of favouring either interflow (FT parameter) or groundwater (GW parameter) to achieve a similar total low flow regime. At the same time, the simulated groundwater recharge can be checked against any existing estimates (DWAF, 2005) and if the range of likely GW parameter values can be restricted to those which simulate appropriate recharge values, then the equifinality associated with the simulation of low flows can be partially resolved.

3.3 Water use parameters

Although the Pitman model is not designed to reproduce all the possible impacts of water resources developments and infrastructure, a limited number of water use components are included. The parameters that can be used to represent some land use changes through changes in interception and evapotranspiration have already been referred to above (AFOR, PI and FF).

The *Irrigation area (km2)* parameter is used to represent direct abstractions from the river for irrigation purposes and the volumes are calculated using the 2nd column of the 'mean monthly distribution data' input (SP 14). *Irrigation return flow* represents a simple fraction of the abstracted irrigation water that returns to the channel in the same month. If the *Effective rainfall fraction* is non-zero, the irrigation depth requirements (mm) are reduced by a fraction of the current monthly rainfall depth (with a check for negative requirements). *Non-irrigation direct demand (m^3 * 10^6 y^{-1})* is assumed to be direct abstractions from the river for purposes other than irrigation and the annual value is distributed by the fractional values in the 3rd column of the 'mean monthly distribution data' input (SP 14).

*Maximum dam storage (m^3 * 10^6)* is the full storage capacity of all the small dams within a single sub-basin. Inflows to this storage are restricted to the simulated flow within a sub-basin and excludes any flows from upstream sub-basins. The *% catchment area above dams* represents the proportion of the sub-area that can contribute to the small dam storage, while *A and B in dam area-volume relationship* are the constant (A) and power (B) parameters in the relationship between reservoir surface area (RA in m^2) and volume (RV in m^3), i.e. $RA = A * RV^B$. The *Irrigation area from dams (km^2)* represents the demand on the small dams and uses the 2nd column of the 'mean monthly distribution data' input (SP 14) to define monthly variations in the same way as direct river abstractions for irrigation.

*Groundwater abstractions (upper and lower slopes in m^3 * 10^6 y^{-1})* represent the annual demands from groundwater storage for abstractions remote from and close to channels (the latter having a more rapid and direct impact on groundwater contributions to stream flow than the former). The 4th column of the 'mean monthly distribution data' input (SP 14) defines the monthly variations.

It is also possible to specify a reservoir at the outlet of any sub-basin, in which case the inflows to storage are made up of the total upstream inflow rather than just the runoff from the specific sub-basin. A separate set of parameters and monthly distributions (SP 13) are then included in the model run.

3.4 Versions of the Pitman model available in SPATSIM

There are three versions of the model available within SPATSIM and all are accessed through a single executable file (SP 16). They all share the same data input/output requirements (SP 17 and SP 18) and parameter inputs that include default values as well as uncertainty information (SP 19 and SP 20). The first version of the model is the single run version and has already been referred to as useful for exploring parameter equifinality and simple manual calibration against observed data. This version is also useful for new model users as they can change parameters and immediately see the impacts on the outputs (using Tsoft).

The second and third options (incremental and cumulative uncertainty: SP 16) are the two parts of the 2-stage uncertainty approach (Figure 3) that was presented in Tumbo and Hughes (2015) and Ndzabandzaba and Hughes (2016). The first stage (incremental uncertainty) of this version runs the model up to 100 000 times only on the incremental sub-basins and compares the simulated outputs to 6 constraint ranges (SP 21) representing mean monthly stream flow ($m^3 * 10^6$) and groundwater recharge (mm), three points on the flow duration curve and the % time of zero flows. The parameter values for each run of the model are independently randomly sampled from the inputs using Normal (defined by the mean and standard deviation) or uniform (defined by the minimum and maximum values) frequency distributions. If a parameter set generates a simulation that satisfies all of the constraints, it is saved to the SPATSIM database. When (typically) 5 000 saved parameter sets have been found, the model terminates. The constraints define the uncertainty in the hydrological response behaviour of each sub-basin (Yadav et al., 2007; Westerberg et al., 2011; Westerberg et al., 2014) and therefore all of the saved parameter sets (combinations of independently sampled individual parameters) represent behavioural responses (Beven, 2012).

The second stage (cumulative uncertainty) randomly samples from the saved parameter sets for those parameters controlling the incremental sub-basin natural hydrological response, as well as independent random sampling of the range of the other parameters (downstream routing and water use) to generate (typically 10 000) ensembles of cumulative stream flow at all sub-basin outlets. The perceived advantage of such an approach is that all of the downstream ensemble outputs are made up of behavioural inputs from each of the sub-basins, where 'behavioural' is defined as being within the range of the constraints used in the first stage. The dependency index (Dep.Index in SP 19) is used to allow groups of sub-basin parameters to follow similar patterns of uncertainty. For sub-basins with the same index value, the parameters (or saved parameter sets) are sampled from a similar part of the total range. In effect this means that generally wetter (or drier) conditions will be simulated for all of the sub-basins with the same index value, while the simulated conditions in other groups of sub-basins will be independent. Figure 4 illustrates the sampling scheme in more detail where the sub-basin groups (j) are equivalent to the dependency index values.

A fourth model option is available to replace the cumulative (second) stage of the 2-stage uncertainty approach. In this model, the parameter sampling approach remains the same but is combined with up to 500 uncertain rainfall inputs. Each rainfall ensemble is combined with up to 500 parameter samples (using the same approach as previously) to generate up to 250 000 ensembles representing both rainfall input and parameter uncertainty. The uncertain rainfall data are compiled separately and can be generated by a stochastic rainfall generator (Srikanthan and Pegram, 2009) or can represent uncertainties in future rainfall regimes based on the outputs from climate models (Hughes, 2015). The fifth model option referred to in SP 16 is an older uncertainty approach and is not discussed further.

Inevitably, all of the uncertainty versions of the model generate a great deal of information and guidelines are often required to assist a user in understanding the outputs. One of the outputs (SP 22) from the 3rd model option is a text file (for each sub-basin) that lists, for every simulated ensemble, all parameter values, summary statistics of the simulated time series and a set of objective functions comparing the simulated data with any observed flows that are available and have been included as one of the model input options (SP 13). These data can be analysed in many different ways within standard spreadsheet packages (e.g. sorting on objective function values, assessing parameter interactions or determining relationships between parameters and either summary output data or objective functions). A further program (SP 23) is available to allow for some analysis and post-processing of the ensemble results (either 10 000 from the 3rd model option and stored in the SPATSIM database, or up to 250 000 from the 4th model option and stored in a binary file).

4. SETTING UP THE 2-STAGE UNCERTAINTY MODEL

The whole purpose of the 2-stage model is for the model results to be driven by the ranges of the 6 hydrological response constraints (SP 21). However, there are 3 critical issues that have to be considered when starting a new model application. The first is to determine the approach to estimating the constraint ranges and how wide their uncertainty ranges should be. The second is to ensure that the constraints are compatible with each other, while the third is to ensure that the parameter uncertainty ranges are compatible with the constraints.

4.1 Estimating constraint ranges

It is almost impossible to provide comprehensive guidelines for estimating the constraint ranges as the approach is likely to vary with each individual basin to be modelled and will depend on the amount of existing information, and/or the level of understanding of the natural hydrological response of different parts of the basin. Tumbo and Hughes (2015) adopted an approach based on analyzing the values of the indices for the available observed data in the Great Ruaha River basin in Tanzania and setting regional values from a somewhat subjective assessment of regional variations in topography, geology and climate. The uncertainties in the constraint ranges were inevitably quite high, particularly in the middle reaches of most tributaries given that most of the stream flow gauges are located either in the headwaters or on the main channel nearer the basin outlet. Further uncertainties were related to quite variable lengths of observed data records, some unquantified water uses upstream of the gauging stations, as well as some problems with apparently non-stationary stage-discharge rating curves.

Ndzabandzaba and Hughes (2016 In Press) adopted a different approach for Swaziland, where an existing set of simulations using a similar version of the Pitman model were available (Midgley et al., 1994). In this study it was assumed that all of the information content of the available observed stream flow data had been incorporated in the previous simulations, but that the information would be uncertain due to difficulties of naturalising the observed data in a region of intensive non-stationary water use, coupled with any observation errors. The constraint indices based on the previous simulations were regionalised using an index of aridity (mean annual potential evaporation/rainfall) and subjective classification of the sub-basins into zones of different topography. The study involved an iterative feedback loop where the ensemble results after step 2 (including water use data where appropriate) were compared to the observed data and the regional constraint ranges modified if necessary. The modifications involved some shifts in the constraint ranges and some narrowing of the ranges (i.e. reduction of uncertainty).

There are a number of other studies where regional analysis of either observed stream flow data or physical basin properties have been used for understanding basin behaviour (Grayson et al., 2002; Wagener et al., 2007; Sawicz et al., 2011), estimating model parameters (Farmer et al., 2003; Pokhrel and Gupta, 2009), assessing model structures (Euser et al., 2013) or setting model output constraints (Nijzink et al., 2016). All of these approaches could be adapted to provide the necessary constraint ranges used for the Pitman model. SP 24 to SP 29 illustrate a regional analysis of the 6 constraints for all of the 1 946 so-called 'quaternary' catchments of South Africa based on the simulated data used in the WR90 study (Midgley et al., 1994) and the groundwater recharge data in DWAF (2005). These diagrams illustrate the regional variation of the constraints over a large area and could be used as a starting point for expanding the Ndzabandzaba and Hughes (2016 In Press) study to the whole of South Africa, Swaziland and Lesotho.

4.2 Compatibility of constraint ranges

To a large extent, ensuring the compatibility of the constraint ranges is one of the outcomes of the regional analysis referred to in the last section. However, there may be little available data for such as the mean monthly recharge constraint and if these values were set too high (or low) it is possible that the simulated low flows would be too high (or low) to match the FDC 90% constraint (SP 21). Under such conditions it is advisable to set the initial recharge constraint range quite high and then adjust it later after some trial runs and an analysis of the results (see next section for more details). A trivial issue is to avoid making obvious errors in setting the constraints, such as having non-zero values for the FDC 90% constraint and values of greater the 10% for the %Zero Flows constraint.

4.3 Compatibility of parameter and constraint ranges

A more difficult task is to establish parameter ranges that match the constraint ranges so that at least some behavioral ensembles are produced. It is possible to start with quite large parameter ranges, but this often leads to relatively few behavioural ensembles as the total parameter space to be sampled is large. A utility is available to explore the saved parameter sets (bottom left button on SP 16), which can also be useful when no behavioural ensembles are found. The supplementary figures SP 30 to SP 33 illustrate how this utility can be used. SP 30 illustrates the general layout of the utility that includes options to select the sub-area and up to 5 parameters for analysis. The first graph (top left) shows the frequency distributions of the constraint values for 5 equally spaced groups in the range between their minimum and maximum values (to identify any bias towards either extreme). The remaining 5 graphs show the frequency distributions of the saved parameter values using 10 equally spaced groups. The latter are used to identify any bias and to indicate if the parameter ranges should be changed to either achieve more behavioural ensembles or to achieve the required number more efficiently by excluding values that are not compatible with the constraint ranges.

SP 31 illustrates how the utility can be used to identify the critical constraints if no behavioral simulations are found. In this case the critical constraint is the mean monthly groundwater recharge and reducing the maximum groundwater recharge parameter (GW) range from 35 to 50 mm month^{-1} to 10 to 25 mm month^{-1} allows 103 behavioural simulations to be achieved out of a total of 1 000 (SP 32). Further progressive reductions in GW, as well as a reduction in the ZMAX parameter affecting surface runoff generation, and an increase in the FT parameter affecting interflow results in 1 000 behavioural simulations from 5 400 total runs (SP 33). The model was re-run with a maximum of 100 000 samples and some 27 000 were required to get the 5 000 behavioural outputs that are considered an appropriate number for the second stage of the model where all the sub-basins are simulated together.

This process therefore represents a form of manual calibration, but not of single parameter values against observed time series (as in the traditional sense), but rather of parameter ranges versus constraint ranges. It is conceivable that a more sophisticated optimization approach (Pechlivanidis, et al., 2011) could be used to determine the most appropriate parameter ranges to match the constraints. However, manually setting the parameter ranges represents a good way for inexperienced users to gain a better understanding of the links between parameter changes and model response, which will always be useful in improving their ability to use the model efficiently. SP 34 to SP 38 provide some very basic guidelines for setting up initial parameter ranges. In some situations, a user may decide to limit the number of parameters that are considered uncertain and focus on those that impact mostly on the constraints (ZMIN, ZMAX, ST, FT, GW, R and Riparian strip width). However, it would always be wise to ensure that the values of the fixed parameters are appropriate and based on either experience or some trial single model runs. In other situations, it may be desirable to allow more parameters to be uncertain and to spend more time examining the effects on the model outputs (SP 30 to SP 33) and progressively refining the parameter ranges to achieve a reasonably efficient solution that generates enough behavioural ensembles.

4.4 Running the 2nd stage of the model under natural and modified conditions

While the uncertainty for the parameters that determine the natural flow regime simulations of each sub-basin has been dealt with during the 1st stage (and saved as parameter sets for use in the 2nd stage), there could be additional uncertainty in the downstream routing (parameters CL and TLGMax: SP 35). However, the key issue with the 2nd stage of the model is to add the values for the water use parameters, with or without uncertainty, so that the results can be compared with downstream observed data that will inevitably include these impacts. SP 39 and SP 40 lists the water use parameters that are available within the model. There are additional options to include the specifications for a large reservoir or a wetland (Hughes et al., 2014) that occurs at the outlet of a sub-area. SP 22 lists the contents of the output text file that is generated during stage 2 for each sub-basin. The objective function statistics within this file can be used to assess the validity of the cumulative flow simulations at any gauging station and if necessary identify any changes that need to be made to the constraint ranges or water use parameters (Ndzabandzaba and Hughes, 2016 In Press). SP 23 refers to the post-processing utility that outputs the ranges of the ensemble simulations and which can be used to compare the simulated and observed flow duration curve characteristics (SP 41).

5. DISCUSSION AND CONCLUSIONS

The development of the 2-stage uncertainty version of the Pitman model was largely driven by a desire to implement uncertainty methods for practical purposes. It was therefore considered essential to keep the concepts reasonably simple and understandable by practitioners within the southern African community, who have traditionally applied the model through manual calibration. The successful application of the method continues to rely on some manual calibration in setting up input parameter ranges that are compatible with the constraint indices. While more complex searching and sampling approaches could be used (Pechlivanidis, et al., 2011), the need for some manual interventions by the model user is believed to be a good learning experience for new users.

In designing the software tools associated with the approach, a key principle was to make the sources of the simulation uncertainties as transparent as possible and completely accessible to the model user (SP 19 to SP 23). A further key principle was to acknowledge that any practical approach needs to generate uncertainty bounds that are realistic and that these bounds will be different under different circumstances, even within a single river basin. The response characteristics of some parts of a basin may be well understood and not very uncertain (due to good quality gauging records, for example), while the understanding of other parts may be quite poor. The suggested approach allows for such flexibility, and variations in the degree of uncertainty are simply determined through the size of the constraint ranges. Arguably, the most difficult part of the 2-stage approach is establishing appropriate constraint ranges. Unfortunately, this is also the part for which it is difficult to offer clear and comprehensive guidelines for new users. The amount, quality and appropriateness of the information that is available to characterise hydrological responses to climate inputs is hugely variable, even within a limited geographic region. However, the perceived advantage of the approach is that it is mainly driven by, and dependent upon, developing an understanding of the response characteristics of the basin being modelled, rather than any mathematical or statistical 'fitting' process. Apart from the fact that such 'fitting' processes are impossible in totally ungauged basins, the authors would argue that mathematical fitting is no substitute for a real, if uncertain, 'hydrological' understanding (Hughes, 2010), particularly in a world that is constantly changing (Montanari et al., 2013).

The main focus of this paper has been on the IWR's version of the Pitman model, the 2-stage uncertainty approach and their implementation in the SPATSIM framework. Most of the applications of this suite of hydrological tools have been in southern Africa, where data scarcity is a key consideration. However, there is no reason to suggest that the tools could not be used in other regions (where snowmelt is absent), nor is there any reason why the simple uncertainty approach adopted for the Pitman model could not be used with other models of a similar type.

SOFTWARE AVAILABILITY

The SPATSIM software and some test applications can be downloaded at no charge from the website of the Institute for Water Research (IWR) at Rhodes University (http://iwr.ru.ac.za/iwr/software/spatsimupdate.php). The software has been developed by the IWR mostly by Prof D A Hughes (d.hughes@ru.ac.za) and Mr D A Forsyth (d.forsyth@ru.ac.za) who can be contacted for further details (preferably by email but the telephone contact is +27 46 6224014). The software is written in Delphi and uses a Paradox database structure for storing data. It will run on any Windows PC platform if the website install instructions are strictly followed. The size of the main program download is 64Mb. The SPATSIM software was originally developed in 2004, but has been continuously updated since then. Most of the recent Pitman model applications were developed during 2015 and 2016.

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List of Figures

Figure 2 Principles of the surface runoff function (a) and the interflow and groundwater recharge functions (b).

Figure 3 Illustration of the 2-stage uncertainty approach using constraints on expected hydrological response.

Figure 4 Parameter sampling scheme for the 2nd part of the 2-stage uncertainty version of the SPATSIM implementation of the Pitman model.

Figure 1

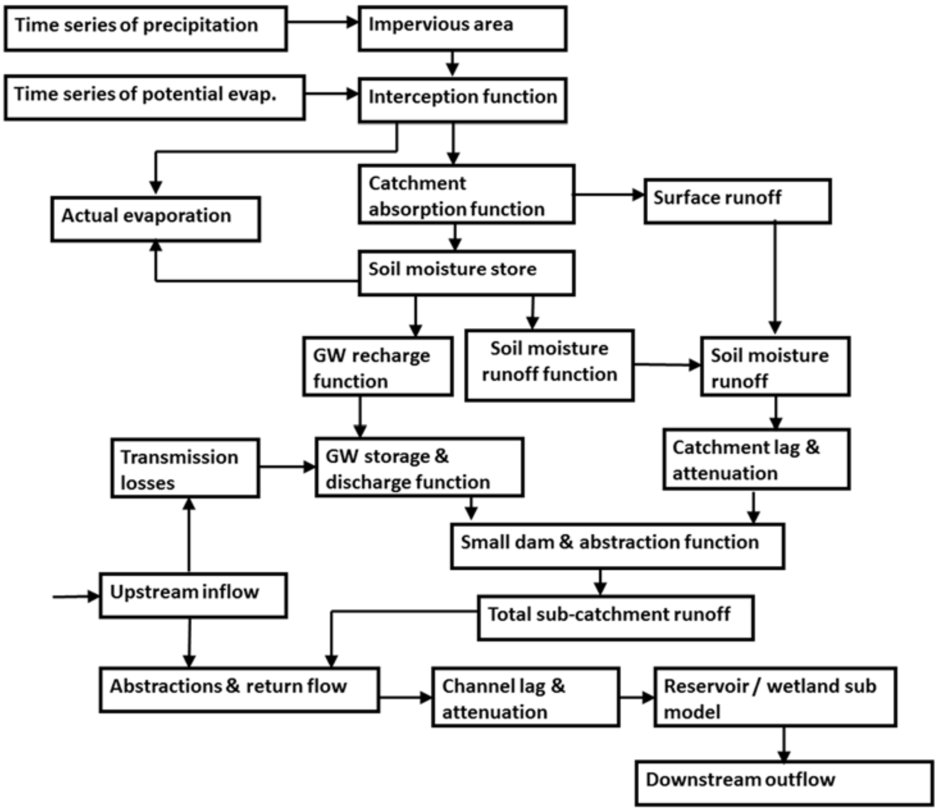

Time series of precipitation
Impervious area
Time series of potential evap.
Interception function
Actual evaporation
Catchment absorption function
Surface runoff
Soil moisture store
GW recharge function
Soil moisture runoff function
Soil moisture runoff
Transmission losses
GW storage & discharge function
Catchment lag & attenuation
Small dam & abstraction function
Upstream inflow
Total sub-catchment runoff
Abstractions & return flow
Channel lag & attenuation
Reservoir / wetland sub model
Downstream outflow

Figure 2

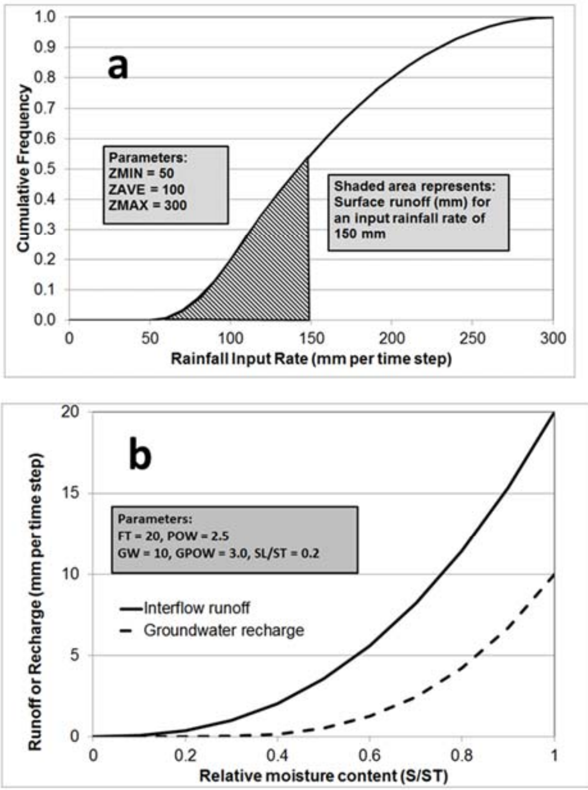

a
Cumulative Frequency
Rainfall Input Rate (mm per time step)
Parameters:
ZMIN = 50
ZAVE = 100
ZMAX = 300
Shaded area represents:
Surface runoff (mm) for
an input rainfall rate of
150 mm
b
Runoff or Recharge (mm per time step)
Relative moisture content (S/ST)
Parameters:
FT = 20, POW = 2.5
GW = 10, GPOW = 3.0, SL/ST = 0.2
Interflow runoff
Groundwater recharge

Figure 3

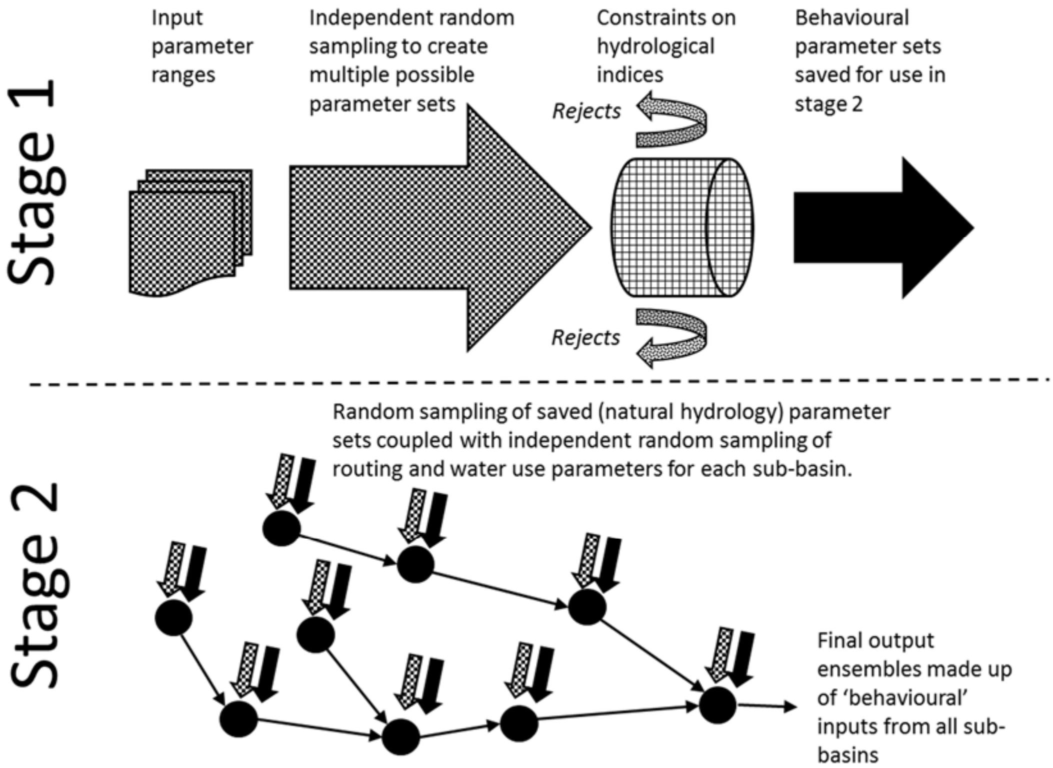
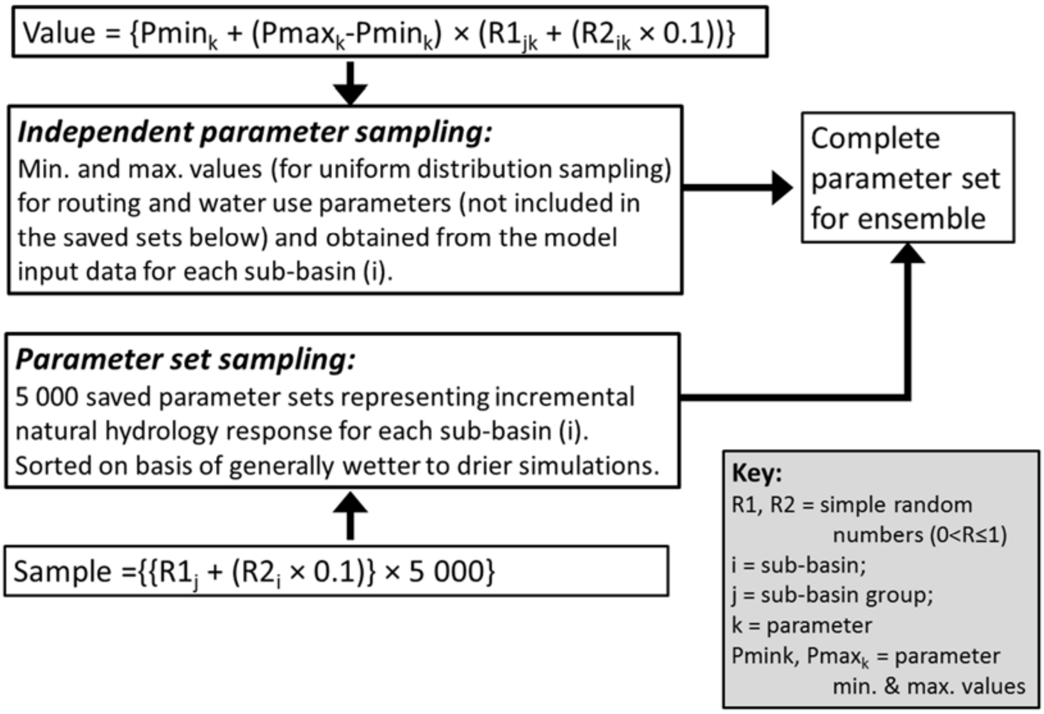

Stage 1
Input parameter ranges
Independent random sampling to create multiple possible parameter sets
Constraints on hydrological indices
Rejects
Rejects
Behavioural parameter sets saved for use in stage 2
Stage 2
Random sampling of saved (natural hydrology) parameter sets coupled with independent random sampling of routing and water use parameters for each sub-basin.
Final output ensembles made up of 'behavioural' inputs from all sub-basins

Figure 4


Value = {$Pmin_k$ + ($Pmax_k$-$Pmin_k$) × ($R1_{jk}$ + ($R2_{ik}$ × 0.1))}
Independent parameter sampling:
Min. and max. values (for uniform distribution sampling) for routing and water use parameters (not included in the saved sets below) and obtained from the model input data for each sub-basin (i).
Complete parameter set for ensemble
Parameter set sampling:
5 000 saved parameter sets representing incremental natural hydrology response for each sub-basin (i). Sorted on basis of generally wetter to drier simulations.
Sample ={{$R1_j$ + ($R2_i$ × 0.1)} × 5 000}
Key:
R1, R2 = simple random numbers (0<R≤1)
i = sub-basin;
j = sub-basin group;
k = parameter
Pmink, $Pmax_k$ = parameter min. & max. values