To Editor

Dear Prof. Gelfan,

Thank you very much for the comments. The manuscript has been further amended to address the issues raised. The point-by-point replies are listed below.

If there are any further questions, please let us know.

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The 1st Referee expressed reasonable concern that the presented results don't allow a reader to evaluate the model's applicability because of short duration of the calibration/validation period (2 years) and suggested prolonging it. I have checked the streamflow data availability for the Vermilion River at Pontiac and found that there are at least 8-year period of continuous daily records from 2009 till 2017. Importantly, this period covers the SMOS satellite data. Thus, I strongly recommend taking into account the criticism of the referee and prolonging the study period.
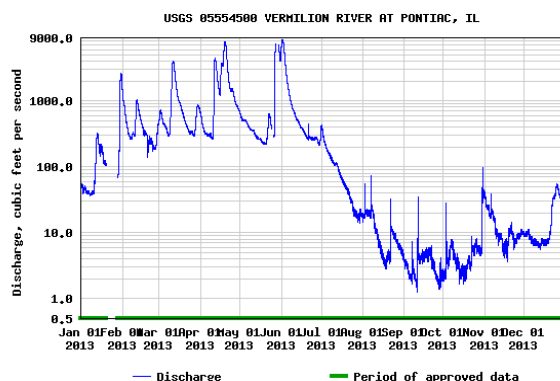
Reply: We thank the editor for the careful checking. In the study catchment, there have been many data gaps from 2013-2017 (see the figures below), and the data quality in 2012 was poor. As a result, only the data in 2010-2011 are consistent and of high quality. As pointed out by Liu and Han (2010), 'Traditionally, hydrologists use rules of thumb to select a certain period of hydrological data to calibrate the models (i.e., 6 year data).' However, their study has shown 'the information content of the calibration data is more important than the data length; thus 6 month data may provide more useful information than longer data series.'   Therefore, the two years of high quality data adopted in the study are better than a longer period of poor quality data. We have added this explanation to the updated manuscript to clarify the issue.

Reference:

J. Liu and D. Han, Indices for calibration data selection of the rainfall-runoff model, *Water Resources Research,* doi:10.1029/2009WR008668, 2010
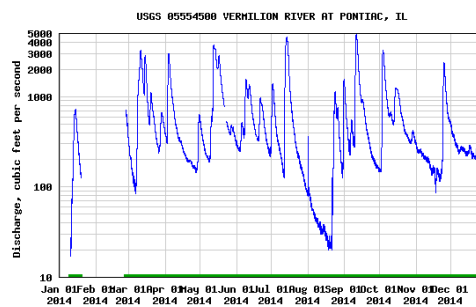
Discharge, cubic feet per second
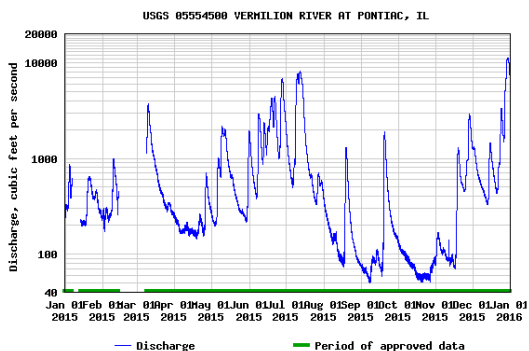Most recent instantaneous value: 1090 05-14-2017 04:45 CST

USGS 05554500 VERMILION RIVER AT PONTIAC, IL

— Discharge   — Period of approved data

Discharge, cubic feet per second
Most recent instantaneous value: 1090 05-14-2017 04:45 CST

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— Discharge   — Period of approved data

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— Discharge   — Period of approved data

Discharge, cubic feet per second
Most recent instantaneous value: 1090 05-14-2017 04:45 CST

USGS 05554500 VERMILION RIVER AT PONTIAC, IL

— Discharge   — Period of provisional data
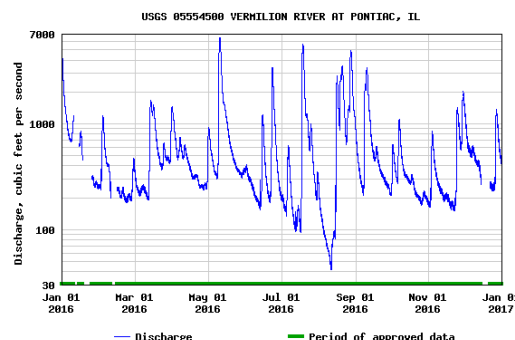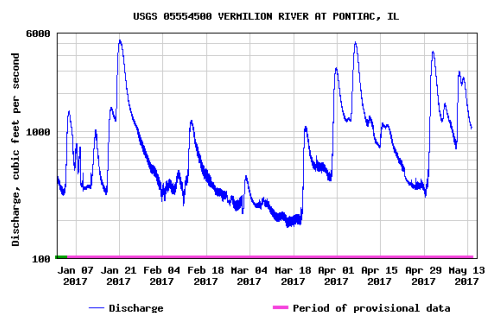
I consider that the next comment of the referee also requires more serious attention. His/her question related to ability of the XAJ model for reproducing soil moisture dynamics under frozen conditions. This ability is important because frequent soil freezing events in winter seasons are specific for the study basin. In their response to this comment, the authors argued that "XAJ model is very good at simulating the flow even during the winter season". In my experience, this argument does not sufficient and good model's performance in reproducing streamflow does not confirm the model's performance in describing water content of frozen soil. Moreover, it is not too difficult tuning the model to short (2 years only) time-series of

streamflow data without considering frozen conditions at all. Unfortunately, I could not find examples of the XAJ model's application for these conditions (the mentioned two-page paper Zhou et al, 2008 can hardly be considered as a convincing example). Thus, I recommend adding more results and discussion confirming ability of the XAJ model for reproducing soil moisture dynamics under frozen conditions

Reply: We agree that this can be misleading. It is better to add some text based on the comments from the editor and reviewer in the updated manuscript to let the readers be aware of the issue.

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The Pontiac catchment is characterized by soil freezing events in winter seasons. During freezing events, soil moisture transfer fundamentally differs from the unfrozen conditions (e.g. Gelfan, 2006). Although the XAJ model has been successfully applied in simulating flows in frozen soil conditions (e.g., see Zhou et al., 2008) as well as in this case study, the lumped XAJ model does not explicitly consider soil freezing, thus SMD simulations can be inaccurate for winter seasons and further research is needed to investigate this issue further.

References:

Gelfan A. N. (2006) Physically based model of heat and water transfer in frozen soil and its parametrization by basic soil data. IAHS Publ., 303, pp. 293-304.

Zhou, S., Li, Y., Zhu, J., 2008. Application of Xin'anjiang model in severe cold region of Niqiu River. Water Resources & Hydropower of Northeast China, 26(9). DOI:10.3969/j.issn.1002-0624.2008.09.016

1   **Multi-source hydrological soil moisture state estimation using data fusion optimisation**

2

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6   **Abstract**

7   Reliable estimation of hydrological soil moisture state is of critical importance in operational

8   hydrology to improve the flood prediction and hydrological cycle description. Although there

9   have been a number of soil moisture products, they cannot be directly used in hydrological

10   modelling. This paper attempts for the first time to build a soil moisture product directly

11   applicable to hydrology using multiple data sources retrieved from SAC-SMA (soil moisture),

12   MODIS (land surface temperature), and SMOS (multi-angle brightness temperatures in H-V

13   polarizations). The simple yet effective Local Linear Regression model is applied for the data

14   fusion purpose in the Pontiac catchment. Four schemes according to temporal availabilities of

15   the data sources are developed, which are pre-assessed and best selected by using the well-

16   proven feature selection algorithm Gamma Test. The hydrological accuracy of the produced

17   soil moisture data is evaluated against the Xinanjiang hydrological model's soil moisture

18   deficit simulation. The result shows that a superior performance is obtained from the scheme

19   with the data inputs from all sources ($NSE = 0.912$, $r = 0.960$, $RMSE = 0.007$ m). Additionally

20   the final daily-available hydrological soil moisture product significantly increases the Nash-

21   Sutcliffe efficiency by almost 50 % in comparison with the two most popular soil moisture

22 products. The proposed method could be easily applied to other catchments and fields with

23 high confidence. The misconception between the hydrological soil moisture state variable and

24 the real-world soil moisture content, and the potential to build a global routine hydrological

25 soil moisture product are discussed.

26 **Keywords**: Hydrological soil moisture state (SMD); Local Linear Regression (LLR); Gamma

27 Test (GT); Soil Moisture and Ocean Salinity (SMOS) multi-angle brightness temperatures;

28 North American Land Data Assimilation System 2 (NLDAS-2); Moderate Resolution Imaging

29 Spectroradiometre (MODIS) land surface temperature

30 **1. Introduction**

31 Soil moisture is a key element in the hydrological cycle, regulating evapotranspiration,

32 precipitation infiltration and overland flow (Wanders et al., 2014). For hydrological

33 applications, the antecedent wetness condition of a catchment is among the most significant

34 factors for accurate flow generation processes (Berthet et al., 2009; Matgen et al., 2012a).

35 (Norbiato et al., 2008) reported that initial wetness conditions are essential for efficient flash

36 flood alerts. Additionally an operational system requires reliable hydrological soil moisture

37 state updates to reduce the time drift problem (Aubert et al., 2003; Berg and Mulroy, 2006;

38 Dumedah and Coulibaly, 2013). However, currently there is no available soil moisture product

39 that can be used directly in hydrology modelling, primarily because soil moisture is difficult to

40 define and there is no single shared meaning in various disciplines (Romano, 2014).

41 Although there have been many soil moisture measuring projects (e.g., satellite missions such

42 as Advanced Scatterometer (ASCAT), Soil Moisture and Ocean Salinity (SMOS), and Soil

43   Moisture Active Passive (SMAP); ground-based networks such as Soil Climate Analysis

44   Network (SCAN), U.S. Surface Climate Observing Reference Networks (USCRN), and

45   COsmic-ray Soil Moisture Observing System (COSMOS)), they are not sufficiently used in

46   hydrology due to the following reasons: 1) misconception between the hydrological soil

47   moisture state variable and the real-field soil moisture content (Zhuo and Han, 2016a); 2)

48   unawareness of data availability and strength/weakness of different data sources; 3) the existing

49   soil moisture products are mainly evaluated against point-based ground soil moisture

50   observations or airborne retrievals which have significant spatial mismatch (both horizontally

51   and vertically) to catchment-scales, and are therefore less applicable to hydrological modelling

52   (Pierdicca et al., 2013); 4) underutilisation of multiple data sources (e.g., multi-angle raw

53   observations by satellite sensors).

54   Some studies have attempted to directly utilise the existing soil moisture products (i.e., data

55   from satellites, land surface models, and in-situ methods directly) for flood prediction

56   improvement, for example (Brocca et al., 2010) explored that utilising the soil water index

57   from ASCAT sensor could improve runoff prediction mainly if the initial catchment wetness

58   conditions were unknown; (Aubert et al., 2003) assimilated in-situ soil moisture observations

59   into a simple rainfall-runoff model and acquired better flow prediction performance ; (Javelle

60   et al., 2010) suggested that estimations of antecedent soil moisture conditions were useful in

61   improving flash flood forecasts at ungauged catchments; contrarily (Chen et al., 2011)'s study

62   showed assimilating ground-based soil moisture observations was generally unsuccessful in

63   enhancing flow prediction; and (Matgen et al., 2012b) revealed that satellite soil moisture

64   products added little or no extra value for hydrological modelling. Clearly those results are

65   rather mixed. Challenges remain in integrating soil moisture estimated outside the hydrological

66   field into hydrological models. We believe if a hydrologically directly applicable soil moisture

67   product could be produced, the aforementioned studies' results would be significantly

68   improved.

69   Therefore the aims of this paper are to clarify the aforementioned misconception between the

70   hydrological model's soil moisture state and the real-world soil moisture, assess the data

71   availabilities for direct hydrological soil moisture state estimation, and fuse those available

72   data sources using a hydrologically relevant approach. It is hoped that the final product has a

73   superior hydrological compatibility over the existing soil moisture products. To achieve these

74   aims, the Xinanjiang (XAJ) (Zhao, 1992) operational rainfall-runoff model is used as a target

75   to simulate flow and soil moisture state information (i.e., soil moisture deficit (SMD)) for the

76   Pontiac catchment in the central United States (U.S.). The reason for adopting XAJ is explained

77   in the following section. For the purpose of hydrological soil moisture state estimation, it is

78   effective to adopt the data driven method, which can map multiple data sources into the desired

79   dataset without computational burden. In this study the Local Linear Regression (LLR) model

80   is used. The multiple data sources applied in this study include the SMOS (Kerr et al., 2010b)

81   multi-angle brightness temperatures (T_bs) with both horizontal (H) and vertical (V)

82   polarizations, the Moderate Resolution Imaging Spectroradiometre (MODIS) (Wan, 2008)

83   land surface temperature, and the soil moisture product by SAC-SMA (Xia et al., 2014). The

84   detail explanations of those datasets are covered in the methodology section. A well-proven

85   feature selection algorithm Gamma Test (GT) (Stefánsson et al., 1997; Zhuo et al., 2016b) is

86   employed to pre-assess the selected data inputs and find the optimal combination of them for

7

87 soil moisture state calculation. In addition, an *M*-test (Remesan et al., 2008) is adopted to

88 explore the best size of the training data. The desired soil moisture product is trained and tested

89 by the XAJ SMD simulation. In total four data-input schemes are developed according to the

90 temporal availability of the selected data inputs, which are then combined to give a daily

91 hydrological soil moisture product.

92 Compared with previous work, our study contains the following new elements: i) a

93 hydrologically directly usable soil moisture product is proposed; ii) the GT and LLR techniques

94 are used for the first time in a data fusion of multiple data sources for hydrological soil moisture

95 state estimation; iii) the use of multiple data sources is useful, which allows data users to

96 analyse the availability of the different products and compare the relative benefits of them.

97 **2. Material and Methods**

98 **2.1 Study Area**

99 In this study, the Pontiac catchment (1,500 km^2, Figure 1) is used for the calibration and the

100 validation of the XAJ model. Pontiac (40.878°N, 88.636°W) lies on the north-flowing

101 Vermilion River, which is a tributary of the Illinois River of the state of Illinois, U.S. The worst

102 flood in this area occurred on December 4, 1982, cresting at 5.84 m above mean sea level

103 (MSL); and the most recent flood occurred on January 9, 2008, cresting at 5.75 m MSL, so this

104 catchment is likely located within a winter-flooding region. Pontiac is covered with moderate

105 canopy (the annual mean Normalized Difference Vegetation Index retrieved from the MODIS

106 satellite is around 0.4), when compared with a densely vegetated catchment, it has more

107 accurate soil moisture estimations from satellites (Al-Bitar et al., 2012). Based on the Köppen-

108   Geiger climate classification, this medium sized catchment is dominated mainly by hot summer

109   continental climate (Peel et al., 2007). With reference to the University of Maryland

110   Department Global Land Cover Classification, it is used primarily for agriculture purpose

111   (Bartholomé and Belward, 2005; Hansen, 1998). The soil mostly consists of Mollisols, which

112   has deep and high organic matter, and the nutrient-enriched surface soil is typically between

113   60-80 cm in depth (Webb et al., 2000). The study period is from January 2010 to December

114   2011. The reason for using this two-year period of data is because there have been many data

115   gaps from 2013-2017, and the data quality in 2012 was poor. As a result, only the data in 2010-

116   2011 are consistent and of high quality. As pointed out by Liu and Han 2010, 'Traditionally,

117   hydrologists use rules of thumb to select a certain period of hydrological data to calibrate the

118   models (i.e., 6 year data).' However, their study has shown 'the information content of the

119   calibration data is more important than the data length; thus 6 month data may provide more

120   useful information than longer data series.' Therefore, the two years of high quality data

121   adopted in the study are better than a longer period of poor quality data.

122   The North American Land Data Assimilation System 2 (NLDAS-2) (Mitchell et al., 2004)

123   provides precipitation and potential evapotranspiration information to run the XAJ model. Both

124   data forces are at $0.125°$ spatial resolution and have been converted to daily temporal resolution.

125   In order to use those distributed forcing into the lumped XAJ model, both forcing have been

126   interpolated with the area-weighted average method instead of the more complicated Kriging

127   approach, because the latter could produce errors if not well controlled (Wanders et al., 2014).

128   The average annual rainfall depth is about 954 mm, and the average annual potential

129 evapotranspiration is approximately 1670 mm. The daily observed flow data are acquired from

130 the U.S. Geological Survey.

131 **2.2 Hydrological Model**

132 The XAJ hydrological model is used for the simulation of SMD and river flow at a daily time

133 step. It is a simple lumped rainfall-runoff model with many applications performed in world-

134 wide catchments (Chen et al., 2013; Gan et al., 1997; Shi et al., 2011; Zhao, 1992; Zhao and

135 Liu, 1995; Zhuo et al., 2016a; Zhuo et al., 2015b). Since XAJ can obtain rather effective flow

136 modelling performances and require only two meteorological forcing (precipitation and

137 potential evapotranspiration) inputs (Peng et al., 2002), it is used more widely than the more

138 complicated semi-distributed/ fully-distributed hydrological models for operational

139 applications.

140 As shown in Figure 2, the XAJ model has three main components: evapotranspiration, runoff

141 generation, and runoff routing. XAJ consists of soil layers (upper, lower and deep) in its

142 evapotranspiration calculations. Because XAJ adopts the multi-bucket variable-size method in

143 its modelling concept, it has unfixed soil depths which is more effective than the fixed depths

144 models (Beven, 2012). Other widely used models such as PDM (Moore, 2007), VIC (Liang et

145 al., 1994), and ARNO (Todini, 1996) also follow this concept.

146 In XAJ, the three-layer soil moisture state variables are all calculated as SMD, which is an

147 important soil wetness variable in hydrology. SMD is defined as the amount of water to be

148 added to a soil profile to bring it to the field capacity (Calder et al., 1983; Rushton et al., 2006).

149 In this study, only the surface SMD (i.e., top layer) referring to the vegetation and the very thin

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150 topsoil, is utilised as a hydrological soil moisture target. This is because the water held in the

151 top few centimetres of the soil has been widely recognised as a key variable associated with

152 water fluxes (Eltahir, 1998; Entekhabi and Rodriguez-Iturbe, 1994). Moreover the current

153 satellite technology is only capable of acquiring the Earth information from the outermost layer

154 of the soil. Therefore as a case study based on the XAJ model, we only focus on the surface

155 soil moisture state investigation here. Future research will focus on the root-zone soil moisture

156 product development by using a similar method proposed in this study.

157 In this study, a modified version of the XAJ model is adopted, and interested readers are

158 referred to (Zhuo and Han, 2016b) for more details. All the XAJ's 17 parameters are used

159 during the model calibration, which are shown in Table 1. In this study, the genetic algorithm

160 (Wang, 1991) is used for parameter optimisation. Based on the genetic algorithm result, minor

161 trial and error adjustments to the parameters *EX*, *B*, *WUM*, *WLM* and *WDM* are also carried out

162 to obtain the best model performance (Chen and Adams, 2006). The calibration and the

163 validation results (during January 2010-April 2011 and May 2011 to December 2011,

164 respectively) of the XAJ model can be found in (Zhuo et al., 2015a). Discussion regarding the

165 river flow and SMD simulation results in this catchment have been published in (Zhuo and

166 Han, 2016b), with Nash-Sutcliffe Efficiency (*NSE*) obtained larger than 0.80 during both the

167 calibration and validation periods. The results are not repeated here.

168 **2.3 Multiple Data Sources for Hydrological Soil Moisture State Estimation**

169 Data sources from SMOS, MODIS and SAC-SMA are used (Table 2). All data sources have

170 been converted into catchment-scale datasets by the area-weighted average method. The detail

171   description of each data source is given as follows. The main reason for choosing those three

172   data sources is due to their Near-Real-Time (NRT) availabilities (MODAPS Services, 2015;

173   Rodell, 2016) (SMOS becomes available in NRT recently (ESA Earth Online, 2016)), which

174   allows fast implementation in flood forecasting.

175   **2.3.1 SMOS Multi-angle Brightness Temperatures (SMOS-T_bs)**

176   The SMOS (1.4 GHz, L-band) Level-3 T_bs data covering the studying period are available from

177   the Centre Aval de Traitement des Données SMOS (CATDS) (Jacquette et al., 2010). The

178   reason for choosing the SMOS satellite is because compare with other satellite techniques (i.e.,

179   optical, and thermal infrared), microwave bands (especially with longer wavelength such as L-

180   band (21 cm)) can penetrate deeper into the soil (~ 5 cm) and have less interruptions from

181   weather conditions (Njoku and Kong, 1977). Additionally SMOS has a relatively longer period

182   of data record compares with other satellite missions such as SMAP. SMOS retrieves the

183   thermal emission from the Earth in both H and V polarizations with a wide ranges of incidence

184   angles from 0° to 60°. The observation depth of SMOS is approximately 5 cm with a spatial

185   resolution of 35-50 km depending on the incident angle and the deviation from the satellite

186   ground track (Kerr et al., 2012; Kerr et al., 2010a; 2001).

187   SMOS provides T_bs retrievals at all incidence angles averaged in 5° -width angle bins, which

188   have been transformed into the ground polarization reference frame (i.e., H, and V

189   polarizations). Therefore the number of the SMOS-T_bs inputs for the hydrological soil moisture

190   estimation can be as high as 24 (12 angle bins per polarization), with the centre of the first

191   angle bin at 2.5^o in both polarizations (Rodriguez-Fernandez et al., 2014). As satellite

192   progresses, any given location on the Earth's surface is scanned a number of times at various

193   incidence angles, depending on the location with respect to the satellite subtrack: the further

194   away, the fewer the angular acquisitions (Kerr et al., 2010b). The data availabilities of the

195   SMOS-T_bs are illustrated in Figure 3 (the availabilities for H and V polarizations are the same).

196   It can be seen that the data availabilities among various incidence angles are rather different.

197   In this study the only angle range that gives the most available record of data is from 27.5^o to

198   57.5^o (i.e., 7 for H and 7 for V polarization), which is therefore chosen for the hydrological soil

199   moisture development. This angle range is in line with the angle selection in (Rodriguez-

200   Fernandez et al., 2014). In addition the SMOS Level-3 soil moisture product from the CATDS

201   (SMOS-SM) is also acquired for a comparison with the estimated soil moisture product.

202   Retrievals that are potentially contaminated with Radio Frequency Interference have been

203   removed. Readers are referred to (Kerr et al., 2012) for a full description of the SMOS

204   retrieving algorithms, and (Njoku and Entekhabi, 1996) for a good knowledge of how passive

205   microwave relates to soil moisture variations.

206   **2.3.2 MODIS Land Surface Temperature (MODIS-LST)**

207   The MODIS/Terra (Earth Observing System AM-1 platform) (Wan, 2008) daily MOD11C1-

208   V5 land surface temperature covering the studying period is downloaded from the Land

209   Processes Distributed Active Archive Centre website. MODIS is chosen among other

210   operational optical satellites for its suitable features, mostly, due to its frequent revisiting time

211   and free NRT data availability. It measures 36 spectral bands between 0.405 and 14.385 μm,

212   and acquires data at three spatial resolutions 250 m, 500 m, and 1,000 m respectively while the

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213 adopted MOD11C1 V5 product incorporates 0.05º (5.6 km) spatial resolution. The benefit of

214 adding land surface temperature information is that previous studies have shown the variations

215 in soil moisture have a strong linkage with land surface temperature (Carlson, 2007; Goward

216 et al., 2002; Mallick et al., 2009). One reason is the changes of land surface temperature are

217 mainly affected by albedo and diurnal heat capacity, and the diurnal heat capacity is mainly

218 controlled by soil moisture (Price, 1980). (Wan, 2008) compared MOD11C1-V5 land surface

219 temperatures in 47 clear-sky cases with in situ measurement and revealed that the accuracy was

220 better than 1 K in the range from −10° to 58 °C in about 39 cases. Cloud-contaminated data

221 have been removed by a double-screening method, and its detail can be found in (Wan et al.,

222 2002).

223 **2.3.3 SAC-SMA Soil Moisture Estimation (SAC-SMA-SM)**

224 The reason for choosing the SAC-SMA land surface modelled soil moisture product is because

225 satellite can often have missing data due to various weather and canopy conditions (e.g., rainfall,

226 frozen weather, and vegetation coverage), so this daily dataset is essential in producing a

227 temporally completed hydrological soil moisture product. In this study, the surface soil

228 moisture (0-10 cm) simulated from the SAC-SMA model is selected. This is because its

229 estimated soil moisture gives a high accuracy against the observational soil moisture and a

230 good correlation with the XAJ SMD (Zhuo et al., 2015b). The daily SAC-SMA-SM is given

231 in a spatial resolution of 0.125º. The dataset can be download from

232 (http://www.emc.ncep.noaa.gov/mmb/nldas/). Readers are referred to (Xia et al., 2012) for a

233 full description of the SAC-SMA data products.

2.3.4 Data Availabilities

As shown in Table 2, the availability of the three data sources is rather different. Unlike SMOS and MODIS, SAC-SMA-2 SM is a model based product which runs in a NRT mode, so it produces valid data every day during the whole studying period. Whereas the two satellites' data are more exiguous depends on weather and surface conditions. Compared with MODIS, the SMOS's retrieval is even sparse and the biggest data shortage normally occurs in the winter season where its returned microwave signal is mostly affected by frozen soils (Zhuo et al., 2015a). Based on the data availability analysis, the proposed hydrological soil moisture product is built from four data-input schemes as presented in Table 3. Those four schemes enable us to test and compare the estimated soil moisture state more comprehensively. Since the continuity of a soil moisture product is essential for any operational applications, SAC-SMA-SM is included in all of the schemes.

2.4 Data Fusion

2.4.1   Gamma Test (GT) for Feature Selection

Before model building, it is important to carry out a feature selection process, because it can simplify the model inputs, shorter training times, and reduce overfitting problems. In this study a proper combination of the incidence angles from the SMOS T_bs is vital for the best soil moisture state calculation. For this purpose, a feature selection method called GT is adopted. It has been effectively used in numerous studies for model inputs selection (Durrant, 2001; Jaafar and Han, 2011; Noori et al., 2011; Remesan et al., 2008; Tsui et al., 2002; Zhuo et al., 2016b). In addition to the feature selection, GT can also give useful indication about the underlying

15

255   model complexity. It is a near-neighbour data analysis routine which determines the minimum

256   mean-squared error (*MSE*) that can be achieved based on the input-output dataset utilising any

257   continuous nonlinear models (Zhuo et al., 2016b). The calculated minimum *MSE* is referred as

258   the Gamma statistics and denoted as Γ. For detailed calculations about the GT algorithm,

259   interested readers are referred to (Koncar, 1997; Pi and Peterson, 1994; Stefánsson et al., 1997).

260   Here only the basic knowledge about the GT is shown:

261     $\{(x_i, y_i), \ 1 \leq i \leq M \}$ (1)

262   here the inputs $x_i \in R^m$ are vectors restricted by a closed bounded set $C \in R^m$, and their

263   corresponding outputs $y_i \in R$ are scalars, *M* stands for the sample points. The outputs *y* are

264   determined by the input vectors *x* that carry predictively useful messages. The only assumption

265   made is that their latent relationship is from the following function:

266     $y = f(x_1 \ldots x_m) + r$ (2)

267   here *f* is built up as a smooth model with *r* representing random noise. Without loss of generality,

268   the assumption of *r* noise distribution is that its mean is always zero, because all the constant

269   bias has been considered within the *f* model. Additionally *r*'s variance ($Var(r)$) is restricted

270   within a set boundary. The observations' potential model is now defined within the class of

271   smooth functions.

272   The Γ is related to $N[i,k]$, which represents as the *k*th ($1 \leq k \leq p$) nearest neighbours of each

273   vector x_i ($1 \leq i \leq M$), written as $x_{N[i,k]}(1 \leq k \leq p)$, where *p* is a fixed integer. In order to

274   determine the Gamma function from the input vectors, the *Delta* function is used:

275 $$\delta_M(k) = \frac{1}{M}\sum_{i=1}^{M}\left|x_{N[i,k]} - x_i\right|^2 \qquad (1 \le k \le p) \qquad\qquad (3)$$

276 here the function $\left|x_{N[i,k]} - x_i\right|$ calculates the Euclidean distance. The Gamma function for its

277 output values is expressed as in Eq. 4, and the Γ can be determined from Eq. 3 and 4:

278 $$\gamma_M(k) = \frac{1}{2M}\sum_{i=1}^{M}\left|y_{N[i,k]} - y_i\right|^2 \qquad (1 \le k \le p) \qquad\qquad (4)$$

279 here $y_{N[i,k]}$ is the corresponding output values for the kth nearest neighbours x_i ($x_{N[i,k]}$). To

280 find Γ a least-squared regression line for the p points ($\delta_M(k)$, $\gamma_M(k)$) is built using the

281 following equation:

282 $$\gamma = A\delta + \Gamma \qquad\qquad (5)$$

283 where Γ can be determined when δ is set as zero. The detailed explanation is:

284 $$\gamma_M(k) \to Var(r), \text{ when } \delta_M(k) \to 0 \qquad\qquad (6)$$

285 Eq. 5 gives us valuable information about the underlying system: not only that the Γ is a useful

286 indicator of the optimal MSE result that any smooth functions can achieve, but its gradient A

287 also provides guidance about the underlying model complexity (i.e., the steeper the gradient

288 the more sophisticated the model should be adopted). In this study, the winGamma^{TM} software

289 is used for GT calculation (Durrant, 2001). The mathematical feasibility of GT has been

290 published in (Evans and Jones, 2002).

291 **2.4.2** *M*-**test for Training Data Size Selection**

292 A common practice in nonlinear modelling is to split the dataset into training and testing parts.

293 However there is no universal solution on how to divide the datasets (i.e., the proportion of

294   each part) so that the best modelling results could be obtained. Here, an M-test is carried out,

295   where M stands for the training data size. M-test is accomplished by calculating the Γ for

296   increasing the M value (i.e., expanding the training data) and exploring the resultant graph to

297   judge whether the Γ approaches a stable asymptote. Such an approach is straightforward and

298   effective in finding the optimal sizes of training and testing datasets, while avoiding overfitting

299   problems and reducing unsystematic attempts.

300   **2.4.3   Local Linear Regression (LLR)**

301   Various data fusion techniques have been developed (Prakash et al., 2012; Srivastava et al.,

302   2013; Wagner et al., 2012), however their methods require high computational time to run and

303   this, in a real-time flood forecasting framework, could not match the operational needs.

304   Comparatively, LLR model is a simpler method and requires relatively low computational time.

305   Therefore it is chosen in order to test if a simple method is able to provide effective

306   performance. LLR is a nonparametric regression model that has been applied in (Liu et al.,

307   2011; Pinson et al., 2008; Sun et al., 2003; Zhuo et al., 2016b) for forecasting and smoothing

308   purposes. LLR builds local linear regression based on the nearest points (p_{max}) of a targeted

309   point, and repeats such a process over the whole training dataset to produce a piecewise linear

310   model. There are many methodologies in selecting the p_{max}, in this study a method called

311   influence statistics is used (Durrant, 2001; Remesan et al., 2008), which is outlined as below.

312   Assume there are p_{max} nearest points, then the Eq. 7 can be built:

313     $Xm = y$ (7)

314   here X is a $p_{\max} \times d$ matrix which shows the d dimensional information of p_{max}, x_i are the

315   nearest points confined between 1 and p_{max}, y is the output vector with p_{max} dimension, and m

316   is a set of parameters formed in a vector, which plays an important role in mapping the solution

317   from X to y. Therefore Eq. 7 can be expanded as

318
$$\begin{pmatrix} x_{11} & x_{12} & x_{13} & \cdots & x_{1d} \\ x_{21} & x_{22} & x_{23} & \cdots & x_{2d} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ x_{p_{\max}1} & x_{p_{\max}2} & x_{p_{\max}3} & \cdots & x_{p_{\max}d} \end{pmatrix} \begin{pmatrix} m_1 \\ m_2 \\ \vdots \\ m_d \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_{p_{\max}} \end{pmatrix} \tag{8}$$

319   In order to solve the equation, the following two conditions are set: a) if X is square and non-

320   singular then Eq. (7) can be simply calculated as $m = X^{-1}y$; b) if X is not square or singular,

321   Eq. (7) needs to be rearranged and m can be get by finding the minimum of:

322    $|Xm - y|^2$ $\hspace{6cm}$ (9)

323   with the distinct solution of:

324    $m = X^{\#}y$ $\hspace{6cm}$ (10)

325   where $X^{\#}$ is the pseudo-inverse matrix of X (Penrose, 1955; Penrose, 1956).

326   **3. Results**

327   In this section, different combinations of input data (Table 3) are adopted to examine their

328   impacts on hydrological soil moisture estimation. XAJ SMD is used as a hydrological soil

329   moisture state benchmark for the training and testing. More discussion about the misconception

330   between the hydrological model's soil moisture state variable and the real-world soil moisture

331   content is covered in Section 4. During GT and M-test processes, all data inputs need to be

332   normalised so that their mean is zero and standard deviation is 0.5. This step is necessary in

333   reducing the impacts of numerical difference from various inputs, hence improves the GT

334   efficiency (Remesan et al., 2008). Five statistical indicators are used for the soil moisture

335   estimation analysis: Pearson product moment correlation coefficient (r), MSE which is the

336   same value as the Gamma statistic Γ, Standard error (SE), NSE (Nash and Sutcliffe, 1970), and

337   Root Mean Square Error ($RMSE$).

3.1 Scheme 1: SMD Estimation Using SAC-SMA-SM as input

339   Although in this scheme, there is no need for data feature selection because only one data input

340   is involved, the GT is still carried out to explore the useful information about the underlying

341   relationship between the XAJ SMD and the SAC-SMA-SM. The calculated Gamma statistics

342   are shown in Table 4. The Γ of 0.072 indicates that the optimal MSE achievable using any

343   modelling technique is 0.072; and the small value of SE means the precision and accuracy of

344   the GT result. Γ is a significant target value in the M-test to find the most suitable training data

345   size. As presented in Figure 4a, when more training data (i.e., M increases in steps of one) is

346   used the Γ changes dramatically. Eventually at $M = 292$, Γ starts to stabilise around 0.072. The

347   M-test allows us to confidently apply the first 292 datasets to build a model of a given quality,

348   in the sense of predicting with a MSE around the asymptotic level. The corresponding Gamma

349   gradient (A) suggests the complexity of the underlying system: the larger the A value is the

350   more complex the system is. For example if A is significantly large, a more complicated model

351   like a Support Vector Machine might be required, but $A = 1.353$ in Scheme 1 is small (Remesan

352   et al., 2008), therefore a LLR model should be able to simulate the system. For LLR modelling,

353   its complexity level is controlled by the p_{max} parameter. As illustrated in Figure 5, p_{max} is

354   identified from a trial and error method. The procedure is by increasing the LLR p_{max} value

355   from 2 to 100 to analyse the variations of their corresponding Γ results. It can be seen from

356   Figure 5 that the smallest Γ is achieved at $p_{max} = 4$, which is therefore adopted for the LLR

357   modelling. The training and testing scatter plots for the LLR modelling are shown in Figure 6a.

358   It is observed that there are some points lying far above the bisector line during the training

359   period signifies higher estimations whereas some points sit far below the bisector line during

360   the testing period indicates under-estimation of the SMD. For the testing results, when XAJ

361   simulated soil moistures state have already reach the total dryness (i.e., XAJ SMD peaks at

362   around 0.080 m) the predicted soil moisture state is still in the drying progress. Figure 7a plots

363   the time series of the estimated and the targeted SMD. The plot shows that the estimated SMD

364   follows the seasonal trend of the soil moisture fluctuations well, so it is wetter during the winter

365   season and exsiccated during the hot summer season. However it is clear to see that the model

366   is not able to capture the extreme situations very well, especially during the wet season when

367   the XAJ SMD becomes smaller (e.g., between Day 300 and Day 350).

368   **3.2 Scheme 2: SMD Estimation Using SAC-SMA-SM and MODIS-LST as inputs**

369   Land surface temperature is the product of the soil temperature multiplied by the emissivity,

370   and the emissivity depends on the dielectric constant of the soil and soil moisture (Rodriguez-

371   Fernandez et al., 2015). Therefore the additional MODIS-LST information could potentially

372   improve the soil moisture estimation. The modelling process is the same as in Scheme 1. In

373   Table 4, it is clear to observe that by adding the MODIS-LST input, the Γ is improved to 0.060

21

374 and its corresponding gradient A is reduced significantly to less than half of the Scheme 1's.

375 Meanwhile the SE value is decreased remarkably as well showing the accuracy of the GT. The

376 M-test in Figure 4b shows the graph settles to an asymptote around 0.060 which is consistent

377 with the calculated Γ result. Training data size of 199 is chosen here because it gives the lowest

378 Γ value. For the LLR modelling, the best p_{max} value is found to be 2 from the trial and error

379 result in Figure 5. The LLR training and testing performances are presented in Figure 6b.

380 Although the problem of underestimation of extremely dry soil still exists (i.e., the points

381 concentrate at the right end of the training and testing plots), overall the model's prediction

382 ability during both phases are better than Scheme 1's (i.e., data points are closer to the 45° line).

383 The improvement can also be seen clearly in the time series plot in Figure 7b. For example, the

384 big disparities between the estimated and the targeted SMDs around DAY 300 and DAY 350

385 are reduced evidently.

386 **3.3 Scheme 3: SMD Estimation Using SAC-SMA-SM and SMOS-T$_b$s as inputs**

387 The multi-angle T$_b$s retrievals are the main data inputs for SMOS soil moisture calculation,

388 therefore their inclusion should also add a positive effect to the hydrological soil moisture

389 estimation. As aforementioned, an efficient feature selection of the SMOS incidence angles is

390 important for the best SMD calculation. In this study all the possible combinations from all

391 inputs variables are examined with the Γ result as the statistical indicator. This method is

392 capable of examining every combination (16383 embeddings in this case) of data inputs to

393 target the optimal combination that gives the smallest absolute Γ value. As discussed in Section

394 2.3.4, SAC-SMA-SM is a compulsory data input, so it is not included in the selecting process.

395   The best set of SMOS-T_bs to retrieve soil moisture state is composed of H polarization at the

396   incidence angles of 27.5°-47.5°, 57.5°, and V polarization at the incidence angles of 27.5°-42.5°,

397   52.5°, 57.5°. This result demonstrates that using a combination of H and V T_bs gives a better

398   soil moisture estimation, which is logically sensible because different polarizations carry

399   distinct information of the Earth surface. However some incidence angles could held common

400   features which when putting together could result in a negative effect to the LLR modelling,

401   and are therefore not included. The detailed investigation of the possible common features is

402   out of the scope of this paper which is mainly due to the SMOS working mechanism.

403   As seen from Table 4, the inclusion of SMOS-T_bs significantly improves the Γ result by 54%,

404   while the gradient A is reduced greatly by 89% as compared with Scheme 1. The small A value

405   illustrates that the underlying system is more straightforward and easier to model than the

406   Scheme 1's. The M-test analysis in Figure 4c produces an asymptotic convergence from 120

407   training data size of Γ value around 0.033. It is interesting to see that the proportion of the

408   required training data is relatively larger than those in Scheme 1 and 2. The potential reason

409   could be explained by the larger amount of data inputs in this scheme. For LLR modelling, the

410   p_{max} that gives the smallest Γ is 7 (Figure 5). The SMD estimations during the training and the

411   testing are presented in Figure 8a. It can be seen that the SMD prediction ability of this scheme

412   is remarkably better than the previous ones, as most of the points lie on the bisector line albeit

413   there are still some under- and over- estimations. The reason SMOS outperforms MODIS in

414   SMD estimation could be due to the long wavelength microwave has, so it presents the top few

415   centimetres of the soil while MODIS LST (thermal infrared) only provides information at the

416   soil surface. The used LLR algorithm has been double checked to filter out the potential of

417 overfitting problem. The checking processes are performed by muddling the SMD target in the

418 testing datasets as well as altering the input file, and its efficiency stays the same. Hence it is

419 believed that the LLR model is very useful in calculating SMD from this scheme. Generally

420 the *NSE*, *r* and *RMSE* statistical indicators show a high agreement during both training and

421 testing phases. For the time series plot in Figure 7c, it is clear to see that most of the estimated

422 points lie closely to the benchmark line. The observed outliers could be partly due to the data

423 shortage in this scheme, so that not all the scenarios are covered in the datasets.

424 **3.4 Scheme 4: SMD Estimation Using SAC-SMA-SM, MODIS-LST, and SMOS-T$_b$s as**

425 **inputs**

426 In this scheme, all the three data sources are used to test if the modelling performance can be

427 further improved. Here the full embedding calculation is again carried out to explore the most

428 suitable incidence angles from the SMOS-T$_b$s. This is because the added MODIS-LST data

429 could carry identical (i.e., redundant) features with some of the SMOS-T$_b$s datasets. As a result

430 of the full embedding calculation, the best set of SMOS-T$_b$s is composed of H polarization at

431 the incidence angles of 37.5°-57.5°, and V polarization at the incidence angles of 37.5°-42.5°,

432 57.5°. As seen in Figure 4d, the total amount of data is significantly reduced due to the shortage

433 of simultanuously available days between the MODIS and the SMOS observations.

434 Interestingly the *M*-test graph vibrates more significantly than the other three schemes, which

435 could be due to the smaller data size and the larger amount of data inputs in this scheme. Here

436 the training data size is chosen as 62 with Γ obtained at around 0.030. The optimal p_{max} is

437 identified to be 5 (Figure 5). The LLR modelling results are shown in Figure 7d and Figure 8b.

438   It is obvious that this scheme further improves the accuracy of the SMD estimation, especially

439   with the high statistical performances achieved during both training and testing phases.

440   Comparatively this scheme is more stable for SMD estimation, albeit it requires more data

441   inputs and is only realisable when both the MODIS and the SMOS observations are available.

3.5 Produce an Unintermitted Soil Moisture Product

443   The data availability of the four schemes varies. As shown in Figure 9, Scheme 1 which has

444   the poorest soil moisture state estimation gives the most data availability, while Scheme 4

445   which has the most accurate soil moisture state estimation owns the least data availability. In

446   order to produce an unintermitted hydrological soil moisture product, the four schemes need to

447   be combined together to complement each other. The combining method is by selecting the

448   best available soil moisture estimation. For example if all the schemes have available data at

449   the same time, the best scheme's soil moisture data is chosen (i.e., scheme 4 in this situation);

450   whereas if just one scheme has data on that day, only that scheme's soil moisture data is used.

451   The performances of the four schemes as well as the combined product are summarised in

452   Table 5. Although the combined soil moisture state is obtained with lower statistical

453   performances than Scheme 3's and 4's, it is still hydrologically very accurate especially when

454   comparing with the SMOS's official soil moisture product (Table 5). The time series of the

455   combined soil moisture state is plotted in Figure 10. It can be seen that the general trend of the

456   produced soil moisture state follows the targeted data very well. However it tends to

457   overestimate some of the wet events during the rainy season and significantly underestimate

458   the dryer soil condition in September 2011. Those poor estimations are mostly from the Scheme

459   1 and 2 where Schemes 3 and 4 are not available. Since more and more microwave satellite

460   observations are becoming obtainable, those new data sources could add extra benefits into the

461   proposed model, and the accuracy of the soil moisture product is expected to be further

462   enhanced.

463   **4. Discussion**

464   - *What is a soil moisture state variable?*

465   This study uses the XAJ's SMD simulation as a target because it is hydrological model directly

466   produced. However it is argued that models with different parameters values can generate

467   equally good flow results named as the equifinality effect, because they are all calibrated based

468   on the observed flow. For this reason, their soil moisture state variables can be distinct among

469   each other.

470   In order to investigate this effect in more details, the XAJ model is manipulated by increasing

471   one of its parameters WUM by 30 %. By doing so, the XAJ's flow simulation remains as

472   effective as its original form (the same NSE values), but its soil moisture state changes

473   significantly from its original values. For a better visualisation, an enlarged plot of the SMD

474   simulations between Day 222 and Day 344 is presented. As seen from Figure 11a although the

475   soil moisture state variables from two equally good calibrations have a wide range of value

476   differences ($NSE = 0.34$), they both follow the same pattern: when it rains they become wet by

477   the similar amount; when there is a dry period they all move into a dryer state in a similar rate

478   to the actual evapotranspiration. Therefore they appear as in parallel movements and the latter

479   plot (Figure 11b) shows a very strong linear correlation ($r = 1.0$) between them. It is important

480   to note that the selection of the dry period (i.e., high SMD values) is because it is the most

481   critical period of time for the need of accurate soil moisture values for hydrological modelling.

482   This is because during the real-time flood forecasting, after a long period of dryness, the

483   accumulation of error in the hydrological models can become larger and larger with time. With

484   accurate soil moisture information, the error could be corrected.

485   Although the absolute values of the models' soil moisture state variables are not quite

486   meaningful and comparable, their variations are the true reflection of the soil moisture

487   fluctuations in the real-world. This clarification is a very important concept, because there has

488   been a wide spread of misunderstanding about the hydrological model's soil moisture state and

489   its connection with the real-world soil moisture.

490   - *Soil moisture state normalisation*

491   One deficiency of this study is that the generated soil moisture state is based on a hydrological

492   model's SMD simulation, so it is model parameter dependent. It is desirable to produce a soil

493   moisture indicator which is independent from model parameters and dimensionless with

494   variables between 0 and 1. Normalised Hydrological Soil Moisture State (NHSMS) indicators

495   are produced as presented in Figure 12 (corresponding to the SMD simulations shown in Figure

496   11). The normalisation method is by adopting the following equation:

497    $$NHSMS = \frac{SMD - \min(SMD)}{\max(SMD) - \min(SMD)}$$ (11)

498   Such an approach is very effective as demonstrated by the almost identical SMD curves

499   between the two XAJ simulations. In the future it is planned to use the same process on other

27

500 hydrological models to test if the normalised soil moisture indicators are not only model

501 parameter independent but also model structure independent. Since all hydrological models are

502 driven by the same physics laws on the conservation of mass, their normalised soil moisture

503 indicators should respond in a similar way (soil becomes wetter when it rains and drier when

504 there is no rain). If this is true a new soil moisture product based on NHSMS could be generated

505 as a routine product by the operational organisations such as NASA and ESA. Such a soil

506 moisture product will also be very useful to the meteorological and hydro-meteorological fields

507 in their land surface modelling because the current land surface models suffer from poor

508 performance in their runoff estimations. As aforementioned, all current soil moisture products

509 such as those from ESA and NASA are not optimised for different application fields. Our study

510 gives an example of simulating the soil moisture data targeted to serve the hydrological

511 community. It is possible other products serving farmers in agriculture, ecologists in the

512 environment, and geotechnical engineers in construction could be produced using the proposed

513 method.

514 - *Application of the produced soil moisture data*

515 Another area needs further work is the hydrological application of the produced data. Generally

516 effective hydrological application of soil moisture data needs three pre-conditions: 1) a good

517 soil moisture data relevant to hydrology; 2) a hydrological model compatible with such data;

518 3) an effective data assimilation scheme. This paper tackles the first point, and the other two

519 points would need further research because there are significant knowledge gaps in them. If all

520 the three points are solved, such a data has a huge potential in operational hydrological

modelling. For example, initialisation of the model could be shortened which reduces the need for model warm up. This is important during real-time flood forecasting when there is not enough data to warm up the model for an imminent flood event. Such a warm-up period could be very long, as demonstrated by the study in (Ceola et al., 2015). In addition the XAJ SMD data used here is based on the calibration of the observed rainfall and flow, so that the targeted SMD is interpolated between observations and there is a minimum time-drift. In the real-time flood forecasting the errors in precipitation and evapotranspiration could accumulate which cause time-drift problems. Therefore a soil moisture product such as the one produced in this study (i.e., based on minimal time-drift SMD) could help avoiding such a problem. The proposed soil moisture data is also valuable for the validation of land surface models, especially useful for their runoff simulations. Due to the limit of time and resources this study has not tackled all the issues, but has laid a good foundation for their future researches.

- *XAJ model under frozen conditions*

The Pontiac catchment is characterized by soil freezing events in winter seasons. During freezing events, soil moisture transfer fundamentally differs from the unfrozen conditions (e.g., (Gelfan, 2006)). Although the XAJ model has been successfully applied in simulating flows in frozen soil conditions (e.g., see Zhou et al. 2008) as well as in this case study, the lumped XAJ model does not explicitly consider soil freezing, thus SMD simulations can be inaccurate for winter seasons and further research is needed to investigate this issue further.

5. Conclusions

29

541   A hydrological soil moisture product is produced for the Pontiac catchment using the GT and

542   the LLR modelling techniques based on four data-input schemes. Three data sources are

543   considered including the soil moisture product from the SAC-SMA model, the land surface

544   temperature retrieved by the MODIS satellite, and the multi-angle brightness temperatures

545   acquired from the SMOS satellite. The four data-input schemes are built from the four

546   combinations of the data sources. The generated soil moisture product (unintermitted with no

547   missing data) for a period of two years (2010-2011) is compared with the XAJ hydrological

548   model's SMD simulation to test its hydrological accuracy. It is concluded that the GT and the

549   LLR modelling techniques together with the chosen data inputs can be used with high

550   confidence to estimate an unintermitted hydrological soil moisture product, and the proposed

551   method could be easily applied to other catchments and fields.

552   In this study it has been found that different data sources have their own unique information

553   contents, so that they can complement each other using data fusion technique. Their synergy

554   can be best achieved to produce an enhanced soil moisture product. In data fusion an important

555   principle is MRmr (Maximum Relevance minimum redundancy). The soil moisture state in

556   this study is generated from a large number of data inputs, and their selection is carried out by

557   the GT which is one of the methods in MRmr. This is the first time that the GT is used in a data

558   fusion of satellite multiple T_bs scans, land surface temperature and external soil moisture

559   information for producing a hydrological soil moisture product. Future studies should explore

560   other MRmr methods in addition to GT, to compare if they are more effective input selection

561   methods. As to the data fusion regression model, LLR is chosen in this study because it is easily

562 applied and very effective. However it is possible there may exist other better models. We

563 encourage the community to apply the proposed methodology using other regression models.

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820

Table 1. The XAJ model parameters used in the Pontiac catchment.

Symbol	Model parameters	Unit	Range
K	Ratio of evapotranspiration	[-]	0.10-1.20
WUM	The areal mean field capacity of the upper layer	mm	30-50
WLM	The areal mean field capacity of the lower layer	mm	20-150
WDM	The areal mean field capacity of the deep layer	mm	30-400
IMP	Percentage of impervious and saturated areas in the catchment	%	0.00-0.10
B	Exponential parameter with a single parabolic curve, which represents the non-uniformity of the spatial distribution of the soil moisture storage capacity over the catchment	[-]	0.10-0.90
C	Coefficient of the deep layer that depends on the proportion of the catchment area covered by vegetation with deep roots	[-]	0.10-0.70
SM	Areal mean free water capacity, which represents the maximum possible deficit of free water storage	mm	10-50
KG	Outflow coefficient of the free water storage to groundwater relationships	[-]	0.10-0.70
KSS	Outflow coefficient of the free water storage to interflow relationships	[-]	0.10-0.70
EX	Exponent of the free water capacity curve	[-]	1.10-2.00
KKG	Recession constant of the groundwater storage	[-]	0.01-0.99
$KKSS$	Recession constant of the lower interflow storage	[-]	0.01-0.99
CS	Recession constant in the lag and route method for routing through the channel system with each sub-catchment	[-]	0.10-0.70
L	Lag in time	[-]	0.00-6.00
V	Parameter of the Muskingum method	m/s	0.40-1.20
dX	Parameter of the Muskingum method	[-]	0.00-0.40

Table 2. General data-input properties relevant for this study.

	SMOS-T_bs	MODIS-LST	SAC-SMA-SM
Product	brightness temperature	land surface temperature	soil moisture
Unit	Kelvin (K)	Kelvin (K)	m^3/m^3
Near-Real-Time (NRT)	Yes	Yes	Yes
Spatial resolution (km)	35-50	5.6	14
Data time-step	~ every three days	~ daily	Daily
Data availability for the studying period (days)	217	458	730

Table 3. Four data-input schemes: scheme 1: SAC-SMA-SM; scheme 2: SAC-SMA-SM and MODIS-LST; scheme 3: SAC-SMA-SM and SMOS-T_bs; scheme 4: SAC-SMA-SM, MODIS-LST, and SMOS-T_bs.

	SAC-SMA-SM	MODIS-LST	SMOS-T_bs
Scheme 1	x		
Scheme 2	x	x	
Scheme 3	x		x
Scheme 4	x	x	x

Table 4. Model statistical performances and modelling information, where Γ is the calculated gamma statistic which is the minimum *MSE* that can be achieved from a modelling method; A is the Gamma gradient; *SE* is the Standard error; p_{max} is the nearest points for LLR modelling; M is the training data size; and SMOS IA is the chosen incidence angles of SMOS-T_bs.

	Γ	A	*SE*	p_{max}	M	SMOS IA
Scheme 1	0.072	1.353	0.004	4	292	-
Scheme 2	0.060	0.568	0.002	2	199	-
Scheme 3	0.033	0.152	0.004	7	120	H: 27.5º-47.5º, 57.5º
						V: 27.5º-42.5º, 52.5º, 57.5º
Scheme 4	0.029	0.119	0.006	5	62	H: 37.5º-57.5º
						V: 37.5º-42.5º, 57.5º

Table 5. Summary of SMD estimation performances. It is noted that *RMSE* is in the unit of metre.

	Training			Testing		
	NSE	*r*	*RMSE*	*NSE*	*r*	*RMSE*
Scheme 1	0.752	0.870	0.011	0.688	0.830	0.014
Scheme 2	0.767	0.877	0.011	0.747	0.865	0.012
Scheme 3	0.928	0.965	0.006	0.876	0.940	0.008
Scheme 4	0.912	0.957	0.007	0.912	0.960	0.007
Combined	-	-	-	0.790	0.889	0.011
SMOS-SM	-	-	-	0.420	0.650	0.017
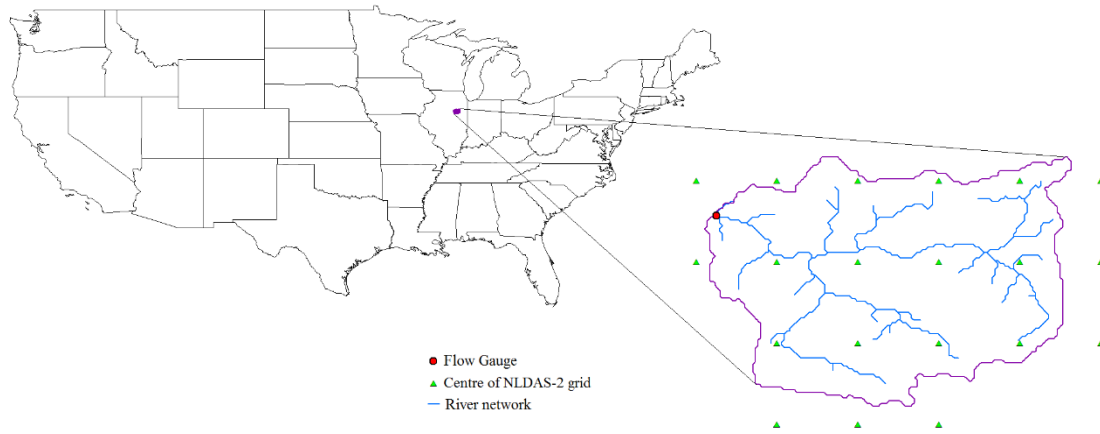
Figure. 1. The location and river network of the Pontiac catchment in the U.S., with the flow gauge and NLDAS-2 central grid points (Zhuo et al., 2015a).
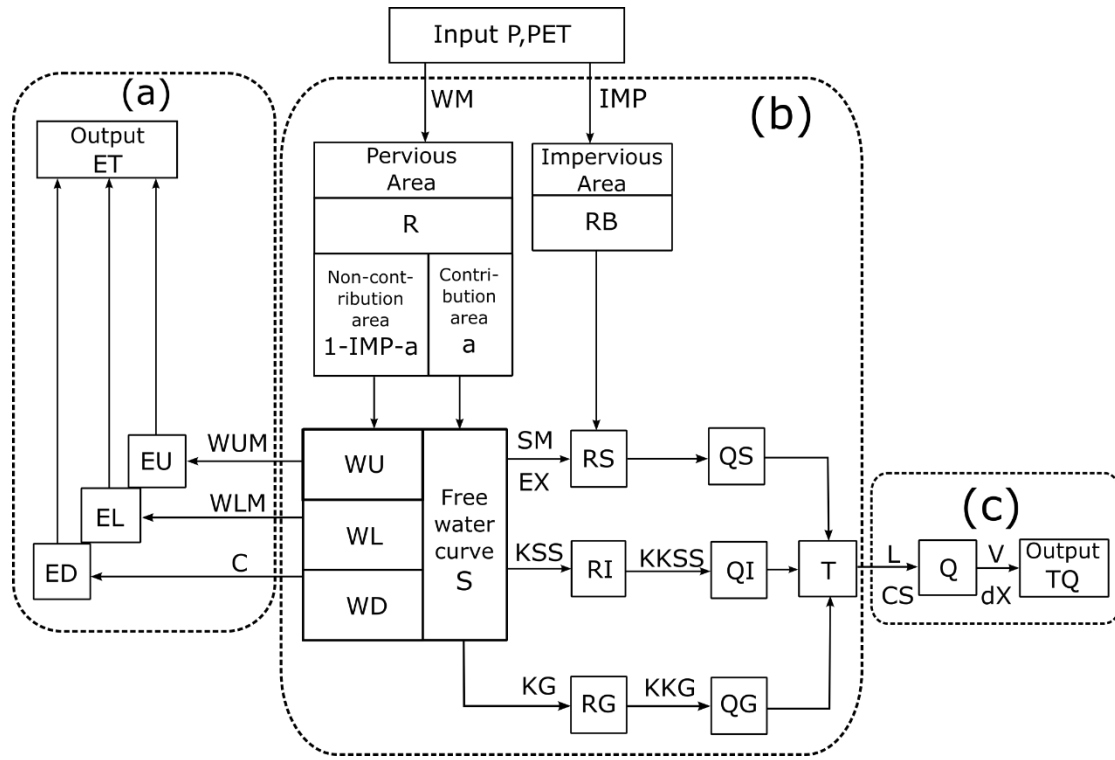
Figure. 2. Adopted flowchart of the XAJ model *(Zhao, 1992)*. The model consists of an evapotranspiration component (a), a runoff generating component (b), and a runoff routing component (c). *P*, *PET*, and *ET* are the precipitation, potential evapotranspiration, and the simulated actual evapotranspiration respectively; *WU*, *WL* and *WD* represent the upper, lower, and deep soil layers' areal mean tension water storage respectively; *WM* is the areal mean field capacity; *EU*, *EL,* and *ED* stand for the upper, lower, and deep soil layers' evapotranspiration output respectively; *S* is the areal mean free water storage; *a* is the portion of the sub-catchment producing runoff; *IMP* is the factor of impervious area in a catchment; *RB* is the direct runoff produced from the small portion of impervious area; *R* is the total runoff generated from the model with surface runoff (*RS*), interflow (*RI*), and groundwater runoff (*RG*) components respectively. These three runoff components are then transferred into *QS*, *QI,* and *QG* and combined as the total sub-catchment inflow (*T*) to the channel network. The flow outputs *Q* from each sub-catchment are then routed to the catchment outlet to produce the final flow result (*TQ*). The rest of the symbols are explained in Table 1.
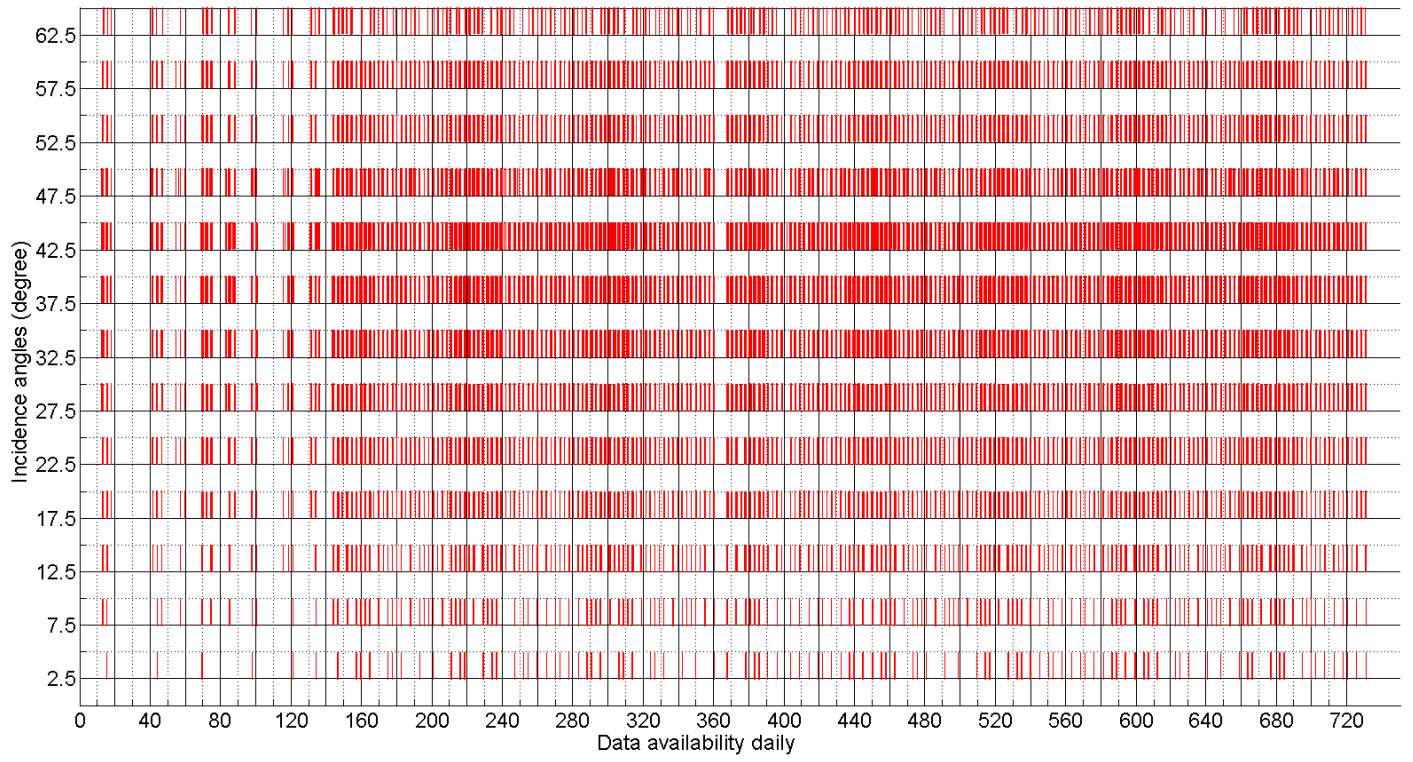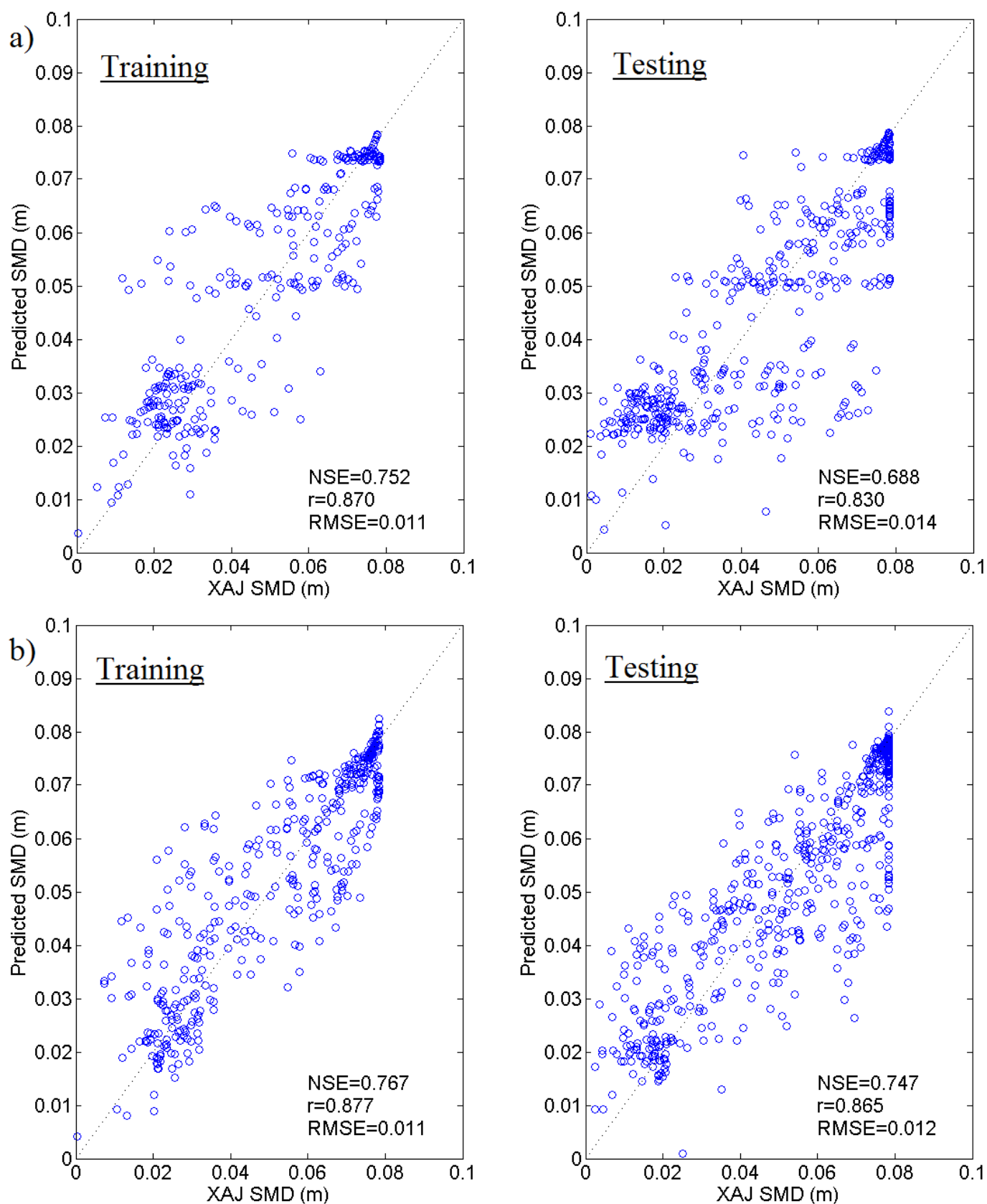
Figure 3. SMOS-T$_b$s data availabilities. It is noted that the available dates for the horizontal and the vertical polarizations are the same, so only one is shown here.
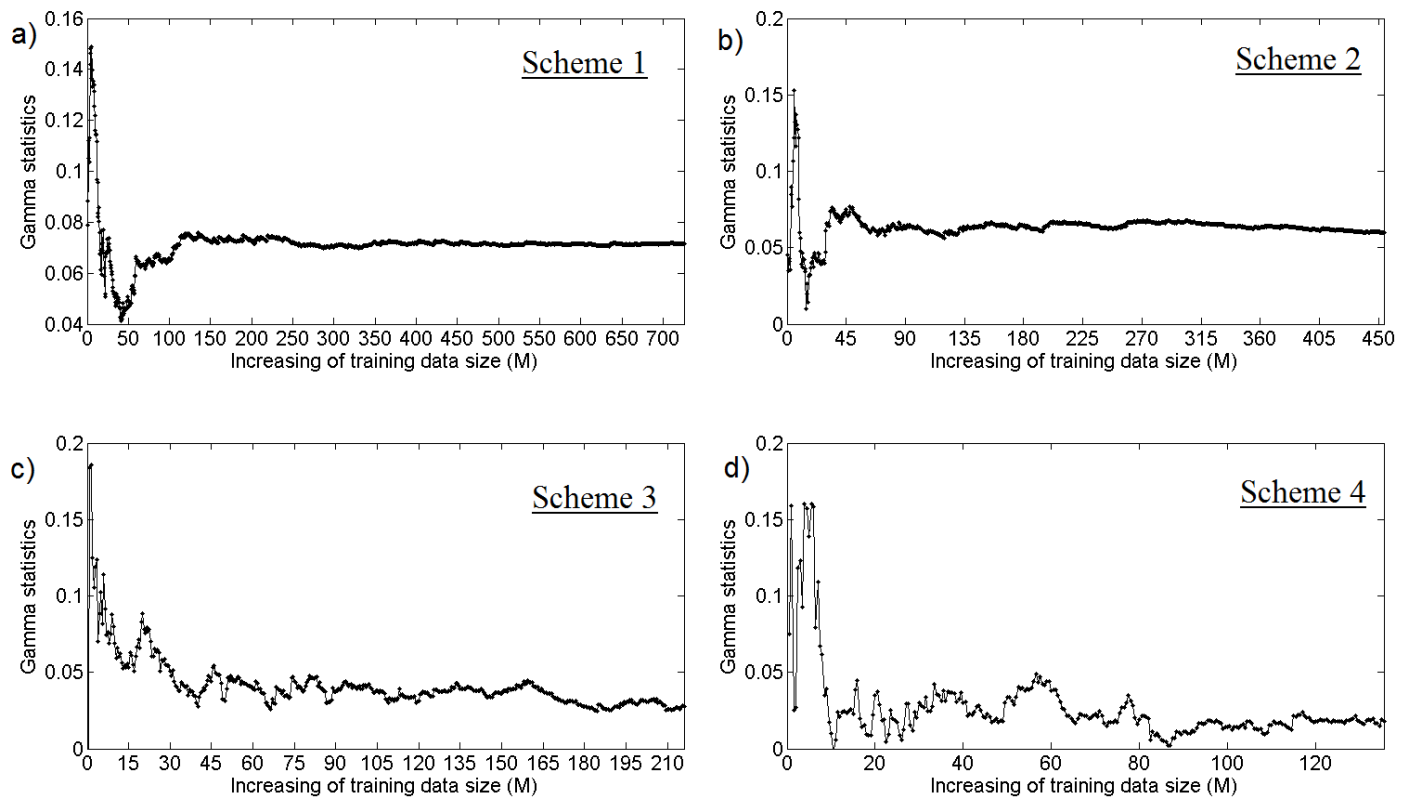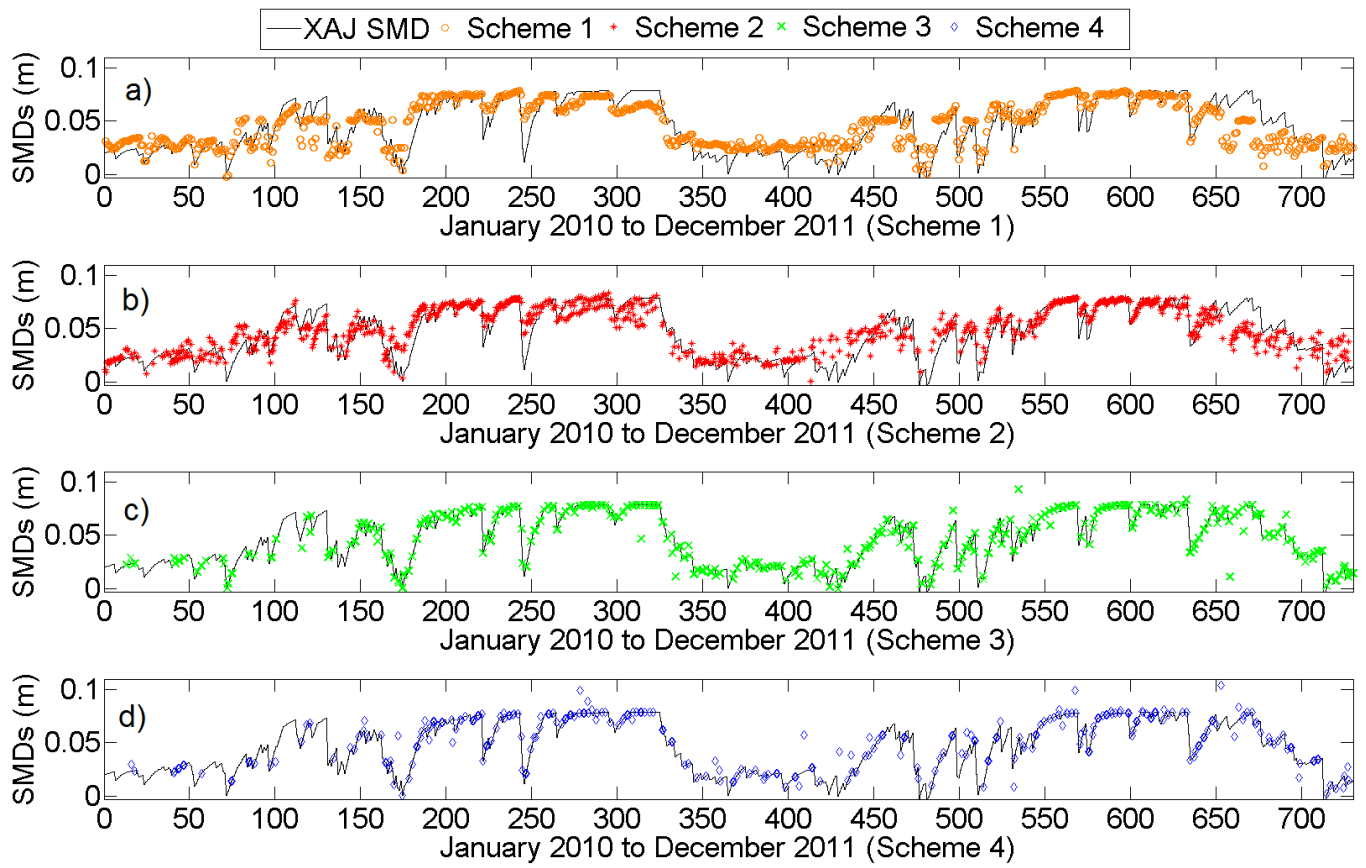
Figure 4. *M*-test, to find the best training data size: a) Scheme 1; b) Scheme 2; c) Scheme 3; and d) Scheme 4.
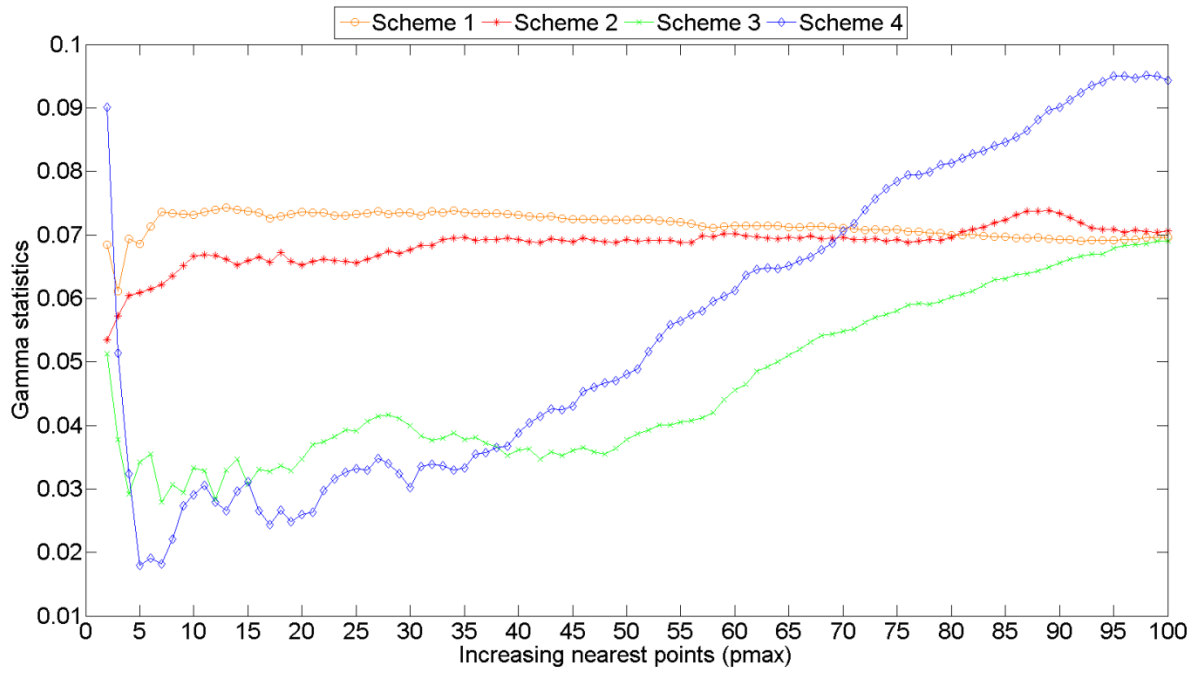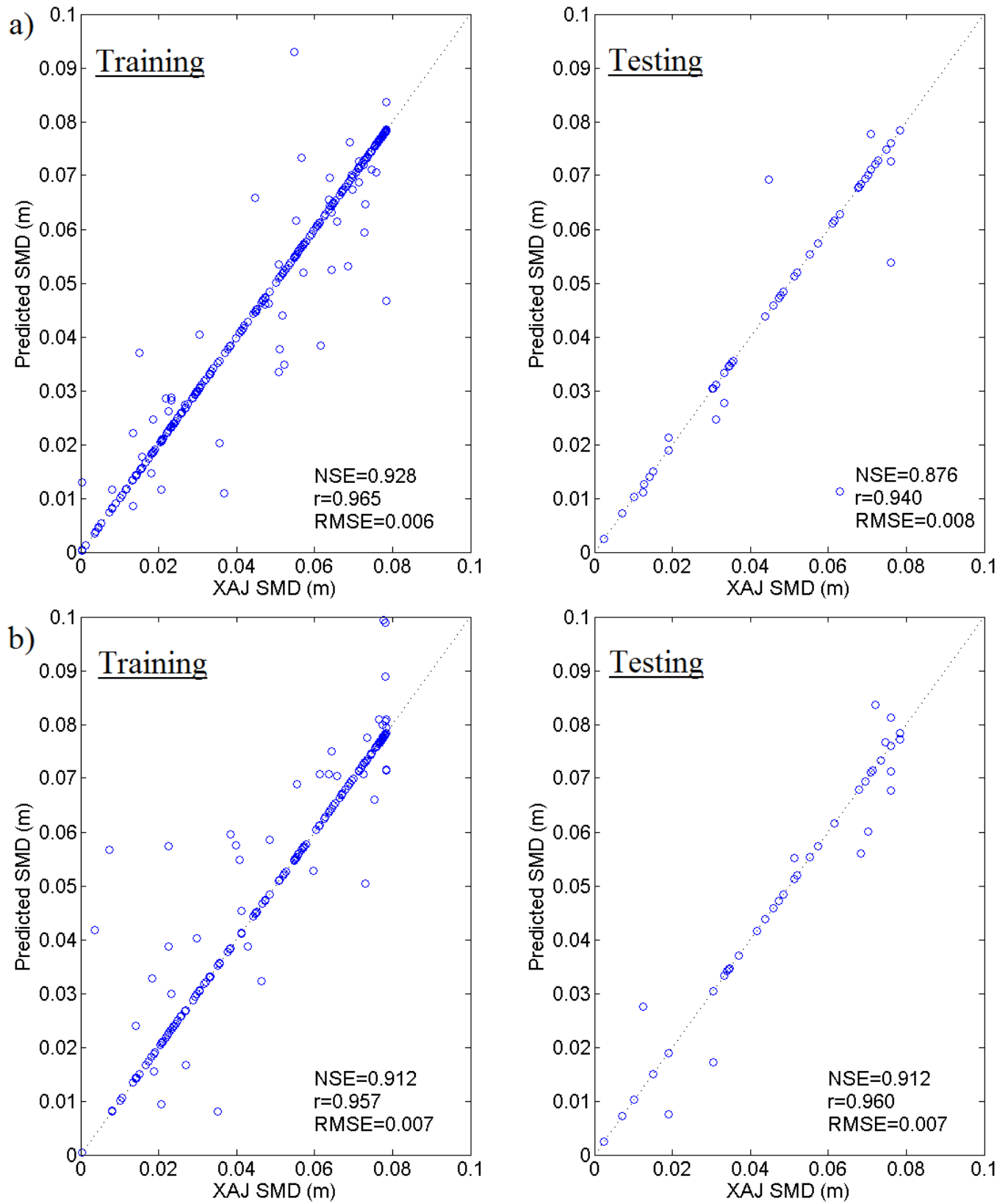
**Figure 5.** Gamma statistic (Γ) variations for increasing the LLR p_{max} value.

**Figure 6.** LLR modelling during the training and testing phases for a) Schemes 1 and b) Scheme 2.

Figure 7. The time series plots of the XAJ SMD and the estimated SMD from the four schemes: a) Scheme 1; b) Scheme 2; c) Scheme 3; and d) Scheme 4.

Figure 8. LLR modelling during the training and testing phases for a) Schemes 3 and b) Scheme 4.
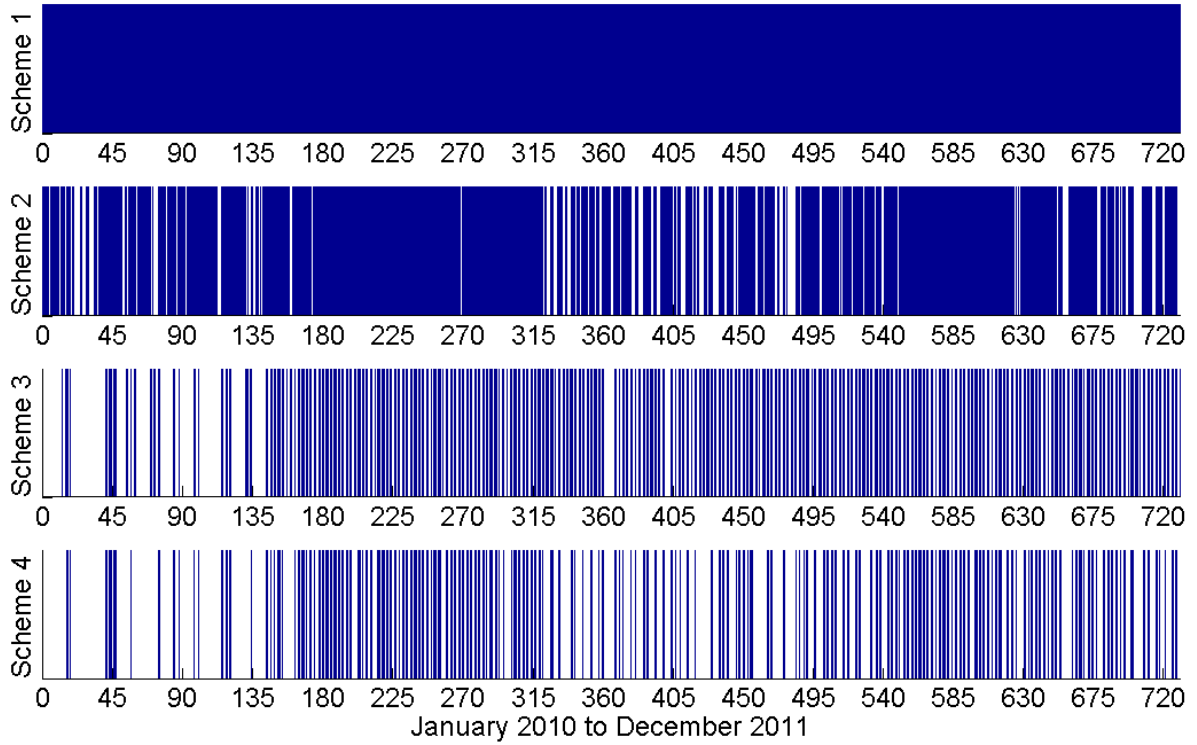
Figure 9. Data availability plots of the four schemes: Scheme 1: SAC-SMA-SM input; Scheme 2: SAC-SMA-SM and MODIS-LST inputs; Scheme 3: SAC-SMA-SM and SMOS-T_bs inputs; Scheme 4: SAC-SMA-SM, MODIS-LST, and SMOS- T_bs inputs. The total available days for the four schemes are 730, 458, 217, and 140 respectively.
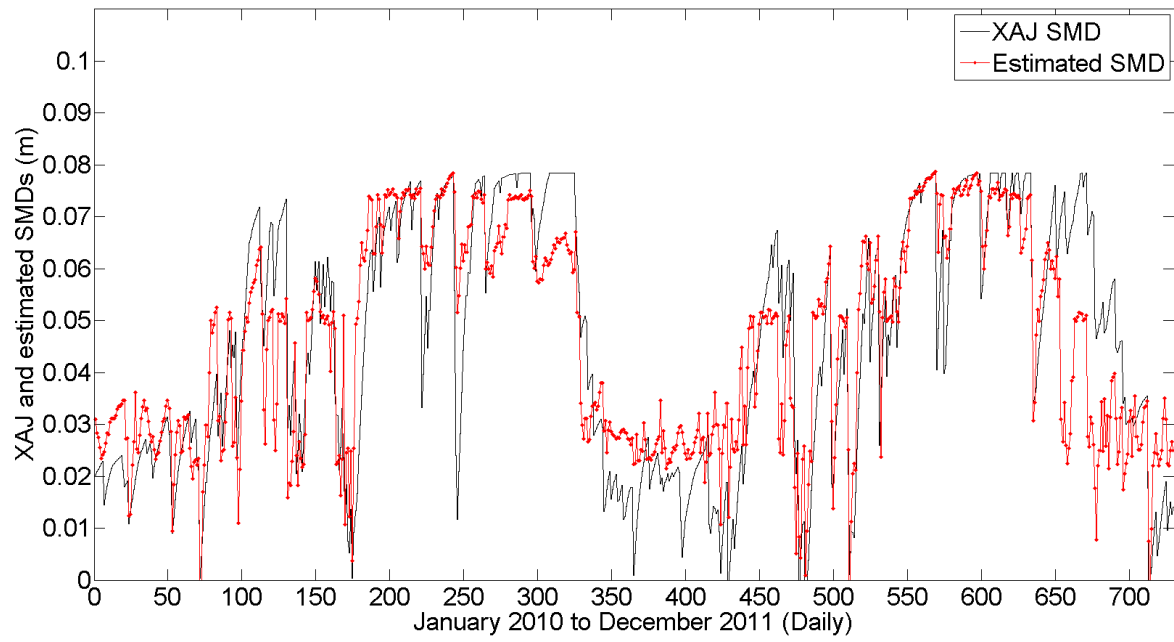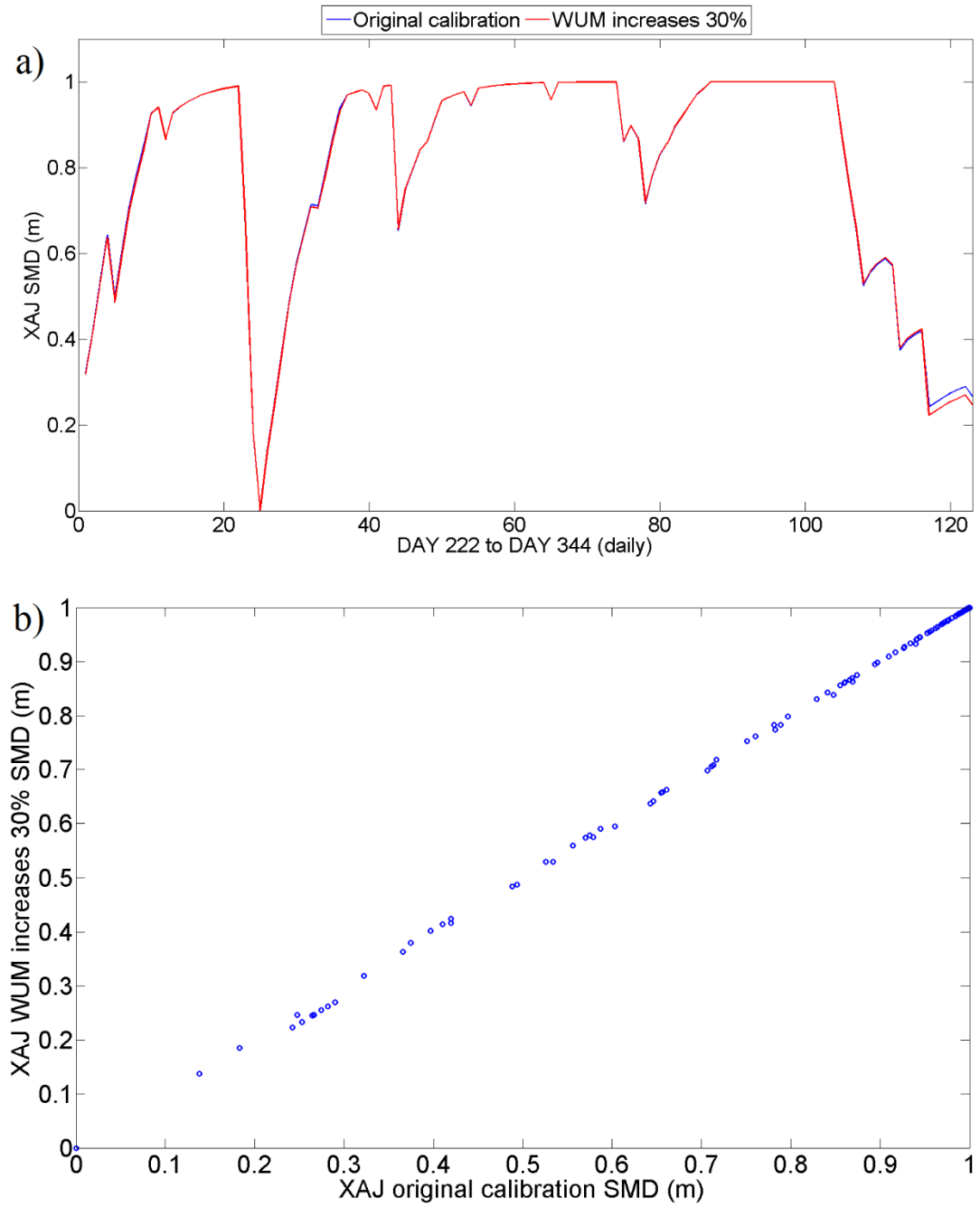
Figure 10. Time series plot of the combined daily hydrological soil moisture state estimations.
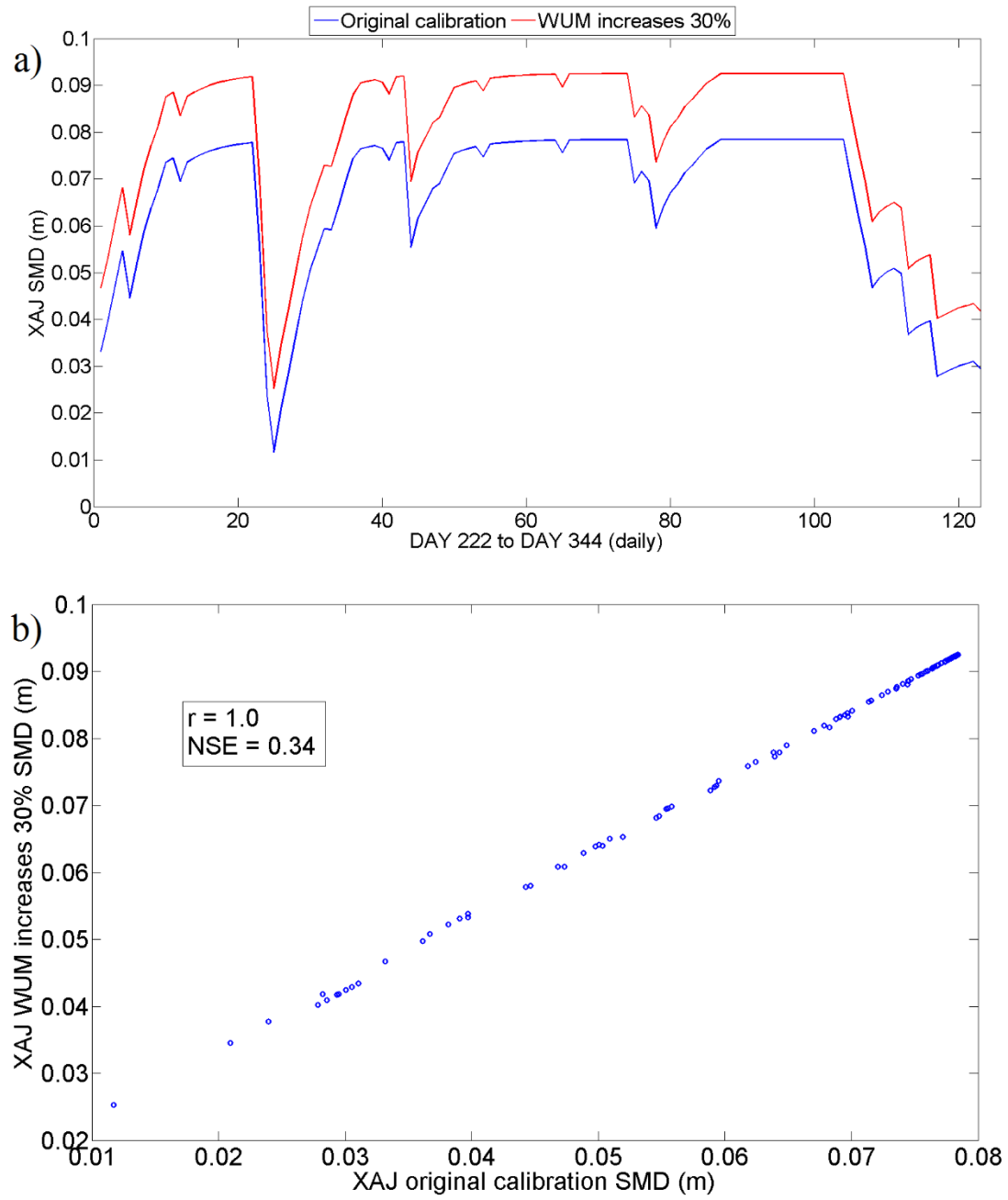
Figure 11. SMD variations from the manipulated XAJ calibration (i.e., the WUM parameter is increased by 30 %) and its original calibration.

Figure 12. Normalised SMD variations from the manipulated XAJ calibration (i.e., the WUM parameter is increased by 30 %) and its original calibration.