

1                   **Diagnosis toward predicting mean annual runoff in ungauged basins**

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6                   **Abstract**

7                   Prediction of mean annual runoff is of great interest but still poses a challenge in ungauged basins.

8                   The present work diagnoses the prediction in mean annual runoff affected by the uncertainty in

9                   estimated distribution of soil water storage capacity. Based on a distribution function, a water

10                  balance model for estimating mean annual runoff is developed, in which the effects of climate

11                  variability and the distribution of soil water storage capacity are explicitly represented. As such,

12                  the two parameters in the model have explicit physical meanings, and relationships between the

13                  parameters and controlling factors on mean annual runoff are established. The estimated

14                  parameters from the existing data of watershed characteristics are applied to 35 watersheds. The

15                  results showed that the model could capture 88.2% of the actual mean annual runoff on average

16                  across the study watersheds, indicating that the proposed new water balance model is promising

17                  for estimating mean annual runoff in ungauged watersheds. The underestimation of mean annual

18                  runoff is mainly caused by the underestimation of the area percentage of low soil water storage

19                  capacity due to neglecting the effect of land surface and bedrock topography. Higher spatial

20                  variability of soil water storage capacity estimated through the Height Above the Nearest Drainage

21                  (HAND) and Topographic Wetness Index (TWI) indicated that topography plays a crucial role in

22                  determining the actual soil water storage capacity. The performance of mean annual runoff

23                  prediction in ungauged basins can be improved by employing better estimation of soil water

24 storage capacity including the effects of soil, topography, and bedrock. It leads to better diagnosis  
25 of the data requirement for predicting mean annual runoff in ungauged basins based on a newly  
26 developed process-based model finally.

27 **Keywords:** mean annual runoff; ungauged; storage capacity; curve number; soil; topography;  
28 bedrock

29

## 30 **1. Introduction**

31 Hydrologists have a long-standing interest in mean annual water balance modeling and  
32 prediction. The factors controlling mean annual runoff have been studied in literature. Mean  
33 climate has been identified as the first order control on mean annual runoff and evaporation and it  
34 has been quantified by climate aridity index, which is defined as the ratio between the mean annual  
35 potential evapotranspiration ( $E_p$ ) and precipitation ( $P$ ) (Turc, 1954; Pike, 1964). Other controlling  
36 factors include the temporal variability of climate (Farmer et al., 2003; Troch et al., 2002; Fu and  
37 Wang, 2019), vegetation (Zhang et al., 2001; Donohue et al., 2007; Gentine et al., 2012; Li et al.,  
38 2013), soil (Atkinson et al., 2002; Yokoo et al., 2008; Li et al., 2014), and topography (Woods,  
39 2003; Abatzoglou and Ficklin, 2017). Mean annual runoff or evaporation has been modeled as a  
40 function of climate aridity index and the equation is usually called as Budyko equation (Budyko,  
41 1958). The effects of other factors are represented by including a parameter to Budyko equation  
42 (Fu, 1981; Yang et al., 2008; Wang and Tang, 2014). Among these factors, climate including its  
43 mean and temporal variability, and soil water storage capacity including its mean and spatial  
44 variability are dominant catchment characteristics controlling mean annual runoff, especially for  
45 those catchments dominated by saturation excess runoff generation (Milly, 1994).

46 Intra- and inter-annual climate variability introduces non-steady state conditions to finer  
47 timescale water balances and the non-steady state effect could propagate to the mean annual runoff.  
48 The effects of seasonal variations of precipitation and potential evaporation on long-term runoff  
49 have been studied in several studies. Milly (1994) showed that seasonality tends to increase mean  
50 annual runoff through a stochastic soil moisture model. The seasonality effects have been  
51 demonstrated through a top-down model by Hickel and Zhang (2006) and a classification study by  
52 Berghuijs et al. (2014). Mean annual water balance also receives impacts from climate variability  
53 at the inter-annual and daily timescales. Li (2014) showed that the inter-annual variability of  
54 precipitation and potential evaporation could increase the mean annual runoff up to 10% based on  
55 a stochastic soil moisture model. Shao et al. (2012) found that daily precipitation with a larger  
56 variation potentially increases mean annual runoff especially in the catchments where infiltration  
57 excess runoff is prevalent. Yao et al. (2020) quantified the relative contribution of daily, monthly  
58 and inter-annual climate variabilities to mean annual runoff and showed that the contribution  
59 decreases, by average, from monthly to inter-annual scale, and then daily scale.

60 Soil water storage capacity is the maximum storage capacity from land surface to bedrock,  
61 which exerts a powerful control on mean annual runoff (Konapala and Mishra, 2016). A smaller  
62 soil water storage capacity creates favorable conditions for runoff generation because the  
63 precipitation in excess of the available storage capacity would be lost as runoff directly, while  
64 catchments with a larger soil water storage capacity could hold more precipitation for evaporation  
65 (Sankarasubramanian and Vogel, 2002; Porporato et al., 2004; Chen et al., 2013). Soil water  
66 storage capacity is closely related to vegetation since the root structure of vegetation could affect  
67 soil water storage capacity significantly. Research has been conducted to reveal the role of soil  
68 water storage capacity through the linkage of vegetation and model parameter (Yang et al., 2008;

69 Chen and Wang, 2015). Gerrits (2009) developed equations for transpiration and interception by  
70 considering the root zone and interception storage capacity as two of the most important catchment  
71 characteristics affecting evapotranspiration. In addition to the magnitude of the average soil water  
72 storage capacity, the spatial variability of soil water storage capacity within a catchment also  
73 influences precipitation partitioning at the event scale, and further influences the cumulative runoff  
74 at the mean annual scale (Moore, 1985; Jothityangkoon et al., 2001; Gao et al., 2016). It has also  
75 been suggested that the spatial variability of soil water storage capacity could suppress the actual  
76 evaporation because the maximum evaporation in areas with soil water storage capacity less than  
77  $E_p$  will be smaller than  $E_p$ ; therefore, the average evaporation over the entire catchment is smaller  
78 than  $E_p$  even though the average storage is greater than  $E_p$ , resulting in more runoff generation  
79 compared to the situation when the soil water storage capacity is spatially uniform (Yao et al.,  
80 2020).

81 Therefore, climate variability and soil water storage capacity need to be explicitly  
82 incorporated into the model for predicting mean annual runoff. The effect of climate variability  
83 could be taken into account by driving the model with daily precipitation and potential evaporation  
84 which are usually available. The spatial distribution of soil water storage capacity could be  
85 modelled by a distribution function, and it is usually modelled by the generalized Pareto  
86 distribution (Moore, 1985; Zhao, 1992). The distribution function includes two parameters, i.e.,  
87 the shape parameter and the maximum storage capacity over the watershed. In ungauged basins,  
88 soil water storage capacity and its spatial variability need to be estimated directly from available  
89 data. Gao et al. (2014) adopted the mass curve technique, which has been used for designing the  
90 storage capacity of reservoir, to estimate the average water storage capacity of the root zone using  
91 precipitation and potential evaporation data. The shape parameter of the distribution function has

92 been estimated from soil data (Huang et al., 2003). However, the estimated parameters from these  
93 methods bring much uncertainty in runoff estimation, and the two parameters of the generalized  
94 Pareto distribution are usually estimated by model calibration using observed streamflow data  
95 (Wood et al., 1992; Alipour and Kibler, 2018, 2019).

96         The objective of this paper is to develop a nonparametric mean annual water balance model  
97 for predicting mean annual runoff in ungauged basins, which has not yet been fully understood  
98 (Blöschl et al., 2013). The mean annual water balance model is forced by daily precipitation and  
99 potential evaporation; therefore, the climate variability at different timescales is represented  
100 explicitly in the climate input. The runoff generation is quantified by a distribution function for  
101 describing the spatial distribution of soil water storage capacity (Wang, 2018). The mean and the  
102 shape parameter of the distribution function need to be estimated from the available data in  
103 ungauged basins. Therefore, the model serves as a diagnosis tool for evaluating the data  
104 requirement for estimating soil water storage capacity. The mean soil water storage capacity is  
105 estimated from curve number and climate because soil water storage capacity consists of the  
106 antecedent soil water storage and the potential maximum soil moisture retention which can be  
107 calculated through SCS curve number method. The estimation of the shape parameter is diagnosed  
108 in terms of the data requirement including soil, land surface topography, and bedrock topography.  
109 Section 2 introduces the new mean annual water balance model and the study watersheds. Results  
110 and discussion are presented in Section 3, followed by Section 4 for conclusions.

## 111 **2. Methodology**

### 112 **2.1 Mean annual runoff model**

113         Climate variability is defined as the temporal variations of precipitation ( $P$ ) and potential  
114 evapotranspiration ( $E_p$ ), including their intra-monthly, intra-annual, and inter-annual variations.

115 For example, the deviations of daily  $P$  or  $E_p$  from its monthly mean values are defined as the intra-  
 116 monthly variations (Yao et al., 2020). As discussed in the introduction section, the mean annual  
 117 runoff model takes daily precipitation and potential evaporation as inputs, therefore, climate  
 118 variability is explicitly included in the model. The developed model calculates daily soil wetting  
 119 (infiltration) and evaporation by tracking the soil water storage. Mean annual runoff is estimated  
 120 by aggregating the daily values. The daily soil wetting is calculated using the concept of saturation  
 121 excess runoff generation by modeling the spatial variability of soil moisture and soil water storage  
 122 capacity. To facilitate the parameter estimation of storage capacity distribution in ungauged basins,  
 123 the following distribution function is used for modeling the spatial distribution of storage capacity  
 124 (Wang, 2018):

$$125 \quad F(C) = 1 - \frac{1}{a} + \frac{C+(1-a)S_b}{a\sqrt{(C+S_b)^2-2aS_bC}} \quad (1)$$

126 where  $F(C)$  is the cumulative distribution function (CDF), representing the fraction of the  
 127 watershed area for which the soil water storage capacity is equal to or less than  $C$ ;  $a$  is the shape  
 128 parameter of the distribution and varies between 0 and 2; and  $S_b$  is the average soil water storage  
 129 capacity over the watershed (i.e., the mean of the distribution). As shown in Wang (2018), this  
 130 distribution function leads to the SCS curve number (SCS-CN) method when the initial storage is  
 131 set to zero. Therefore, there is a linkage between  $S_b$  and the “potential maximum retention after  
 132 runoff begins” in the SCS-CN method, denoted as  $S_{CN}$ .

133 Daily soil wetting and runoff generation is computed as a function of daily precipitation  
 134 ( $P$ ), initial storage ( $S_0$ ),  $a$ , and  $S_b$ . As shown in Wang (2018), the average soil wetting ( $W$ ) is  
 135 computed by:

$$136 \quad W = \frac{P+S_b\sqrt{(m+1)^2-2am}-\sqrt{[P+(m+1)S_b]^2-2amS_b^2-2aS_bP}}{a} \quad (2)$$

137 where  $m = \frac{S_0(2S_b - aS_0)}{2S_b(S_b - S_0)}$ . Setting  $S_0 = 0$  and dividing  $P$  on both sides of Equation (2), a Budyko-  
 138 type equation, representing  $\frac{W}{P}$  as a function of  $\frac{S_b}{P}$ , is obtained (Wang and Tang, 2014), which has  
 139 been used to model long-term soil wetting (Tang and Wang, 2017). Therefore, Equation (2) can  
 140 be interpreted as a non-steady state Budyko equation which accounts for the effect of water storage.  
 141 Daily evaporation ( $E_d$ ) is computed as (Yao et al., 2020):

$$142 \quad E_d = \frac{W + S_0}{S_b} \frac{E_p + S_b - \sqrt{(E_p + S_b)^2 - 2aS_bE_p}}{a} \quad (3)$$

143 The first component on the right-hand side of Equation (3),  $\frac{W + S_0}{S_b}$ , is the percentage of storage, and  
 144 the second component is the evaporation for the condition when the entire watershed is saturated,  
 145 i.e., the spatial distribution of soil water storage is same as that of storage capacity (Yao et al.,  
 146 2020). Dividing  $W + S_0$  on both-hand sides, Equation (3) represents  $\frac{E_d}{W + S_0}$  as a function of  $\frac{E_p}{S_b}$ , and  
 147 the function is same as the Budyko-type equation derived by Wang and Tang (2014). Mean annual  
 148 evaporation ( $\bar{E}$ ) is computed by aggregating the daily evaporation, and mean annual runoff ( $\bar{Q}$ ) is  
 149 computed as the difference of mean annual precipitation and evaporation:

$$150 \quad \bar{E} = \frac{\sum_{y=1}^Y \sum_{d=1}^{D_y} E_d}{Y} \quad (4)$$

$$151 \quad \bar{Q} = P - \bar{E} \quad (5)$$

152 where,  $Y$  is the number of years, and  $D_y$  is the number of days in  $y^{\text{th}}$  year;  $y$  and  $d$  represent the  
 153  $y^{\text{th}}$  year and  $d^{\text{th}}$  day, respectively. Note that the mean annual runoff includes surface runoff and  
 154 baseflow, and both are impacted by climate variability (e.g., intra-annual variability) (Berghuijs et  
 155 al., 2014; Fan et al., 2007).

156 This mean annual water balance model applies two non-steady Budyko-type equations at  
 157 the daily scale, one for daily soil wetting and the other for daily evaporation. Runoff routing is

158 not necessary since the model is prepared for long-term water balance analysis. As a result, the  
159 mean annual water balance model includes two parameters, i.e., the shape parameter ( $\alpha$ ) and the  
160 average soil water storage capacity ( $S_b$ ). For studies where a one-parameter Budyko equation is  
161 applied to long-term scale directly, the effects of climate variability (seasonality, inter-annual  
162 variability, and daily storminess) on mean annual water balance are attributed to the single  
163 parameter of Budyko equation (e.g., Fu, 1981; Zhang et al., 2001). This creates the challenge to  
164 estimate the single parameter in ungauged basins; whereas, the mean annual water balance model  
165 used in this paper takes daily precipitation and potential evaporation as inputs, and the effects of  
166 climate variability are taken into account explicitly. To achieve the goal of predicting mean annual  
167 runoff in ungauged basins,  $\alpha$  and  $S_b$  need to be estimated in ungauged basins.

## 168 **2.2 Parameter estimation**

### 169 **2.2.1 Average soil water storage capacity**

170 Under a given soil moisture condition, soil water storage capacity is the sum of actual water  
171 storage and the remaining (or effective) storage capacity. The effective storage capacity  
172 corresponding to the normal antecedent moisture condition defined in the SCS-CN method,  $S_{CN}$   
173 (mm), is computed as a function of CN (SCS, 1972; Bartlett et al., 2016):

$$174 \quad S_{CN} = 25.4(1000/CN - 10) \quad (6)$$

175 where CN is the composite curve number based on land use and land cover (LULC) and hydrologic  
176 soil group (HSG) for each watershed. The LULC data can be obtained from the National Land  
177 Cover Database (Homer et al., 2015), and the HSG data can be extracted from the Gridded Soil  
178 Survey Geographic (gSSURGO) database with a spatial resolution of 10 m (USDA, 2014). In  
179 HSG, soils are assigned to one of the four groups (A, B, C, and D) and three dual classes (A/D,  
180 B/D, and C/D) according to the rate of infiltration when the soils are not protected by vegetation



181 and receive precipitation from long-duration storms. For the cells characterized by dual classes,  
182 the CN value is calculated as the average of the two CN values corresponding to the two soil  
183 groups.

184 The average soil water storage capacity ( $S_b$ ) is the sum of the actual storage under the  
185 normal condition ( $\bar{S}$ ) and its corresponding effective storage capacity:

$$186 \quad S_b = \bar{S} + S_{CN} \quad (7)$$

187 The physical meaning of  $S_b$  is the mean value of the soil water storage capacity over a watershed  
188 which is defined as the maximum storage from land surface to bedrock in this study rather than  
189 the storage capacity from shallow soils. Since the “normal antecedent moisture” can be interpreted  
190 as the steady-state soil moisture condition,  $\bar{S}$  is the long-term average storage over the watershed.

191 The values of  $\bar{S}$  for 59 MOPEX (MOdel Parameter Estimation Experiment) watersheds are  
192 estimated based on the long-term water balance model in Yao et al. (2020); and these watersheds  
193 do not include any watersheds studied in this paper. The long-term water balance model used in  
194 their study has a same model structure but the two parameters, i.e., the mean value of the soil water  
195 storage capacity and its shape parameter in the distribution function, were obtained by model  
196 calibration. The ratio between  $\bar{S}$  and  $S_b$  is defined as the long-term storage ratio  $\left(\frac{\bar{S}}{S_b}\right)$ . It is found

197 that the values of  $\frac{\bar{S}}{S_b}$  for all the watersheds were larger than 0.5. As shown in Figure 1,  $\frac{\bar{S}}{S_b}$  has a  
198 linear relationship with the climate aridity index:

$$199 \quad \frac{\bar{S}}{S_b} = -0.46\Phi + 1.2 \quad (8)$$

200 where  $\Phi$  is the climate aridity index. Substituting Equations (6) and (7) into Equation (8), one can  
201 estimate the average soil water storage capacity as a function of curve number and climate aridity  
202 index:

203 
$$S_b = \frac{S_{CN}}{0.46\Phi - 0.2} \quad (9)$$

204 **2.2.2 Shape parameter**

205 The spatial variability of storage capacity is determined by the spatial distribution of point-  
 206 scale pore space across the watershed. The volume of soil pores at point scale can be determined  
 207 by soil thickness and porosity in different soil layers. The porosity ( $\theta_s$ ) for each layer is calculated  
 208 from the soil bulk density:

209 
$$\theta_s(j) = 1 - \frac{\rho_b(j)}{\rho} \quad (10)$$

210 where  $j$  denotes the  $j^{th}$  soil layer;  $\rho_b(j)$  is the bulk density of the  $j^{th}$  soil layer;  $\rho$  is the particle  
 211 density (2.65 g/cm<sup>3</sup>). After obtaining the porosity, the point-scale storage capacity can be  
 212 calculated as the following equation (Huang et al., 2003):

213 
$$C = \sum_1^n z_j \cdot \theta_s(j) \quad (11)$$

214 where  $C$  is the point-scale soil storage capacity;  $n$  is the number of soil layers;  $z_j$  and  $\theta_s(j)$  are the  
 215 thickness and porosity of the  $j^{th}$  soil layer, respectively. In the gSSURGO database, the soil  
 216 thickness and bulk density for each layer are available for shallow soil from the land surface to ~  
 217 2 m soil depth.

218 The total soil thickness at each point is the elevation difference from land surface to fresh  
 219 bedrock. However, the bedrock topography is difficult to obtain especially at the watershed scale.  
 220 Alternatively, it is assumed that the spatial distribution of the actual soil water storage capacity is  
 221 same as the spatial distribution of water storage capacity computed from the gSSURGO database.  
 222 In order to compare the shape parameter evaluated from the soil data with its counterparts  
 223 evaluated from other methods, the point-scale storage capacity is normalized with the average  
 224 storage capacity over the watershed, and Equation (1) is rewritten as:

225 
$$F(x) = 1 - \frac{1}{a} + \frac{x+(1-a)}{a\sqrt{(x+1)^2-2ax}} \quad (12)$$

226 where  $x$  is the normalized storage capacity  $\left(\frac{C}{S_b}\right)$  at point scale;  $a$  is the shape parameter describing  
227 the spatial variability of soil water storage capacity. The shape parameter  $a$  is then estimated by  
228 fitting the point-scale storage capacity data obtained from Equation (11). A nonlinear  
229 programming solver using derivative-free method (i.e., Matlab function “fminsearch”) was used  
230 to calculate the optimal shape parameter by minimizing the root mean square error (RMSE). To  
231 demonstrate the sensitivity of mean annual runoff to the value of shape parameter, Figure 2  
232 presents mean annual runoff versus shape parameter based on the mean annual water balance (Yao  
233 et al., 2020). It can be found that mean annual runoff decreases significantly as the shape parameter  
234 increases, especially when shape parameter approaches its upper limit (i.e., 2). The negative  
235 relationship between the mean annual runoff and the shape parameter can be attributed to the fact  
236 that the larger shape parameter indicates that less watershed area has small values of point-scale  
237 storage capacity (Wang, 2018) and more precipitation could be retained underground for  
238 evaporation.

### 239 **2.3. Study watersheds**

240 The estimations of mean annual runoff in 35 watersheds are diagnosed in this paper. The  
241 number of 35 was determined due to the consideration of the data availability including soil  
242 (hydrologic soil group), land cover and land use, DEM as well as the minimum snow effect and  
243 human activities (Wang and Hejazi, 2011), and to keep the efforts of gSSURGO data processing  
244 to a reasonable level while still to have a sufficient number of sample of watersheds. The drainage  
245 area of the watersheds varies from 2044 to 9889 km<sup>2</sup>. Table 1 shows the USGS gauge number and  
246 climate aridity index of these watersheds. The saturation excess is the dominated runoff generation

247 in these watersheds. Daily precipitation and streamflow data during 1948 – 2003 are extracted  
248 from the MOPEX dataset (Duan et al., 2006), and the daily potential evaporation during this period  
249 is calculated based on the Hargreaves method (Hargreaves and Samani, 1985) by using the daily  
250 maximum, minimum, and mean temperature. The average soil water storage capacity and the  
251 shape parameter for these watersheds are estimated from the available data of climate, LULC, soil,  
252 and topography, and the predictions of mean annual runoff are diagnosed.

### 253 **3. Results and discussion**

#### 254 **3.1. Estimated average soil water storage capacity**

255 The potential maximum retention ( $S_{CN}$ ) is calculated based on the average CN in each  
256 watershed (Table 1). The average CN is computed based on LULC and hydrologic soil group.  
257 For examples, Figure 3a shows the LULC map for the Fox River watershed in Wisconsin and  
258 Figure 3d shows the LULC map for the Spoon River watershed in Illinois. The dominant land  
259 uses are agriculture (49%) and forest (33%) in the Fox River watershed, and agriculture (77%) and  
260 forest (15%) in the Spoon River watershed. The hydrologic soil groups are shown in Figure 3b  
261 (Fox River watershed) and Figure 3e (Spoon River watershed). Given the same LULC, the  
262 hydrologic soil group D is more favorable for runoff generation compared with group A. The  
263 dominant hydrologic soil groups are group A (31%) and group B (19%) in the Fox River watershed,  
264 and group C/D (49%) and group B/D (20%) in the Spoon River watershed. The calculated CN for  
265 each grid cell is shown in Figure 3c (Fox River watershed) and Figure 3f (Spoon River watershed).  
266 The average CN is 61.0 for the Fox River watershed and 78.1 for the Spoon River watershed.  
267 Since the Spoon River watershed has a higher percentage of agricultural land and lower soil  
268 permeability, its average CN is higher than that for the Fox River watershed. Correspondingly,  
269 the calculated  $S_{CN}$  in the Fox River watershed (162 mm) is higher than that in Spoon River

270 watershed (71 mm). The values of  $S_{CN}$  over the study watersheds vary from 56 mm (Auglaize  
271 River watershed) to 182 mm (Chattahoochee River watershed) as shown in Table 1.

272 The average soil water storage capacity is estimated based on the computed  $S_{CN}$  and  
273 climate aridity index shown in Equation (8). For examples, the climate aridity index in the Fox  
274 River watershed is 1.12 which is the same as that in the Spoon River watershed. The estimated  $S_b$   
275 is 721 mm in the Fox River watershed and 314 mm for the Spoon River watershed. As shown in  
276 Table 1, the estimated  $S_b$  varies from 177 mm (Chikaskia River watershed) to 1559 mm  
277 (Chattahoochee River watershed) over the study watersheds. Figure 4a shows the spatial  
278 distribution of the estimated  $S_b$ . Watersheds with higher  $S_b$  are mostly distributed in the eastern  
279 US, where the aridity index is relatively lower than that in the other watersheds.

### 280 **3.2. Estimated shape parameter**

281 The shape parameter ( $a$ ) for the distribution of soil water storage capacity is estimated  
282 based on the soil data in the gSSURGO database. For examples, the black circles in Figure 5 show  
283 the normalized storage capacity for the Fox River watershed (Figure 5a) and the Spoon River  
284 watershed (Figure 5b) based on the soil data in the gSSURGO database. As shown in Figure 5,  
285 the normalize CDF for both watersheds shows an S-shape. The estimated shape parameter is 1.996  
286 for the Fox River watershed (RMSE = 0.58) and 1.990 for the Spoon River watershed (RMSE =  
287 1.27) by fitting to the soil data. Higher value of shape parameter indicates less spatial variability;  
288 therefore, the spatial variability in the Spoon River watershed is higher than that in the Fox River  
289 watershed. The mean value of RMSE for the 35 study watersheds is 0.06. Figure 4b shows the  
290 estimated shape parameters for the study watersheds, which vary from 1.830 to 1.998.

### 291 **3.3. Diagnosing mean annual runoff prediction**

292 The estimated values of  $S_b$  and  $a$  based on climate, LULC, and soil data are applied to the  
293 mean annual water balance model. The comparison of simulated and observed mean annual runoff  
294 for the study watersheds is shown in Figure 6a. The RMSE for estimated mean annual runoff is  
295 80 mm/yr. The water balance model captures 88.2% of the mean annual runoff across the 35 study  
296 watersheds; therefore, the methods for estimating  $S_b$  and  $a$  based on the available data are  
297 promising for predicting annual runoff in ungauged basins.

298 The water balance model with the estimated values of  $S_b$  and  $a$  underestimates the mean  
299 annual runoff in some watersheds, and the relative underestimation error is 11.8% on average  
300 among all the study watersheds. The underestimation of mean annual runoff could be due to the  
301 biased estimation of the shape parameter. As described in Section 3, the spatial variability of soil  
302 water storage capacity is assumed to be equal with the spatial variability of the pore space in the  
303 shallow soil. The pore space at the point scale is calculated through the porosity and soil thickness.  
304 The thickness of the shallow soil in the gSSURGO database is quite uniformly distributed across  
305 the watershed, i.e., around 2 m; whereas, the actual soil thickness including the weathered bedrock  
306 is the elevation difference between the land surface and fresh bedrock, and can be highly  
307 heterogeneous due to the variable land surface and bedrock topography over the watershed.

308 To diagnose the effect of land surface and bedrock topography on mean annual water  
309 balance, the shape parameter is calibrated using the observed streamflow. The streamflow data  
310 during 1948-2003 are divided into three periods: 1) the warm-up period (1948-1953); 2) the  
311 calibration period (1954-1973); and 3) the validation period (1974-2003). During the calibration,  
312 the estimated  $S_b$  based on CN is used, and  $a$  is the only free parameter to be calibrated. The  
313 calibration is conducted by minimizing the absolute error of the observed and simulated mean  
314 annual runoff through a global optimization method, i.e., Shuffled Complex Evolution Method

315 (Duan et al., 1992). As shown in Figure 6b, most of the calibrated  $a$  are smaller than the estimated  
316  $a$  based on soil data only. The performance of predicted mean annual runoff (during the validation  
317 period) is improved with the calibrated shape parameter (Figure 6c). The average of absolute error  
318 for the mean annual runoff is 7.1%.

319 The overestimation of shape parameter based on the soil porosity data underestimates the  
320 area percentage of low soil water storage capacity compared with the calibrated one as shown in  
321 Figure 5a for the Fox River watershed and Figure 5b for the Spoon River watershed. The slope at  
322 the normalized soil water storage capacity around 1 for the estimated shape parameter is higher  
323 than that for the calibrated one. Therefore, the calibrated shape parameter indicates a larger spatial  
324 variability. The underestimation of catchment area with low soil water storage capacity could be  
325 resulted from neglecting the effect of land surface and bedrock topography which cannot be  
326 referred from the soil database (gSSURGO) where the point-scale soil thickness is around 2 m.

327 To explore the impact of land surface topography on the spatial distribution of soil water  
328 storage capacity, the soil data (i.e., porosity) is combined with the Height Above the Nearest  
329 Drainage (HAND) method proposed by Gao et al. (2019). HAND is the vertical elevation  
330 difference from a point to its nearest drainage point. The distribution of HAND was used for  
331 estimating the shape parameter of the spatial distribution of storage capacity. Therefore, the  
332 HAND method uses land surface topography data only for estimating the shape parameter. In our  
333 analysis, the porosity of the soil beyond the bottom layer in the soil database is assigned with the  
334 same value as the bottom layer. For example, if the HAND for a grid cell is 10.0 m and the porosity  
335 and depth of the bottom soil layer in the gSSURGO database is 0.2 and 2.0 m, respectively, the  
336 porosity for the soil from 2.0 m to 10.0 m depth is assigned with 0.2. Finally, the total volume of

337 pores is calculated for each grid cell based on the soil porosity obtained from the gSSURGO  
338 database and the HAND value based on land surface topography.

339 The control of land surface topography on the hydrologic process has also been widely  
340 quantified through topographic wetness index (TWI) of TOPMODEL (Beven and Kirkby, 1979).  
341 The spatial variability of soil storage capacity based on the TOPMODEL assumption has been  
342 demonstrated as a beneficial representation of the conceptual model (Sivapalan et al., 1997).  
343 Therefore, the heterogeneity of TWI in a watershed was proposed to be another surrogate of the  
344 heterogeneity of the soil storage capacity in this study, and the shape parameter estimated by fitting  
345 TWI against Equation (12) through minimizing the root mean square error (RMSE) for the  
346 Maquoketa River in Iowa was compared with those obtained from other methods.

347 The dashed blue line in Figure 7 shows the porosity-HAND based CDF of normalized soil  
348 water storage capacity for the Maquoketa River in Iowa (gauge #05418500). The stream initiation  
349 threshold used for calculating HAND is  $40 \text{ km}^2$  which is 1% of the maximum flow accumulation  
350 (Maidment, 2002). The threshold affects the value of HAND but this is beyond the scope of this  
351 paper. The best fit value of  $a$  for the porosity-HAND based CDF is 1.779, which overestimates  
352 the spatial variability of storage capacity compared with the calibrated shape parameter ( $a=1.905$ ).  
353 This is due to the assumption of the HAND method that the bedrock between a specific point and  
354 its nearest drainage point is horizontal and intercepts with the channel bed. However, the bedrock  
355 topography may have various slopes in a watershed (Troch et al., 2002). Therefore, the true value  
356 of  $a$  (indicated by the calibrated one) potentially falls between the  $a$  obtained from soil data and  
357 the  $a$  based on soil and HAND. The bedrock topography from observation or models is needed to  
358 accurately estimate the shape parameter. The dashed dot red line in Figure 7 displays the CDF of  
359 the normalized soil storage capacity based on TWI, and the corresponding value of  $a$  is 1.967. The



360 TWI-based  $a$  value also presents a larger spatial variability than that derived from soil data solely,  
361 confirming the importance of topography in determining the heterogeneity of soil water storage  
362 capacity. The deviation of the TWI-based  $a$  value from its calibrated counterpart could be due to  
363 the fact that the bedrock topography is not considered in TWI.

#### 364 **4. Conclusion**

365 A mean annual water balance model based on the concept of saturation excess runoff  
366 generation is used for diagnosing the potential for nonparametric modeling of mean annual runoff  
367 in ungauged basins. The model takes the effect of climate variability into account explicitly since  
368 it is driven by daily precipitation and potential evapotranspiration at the daily time step. The  
369 distribution function, which leads to the SCS curve number method, is used for describing the  
370 spatial distribution of soil water storage capacity. The mean (i.e., average soil water storage  
371 capacity) and the shape parameter (i.e., the spatial variability of soil storage capacity over the  
372 watershed) of the distribution function can be estimated from the available data. Based on the  
373 linkage of the distribution function and the SCS curve number method, a new method based on  
374 the existing observed data of watershed characteristics is proposed for estimating the average soil  
375 water storage capacity. The average soil water storage capacity ( $S_b$ ), as one of the parameters in  
376 the model, was estimated as a function of climate aridity index and curve number which is  
377 calculated based on land cover and soil data.

378 The developed mean annual water balance was applied to diagnose the estimation of shape  
379 parameter ( $a$ ) in this study. The shape parameter, describing the spatial variation of soil water  
380 storage capacity, was first estimated based on the porosity and soil thickness data in the soil  
381 database (gSSURGO). The estimated values of  $a$  were tested in 35 watersheds. The results  
382 showed that the model with the estimated values of  $S_b$  and  $a$  underestimated the mean annual

383 runoff by 11.8% on average over all the study watersheds. The underestimation of runoff is mainly  
384 caused by the underestimation of the spatial heterogeneity of soil thickness over the watershed.  
385 The Height Above the Nearest Drainage (HAND) was then calculated as the total soil thickness  
386 for estimating the total volume of the pore space. The result showed that topography is of great  
387 importance for determining the spatial variability of soil water storage capacity. The estimated  
388 shape parameter from porosity-HAND overestimated the spatial variability of the storage capacity  
389 compared with the calibrated  $\alpha$ , which may result from the assumed bedrock in the HAND method.  
390 The Topographic Wetness Index (TWI) based shape parameter further indicated the importance  
391 the topography including the land surface topography and bedrock topography. Future research  
392 will investigate alternative methods for better estimating the spatial variability of soil water storage  
393 capacity over watersheds, and quantify the impacts of vegetation and climate variability (e.g.,  
394 distribution of rainy days, the magnitude and the seasonality of climate variables).

395

396 **Data availability**

397 The soil and land use and land cover data that support the findings of this study are openly available  
398 at: <https://websoilsurvey.sc.egov.usda.gov/App/WebSoilSurvey.aspx> (Natural Resources  
399 Conservation Services, United States Department of Agriculture), and:  
400 [https://www.mrlc.gov/data?f%5B0%5D=category%3Aland%20cover&f%5B1%5D=region%3A](https://www.mrlc.gov/data?f%5B0%5D=category%3Aland%20cover&f%5B1%5D=region%3Aconus)  
401 [conus](https://www.mrlc.gov/data?f%5B0%5D=category%3Aland%20cover&f%5B1%5D=region%3Aconus) (National Land Cover Database, United States Geological Survey), respectively.

402 Daily precipitation, streamflow, and temperature data are available from 1948 to 2003 through the  
403 MOPEX website at [https://hydrology.nws.noaa.gov/pub/gcip/mopex/US\\_Data/](https://hydrology.nws.noaa.gov/pub/gcip/mopex/US_Data/).

404

405 **Author contributions**

406 Dingbao Wang designed the study, contributed to the methods, results discussion and modified  
407 the text. Yuan Gao quantified the parameters of the model and prepared the manuscript with  
408 contributions from all co-authors. Lili Yao developed the model code, quantified the parameters,  
409 performed the simulations and prepared the manuscript with contributions from all co-authors. Ni-  
410 Bin Chang contributed to the introduction and modified the text.

411

#### 412 **Competing interests**

413 The authors declare that they have no conflict of interest.

414

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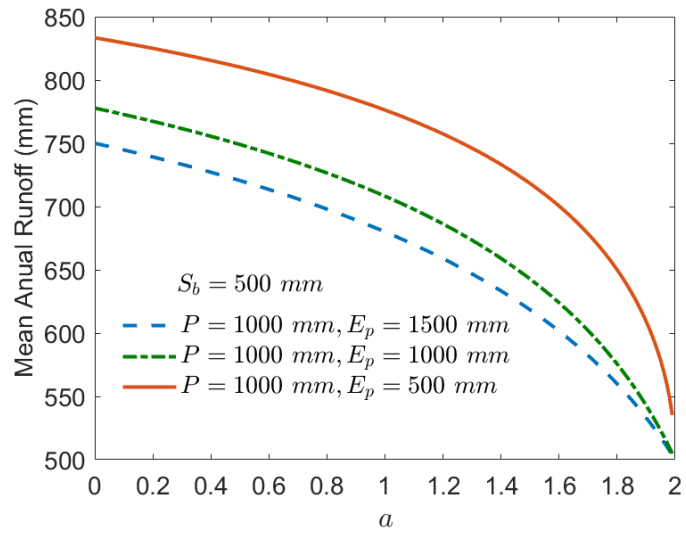
579

580 Table 1: The USGS gage stations, climate aridity index, the estimated potential maximum  
 581 retention of curve number method ( $S_{CN}$ ), and the average soil water storage capacity ( $S_b$ ) for the  
 582 study watersheds.

Index	Station Name	State	USGS Gauge Number	Climate Aridity Index	$S_{CN}$ (mm)	$S_b$ (mm)
1	Susquehanna River	NY	01503000	0.69	100	862
2	Chemung River	NY	01531000	0.84	95	518
3	Juniata River	PA	01567000	0.85	134	714
4	Rappahannock River	VA	01668000	0.85	152	792
5	Yadkin River	NC	02116500	0.71	153	1221
6	Chattahoochee River	GA	02339500	0.69	182	1559
7	Escambia River	FL	02375500	0.73	143	1075
8	Allegheny River	NY	03011020	0.68	153	1369
9	New River	VA	03168000	0.69	177	1494
10	Great Miami River	OH	03274000	0.89	63	301
11	Eel River	IN	03328500	0.92	68	304
12	East Fork White River	IN	03364000	0.83	68	378
13	Little Wabash River	IL	03381500	0.96	68	279
14	Fox River	WI	04073500	1.12	162	520
15	Auglaize River	OH	04191500	0.98	56	225
16	Maquoketa River	IA	05418500	1.19	72	209
17	Wapsipinicon River	IA	05422000	1.16	69	210
18	Rock River	WI	05430500	1.11	98	316
19	Pecatonica River	IL	05435500	1.11	66	214
20	Kishwaukee River	IL	05440000	1.03	70	255
21	Green River	IL	05447500	1.10	75	247
22	Iowa River	IA	05454500	1.18	65	191
23	Cedar River	IA	05458500	1.17	65	193
24	Kankakee River	IL	05520500	0.93	101	448
25	Fox River	IL	05552500	1.04	88	321
26	Spoon River	IL	05570000	1.12	71	227
27	Kaskaskia River	IL	05592500	0.99	67	263
28	Blue River	KS	06884400	1.70	74	127
29	Thompson River	MO	06899500	1.16	65	195
30	Meramec River	MO	07019000	0.95	109	460
31	Chikaskia River	OK	07152000	1.82	77	121
32	Neosho River	KS	07183000	1.42	63	140
33	Deep Fork River	OK	07243500	1.40	87	197
34	Neches River	TX	08033500	1.14	174	540
35	Elm Fork Trinity River	TX	08055500	1.63	87	159

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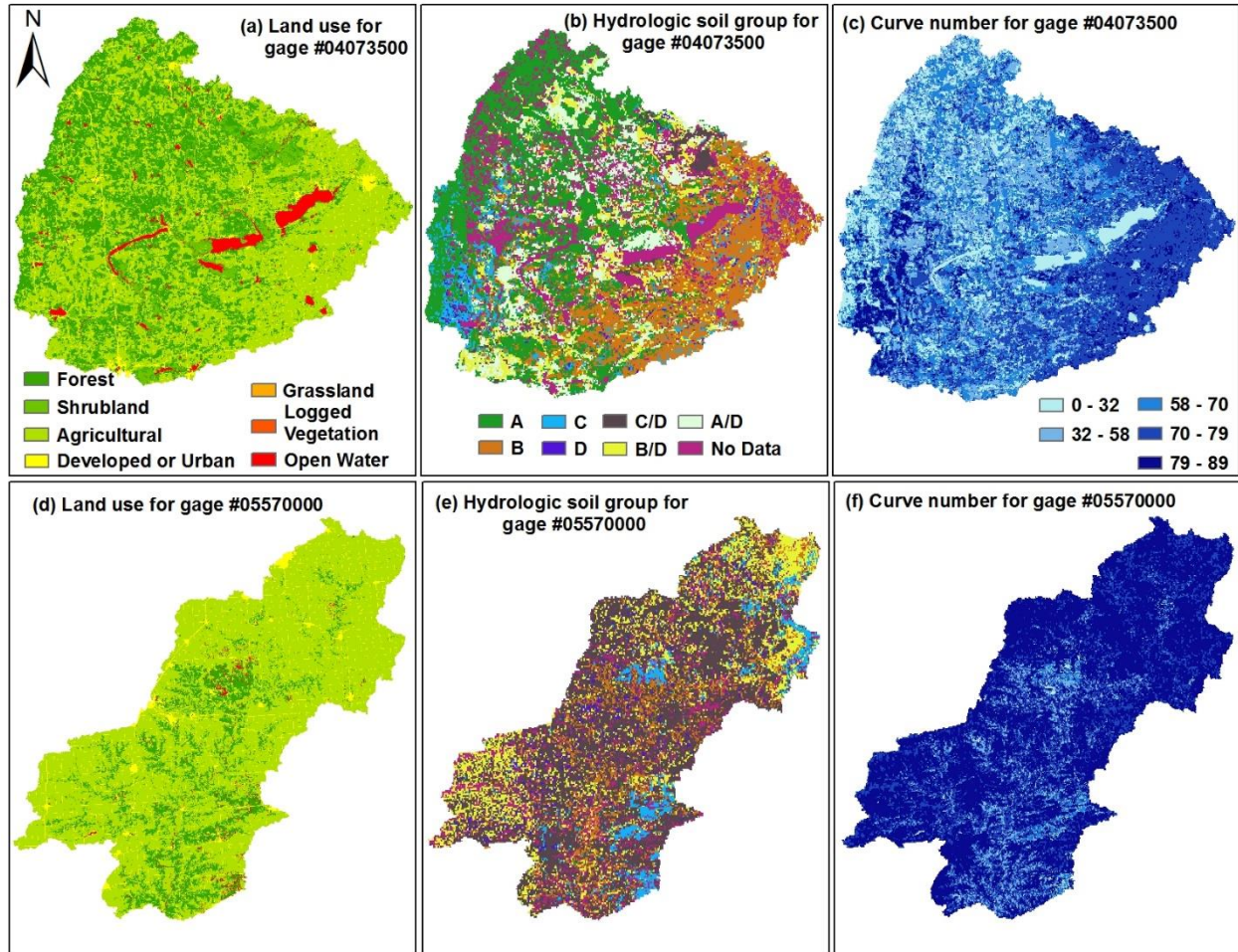


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Figure 2: The sensitivity of mean annual runoff ( $Q$ ) to the value of shape parameter ( $a$ ).

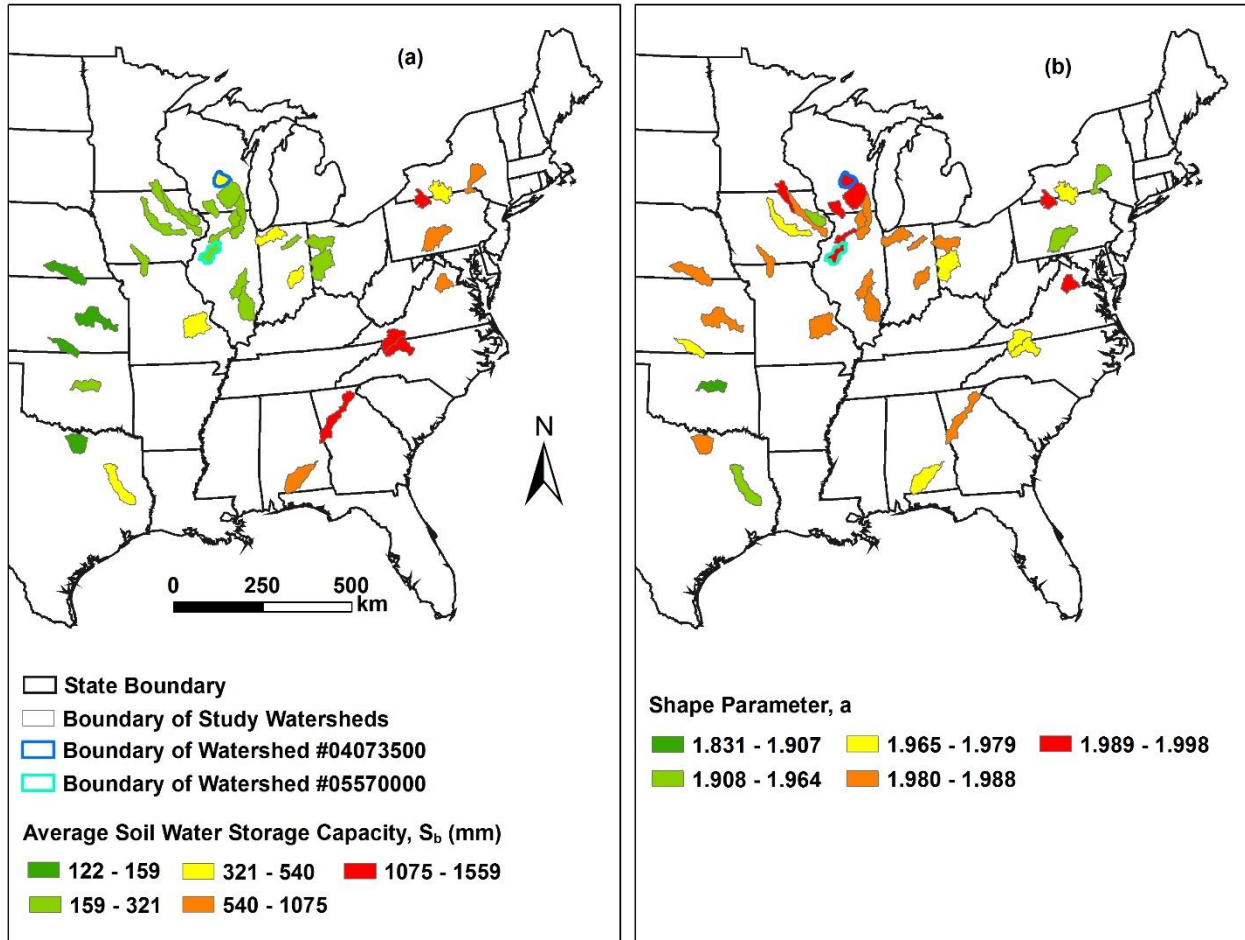
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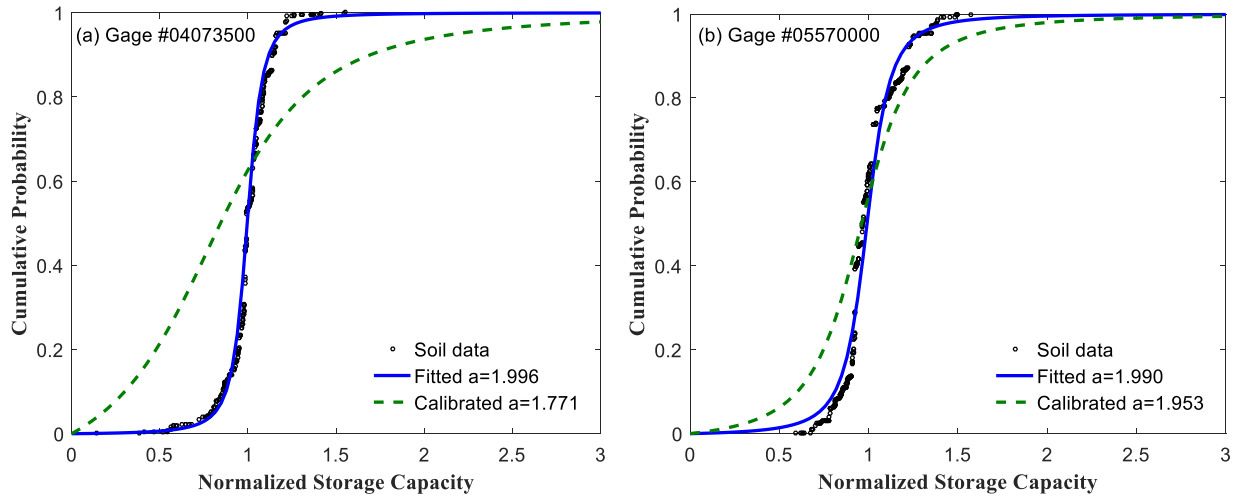
592 Figure 3: The spatial distribution of land use and land cover for Fox River watershed in  
 593 Wisconsin (a) and Spoon River watershed in Illinois (d), the hydrologic soil groups for Fox  
 594 River watershed (b) and Spoon River watershed (e), and the curve numbers for Fox River  
 595 watershed (c) and Spoon River watershed (f).

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 598 Figure 4: The estimated average soil water storage capacity ( $S_b$ ) as a function of  $S_{CN}$  and climate  
 599 aridity index (a) and shape parameter from soil data (b).

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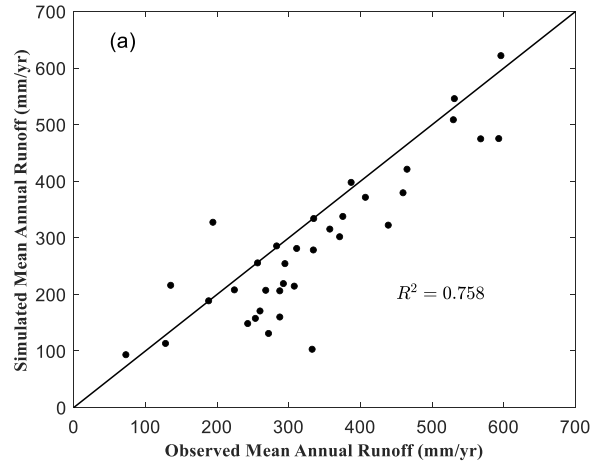
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602 Figure 5: The estimated shape parameter for the spatial distribution of soil water storage capacity  
 603 based on soil data and the calibrated shape parameter based on mean annual water balance in the  
 604 Fox River watershed (a) and the Spoon River watershed (b).

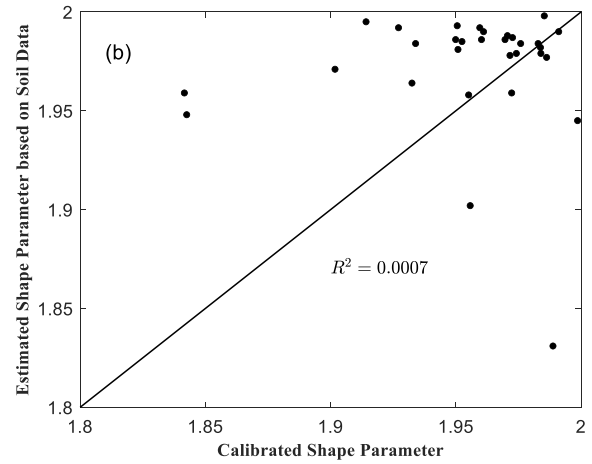
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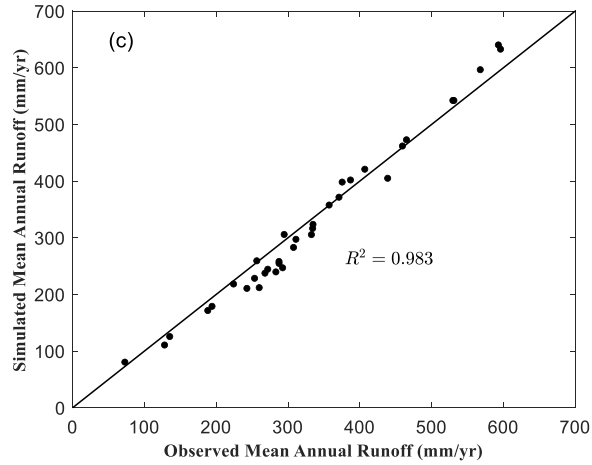
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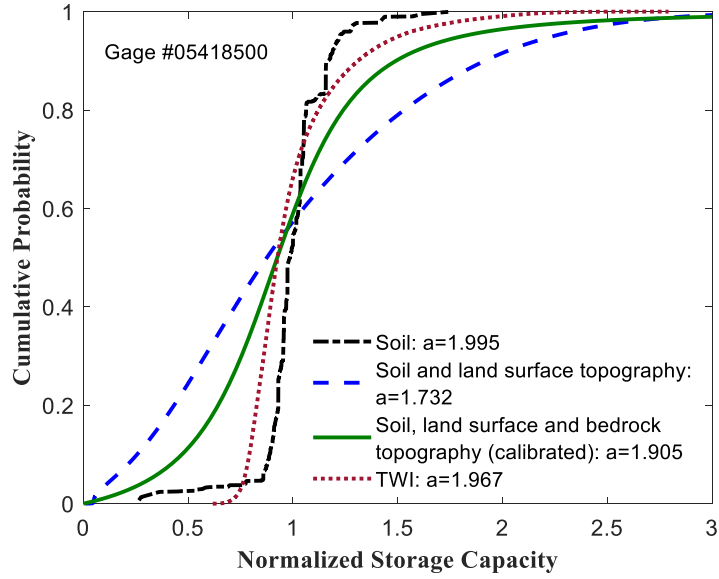


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Figure 6: (a) Observed versus simulated mean annual runoff using shape parameter based on soil data; (b) Soil data-based versus calibrated shape parameter; and (c) Observed versus simulated mean annual runoff using shape parameter based on calibration.



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Figure 7: The effects of soil, land surface topography, bedrock topography, and topographic wetness index (TWI) on the shape parameter of the spatial distribution of soil water storage capacity.

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