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Misrepresentation and amendment of soil moisture in conceptual hydrological modelling

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Abstract

Although many conceptual models are very effective in simulating river runoff, their soil moisture schemes are generally not realistic in comparison with the reality (i.e., getting the right answers for the wrong reasons). This study reveals two significant misrepresentations in those models through a case study using the Xinanjiang model which is representative of many well-known conceptual hydrological models. The first is the setting of the upper limit of its soil moisture at the field capacity, due to the ‘holding excess runoff’ concept (i.e., runoff begins on repletion of its storage to the field capacity). The second is neglect of capillary rise of water movement. A new scheme is therefore proposed to overcome those two issues. The amended model is as effective as its original form in flow modelling, but represents more logically realistic soil water processes. The purpose of the study is to enable the hydrological model to get the right answers for the right reasons. Therefore, the new model structure has a better capability in potentially assimilating soil moisture observations to enhance its real-time flood forecasting accuracy. The new scheme is evaluated in the Pontiac catchment of the USA through a comparison with satellite observed soil moisture. The correlation between the XAJ and the observed soil moisture is enhanced significantly from 0.64 to 0.70. In addition, a new soil moisture term called SMDS (Soil Moisture Deficit to Saturation) is proposed to complement the conventional SMD (Soil Moisture Deficit).

Keywords: Satellite soil moisture observations, Holding excess runoff, Soil moisture deficit (SMD), Soil Moisture Deficit to Saturation (SMDS), Xinanjiang (XAJ), Soil Moisture and

1. Introduction

Overestimation and underestimation of flood peaks are common in hydrological modelling, especially in operational flood forecasting due to the errors in antecedent soil moisture estimation ([Huza et al., 2014](#)). This is usually caused by the accumulated errors in the model's soil moisture state variable which is difficult to rectify until the flood peaks are passed (by that time, it is too late for practical purposes). Therefore, it is important to assimilate the soil moisture observation data into an operational hydrological model to reduce error accumulation ([Berthet et al., 2009](#); [Brocca et al., 2012](#); [Ottlé and Vidal-Madjar, 1994](#); [Ridler et al., 2014](#); [Wagner et al., 2007](#); [Wanders et al., 2014](#)).

Among all the operational hydrological model types, conceptual rainfall-runoff models have shown their superiority and popularity in real-time flood forecasting compared with other types of models used in an operational context ([Christian, 1997](#); [Perrin et al., 2001](#); [Reed et al., 2004](#); [Wood et al., 1997](#); [Zhuo et al., 2014](#)). This is because they are simple yet effective in modelling the most important features of the river flow ([Kitanidis and Bras, 1980a](#); [1980b](#); [Zhao and Liu, 1995](#)). However many conceptual models based on the variable soil water storage curve (to be explained later) have misrepresented soil moisture variable. This soil moisture misrepresentation can significantly reduce the model's capability in data assimilation during operational mode, because of its incompatibility with the observed soil moisture information. A number of attempts have been made by various studies to assimilate soil

moisture observations in conceptual hydrological models. For example, [Aubert et al. \(2003\)](#) used a sequential assimilation procedure by introducing ground measured soil moisture data into a conceptual rainfall-runoff model and obtained improved flow prediction results; [Brocca et al. \(2010\)](#) revealed that adopting the Advanced SCATterometer (ASCAT) soil moisture index into a rainfall-runoff model could improve model's runoff prediction; contrarily [Parajka et al. \(2006\)](#) showed that assimilating the European remote sensing satellite (ERS) derived soil moisture data into a conceptual hydrological model would not improve the runoff model efficiency; [Matgen et al. \(2012\)](#) presented that coarse-resolution remotely sensed soil moisture data added little or no extra value for runoff prediction. It is clear the effect of soil moisture assimilation in flow modelling is mixed. Interestingly [Matgen et al. \(2012\)](#) raised an open research question in the study of whether the assimilation results could mainly be attributed to errors in the soil moisture estimates, or if it was mainly related to the hydrological model itself. Currently, no particular attention has been given to improve the soil moisture scheme in the conceptual hydrological models so that they can be more compatible with the observed soil moisture information. Therefore, an improved scheme is proposed in this study to rectify the weaknesses of the existing soil moisture accounting scheme in a widely used conceptual hydrological model called Xinanjiang (XAJ) ([Zhao, 1980](#); [1992](#); [Zhao and Liu, 1995](#)) as a representative conceptual model. This is because there are many similar models to XAJ (such as PDM, HBV, etc.) so the result from XAJ would be of interest to a wide range of the hydrological modelling community. More detailed reasons for choosing XAJ as a representative model is presented later.

The new scheme includes two steps, which are discussed via a case study in the Pontiac catchment, through a comparative analysis with the observed soil moisture datasets. It is clear that field measurements do not easily suit operational conditions ([Corradini, 2014](#)) and soil moisture information derived from satellite earth observation data would significantly ease data acquisition ([Aubert et al., 2003](#)). There have been enormous investments by various organisations such as ESA (European Space Agency) and NASA (National Aeronautics and Space Administration), in a wide range of soil moisture observational programs (e.g., satellite missions such as ENVISAT (Environmental Satellite), SMOS (Soil Moisture and Ocean Salinity), SMAP (Soil Moisture Active Passive), and so on. The availability of those modern satellite soil moisture data provides a great opportunity, but also poses a challenge to hydrological modellers on how to assimilate such information in hydrological models that have not been designed for them. Therefore in this study, an attempt has been made by correlating the modified XAJ soil moisture scheme through the comparison with the SMOS ([Kerr et al., 2010](#)) satellite retrieved soil moisture.

The novelty of this study is to improve the XAJ model's soil moisture accounting representation while keeping its high flow modelling accuracy. Maintaining flow modelling effectiveness is important because XAJ has been successfully and widely applied globally (see more detail in the model description section). It is expected that the amended scheme is more realistic in representing the soil moisture information, and hence improves the model's compatibility with the satellite soil moisture observations, as well as other soil moisture data types.

In this context, the overall methodology of this study is to first analyse the original concept and structure of the XAJ model, test the existing XAJ model over a selected catchment, and explore the issues in its current soil moisture scheme through a comparative analysis with the SMOS retrieved soil moisture. The XAJ model is then amended accordingly to overcome its soil moisture misrepresentations, and re-tested over the selected catchment to evaluate the modified model's flow performance, as well as its soil moisture representation (through the comparison with the SMOS retrieved soil moisture).

2. Data and methodology

2.1 Study area and datasets

The case study is carried out in the Vermilion River at the Pontiac catchment, mid-Illinois, in the United States (U.S.) (40.878°N, 88.636°W). The reason for choosing this catchment is because of its moderate vegetation coverage (the annual averaged Normalized Difference Vegetation Index retrieved from the MODIS (Moderate Resolution Imaging Spectroradiometer) satellite is around 0.4) which should give a better satellite soil moisture retrieval result than densely vegetated catchments ([Al Bitar et al., 2012](#)). Furthermore this medium-sized catchment (1,500 km²) has a similar spatial scale with the SMOS footprint, therefore there is no spatial mismatch between them. However if the satellite footprint is much smaller or larger than the catchment area, further studies are required such as using the spatial downscaling method. Pontiac is dominated mainly by hot summer continental climate ([Peel et al., 2007](#)), and is used primarily for agriculture purposes ([Bartholomé and Belward, 2005](#); [Hansen, 1998](#))

with Mollisols soil type ([Webb et al., 2000](#)). The average annual rainfall depth is about 954 mm, and the average annual potential evapotranspiration demand is approximately 1670 mm. The layout of the Pontiac catchment is shown in Fig. 1 along with the location of its flow gauge, the National Aeronautics and Space Administration (NASA) Land Data Assimilation Systems 2 (NLDAS-2) grid points (a total of 20 $0.125^{\circ} \times 0.125^{\circ}$ NLDAS-2 grids with their central points shown in the figure) and river network.

The observed daily flow data is obtained from the U.S. Geological Survey for the period from January 2010 to December 2011. The data from the first two-thirds of the period (January 2010-April 2011) is used for the calibration of the XAJ model and the remaining one-third of the data (May 2011 to December 2011) is employed for the validation purpose. The reason for using this two-year period of data is due to the limitation of the flow records in this catchment, and the selected period provides the most continuous flow dataset. The XAJ model's hydrological forcing ([Peng et al., 2002](#)) is provided by the NLDAS-2 ([Mitchell et al., 2004](#)). It includes precipitation (P) ([Daly et al., 1994](#)) and potential evapotranspiration (PET) at 0.125° spatial resolution and daily temporal resolution (converted from hourly resolution). Both PET and P datasets have been transformed into one catchment-scale dataset using the area-weighted average method to operate the lumped XAJ model. Readers are referred to [Xia et al. \(2012\)](#) for a full description of the NLDAS-2 data products. The SMOS level-3 soil moisture dataset (both ascending and descending orbits) used in this study is from the SMOS Barcelona Expert Centre (SMOS-BEC) ([SMOS-BEC, 2014](#)), covering the period between January 2010 and December 2011. The retrieved soil moisture dataset has been converted into a catchment-scale dataset by

the same weighted average method.

2.2 SMOS soil moisture monitoring system

Compared with in-situ soil moisture measurement, satellite monitored soil moisture is more representative in a catchment-scale analysis, because of its large footprint ([Fang and Lakshmi, 2014](#); [Srivastava et al., 2013a](#); [2014](#)). Among all the satellite soil moisture techniques (i.e., optical, thermal infrared and microwave bands), microwave bands (especially with longer wavelength such as L-band (21 cm)) show advantages in penetrating into deeper soil (~5 cm) and have more capability in passing through cloud and some vegetation cover ([Njoku and Kong, 1977](#)). Therefore in this study, the microwave-banded SMOS (1.4 GHz, L-band) satellite is selected. The reason for choosing SMOS is not only because it is designed particularly for soil moisture monitoring, but also because it has a relatively long period of soil moisture data record since its launch in 2009 ([Kerr et al., 2010](#)). Furthermore, there have been a number of studies addressing the accuracy of the SMOS soil moisture in which the observations are able to provide useful information for catchment-scale research ([Al Bitar et al., 2012](#); [Djamai et al., 2015](#); [Louvet et al., 2015](#); [Srivastava et al., 2013a](#)). The SMOS retrieved soil moisture observation has a spatial resolution of 35-50 km ([Kerr et al., 2010](#); [2001](#)) with its unit in m^3/m^3 . SMOS has a global coverage at the equator crossing times of 6 am at the local solar time (LST) (ascending) and 6 pm (LST, descending) ([Kerr et al., 2012](#)). Readers are referred to [Kerr et al. \(2012\)](#) for a full description of the SMOS soil moisture retrieving method.

Both the ascending and the descending overpasses are firstly compared with the XAJ soil moisture deficit (SMD), as discussed in [Zhuo et al. \(2015a\)](#). For this selected catchment, there is a better correlation with the SMOS descending orbit than with the ascending orbit. Hence, only the descending observations are used in the following study.

2.3 XAJ hydrological model

There are common features among conceptual hydrological models as demonstrated by PDM ([Moore, 2007](#)), ARNO ([Todini, 1996](#)), HBV ([Geris et al., 2014](#)), and Xinanjiang (XAJ) ([Zhao, 1980](#); [1992](#); [Zhao and Liu, 1995](#)), such as using multi-bucket concepts, and unrealistic modelling of their soil moisture (e.g., their maximum soil moisture is set at the field capacity). Among them, XAJ is the first model with the multi-bucket variable-size concept in its model structure and has been followed by other models ([Beven, 2012](#)). XAJ is a widely used conceptual rainfall-runoff model. The model has been shown to be effective in simulating river flow in humid, semi-humid, and even arid catchments ([Chen et al., 2013](#); [Gan et al., 1997](#); [Shi et al., 2011](#); [Zhao, 1992](#); [Zhao and Liu, 1995](#); [Zhuo et al., 2015b](#)).

The XAJ model's main concept is runoff production via the field capacity excess runoff mechanism, which means that runoff is not generated until the soil water reaches the field capacity ([Zhao, 1992](#)). In the past, such a process has been wrongly named as Dunne's saturation excess overland runoff ([Dunne, 1978](#)). People often erroneously believe that the runoff in XAJ and other similar models such as HBV and PDM only occurs when the water content reaches the complete saturation in the soil. Here we introduce a new term called

‘holding excess runoff’ to represent the runoff above the field capacity, and to correct this misunderstanding. In XAJ, HBV, PDM and other similar models the runoff concept is that any water above the field capacity is free moving water and can only be held in the soil temporarily before it flows away as runoff. To apply such a concept in the XAJ hydrological modelling, once the soil water storage is filled up with the effective rainfall (rainfall subtracted by evapotranspiration) above the field capacity, the holding excess water will be moved immediately into the model’s free water storage for a detailed runoff calculation ([Zhao, 1980; 1992; Zhao and Liu, 1995](#)). However in reality, the holding excess water is temporarily retained in the soil for a gradual release as runoff instead of being moved immediately to the separate free water storage as represented in XAJ. This unrealistic representation of soil water would result in a negative impact on its soil moisture state, and hence lower its operational performance when soil moisture observations are assimilated. Furthermore in the XAJ model, no water movement is considered between soil layers (e.g., the capillary action is ignored), and the evapotranspiration mainly depends on the remaining soil moisture content in individual soil layers. More explanations of these two misrepresentations are provided below with relevant formulas and diagrams.

As illustrated in Fig. 2, the XAJ model consists of three key components: an evapotranspiration component, a runoff generating component and a runoff routing component. The model includes three soil layers (upper, lower and deep) which represent the three evapotranspiration parts. The upper layer refers to the vegetation and the very thin topsoil. The lower layer refers to the soil in which the vegetation roots dominate and the deep layer refers to the soil that

comprises vegetation's deep roots ([Jayawardena and Zhou, 2000](#)). Replenishment and depletion of the soil water storage in the XAJ model are driven by the P and PET forcing. In the upper layer, evapotranspiration occurs at the potential demand if there is any soil water. In other words, on exhaustion of the soil moisture from the upper layer, evapotranspiration will continue from the lower layer at a reduced demand which is proportional to the soil moisture content of that layer. Once the lower layer soil water is depleted, the deep layer will commence to evaporate ([Jayawardena and Zhou, 2000](#); [Zhao and Liu, 1995](#); [Zhuo et al., 2015a](#)). The three-layer evapotranspiration processes have been categorised into four situations and calculated using the following equations.

$$\text{If } P_{\Delta t} + WU_t \geq PET_{\Delta t} \begin{cases} EU_{\Delta t} = PET_{\Delta t} & WU_{t+1} = WU_t + P_{\Delta t} - PET_{\Delta t} \\ EL_{\Delta t} = 0 & ; WL_{t+1} = WL_t \\ ED_{\Delta t} = 0 & WD_{t+1} = WD_t \end{cases} \quad (1)$$

where Δt stands for the model time step, and in this study it is 24 hours (i.e., daily time step); t means the time at the beginning of a time step, and $t+1$ is the time at the end of a time step; P is rainfall in mm, WU , WL and WD represent the upper, lower and deep soil layers' areal mean tension water storage respectively in mm; PET is the potential evapotranspiration in mm; EU , EL , and ED stand for the upper, lower and deep soil layers' evapotranspiration respectively in mm. In Eq. 1, if there is sufficient water in the upper layer (i.e., $P + WU$ is equal to or greater than the PET), EU will be equal to PET in this layer, and there will be no evapotranspiration from the lower two layers.

$$\text{if } \begin{cases} P_{\Delta t} + WU_t < PET_{\Delta t} \\ WL_t \geq C \times WLM \\ WL_t \geq C(PET_{\Delta t} - EU_{\Delta t}) \end{cases} \begin{cases} EU_{\Delta t} = P_{\Delta t} + WU_t & WU_{t+1} = 0 \\ EL_{\Delta t} = (PET_{\Delta t} - EU_{\Delta t}) \frac{WL_t}{WLM} & WL_{t+1} = WL_t - EL_{\Delta t} \\ ED_{\Delta t} = 0 & WD_{t+1} = WD_t \end{cases} \quad (2)$$

where C is a coefficient of the deep soil layer that depends on the proportion of the catchment area covered by vegetation with deep roots; WLM is the areal mean field capacity of the lower layer in mm. In Eq. 2, if there is insufficient water in the upper layer to satisfy the PET , but there is more water in the lower layer than the specified thresholds ($C \times WLM$ and $C(PET_{\Delta t} - EU_{\Delta t})$), all the water in the upper layer is initially depleted, and then evapotranspiration will occur from the lower layer at a reduced demand of $(PET_{\Delta t} - EU_{\Delta t}) \frac{WL_t}{WLM}$, and there will be no evapotranspiration from the deep layer.

$$\text{if } \begin{cases} P_{\Delta t} + WU_t < PET_{\Delta t} \\ C(PET_{\Delta t} - EU_{\Delta t}) \leq WL_t < C \times WLM \end{cases} \begin{cases} EU_{\Delta t} = P_{\Delta t} + WU_t & WU_{t+1} = 0 \\ EL_{\Delta t} = C(PET_{\Delta t} - EU_{\Delta t}) & WL_{t+1} = WL_t - EL_{\Delta t} \\ ED_{\Delta t} = 0 & WD_{t+1} = WD_t \end{cases} \quad (3)$$

In Eq. 3, if there is insufficient water in the upper layer, and there is less water in the lower layer than a specified threshold ($C \times WLM$) but more than $C(PET_{\Delta t} - EU_{\Delta t})$, all the water in the upper layer is initially depleted, and the evapotranspiration will occur from the lower layer at the demand of $C(PET_{\Delta t} - EU_{\Delta t})$, and there will be no evapotranspiration from the deep layer..

$$\text{if } \begin{cases} P_{\Delta t} + WU_t < PET_{\Delta t} \\ WL_t < C(PET_{\Delta t} - EU_{\Delta t}) \end{cases} \begin{cases} EU_{\Delta t} = P_{\Delta t} + WU_t & WU_{t+1} = 0 \\ EL_{\Delta t} = WL_t & WL_{t+1} = 0 \\ ED_{\Delta t} = C(PET_{\Delta t} - EU_{\Delta t}) - EL_{\Delta t} & WD_{t+1} = WD_t - ED_{\Delta t} \end{cases} \quad (4)$$

In Eq. 4, if there is insufficient water in the upper and lower layers, all the water in the top two layers is depleted, and evapotranspiration will occur from the deep layer at the further reduced demand of $C(PET_{\Delta t} - EU_{\Delta t}) - EL_{\Delta t}$.

During rainfall events, PET is first subtracted and the water replenishment process at the soil column is based on storage capacities (i.e., the field capacity) of the soil layers. Any excess rainfall is numerically moved to a free water storage detached from the layers (represented by the shaded F area in Fig. 3. More discussion is provided later on). The free water in the free water storage is then separated into three runoff components (surface runoff (RS), interflow (RI) and groundwater (RG)) which are calculated by using the following equations.

if $P_{\Delta t} - PET_{\Delta t} + AU_{t-1} < SMM$,

$$\begin{cases} RS_{\Delta t} = a[P_{\Delta t} - PET_{\Delta t} + S_t - SM + SM(1 - \frac{P_{\Delta t} - PET_{\Delta t} + AU_{t-1}}{SMM})^{EX+1}] \\ S_{t+1} = S_t + P_{\Delta t} - PET_{\Delta t} - RS_{\Delta t} \\ RI_{\Delta t} = KSS \times S_{t+1} \times a \\ RG_{\Delta t} = KG \times S_{t+1} \times a \end{cases} \quad (5)$$

if $P_{\Delta t} - PET_{\Delta t} + AU_{t-1} \geq SMM$,

$$\begin{cases} RS_{\Delta t} = a(P_{\Delta t} - PET_{\Delta t} + S_t - SM) \\ S_{t+1} = S_t + P_{\Delta t} - PET_{\Delta t} - RS_{\Delta t} \\ RI_{\Delta t} = KSS \times S_{t+1} \times a \\ RG_{\Delta t} = KG \times S_{t+1} \times a \end{cases} \quad (6)$$

$$\text{where } SMM = \frac{SM}{EX + 1} \quad (7)$$

$$S_t = \int_0^{AU_{t-1}} (1 - \frac{S}{SMM})^{EX} dS = SM - SM(1 - \frac{AU_{t-1}}{SMM})^{EX+1} \quad (8)$$

$$AU_t = SMM \left[1 - (1 - \frac{S_t}{SM})^{\frac{1}{EX+1}} \right] \quad (9)$$

where a is the portion of the sub-catchment producing runoff; S is the free water in mm which can be calculated by Eq. 8; SM is the areal mean free water capacity which represents the

maximum possible deficit of free water storage in mm; EX is the exponent of the free water capacity curve; RS , RI and RG are the surface runoff, interflow and groundwater runoff, respectively in mm; KSS is the outflow coefficient of the free water storage to interflow relationship; KG is the outflow coefficient of the free water storage to groundwater relationship; SMM , and AU are the parameters related with the free water capacity curve which can be calculated from Eq. 7 and 9. Eq. 5-6 illustrate the separation of runoffs RS , RI and RG under different conditions. For more details about their derivations, readers are referred to [Zhao \(1992\)](#). Since the free water storage capacity within a catchment is non-uniform, Eq. 7 describes the maximum value. Eq. 8 represents the amount of free water. Eq. 9 is the free water in depth over a variable area depending on the distribution of the free water storage (as represented by the ‘free water curve S’ box in Fig. 2. There are several options for this curve such as exponential and Pareto, and the exponential curve is used in this study). The generated runoff components are then routed to the outlet of the catchment by the convolution of time through solving the Muskingum river routing method ([Gill, 1978](#)).

Although XAJ is already recognised as useful in simulating river hydrographs, its soil moisture is not realistically calculated based on soil water’s general movement principles. First XAJ assumes that there is no capillary rise of water from lower to upper layers (as shown in Eq. 1–4) which is clearly not true in the real field situation; second the model numerically removes the excess rainfall above the field capacity from the soil into an imaginary free water storage (as illustrated in Fig. 2 and 3, the free water amount is calculated from Eq. 5-9). Albeit these misrepresentations have little influence on the model’s flow simulation (because the water

balance is not affected), they clearly reduce the accuracy of the model's soil moisture simulation, and hence its utilisation capability of soil moisture observations during real-time flood forecasting. Therefore an amendment to the XAJ soil moisture scheme is necessary.

The XAJ's three-layer soil moisture fluctuations are represented by the SMDs in the unit of metre. SMD is an important soil moisture indicator in hydrology, which shows the amount of water to be added to a soil profile to bring it to the field capacity ([Calder et al., 1983](#); [Rushton et al., 2006](#)). The SMD can be expressed as the following formula ([Srivastava et al., 2013b](#)).

$$SMD = FC - SMC \quad (10)$$

where FC is the field capacity in metre, which is normally considered as the upper limit in hydrological modelling for soil water storage (obtained through the hydrological model calibration); SMC is the soil moisture content in metre (e.g., $WU/1000$ from Eq. 1-4 for the surface layer). In this study only the SMD from the upper soil layer is utilised (referred to as SMD hereafter) for the analysis, because it is the most scale-matched with the satellite soil moisture depth (~5 cm).

2.4 Statistical indicators

In order to evaluate the performance of the XAJ model in flow simulation, as well as to compare its soil moisture output with the SMOS soil moisture measurements, two statistical indicators are employed (Table 1). Nash-Sutcliffe Efficiency (NSE) ([Nash and Sutcliffe, 1970](#)) is used as an objective function for the XAJ calibration and validation because it is the most

widely applied indicator for examining the performance of the hydrological models ([Krause et al., 2005](#)). Pearson product moment correlation coefficient (r) is utilised to evaluate the correlation between the XAJ simulated soil moisture and the SMOS observed soil moisture.

3. Results and suggested improvements

3.1 XAJ flow simulation result

The automatic calibration and validation of the XAJ model are carried out by using the daily rainfall-runoff data (i.e., P , PET and observed flow) from 2010 to 2011. In this study, the Genetic Algorithm ([Wang, 1991](#)) is used for optimising the XAJ model's 16 parameters. Upon completing the automatic parameter optimisation, minor adjustments of the model parameter values (i.e., EX , B , WUM , WLM and WDM) are made by the trial and error method ([Chen and Adams, 2006](#)). The calibration procedure focuses especially on the modelling of the actual evapotranspiration and the partition of total runoff (i.e., surface runoff, interflow and groundwater) based on a good agreement between the estimated and the observed flow. The calibrated parameters are described in Table 2 with the ranges used and the optimal values. Fig. 4 shows that the XAJ model in this catchment is capable of producing an acceptable river hydrograph in terms of NSE results (> 0.80 during both calibration and validation phases) ([Moriasi et al., 2007](#)). Further details on calibration and validation of the XAJ model in this catchment are discussed by [Zhuo et al. \(2015a\)](#).

3.2 Misrepresentations of XAJ soil moisture scheme

To better understand the misrepresentations of the XAJ soil moisture scheme, the SMOS soil moisture observations are used for the comparison. The time series of the XAJ SMD and the SMOS soil moisture observations, as well as the associated hydrological forcing (i.e., P and PET) are shown in Fig. 5. In addition a scatter plot of the XAJ SMD against the SMOS soil moisture observations is also presented in Fig. 6. It can be seen that the correlation between the SMOS soil moisture and the XAJ SMD in terms of r (-0.64) is acceptable as compared with the published results ([Srivastava et al., 2013b](#)), however the movement of the SMD is rather misleading as seen in Fig. 5. For a better visualisation effect, a typical heavy rainfall event between Day 460 and Day 495 is presented in Fig. 7. It is clear to see that after a heavy rainfall event, the soil moisture in the XAJ only peaks at the field capacity line (as indicated by the dashed black line). However in reality, it should go up until the complete saturation occurs. In order to better understand this misrepresentation in the XAJ model, Fig. 3 illustrates its distribution of the water holding capacity based on the multi-bucket concept, as well as its connection with the three critical soil moisture states in the real field situation. It is obvious to see that in reality the wettest soil moisture is at the complete saturation point rather than the field capacity as adopted in the XAJ model. In other words, after a heavy rainfall event the upper soil layer should become completely saturated fairly quickly, and then take approximately a few days for the excess water (i.e., the holding excess runoff) to be gradually drained away to reach the field capacity point ([Rubin, 1966](#); [Veihmeyer and Hendrickson, 1931](#)). To explain this process in detail, Fig. 8 is illustrated. It can be seen that after a heavy rainfall event (when precipitation level is higher than the infiltration capacity),

surface runoff will occur immediately; because the infiltration capacity at the upper soil layer (f_s) is larger than the infiltration capacity at the lower soil layer (f_d) ([Zhao and Liu, 1995](#)), some free water is aggregated at the upper layer, however this amount of water has been subtracted from the upper soil in the conventional XAJ model. In another word, if soil water is at or above FC, all the excess rainfall (i.e., the amount of water above FC; shown as the shaded area marked with F in Fig. 3) is numerically moved to a free water storage detached from the soil layers; however part of this excess should be retained in soil and then be gradually released from the soil pores.

Another misrepresentation of the XAJ soil moisture scheme is that the upper soil layer tends to dry up faster than in reality during soil drying periods, which is unlike the real world situation where water can move from the lower layer to the upper layer through the capillary action ([Moore and Cole, 1939](#)). In the XAJ model, water movement between soil layers is not considered. As presented in Eq. 1-4, soil water in the upper layer is forced to evaporate at the full potential demand until it is totally depleted, and only then the water from the lower soil layers will start to contribute to further evapotranspiration. Although this method has little impact on the total water balance, its unrealistic mechanism leads to the abrupt soil moisture drying phenomenon as indicated in Fig. 9 (i.e., during two typical drying events).

Although the XAJ's soil moisture is misrepresented, it can still simulate river hydrograph rather effectively, but its soil moisture accounting scheme limits its compatibility with the measured soil moisture dataset in data assimilation during real-time flood forecasting.

Therefore the XAJ soil moisture scheme needs to be amended accordingly, and a proposed method is discussed in the following section.

3.3 Amendment to the XAJ soil moisture scheme

In order to rectify the XAJ model's soil moisture accounting scheme, a new approach comprising two steps is proposed as follows.

First step: the upper limit of soil moisture in the model is increased from FC to complete saturation (CS). An alternative soil moisture deficit term is created as Soil Moisture Deficit to Saturation (SMDS), which is complementary to SMD but hydrologically more realistic for soil moisture representation:

$$SMDS = CS - SMC \quad (11)$$

where CS is in the unit of metre, which is now considered as the upper limit in the amended XAJ model for its soil water storage (calibrated FC + upper layer's free water). The amendment method is to add upper part of the free water ($CS-FC$) back to the upper soil. However because the XAJ free water storage covers all the three soil layers, it is currently a challenge to divide the free water into three soil layers. Since the interflow in reality is mainly in the upper layer and in proportion to the upper free water, in this study RI in Eq. 5-6 is used as a proxy for the upper free water. In the future, further research may be needed to develop a new three-layer free water scheme (However it should be noted that such a scheme may deteriorate the XAJ's flow simulation so it is not an easy task). To check the effectiveness of this proposed

first step, an evaluation has been carried out (a recalibration is not required, because this approach does not affect the model's flow simulation) and it has been found that after the rectification the correlation between the XAJ SMDS and the SMOS soil moisture has been improved significantly from $r = -0.64$ to $r = -0.69$ (Fig. 10-step 1), while the flow simulation remains as effective as its original model ($NSE = 0.81$ for calibration and $NSE = 0.80$ for validation). Therefore, the proposed scheme is effective albeit there is room for improvement.

Second step: in order to simulate the capillary action of the water rises from the lower soil layer, a part of the lower-layer soil moisture should be added to the upper soil layer. Although this is clear in concept, it is not easy to calculate the exact contribution in practice. In this study, a ratio related to the lower soil water content is used to represent the capillary action's contribution. In order to find the optimal *ratio*, a trial and error method is proposed as shown in Fig. 11. The trial and error illustration presents the correlation between the modified XAJ soil moisture (the *RI* portion of the free water has been added from the first modification step and the capillary rise water from the lower soil layer is changed based on the different ratios trialed) and the SMOS retrieved soil moisture, at each trial and error step. It is interesting to observe that the change of the capillary rise water amount from the lower soil layer can have a dramatic impact on the soil moisture, as r can range from as low as $r = -0.67$ when all the second soil water is added to as high as $r = -0.70$ when 27% of the lower soil water is included. This particular ratio could be partly related to the soil hydraulic conductivity based on Darcy's law ([Lu and Likos, 2004](#)).

As illustrated in Fig. 10-step 2 (during the whole monitoring period) and Fig. 12 (two enlarged plots of Fig. 10-step 2), the XAJ soil moisture is now wetter than the field capacity (the modified XAJ soil moisture in a green line can now go beyond the field capacity in the dashed black line) and shows more moderate drying process during the drying periods (the modified XAJ soil moisture in a green line dries at a slower rate than the original XAJ soil moisture shown in the red line). As a result, the fluctuation of the modified XAJ soil moisture is more compatible with the SMOS soil moisture variations, as also agreed by the increased r value shown in Table 3. Meanwhile the XAJ model's effectiveness in flow simulation remains the same (i.e., $NSE > 0.80$), because the amendment does not change the flow calculations in the model. Although the trial and error result depends on catchment soil properties ([Lu and Likos, 2004](#)), this method should be easily applied and generalised under various catchment conditions. The scatter plot between the proposed XAJ SMDS and the SMOS soil moisture is presented in Fig. 13. Compared with Fig. 6, the number of soil total dryness points in the proposed XAJ soil moisture representation is significantly reduced. Besides it is interesting to see in Fig. 10- step 2 that when the XAJ model has exhausted its upper soil water, the SMOS's soil moisture is still greater than $0 \text{ m}^3/\text{m}^3$. This could be explained by the soil depth difference between the XAJ model and the SMOS satellite observation, because both of the soil depths are not fixed. Unlike a bucket model with a fixed size, XAJ conceptualises that a catchment should be made of an infinite number of buckets with different sizes in each soil layer (represented by the holding capacity curve). This particular design has significantly improved the stream flow modelling result ([Beven, 2012](#)). This is because a catchment is not horizontally flat, so the

slope of a catchment leads to uneven soil moistures holding capacities. For example, soil usually tends to be wetter and deeper near the bottom of a catchment, while it is drier and thinner at higher elevations. Hence a fixed soil layer tends to work poorly in conceptual hydrological models ([Beven, 2012](#)). Another issue is that there are no parameters to describe the XAJ soil layer thicknesses directly. Instead, they are only represented by the proxy parameters (i.e., *WUM*, *WLM*, and *WDM*). On the other hand, satellite observation soil depth is affected by many factors such as soil moisture, land surface temperature, satellite sensor frequency, incident angle, polarization, surface roughness, soil properties and vegetation cover ([Schmugge, 1980](#)) (e.g., the drier the soil, the deeper the sampling depth, and vice versa ([Escorihuela et al., 2010](#); [Ulaby et al., 1986](#))). Thus even if the hydrological model's soil depth is known and fixed, it is still difficult to match it with the satellite soil moisture depth. Nevertheless it has been shown in various literatures that as long as a good correlation can be built between the hydrological soil moisture state variable and the soil moisture observations, it should be possible to apply such a correlation in real-time flood forecasting ([Al - Shrafany et al., 2013](#); [Lacava et al., 2012](#); [Srivastava et al., 2013b](#); [2014](#)).

4. Discussion

There are several potentially controversial issues in this study that should be further clarified.

4.1 The right answers for the right reasons

Although both the original and the amended models have the same flow accuracy, the amended model has simulated flow effectively with the right reason (i.e., more realistic soil moisture

representation). A major issue in hydrological modelling is equifinality as emphasised by Keith Beven ([Beven, 2012](#)), because many hydrological models are able to simulate similar flow results with different parameter sets, but not all the model parameters are hydrologically sensible. Currently there is a trend in hydrological research to emphasise that it is not sufficient to just accurately simulate the river discharge; it is also important the model should represent the internal hydrological processes correctly and accurately. For example a black-box model such as ANN is able to model rainfall-runoff very effectively, but it has no physical meanings with its neuron weights and connections. Hence it will be difficult for an ANN model to assimilate soil moisture observations.

A well-known paper written by James W. Kirchner ([Kirchner, 2006](#)) calling for “getting the right answers for the right reasons”, where he pointed out: “for many routine operational purposes, one just needs methods that get the right answers”. For example the XAJ model is designed for operational flow modelling, and it does a very good job albeit its soil moisture is misrepresented. Therefore the aim of our study is to produce a hydrological model with not only good flow simulation, but also accurate internal processes representations (i.e., soil moisture). In addition, as pointed out by Kirchner ‘Furthermore, getting the right answers for the right reasons could be crucial for getting the right answers at all’. We argue that in real-time flood forecasting, a hydrological model with more realistic soil moisture representation is able to assimilate soil moisture observations more effectively and as a result, its flood forecasting accuracy will be improved over the model which only gets the right answers but with wrong reasons (i.e., poor soil moisture representation).

4.2 Soil moisture representation and observation

The second one is what the soil moisture state is about in a conceptual hydrological model, and whether it is possible to measure it. A soil moisture state variable is used to serve the purpose of flow simulation, but itself cannot be validated by observations because they are not the same due to the difference in depth, spatial coverage, and model formulation. One may argue a comparison between them is like comparing an apple with an orange.

It is believed that a better analogy can be made about inner body temperature checked by doctors. The inner body temperature is an important indicator about the human body health, however it is not possible to measure it. Instead, a thermometer is used to measure the external temperature such as under the armpit. Although they are not the same thing, there is a good correlation between them. Therefore medical doctors can still use such information for diagnoses. Since both observed soil moisture and the model's soil moisture are driven by the same hydrological processes (precipitation, evapotranspiration and runoff), they are physically correlated to each other albeit the model is a simplification of the reality.

4.3 'True' soil moisture?

Now the question is what is the true catchment soil moisture. Soil moisture is difficult to define because it does not have a single shared meaning in different disciplines ([Romano, 2014](#)). For example, to a farmer, she/he is only interested in the root zone soil moisture; to remote sensing scientists, they are only interested in the surface soil moisture; to hydrologists, it is the aquifer (including both confined and unconfined aquifers) that is important which covers the surface

soil moisture, the root zone soil moisture and beyond. Therefore it is challenging to define what the true soil moisture is.

Currently the surface soil moisture can be measured by in-situ ground based measurements and remote sensing technology. The deeper root zone soil moisture can only be measured by in-situ sensors, but it still suffers from spatial representation. The soil water in aquifer is more challenging because it changes over different locations and it can be confined or unconfined. Therefore it is still challenging to measure the soil moisture over the whole aquifer and all the current measurement techniques are not commensurate with the aquifer soil water, but mainly surface or/and root zone soil moisture. However since most water movement happens from the ground surface to the root zone, the information at this depth is usually sufficient for hydrological modelling.

4.4 Issues with current satellite soil moisture observations

The final issue is about the accuracy of satellite soil moisture that may not be good enough for hydrological modelling purpose. As aforementioned, the hydrological model's soil moisture and observed soil moisture are two different things (but related). Therefore a conversion between them is required. The higher the correlation, the better the conversion can be carried out. There are three problems that need to be addressed:

- The first one is the current satellite soil moisture products are calibrated by in-situ soil moisture observations, hence they are less relevant to hydrological modelling's soil moisture state variable. It has been found by converting the raw satellite brightness

temperature data at multiple angles into hydrologically compatible soil moisture can achieve significant improvement in accuracy, in comparison with the standard satellite soil moisture products. This result has been submitted to a hydrological journal which is currently under review.

- Second, the existing hydrological model is not compatible with the surface soil moisture as described in this paper, so an improvement to the hydrological model is required, which is the main purpose of this paper.
- The third is the lack of reliable data assimilation technologies, because the observed soil moisture data cannot be inserted directly into the hydrological model in an operational mode. The performance of data assimilation depends on the research carried out in the first and second problems. The novel contribution of this paper in the first and second problems will lay a good foundation to this third problem.

We believe those are the main potential reasons for the satellite soil moisture products not showing a robust and high quality behaviour in operations. Therefore, we hope this study will attract attention from the hydrological community on those problems and encourage more research to solve them in the future.

5. Conclusions

A modification scheme to the XAJ model has been proposed in this study which is evaluated from the SMOS observation to be very effective in amending its soil moisture misrepresentations while keeping its excellent flow simulation performance. In addition, a

term called the holding excess runoff has been introduced to illustrate the computational runoff mechanism in the XAJ and other similar models, which helps to clarify the difference between the runoff in reality and the modelled runoff. Another term called SMDS (Soil Moisture Deficit to Saturation) is proposed to complement the conventional SMD. The study shows that SMDS is hydrologically more realistic for soil moisture representation than SMD based on general soil water movement principles. As an answer to [Matgen et al. \(2012\)](#) based on this study, many conceptual hydrological models' soil moisture schemes should be improved so that they are more compatible with the soil moisture observations. Hence better soil moisture data assimilation performances can be obtained during operational flood forecasting. The methods discussed in this paper are only a first step towards a comprehensive soil moisture modification procedure. Therefore more studies with longer time periods in a larger number of catchments should be carried out. Furthermore if there are alternative soil moisture observations available (e.g., new soil moisture monitoring networks), the proposed methodology should also be easily applied to those data types.

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(<http://www.smos-bec.icm.csic.es/>).

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