1 **Quantifying the Space – Time Variability of Water Balance Components in** 2 **an Agricultural Basin using a Process-Based Hydrologic Model and the** 3 **Budyko Framework**

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9 **Abstract**

10 Process-based distributed hydrologic models (PBHMs), which link watershed 11 characteristics with process representations, are useful tools to evaluate both the distributed 12 and ensemble hydrologic responses of a basin to climate inputs. However, complexities 13 associated with parameter interactions and their spatial heterogeneities may produce high 14 uncertainties in the parameterization of a PBHM. The Budyko curve framework presented in 15 this work offers an effective approach for evaluating variabilities in the water balance 16 components using a PBHM and explores the link between model performance with parameter 17 heterogeneities and the Budyko curve characteristics. The PBHM was calibrated using a multi-18 site calibration strategy (MLT), which was built upon a step-wise calibration algorithm 19 combined with multiple calibration targets including river discharges, evapotranspiration and 20 ground water heads to reduce the compensation errors caused by component interactions. This 21 strategy was tested for the Kalamazoo River watershed in Michigan, USA, with obvious 22 physiographic and land surface heterogeneities. The Budyko framework characterized the 23 water balance variability at the sub-watershed scale; two empirical methods are employed to 24 evaluate calibrated parameters using Budyko-estimated values and to assess the physical 25 relevance of parameters. The relative infiltration capacity is found to play an important role in 26 affecting the spatial variability of the annual water balances of this watershed. This work brings 27 out the importance of optimizing calibration strategies by linking catchment heterogeneities 28 with processes reasoning in order to understand the underlying hydrologic controls.

29 *Keywords: hydrologic models, model calibration, water budgets, Budyko curve*

30 **1. Introduction**

31 Water resources management in an era of global change requires hydrologists to provide

32 reliable predictions of water fluxes and to analyze and interpret their distributed and evolving

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33 roles (Wagener et al., 2010; McDonnell and Beven, 2014). At the catchment scale, it is of great 34 interest to link the structure of a watershed to its response to climate variability and to evaluate 35 water budget components and their variability (Sivapalan, 2006). Two approaches have been 36 used in the past decades to study annual water budgets and their inter-annual variability: (a) 37 the empirical approach and (b) process-based modeling (Sivapalan et al., 2011). One classic 38 example of an empirical approach is Budyko's work (Budyko, 1974), which assumes that the 39 partition of precipitation into evaporation and runoff could be determined from available water 40 measured with precipitation (*P*) and available energy measured with potential 41 evapotranspiration (*PET, Ep*). Based on the Budyko hypothesis, the ratio of actual 42 evapotranspiration over precipitation (*ET/P*), i.e., the evaporation ratio, is fundamentally 43 related to the ratio of potential evapotranspiration over precipitation (E_p/P) , i.e., the climate 44 dryness index (Budyko, 1974):

45
$$
\frac{ET}{P} = \left[\frac{E_p}{P} \tanh\left(\frac{E_p}{P}\right)\left\{1 - \cosh\left(\frac{P}{E_p}\right) + \sinh\left(\frac{P}{E_p}\right)\right\}\right]^{0.5}
$$
(1)

46 The Budyko framework was used to evaluate the inter-annual variability of annual water 47 balances as well as water balances at seasonal time scales. For example, Yang et al. (2007) 48 evaluated long time series of climate data and discharge in 108 non-humid catchments of China 49 using the Budyko framework and found that the inter-annual variability of water-energy 50 balance can be expressed with infiltration capacity, soil water storage capacity and the average 51 ground surface slope. Wang (2012) studied effects of annual water storage changes on the inter52 annual water balances of 12 watersheds in Illinois based on long-term soil moisture and 53 groundwater level observations using the Budyko framework. The observed deviations of 54 Budyko-type curves for different watersheds can reflect the ensemble effects of the climate 55 fluctuations (Milly, 1994) and watershed characteristics such as storage (Fang et al., 2016) and 56 soil moisture capacity, topography and soil properties (Yokoo et al., 2008), vegetation type and 57 dynamics (Zhang et al., 2001; Oudin et al., 2008; Domohue et al., 2012) on the mean annual 58 water balances. However, as with most empirical approaches, the derivation of Budyko-type 59 curves lacks the explicit representations of interactions of climate inputs and various 60 hydrologic processes. It is difficult for empirical approaches to distinguish the effects of 61 different hydrologic processes, especially when considering the intra-annual (e.g. daily) 62 variability of water balances (Chen et al., 2013; Fang et al., 2016).

63 PBHMs, on the other hand, describe the hydrologic processes explicitly and provide a 64 direct link between catchment structures and response behaviors. Simulations based on PBHMs 65 are suitable for distinguishing the distributed flow pathways (Beven, 2002), quantifying the 66 water storage changes in hydrologic systems (Niu et al., 2014) and understanding the physical 67 processes in controlling the hydrologic responses (Shen et al., 2013). They require, however, a 68 large amount of input data in representing the physical processes and abundant observed data 69 to calibrate the parameters (Beven and Binley, 1992; Ragettli and Pellicciotti, 2012). Co-70 evolution of water budget components in a PBHM with various parameter suits may contribute 71 to similar ensemble predictions; this phenomenon has been famously generalized by (Beven, 72 1993; and Beven and Freer 2001) as the equifinality problem. Calibration against a single target 73 (e.g., stream discharge) does not guarantee that internal processes are all correctly simulated; 74 compensation errors could be produced with discrepancies coexisting in more than one 75 hydrologic component representing the processes. For example, ungauged infiltration and 76 lateral groundwater flow processes may cause underestimated (overestimated) groundwater 77 supply while compensated by overestimated (underestimated) surface runoff to achieve 78 comparable stream discharge results (Ragettli and Pellicciotti, 2012). An effective method for 79 reducing uncertainty in parameter identification in PBHMs might be through evaluations 80 against a number of responses representing different hydrological components (Anderton et al.*,* 81 2002). Multistep, multi-site, and multivariable calibration methods are being widely applied by 82 calibrating different internal processes to improve both the overall and distributed model 83 performances (Ragettli and Pellicciotti, 2012; Stahl et al., 2008; Sutanudjaja et al., 2014; Choi 84 et al., 2015), e.g., step-wise optimization using stream discharge, groundwater heads, and 85 remotely-sensed soil moisture data as the optimization objectives; and calibration to data from 86 multiple gauging stations in different sub-watersheds.

87 The objectives of this paper are to: (1) quantify the spatial and temporal variability of 88 annual water balances in a semi-humid watershed in Michigan, USA using a PBHM; (2) use a 89 multi-site calibration strategy combined with multiple criteria evaluations to understand how 90 parameters, process representations and water budget results change across scales; and (3) 91 evaluate calibrated parameters with Budyko-estimated values to assess the physical relevance 92 of parameters and to identify deficiencies in each methodology. Briefly, we addressed the

93 question of how different empirical equations for the parameter *ω* in the Budyko curve 94 formulation compare with simulated results based on a PBHM in a Great Lakes watershed.

95 To address these questions, we use a PBHM, PAWS (Process-based Adaptive Watershed 96 Simulator, *Shen and Phanikumar* (2010)). The model can simulate different hydrologic 97 components and states including surface runoff, channel flow, groundwater, ET, soil moisture, 98 soil temperature and changes in storage. Vegetation growth dynamics are also simulated by 99 coupling PAWS with the land surface model CLM 4.0 as described in Shen et al. (2013; 2014). 100 We first establish a calibration procedure to ensure that stream discharge and other important 101 hydrologic components such as ET and groundwater are correctly simulated. A stepwise 102 calibration method was applied to reduce the compensation errors. For reducing uncertainty in 103 scaled heterogeneity, a multi-site calibration (MLT) method is employed and combined with 104 multi-criteria evaluations. For the second effort, instead of attempting to elaborate on the 105 heterogeneity within each process, we focus on inter-annual water balances at sub-watershed 106 scale and study the ensemble catchment performances using the Budyko framework.

107 **2. Methods**

108 **2.1 The Model**

109 Governing equations and numerical details of the PAWS model have been explained in 110 Shen and Phanikumar (2010) and presented in Table 2 of Niu et al. (2014). The coupling details 111 of PAWS with CLM 4.0 have been extensively discussed and evaluated earlier (Shen et al., 112 2013; Riley and Shen, 2014; Niu et al., 2014; Niu and Phanikumar, 2015; Qiu et al., 2019).

113 Briefly, PAWS includes key hydrologic processes in the domains of surface flow, surface 114 ponding, channel flow, unsaturated vadose zone and saturated groundwater flow. PAWS uses 115 a structured grid and the finite-volume method to solve the governing partial differential 116 equations in different hydrologic units. The overland flow governed by diffusive wave equation 117 occurs in the surface flow domain while infiltration and evaporation happen in the ponding 118 domain. Runoff occurs when the water depth of ponding domain is in excess of the interception 119 depth. Water may also backfill into the ponding domain during flood conditions. The overland 120 flow in the surface flow domain interacts and exchanges water with river segments. Channel 121 flow is simulated using the diffusive wave equation and its exchange with groundwater is 122 modeled based on the leakance concept (Gunduz and Aral, 2005). The vadose zone is simulated 123 in 1-D columns connected to land surface cells at the top and saturated groundwater flow cells 124 at the bottom. PAWS conceptualizes the unsaturated vadose zone as an array of vertical soil 125 columns on the assumption that lateral fluxes in this domain are negligible. The saturated - 126 unsaturated soil water flow is governed by the Richards equation with the vegetation uptake as 127 a sink term. PAWS uses the concept of root water efficiency (Lai and Katul, 2000) to adjust 128 the vegetation root water uptake fluxes along the soil column. The van Genuchten formulation 129 is employed for soil water retention calculations. Field capacity, saturated water content and 130 wilting point are set in correspondence to the soil properties. Phase change is also considered 131 by applying the freezing-point depression formula in (Niu and Yang, 2006) to reduce hydraulic 132 conductivities in freezing soils. The last computational cell of the soil column, whose thickness 133 changes as the water table fluctuates, serves as the linkage between vadose zone and 134 groundwater. Quasi- 3D Groundwater equation derived from Darcy's law is employed for 135 solving groundwater flow. The vegetation dynamics, energy cycling, and carbon/nutrient 136 cycling are incorporated through CLM (Oleson et al., 2010).

137 **2.2 Sites and Data Sources**

138 **2.2.1 Site descriptions**

139 The Kalamazoo River Watershed (KRW) is located in the southwest portion of the lower 140 peninsula of Michigan (Figure 1). This watershed has a drainage area of approximately 2,020 141 square miles (5,200 km²) and it drains portions of nine counties in Michigan. The Kalamazoo 142 River stretches 130 miles (210 km) from the junction of its north and south branches to its 143 outlet at Lake Michigan. Based on the 10-digit Hydrologic Unit Code (HUC), the KRW is 144 divided into 9 sub-watersheds (Figure. 1). Substrates in the headwaters and upstream segment 145 consist of mostly sand, gravel and some cobble. The substrates in the streams of the middle 146 segment are dominated by gravel and cobble. In contrast, the substrates in the mouth segment 147 streams are mostly composed of sand and silt. Annual mean precipitation in this area averages 148 ~970 mm and there is an increase of annual snowfall from the head waters to the mouth area 149 due to the lake effect (Wesley, 2005). Average growing season increases from ~150 days at the 150 eastern end of the watershed to ~180 days near Lake Michigan. The land surface elevation 151 ranges from 175 to 380 meters above the sea level and varies distinctly in different sub-basins. 152 Seasonal ET demands vary throughout the year as the solar radiation and air temperature 153 change. The bedrock is mainly cold-water shale, overlain by the glacial deposits composed of 154 outwash sand and gravel, which form the unconfined aquifer. Dominance of the soil types in 155 the watershed includes clay, silt, sand, and organic materials. The land use and land cover 156 (LULC) types for this watershed are occupied by approximately 47% agriculture (dominated 157 by corn and soybeans), 21% forest, 9% open land, and 7% urban (Figure 2). Varied topography 158 and heterogeneous subsurface properties, diverse vegetation and land use types render the 159 watershed well suited for our study. We use a relatively fine grid resolution of 400m×400m for 160 horizontal discretization which produces a 247×366 mesh for the whole watershed and 20 161 vertical layers to simulate the vadose zone dynamics and 2 layers for the groundwater domain 162 (unconfined and confined aquifers).

163 **2.2.2 Data sources**

164 Details of data assimilation and data integration algorithms of PAWS are available in 165 (Shen et al., 2014) thus we simply introduce the basic data input and processing information in 166 this section. For river network simulation, National Hydrography Dataset (NHD) 167 (https://nationalmap.gov/hydro.html) from U.S. Geological Survey (USGS) is used and 168 reorganized as 'river segments' with a length of 400m in correspondence to our grid resolution. 169 The 30 m resolution National Elevation Dataset (NED) from USGS serves as the Digital 170 Elevation Model (DEM) for topographic calculations (e.g. surface slope and overland flow). 171 To avoid possible compensation errors from other hydrologic components resulting from 172 reduced channel density (Wang and Wu, 2013), we keep a relatively high river network density 173 and include up to level-5 rivers (Figure. 1). NHD is overlaid on the NED model to extract a 174 profile of elevations simulated as the riverbank elevations. A 30 m resolution raster data 175 provided by the Michigan Department of Natural Resources (MDNR), i.e., the Integrated 176 Forest Monitoring Assessment and Prescription (IFMAP) data set (*MDTMB: Michigan* 177 *Department of Technology*, *Management & Budget*, 2016) is employed as the Land use and 178 Land cover layout. PAWS regroups the land use and land cover using a hierarchical stochastic 179 selection method to do reclassifications while preserving the proportionality between the land 180 use types of the original dataset (Shen et al., 2014). Soil type and properties information are 181 obtained from Soil Survey Geographic (SSURGO) (Soil Survey Staff) database from the U.S. 182 Department of Agriculture, Natural Resources Conservation Services (NRCS). Spatially 183 distributed soil parameters are processed by the pedotransfer functions provided in Rosetta 184 (Schaap et al., 2001) with an Artificial Neutral Network method to provide information of van 185 Genuchten parameters and to calculate soil water retention properties and unsaturated 186 conductivities. Climate data (e.g., precipitation, snowfall, daily maximum temperature and 187 minimum temperature, and wind speed) are acquired from National Climatic Data Center 188 (NCDC, 2010) of the National Oceanic and Atmospheric Administration (NOAA) and 189 Michigan Automated Weather Station Network (MAWN) (Enviro-weather, 2016). The nearest 190 neighbor interpolation scheme is used for spatial interpolation of climate data sets. Locations 191 of meteorological stations are shown on Figure 1, marked as NCDC and MAWN stations 192 respectively. We downloaded the evapotranspiration data from Moderate Resolution Imaging 193 Spectroradiometer (MODIS) Global Evapotranspiration Project (MOD16) 194 (http://www.ntsg.umt.edu/project/mod16), which is part of a NASA/EOS project to estimate 195 global terrestrial ET from earth land surface using remote sensing.

196 **2.3 Step-wise calibration**

197 Instead of calibrating to river discharge data exclusively, the calibration procedure 198 employed in this work uses several state variables involved in the quantification of major 199 hydrologic fluxes. Besides the parameters of the PAWS model described in Shen et al. (2013), 200 we estimate several additional parameters that are listed in Table S1 in Supporting Information 201 (SI). To estimate spatially varied parameters such as hydraulic conductivity and to honor 202 geology and the raw data, we use a linear transformation of the form $y = a x + b$ to adjust the 203 parameters where **x** represents the original parameters which vary spatially, **y** is the 204 transformed variable and *a* and *b* are constants. Based on the physical meaning and scale effect 205 of each parameter, the parameters are adjusted as shown in Table 1 using operators which are 206 either pure multipliers noted with a \times (non-zero value of *a* and $b = 0$ in the above equation) or 207 purely additive constants added to the original value noted with $a + (that is, a = 1$ and a non-208 zero value of *b*). The parameters are separated into three groups according to their relevance to 209 certain processes in controlling the water fluxes, following similar approaches used by Stahl et 210 al. (2008), Huss et al. (2008), and Ragettli and Pellicciotti (2012).

211 This procedure starts with adjusting the annual ET outputs in correspondence to MOD16 212 products. The aim of this step is to constrain the largest water flux in the model first, as the 213 annual ET is approximately 55% to 75% of the total annual precipitation in this region 214 (Kalamazoo River Watershed Council, 2011). Since we do not have spatially distributed soil 215 moisture observations to constrain our vadose zone simulations, we also employ the annual 216 average ET for controlling land surface processes (e.g., interception depth) and the plant soil-217 uptake processes using a tunable parameter γ in root water uptake efficiency (Lai and Katul, 218 2000) and other soil properties. Since the data integration schemes of PAWS have already 219 incorporated the heterogeneity of vegetation types and soil properties, the van Genuchten soil 220 parameters are slightly adjusted based on the initial parameters generated by Rosetta (A newer 221 version Rosetta 3 is also available, Zhang and Schaap, 2017). In the second step, we focus on 222 improving the comparisons of stream discharge calibrated to the USGS gauging observations 223 at the outlet for each sub-watershed by adjusting the values of river bed conductivity, length of 224 flow paths for runoff contribution to overland flow domain, and river bed elevation, all of 225 which have uncertainties associated with. The river bed conductivity parameter (K_r) is spatially 226 heterogeneous, and is initially estimated as $K_r = \sqrt{K_1 K_s}$ for each river segment grid (Shen et 227 al., 2016), where K_l is the first layer groundwater hydraulic conductivity from the well logic 228 database, K_s is the soil vertical saturated hydraulic conductivity derived from SSURGO 229 database. The final step is to calibrate the model for the steady state groundwater heads by 230 adjusting the groundwater hydraulic conductivities. The differential evolution algorithm (Price 231 et al., 2005) is finally employed to optimize the parameters by minimizing the objective 232 function $f(x)$, which represents model errors relative to observed values (Eqs. $(2) - (6)$). Details 233 of the calibration procedure are illustrated in Figure 3. The upper and lower limits of the 234 parameters were constrained within the scope of reasonable physical reasoning and were 235 gradually adjusted during the calibration. The model performance was evaluated using the 236 Nash-Sutcliffe efficiency metric (NASH) (Eq. 3), the absolute bias (APB) (Eq. 7), and the root 237 mean squared error (RMSE) (Eq. 8). The RNASH metric is used for calibrating stream 238 discharge to emphasize the baseflow contribution (Shen and Phanikumar, 2010), as shown in

239 Eq. (4). For ET and groundwater heads, NASH is used to calculate f_i , as shown in Eq. (3).

240
$$
f(x) = \sum_{i=1}^{N} w_i f_i
$$
 (2)

241
$$
NASH = 1 - \frac{\sum_{j=1}^{n} (O_j - P_j)^2}{\sum_{j=1}^{n} (O_j - \overline{O}_j)^2}
$$
 (3)

242
$$
RNASH = 1 - \frac{\sum_{j=1}^{n} (\sqrt{O}_{j} - \sqrt{P}_{j})^{2}}{\sum_{j=1}^{n} (\sqrt{O}_{j} - \overline{\sqrt{O}}_{j})^{2}}
$$
(4)

$$
f_i = 1 - \text{NASH}_i \tag{5}
$$

244 or, alternatively
$$
f_i = 1 - \left[\frac{NASH_i + RNASH_i}{2} \right]
$$
 (6)

245
$$
APB = \frac{\sum_{j=1}^{n} (O_j - P_j) \times 100}{\sum_{j=1}^{n} O_j}
$$
 (7)

246
$$
RMSE = \sqrt{\sum_{j=1}^{n} \frac{1}{n} (O_j - P_j)^2}
$$
 (8)

247 Here *x* denotes the vector of parameters; f_i denotes the objective functions and w_i denotes the 248 weights; *i* equals unity for ET and steady groundwater head or denotes the *i*-th stream gauging 249 stations (*i = 1, 2, …, N*) for the stream discharge. O*j* and P*j* denote observations and simulations 250 respectively. *j* is the *j*-th year for ET and groundwater heads or the *j*-th simulated day for stream 251 discharge.

252 **2.4 Multi-site calibration**

253 To further examine the effects of local heterogeneity on the overall model performance, 254 we divided the whole KRW into 4 sub-areas (Figure 1) and regionalized the parameter groups 255 accordingly. This division was based not on the drainage areas corresponding to each of the 256 gauging stations but on the distinct geologic and hydrologic characteristics of the watershed 257 described in section 2.2.1. Each of the four sub-areas is loosely referred to as sub-watershed 258 (SW) in this paper since they were formed by combining different 10-digit Hydrologic Unit 259 Code (HUC) sub-watersheds. North Branch and South Branch KRWs are grouped into one 260 region (SW1). Battle Creek watershed formed SW2 while Morrow Lake and Spring Brook 261 watersheds are grouped into SW3. Gun river watershed, Rabbit River watershed and small 262 KRW are grouped as SW4. Each SW is marked with a distinct color in Figure 1. The MLT 263 calibration for all of the four SWs followed the step-wise calibration procedure described above. 264 In particular, the stream discharge of each SW was calibrated to the observations from the 265 stream gauging stations within the SW domain with equal weights assigned to all gauges within 266 the SW.

267 **2.5 Empirical equation for** ^ω

268 Different mathematical formulations based on climate and catchment characteristics have 269 been developed for the Budyko framework in the past (Budyko, 1974; Fu, 1981; Choudhury, 270 1999; Wang et al., 2009; Donohue et al., 2012; Xu et al., 2013; Liang et al., 2015). *Fu*'s 271 equation is used in this work, which provides a relation between the dryness index and the 272 evaporation ratio with an adjustable parameter ω ($1 \le \omega \le \infty$) that represents catchment 273 characteristics (Fu, 1981):

274
$$
\frac{ET}{P} = 1 + \frac{E_p}{P} - \left[1 + \left(\frac{E_p}{P}\right)^{\omega}\right]^{1/\omega}
$$
 (9)

275 Yang et al. (2007) found that the parameter ω in Fu's equation is closely correlated with

276 three dimensionless landscape characteristics, i.e., the relative infiltration capacity (Berger and

277 Entekhabi, 2001), the relative soil water storage and the average ground surface slope.

278 Similarly, Xu et al. (2013) proposed an equation for *ω* based on data for 224 MOPEX (Model

279 Parameter Estimation Experiment) watersheds. 280 In order to identify the controlling factors contributing to differences in the Budyko curves 281 for the four SWs, we used empirical equations proposed by Yang et al. (2007), i.e. Eqs. (11) 282 and (12) and Xu et al. (2013), i.e. Eq. (13), to estimate the ω values in Eq. (9). Three 283 dimensionless variables were evaluated by *Yang et al.* (2007) as the key descriptors of a 284 catchment to estimate the parameter ω, i.e., the relative infiltration capacity (Berger and 285 Entekhabi, 2001), the relative soil water storage and the average ground surface slope. The 286 relative infiltration capacity used in the Eqs. (11) and (12) in Yang et al. (2007) is defined as 287 the ratio of saturated hydraulic conductivity K_s (mm hour⁻¹) to the mean precipitation intensity 288 *i_r* (mm hour⁻¹) and represents infiltration excess. The mean precipitation intensity i_r is 289 averaged over the rainy hours of the simulation period. To represent the effect of vegetation 290 and soils on the annual water balance, the plant extractable water capacity, *Smax* (Dunne and 291 Willmott, 1996) is employed and scaled by the mean annual potential evapotranspiration (E_p) 292 in a dimensionless form, i.e., the relative soil water storage (S_{max}/E_p). S_{max} is calculated as:

$$
S_{\text{max}} = (\theta_f - \theta_w) \times d_{\text{root}} \tag{10}
$$

294 where θ_f and θ_w are the soil moisture contents at field capacity and wilting point respectively; 295 $d_{\text{root}} = \min (d_{\text{Top}}^-, d_{\text{max}}^-,$ where $d_{\text{Top}}^-,$ is the top soil depth and d_{max} is the maximum root depth 296 of each vegetation type. *d*root is also the most direct parameter representing the vegetation type 297 affecting the *ω* value. Another dimensionless parameter is the average ground surface slope 298 (*tan β*). They used an empirical non-linear functional form as Eqs. (11) and (12), considering 299 the correlations of the parameter ω with the three descriptors. A stepwise regression analysis 300 of the data from 108 non-humid catchments in China was used to estimate the functional form 301 and was generalized as Eq. (12).

302
$$
\omega = 1 + f_1 \left(\frac{K_s}{i_r}\right) f_2 \left(\frac{S_{\text{max}}}{\overline{E_0}}\right) f_3(\tan \beta) \tag{11}
$$

303
$$
\omega = 1 + 8.652 \left(\frac{K_s}{\overline{i}_r}\right)^{-0.368} \left(\frac{S_{\text{max}}}{\overline{E_0}}\right)^{0.436} \exp(-4.464 \tan \beta) \tag{12}
$$

304 Xu et al. (2013) proposed the following equation for ω for basins with area 100 - 10,000 km²:

$$
\omega = 5.05722 - 0.09322(lat) + 0.13085(CTI)
$$

+1.31697(NDVI) + 0.00003(A) - 0.00018(elev) (13)

306 Where *lat* is the basin center latitude, $CTI = ln[A_s / tan\beta]$ is the compound topographic index, 307 also called the topographic wetness index (Sørensen et al., 2006; Gessler et al., 1993), *A^s* is the 308 specific catchment area (m²) per unit width orthogonal to the flow direction and β is the 309 slope angle in radians. *NDVI* is the normalized difference vegetation index, *A* is the catchment 310 $\arctan(km^2)$ and *elev* is the elevation (m).

311 We used Eqs. (12) and (13) to estimate the *ω* values for the four SWs and the whole 312 KRW. In addition, we used our simulated results to calculate the fitted values of *ω* following 313 the Budyko framework in Eq. (9). The sets of *ω* values are then compared to assess the physical 314 relevance of parameters to identify any deficiencies in each methodology. The values of *θf* and 315 θ_w are directly obtained from the SSURGO database; for K_s we used the calibrated data sets. 316 *dTop* values are obtained from a 5 min resolution data set (Food and Agricultural Organization, 317 2003), following the same approach of Yang et al., (2007); *drmax* values are obtained for each 318 vegetation as described in Zeng (2001) and weighted with the percentage of the corresponding 319 vegetation. *NDVI* values are obtained from the NASA Earthdata website 320 (https://earthdata.nasa.gov/).

321 **3. Results and Discussion**

322 In this section, we present the results for major hydrologic fluxes following the same order 323 we used for the calibration procedures. Inter-annual water balances of a watershed can be 324 described using the equation:

$$
\Delta S = P - Q - E \tag{14}
$$

326 where *P* is precipitation, *Q* is runoff and *E* is evapotranspiration. Δ*S* denotes the change of 327 storage over the simulation period (i.e., the difference between the amount of water storage 328 over the simulation period). All variables are annual average fluxes (mm yr^{-1}). The calibrated 329 parameters are tabulated in Table 1. The parameters here are the multipliers or the additive or 330 multiplicative constants used to change the initial model parameters. The real parameter values 331 after the calibrations are tabulated in Table 2. For spatially heterogeneous parameters, we list 332 the minimum, the maximum, the mean and the median values of the optimized parameters for 333 each (sub-) watershed. For spatially homogeneous parameters, we simply list the values. All 334 water balance components are expressed in mm yr^{-1} while conductivity values are expressed in 335 mm hr⁻¹. The riverbed conductivity (K_r) values are low compared to the aquifer hydraulic 336 conductivity values. This observation and the ranges of *Kr* values are supported by data based 337 on geophysical surveys and temperature modeling reported for sites along the Great Miami 338 River in Ohio (Wojnar et al., 2013).

339 **3.1 The spatial and temporal ET results**

340 Figures 4 (a) and (b) show the annual-average spatial maps of ET based on the simulations 341 and MODIS16 data respectively. The spatial maps of ET from simulations and MODIS data 342 generally follow a similar pattern. The results of the linear correlation analysis for the spatially 343 distributed ET simulated values against the LULC types and soil types are summarized in 344 section S1 and Table S2. The PAWS model outputs resolved the ET heterogeneity better than 345 did the remotely sensed MODIS data. The major land cover in northwestern KRW is forest and 346 there are many lakes and reservoirs located in the middle of the watershed. Therefore, we 347 expect high ET values within this area as shown in simulated ET maps. The south-central areas 348 of Kalamazoo (where the MODIS data are blank) are urban areas, which correspond to the low 349 ET values in PAWS output (colored blue). Details related to the spatial variability of ET are 350 further studied in the analysis based on Budyko framework in a later section. 351 Annual average ET of the 7-year simulation period is 583.43 mm yr^{-1} , which is comparable

352 to the MODIS value, 559.89 mm yr^{-1} . To further evaluate simulated ET, the monthly ET time 353 series (averaged over the entire watershed) is compared with MODIS16 data in Figure 5. The 354 simulated monthly ET is similar compared with MODIS 16 data. The most obvious deviations 355 are during winter months when the model underestimates, whereas in most summer months the 356 model overestimates MODIS ET data. The mismatch between MODIS and simulation is 357 probably due to the different algorithms used. PAWS (via CLM) uses a resistance approach to 358 describe ET based on the two-big leaf model (Dai et al., 2004), while the MODIS product is 359 based on the Penman-Monteith formulation (Mu et al., 2011).

360 **3.2 Stream flow comparisons**

361 Figure 6 shows the 7-year stream flow comparisons between simulations and observations 362 from 6 different USGS gauging stations in the KRW. The NASH values range from 0.57 to 363 0.87, as tabulated in Table S3, which showed fairly well performance. At Gauging station 364 04105000, the optimized river bed conductivity values for all (sub-)watersheds are not 365 significantly different compared with the first set of values used in (*Shen et al.* 2016), which 366 has a log mean of 0.12 m/day in another watershed in Michigan. While *Hoaglund et al.* (2002) 367 assigned a uniform value of 0.086 m/day to the riverbed conductivity for all rivers in a regional 368 groundwater modeling study of Michigan. At the outlet gauging station 04108660 of the whole 369 KRW, outputs show almost similar performance as the heaviest weight of the optimization 370 strategy is laid on the outlet gauging station. Thus, the multi-site strategy helped in quantifying 371 the overall stream flow values by preventing simulation compensation errors from other 372 processes.

373 **3.3 Steady state groundwater head comparisons**

374 The plots of simulated versus observed depths to groundwater table from the Michigan 375 Wellogic database (State of Michigan, 2016) for each computational grid cell are shown in 376 Figure 7. The overall NASH values, as tabulated in Table 3, are over 0.91 showing a spatially 377 good match. These values are comparable to or better than the reported NASH values for water 378 table comparisons (e.g., Niu et al., 2014, Shen et al., 2013). The simulated annual groundwater 379 recharge values are within the range of $176 - 351$ mm yr⁻¹ which was estimated with a tritium 380 interface method by *Delcore and Larson* (1987) in the same watershed.

381 **3.4 Soil Moisture and Soil Temperature Comparisons**

382 Figures 8 and 9 show the 10 cm soil moisture and soil temperature comparisons at two 383 MAWN stations. It should be noted that the observed data represent a point measurement as 384 data were collected using a Campbell Scientific CS616 water content reflectometer (WCR) 385 whereas our simulated results represent an average of a grid cell domain with area of 400×400 386 m². At station Albion (Figure 8 (a)), simulated soil moistures show almost the same trend 387 comparing with observations but generally lower in winter and higher in summer. For example, 388 around February 2004, the simulated soil moisture values are below 0.1 while the observed soil 389 moisture values are between 0.2 and 0.25. Around July 2005, the simulated soil moistures are 390 above 0.1 while the observations are slightly lower. At Michigan State University Kellogg 391 Biological station (MSUKBS) (Figure 8 (b)), the relatively higher soil moistures could not be 392 simulated accurately in February 2009, which may due to the underestimated rainfall intensity 393 during this period. For the soil temperature simulations (Figure 9), the simulated results 394 generally show a good performance at both stations compared with observations except that

395 more fluctuations in simulated results are noted when temperature is below 0° C during winter. 396 The static temperatures around 0° C measured by the WCRs during winter time are possibly 397 because of the frozen soil. It was found by several researchers that the responses of WCRs such 398 as the CS616 are sensitive to temperature and soil type (Benson et al., 2006; Saravanathiiban, 399 2014). Considering these differences, the comparisons of soil moisture and soil temperature 400 are considered acceptable for vadose zone simulations.

401 **3.5 Analysis based on the Budyko framework**

402 Annual water budgets based on Eq. (14) for the whole KRW and four SWs are listed in 403 Table 4. The plots of annual *E/P* versus *Ep/P* (termed Budyko pairs) in the Budyko framework 404 for the four SWs and the whole KRW are shown in Figure 10 for the 7- year simulation period 405 (2003 - 2009). All the Budyko curves in the section refer to the Budyko-type curves are 406 generated by Eq. (9) using simulated results. For the whole KRW, the annual ET value is 407 calculated using three methods (Chen et al., 2013; Condon and Maxwell, 2017): 1) direct ET, 408 simulated ET values are used; 2) inferred ET, assuming the annual storage change is negligible, 409 ET is computed as: $ET = P - Q$ in Eq. (9) and 3) effective precipitation, *P* is replaces by $P - \Delta$ 410 *S* in Eq. (9). The alfalfa (mature, 40cm canopy height) reference ET values are calculated as 411 the *Ep* values, using the Penman - Monteith equation (Dingman, 2008). In this figure, the 412 horizontal straight line indicates the arid or water-limited conditions, while the 1 to 1 line 413 indicates the humid or energy-limited upper bound. The fitted ω values and the R² values for 414 the curve fitting using Eq. (9) are tabulated in Table 5. While the *ω* values using the three 415 different methods are slightly changed due to the partitions of water storage (Istanbulluoglu et 416 al. 2012; Wang, 2012), the ranks of *ω* values among the four SWs and whole KRW are the 417 same. Therefore, the rest part of Budyko curve analyses are based on results of effective 418 precipitation to simplify our discussion.

419 The average Mahalanobis distance *D* (*Mahalanobis*, 1936) of each SW was calculated 420 using the whole KRW results as a reference sample (see Table 6) to represent the dissimilarity 421 of each SW from the averaged pattern. The Mahalanobis distance is a measure of distance in a 422 multidimensional parameter space, which is similar to the Euclidean distance but takes into 423 account the covariance among dimensions of the reference sample. Large *D* indicates more 424 dissimilarity. SW4 shows the most obvious dissimilarities from the KRW, and this is also 425 apparent from Figure 10 - SW4 has consistently higher *E/P* values compared to other sub-426 basins, given similar *Ep/P*.

427 The *ω* values of the four SWs and the whole KRW calculated by Eqs. (12) and (13) and 428 the parameters involved are tabulated in Table 6. All the parameters are calculated within each 429 grid cell and are averaged across the watershed. The *ω* values calculated by Yang's method for 430 the 4 SWs and whole KRW are generally lower compared with the fitted *ω* values in Budyko's 431 framework for the 7-year simulation period, with an average deviation around 8.5%. Five major 432 factors could be identified as the reasons for the uncertainties of calculating *ω* using *Yang*'s 433 method here. First, there are errors in calculating the parameters (for example, there are 434 uncertainties in calculating the average ground surface slope). Second, although *Yang*'s method 435 has considered relative infiltration capacity and relative soil water storage, it overlooked the 436 effects of groundwater flow which also play an important role in water storage and stream 437 discharge contribution (Wang, 2012; Shen et al., 2013; Condon and Maxwell, 2017). Third, 438 the climate conditions of 108 catchments used to generate the empirical equation of *Yang*'s 439 method are different from the climate of KRM; there are uncertainties in the coefficients 440 considering the climate variations. Fourth, there may be parameter inversion errors during the 441 parameter generation processes of Yang's and Xu's methods. Fifth, open water ET plays an 442 important role in SW4, however, this factor is not included in the three indicators suggested by 443 *Yang*'s method. This is also an important reason *ω* is underestimated using *Yang*'s method for 444 SW4. *Xu*'s method, however, overestimate the *ω* values with an average deviation around 445 10.5%, especially for the whole KRW. *Xu*'s method utilizes the catchment area as an indicator 446 which is positively correlated with *ω*. This may create a discrepancy to differentiate the *ω* 447 values between whole watershed and SWs. Since the area for the whole watershed is larger 448 than each SW, which indicates larger *ω* value for the whole watershed, whereas its *ω* values 449 should fall between the ranges of those of all SWs based on water budgets. In addition, the *ω* 450 values obtained using *Xu*'s method for the four SWs are not as different as *ω* values obtained 451 from using *Yang*'s method and the simulated data. This could be due to the climate conditions, 452 i.e. the rainfall intensities, are not explicitly expressed in *Xu*'s method. Besides the possible 453 uncertainties in estimating the values of *ω* in *Yang*'s and *Xu*'s methods, any errors in the model 454 outputs of the ET and the estimation errors of *Ep* could also shift the Budyko pairs to some 455 extent compared with the two empirical methods.

456 The *ω* values of the four sub-watersheds do not change much and generally fall within 457 the range of $2 \sim 3$, and one major reason is that the vegetation types and percentages do not 458 vary significantly among the four SWs. This information is represented as the indicators of root 459 depth in *Yang*'s method and *NDVI* in *Xu*'s method. Although the *ω* values produced by the 460 three methods (two empirical equations and numerical simulation based on the PAWS model) 461 are different, SW4 has the highest value of *ω* among all four sub-watersheds., and the most 462 significant influencing factor is the mean precipitation intensity in *Yang*'s method and the 463 watershed elevation in *Xu*'s method. Compared to the other SWs, SW4 had a relative higher 464 precipitation intensity, which decreases the relative infiltration capacity accordingly. 465 Relatively less infiltration capacity translates to more surface ponding, which produces higher 466 actual ET. Some previous studies (e.g., Schenk and Jackson, 2002) suggested that rooting depth 467 increases with precipitation (at least in water-limited ecosystems). Results shown in Table 6 468 suggest that SW 4 has the highest precipitation and root depth values, although the differences 469 of root depth values are not significant. The lake effect may be responsible for the higher 470 precipitation intensity at SW4, which is also implicitly reflected in the elevation indicator of 471 *Xu*'s method. In contrast, SW3 shows the lowest *ω* value, and higher averaged soil saturated 472 hydraulic conductivity increases the relative infiltration capacity, which tends to generate lower 473 actual ET. In addition, SW3 has higher ground surface slope and accordingly lower CTI, which 474 indicates higher potential to produce surface runoff with less water retained for 475 evapotranspiration (Hjerdt et al., 2004, Yang et al., 2019). Another factor influencing the ET 476 of SW3 could be its largest urban area ratio among all the SWs; this information was 477 incorporated in the data integration algorithm during the model construction (Shen et al., 2013). 478 These calculated *ω* values are also in correspondence to *D* values discussed above when 479 considering the deviations of *ω* values of the four SWs from that of the whole KRW. 480 Considering all the possible errors in estimating the values of ω, the dominant heterogeneous 481 characteristics controlling the water budgets are effectively identified within the indicators of 482 the two empirical methods at SW scale, which indicates the usefulness of the two empirical 483 methods in predicting the interannual variability of regional water balances over a long period. 484 The advantage of the Budyko approach lies in its ability to predict changes in long term 485 ET or water yields due to changes in vegetation (e.g. replacing traditional crops with biofuel 486 crops) based on multiple observations. The Budyko approach could efficiently generate the 487 general functional patterns of catchments and inform controlling hydrologic parameters based 488 on empirical relationships. These results reveal the possibility of using Budyko approach to 489 guide the calibration of PBHM models, to recognize the controlling processes, and to constrain 490 individual processes in the integrated system.

491 **4. Conclusions**

492 In order to accurately quantify the spatial and temporal inter-annual water balances for a 493 heterogeneous catchment, in this work, we used a step-wised calibration method combined 494 with a multisite calibration strategy to optimize a PBHM. The calibration objectives are not 495 limited to stream discharge exclusively, while also include ET and groundwater heads to 496 resolve the equifinality issue. This calibration strategy successfully converged, and the 497 calibrated results showed good comparisons with the observed data for different SWs. The 498 Budyko curves based on the simulated water balance components and two empirical equations 499 (Yang et al. (2007) and Xu et al, (2013)) are employed to quantify the variabilities of inter-

509 **References**

510 Anderton, S., Latron, J., Gallart, F., 2002. Sensitivity analysis and multi-response, multi-511 criteria evaluation of a physically based distributed model. Hydrol. Process. 16, 333–353. 512 doi:10.1002/hyp.336

513 Benson, C. H., and Wang, X, 2006. Temperature-Compensating Calibration Procedure for 514 Water Content Reflectometers. Proc. TDR 2006, Purdue University, West Lafayette, 515 USA, Sept. 2006, Paper ID 50, 16 p., https://engineering.purdue.edu/TDR/Papers

- 516 Berger, K.P., Entekhabi, D., 2001. Basin hydrologic response relations to distributed 517 physiographic descriptors and climate. J. Hydrol. 247, 169–182. doi:10.1016/S0022- 518 1694(01)00383-3
- 519 Beven, K.J., Binley, A., 1992. The future of distributed models: Model calibration and 520 uncertainty prediction. Hydrol. Process. 6, 279–298. doi:10.1002/hyp.3360060305
- 521 Beven, K.J., 1993. Prophecy, reality and uncertainty in distributed hydrological modelling. 522 Advances in Water Resources, Research Perspectives in Hydrology 16, 41–51. 523 doi:10.1016/0309-1708(93)90028-E

- 558 Fang, K., Shen, C., Fisher, J.B., Niu, J., 2016. Improving Budyko curve-based estimates of 559 long-term water partitioning using hydrologic signatures from GRACE. Water Resour. 560 Res. 52, 5537–5554, doi:10.1002/2016WR018748.
- 561 Food and Agricultural Organization, 2003. Map of world soil resources, Rome.
- 562 Fry, L.M., Hunter, T.S., Phanikumar, M.S., Fortin, V., Gronewold, A.D., 2013. Identifying 563 streamgage networks for maximizing the e_ectiveness of regional water balance 564 modeling. Water Resources Research 49, 2689-2700. doi:10.1002/wrcr.20233.
- 565 Fu, B. P., 1981. On the calculation of the evaporation from land surface. Chinese Journal of 566 Atmospheric Sciences (in Chinese), 5(1), 23-31. doi:10.3878/j.issn.1006- 567 9895.1981.01.03.
- 568 Gessler, P.E., Moore, I.D., McKenzie, N.J., Ryan, P.J., 1993. Soil-landscape modelling and 569 spatial prediction of soil attributes. International Journal of Geographical Information 570 Systems 9(4), 421-432. doi:10.1080/02693799508902047.
- 571 Gunduz, O., Aral, M.M., 2005. River networks and groundwater flow: a simultaneous 572 solution of a coupled system. J. Hydrol. 301, 216–234. 573 doi:10.1016/j.jhydrol.2004.06.034
- 574 Hjerdt K. N., McDonnell J. J., Seibert J. and Rodhe A., 2004. A new topographic index to 575 quantify downslope controls on local drainage. Water Resources Research, 40(5), 576 doi:10.1029/2004WR003130.
- 577 Hoaglund, J.R., Huffman, G.C., Grannemann, N.G., 2002. Michigan basin regional ground 578 water flow discharge to three Great Lakes. Ground Water, 40(4), 390–405.
- 579 Huss, M., Bauder, A., Funk, M., Hock, R., 2008. Determination of the seasonal mass balance 580 of four Alpine glaciers since 1865. J. Geophys. Res. 113, F01015. 581 doi:10.1029/2007JF000803
- 582 Huss, M., Bauder, A., Funk, M., Hock, R., 2008. Determination of the seasonal mass balance 583 of four alpine glaciers since 1865. J. Geophys. Res. 113(F01015.). 584 doi:10.1029/2007JF000803.
- 585 Harman, C., Troch, P.A, 2013. Darwinian hydrology: can the methodology Charles Darwin 586 pioneered help hydrologic science? Hydrology and Earth System Sciences Discussions. 587 10, 6407–6444, doi:10.5194/hessd-10-6407-2013.

588 Istanbulluoglu, E., Wang, T., Wright, O.M., Lenters, J.D., 2012. Interpretation of hydrologic 589 trends from a water balance perspective: The role of groundwater storage in the Budyko 590 hypothesis. Water Resour. Res. 48, W00H16. doi:10.1029/2010WR010100

- 625 GRACE, MODIS products. Water Resour. Res. 50, 7359–7377. 626 doi:10.1002/2014WR015589
- 627 Oleson, K.W., Lawrence, D.M., Gordon, B., Flanner, M.G., Kluzek, E., Peter, J., Levis, S., 628 Swenson, S.C., Thornton, E., Feddema, J., others, 2010. Technical description of version 629 4.0 of the Community Land Model (CLM) (No. NCAR/TN-478+STR), NCAR Technical 630 Note. National Center for Atmospheric Research, Boulder, Colorado.
- 631 Oudin, L., Andréassian, V., Lerat, J., Michel, C., 2008. Has land cover a significant impact 632 on mean annual streamflow? An international assessment using 1508 catchments. J. 633 Hydrol. 357, 303–316. doi:10.1016/j.jhydrol.2008.05.021
- 634 Price, K., Stone, R., and Lampinen, J. (2005), Differential Evolution: A Practical Approach to 635 Global Optimization, Springer, Berlin.
- 636 Qiu, H., P. Blaen, S. Comer‐Warner, D.M. Hannah, S. Krause, M.S. Phanikumar, Evaluating 637 a coupled phenology – surface energy balance model to understand stream – subsurface 638 temperature dynamics in a mixed‐use farmland catchment, Water Resources Research, 639 vol. 55, doi:10.1029 / 2018WR023644 (2019)
- 640 Riley, W.J., Shen, C., 2014. Characterizing coarse-resolution watershed soil moisture 641 heterogeneity using fine-scale simulations. Hydrol. Earth Syst. Sci. 18, 2463–2483. 642 doi:10.5194/hess-18-2463-2014
- 643 Ragettli, S., Pellicciotti, F., 2012. Calibration of a physically based, spatially distributed 644 hydrological model in a glacierized basin: On the use of knowledge from 645 glaciometeorological processes to constrain model parameters. Water Resour. Res. 48, 646 W03509. doi:10.1029/2011WR010559
- 647 Saravanathiiban, D. S., 2014. Preferential flow through earthen landfill covers: Field 648 evaluation of root zone water quality model and laboratory validation of lattice 649 Boltzmann method, PhD dissertation, Dep. of Civ. Environ. Eng., Mich. State Univ., 650 East Lansing.
- 651 Schaap, M.G., Leij, F.J., van Genuchten, M.T., 2001. rosetta: a computer program for 652 estimating soil hydraulic parameters with hierarchical pedotransfer functions. J. Hydrol. 653 251, 163–176. doi:10.1016/S0022-1694(01)00466-8
- 654 Schenk, H., Jackson, R., 2002. Rooting depths, lateral root spreads and below-ground/above-655 ground allometries of plants in water-limited ecosystems. Journal of Ecology 90(3), 480- 656 494. doi:10.1046/j.1365-2745.2002.00682. x.
- 657 Shen, C., Niu, J., Phanikumar, M.S., 2013. Evaluating controls on coupled hydrologic and 658 vegetation dynamics in a humid continental climate watershed using a subsurface-land 659 surface processes model. Water Resour. Res. 49, 2552–2572. doi:10.1002/wrcr.20189
- 660 Shen, C., Niu, J., Fang, K., 2014. Quantifying the effects of data integration algorithms on the 661 outcomes of a subsurface–land surface processes model. Environmental Modelling & 662 Software 59, 146–161. doi:10.1016/j.envsoft.2014.05.006 663 Shen, C., Phanikumar, M.S., 2010. A process-based, distributed hydrologic model based on a 664 large-scale method for surface–subsurface coupling. Advances in Water Resources 33, 665 1524–1541. doi: 10.1016/j.advwatres.2010.09.002 666 Shen, C., Riley, W.J., Smithgall, K.R., Melack, J.M., Fang, K., 2016. The fan of influence of 667 streams and channel feedbacks to simulated land surface water and carbon dynamics. 668 Water Resour. Res. 52(2), 880 { 902. doi:10.1002/2015WR018086. 669 Sivapalan, M., 2006. Pattern, process and function: elements of a unified theory of hydrology 670 at the catchment scale. Encyclopedia of hydrological sciences, 193–219, John Wiley, 671 Chichester, U. K., doi:10.1002/0470848944.hsa012. 672 Sivapalan, M., Yaeger, M.A., Harman, C.J., Xu, X., Troch, P.A., 2011. Functional model of 673 water balance variability at the catchment scale: 1. Evidence of hydrologic similarity and 674 space-time symmetry. Water Resour. Res. 47, W02522. doi:10.1029/2010WR009568 675 Sørensen, R., Zinko, U., Seibert, J., 2006. On the calculation of the topographic wetness 676 index: Evaluation of different methods based on field observations. Hydrology and Earth 677 System Sciences 10, 101-112. 678 Soil Survey Staff, Survey Geographic (SSURGO) Database for Michigan. Natural Resources 679 Conservation Service, United States Department of Agriculture. Available online at 680 <http://soildatamart.nrcs.usda.gov> (accessed 06.01.10). 681 Stahl, K., Moore, R.D., Shea, J.M., Hutchinson, D., Cannon, A.J., 2008. Coupled modelling 682 of glacier and streamflow response to future climate scenarios. Water Resour. Res. 44, 683 W02422. doi:10.1029/2007WR005956 684 State of Michigan, 2016. Wellogic digital water well dataset, Michigan GIS open data portal, 685 State of Michigan. URL http://gis.michigan.opendata.arcgis.com/datasets? 686 q=wellogic&sort by=relevance. Accessed on June 21, 2016. 687 Sutanudjaja, E.H., van Beek, L.P.H., de Jong, S.M., van Geer, F.C., Bierkens, M.F.P., 2014. 688 Calibrating a large-extent high-resolution coupled groundwater-land surface model using
- 689 soil moisture and discharge data. Water Resour. Res. 50, 687–705. 690 doi:10.1002/2013WR013807
- 691 Wagener, T., Sivapalan, M., Troch, P.A., McGlynn, B.L., Harman, C.J., Gupta, H.V., Kumar, 692 P., Rao, P.S.C., Basu, N.B., Wilson, J.S., 2010. The future of hydrology: An evolving 693 science for a changing world. Water Resour. Res. 46, W05301.
- 694 doi:10.1029/2009WR008906
- 695 Wang, D., 2012. Evaluating interannual water storage changes at watersheds in Illinois based 696 on long-term soil moisture and groundwater level data. Water Resour. Res. 48, W03502. 697 doi:10.1029/2011WR010759
- 698 Wang, D., Wu, L., 2013. Similarity of climate control on base flow and perennial stream 699 density in the Budyko framework. Hydrol. Earth Syst. Sci. 17, 315–324. 700 doi:10.5194/hess-17-315-2013
- 701 Wang, T., Istanbulluoglu, J.L., Scott, D., 2009. On the role of groundwater and soil texture in 702 the regional water balance: An investigation of the Nebraska Sand Hills, USA. Water. 703 Resour. Res. 45. doi:10.1029/2009WR007733.
- 704 Wesley, J.K., 2005. Kalamazoo River Assessment. Fisheries Division Special Report. 705 Michigan Department of Natural Resources, Michigan, USA. Available online at 706 http://www.michigan.gov/dnr/0,4570,7-153-10364_52259_19056-46270--,00.html
- 707 Wojnar, A.J., Mutiti, S., Levy, J., 2013. Assessment of geophysical surveys as a tool to 708 estimate riverbed hydraulic conductivity. Journal of Hydrology 482, 40-56. 709 doi:10.1016/j.jhydrol.2012.12.018.
- 710

714

- 711 Xu, X., Liu, W., Scanlon, B.R., Zhang, L., Pan, M., 2013. Local and global factors control 712 water-energy balances within the Budyko framework. Geophys. Res. Lett. 40, 6123 - 713 6129.
- 715 Yang, D., Sun, F., Liu, Z., Cong, Z., Ni, G., Lei, Z., 2007. Analyzing spatial and temporal 716 variability of annual water-energy balance in nonhumid regions of China using the 717 Budyko hypothesis. Water Resour. Res. 43, W04426. doi:10.1029/2006WR005224
- 718 Yang, D., Yang, A., Qiu, H., Zhou, Y., Herrero, H., Fu, C.-S., Yu, Q. and Tang, J., 2019. A 719 Citizen-Contributed GIS Approach for Evaluating the Impacts of Land Use on 720 Hurricane-Harvey-Induced Flooding in Houston Area, Land, 8(2), 25, 721 doi:10.3390/land8020025.
- 722 Yokoo, Y., Sivapalan, M., Oki, T., 2008. Investigating the roles of climate seasonality and 723 landscape characteristics on mean annual and monthly water balances. J. Hydrol. 357, 724 255–269. doi:10.1016/j.jhydrol.2008.05.010
- 725 Zeng, X., 2001. Global Vegetation Root Distribution for Land Modeling. J. Hydrometeor 2, 726 525–530. doi:10.1175/1525-7541(2001)002<0525:GVRDFL>2.0.CO;2
- 727 Zhang, L., Dawes, W.R., Walker, G.R., 2001. Response of mean annual evapotranspiration to 728 vegetation changes at catchment scale. Water Resour. Res. 37, 701–708. 729 doi:10.1029/2000WR900325

730 **Figures**

- 731 **Figure 1.** Map of the Kalamazoo River watershed. Elevation is shown as the color gradient.
- 732 National Hydrography Dataset (NHD) rivers, U.S. Geological Survey (USGS) gauges,
- 733 National Climatic Data Center (NCDC) weather stations and Michigan Automatic Weather
- 734 Network (MAWN) stations are shown.
- 735 **Figure 2.** Land Use and Land Cover map for the Kalamazoo River Watershed.
- 736 **Figure 3.** Flow chart of the calibration procedure. See Table S1 for an explanation of 737 variables and their meaning.
- 738 **Figure 4.** Spatial map of yearly averaged evapotranspiration for the Kalamazoo River 739 watershed for the 7-year period (2003–2009) of (a) simulated output and (b) MODIS data.
- 740 **Figure 5.** Monthly ET comparisons of simulated outputs with MODIS data for the 7-year
- 741 simulation period (2003–2009). NASH is the Nash-Sutcliffe efficiency metric; APB is the
- 742 absolute bias; RMSE is the root mean squared error.
- 743 **Figure 6.** River discharge comparisons of simulated outputs with observations at different 744 U.S. Geological Survey (USGS) gauge stations. Sim is the simulated; Obs is the USGS 745 observations. NASH is the Nash-Sutcliffe efficiency metric. The model performance for each 746 gauge is summarized in Table S3.
- 747 **Figure 7.** Plots of simulated versus observed depth to groundwater table (from Wellogic 748 data set) for each computation grid cell. SW1, SW2, SW3, SW4 are the simulated results 749 within each SW.
- 750 **Figure 8.** 10 cm Soil Moisture comparisons of simulated outputs with MAWN (Michigan 751 Automatic Weather Network) station observations at (a) Albion and (b) MSUKBS. Sim is the 752 simulated outputs; Obs is the MAWN station observations.
- 753 **Figure 9.** 10 cm Soil Temperature comparisons of GLB and MLT simulated outputs with 754 MAWN (Michigan Automatic Weather Network) station observations at (a) Albion and (b)
- 755 MSUKBS. Sim is the simulated outputs; Obs is the MAWN station observations.
- 756 **Figure 10.** Budyko Curve Analysis for the 4 SWs and the whole Kalamazoo River
- 757 watershed for a 7-year simulation period from 2003 to 2009 using a) direct ET, b) inferred
- 758 ET and (c) effective precipitation.

Discharge (m Discharge (m³/s)

Date (MM/DD/YY)

	optimized operator values					
Symbol(Unit)	optimization type	SW1	SW ₂	SW ₃	SW4	
γ	\times	4.10×10^{-2}	4.30×10^{-2}	3.68×10^{-2}	1.68×10^{-2}	
a_{ice}	$^{+}$	0.45	-0.20	0.64	0.53	
K_I	×	1.27	0.78	1.39	0.99	
K_2	×	1.07	1.2	2.19	1.86	
K_{s}	X	1.46	0.96	0.81	1.26	
N	$\ddot{}$	-0.14	-0.26	-0.15	0.08	
$A(1 m^{-1})$	×	0.86	0.88	0.81	1.43	
L(m)	$^{+}$	-35	-6	-54	-44	
$h_o(m)$	$^{+}$	4.24×10^{-2}	4.45×10^{-2}	4.38×10^{-2}	3.98×10^{-2}	
K_r (m day ⁻¹)	\times	1.10×10^{-2}	7.39×10^{-3}	2.15×10^{-2}	1.01×10^{-1}	
$h_r(m)$	\pm	0.14	0.21	θ	θ	

1 **Table 1.** Calibrated parameter operator values and the optimization types

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	SW1	SW ₂	SW ₃	SW4
Parameter (Unit)	min-max(mean, median)	min-max(mean, median)	min-max(mean, median)	min-max(mean, median)
γ	4.1×10^{-2}	4.3×10^{-2}	3.68×10^{-2}	1.68×10^{-2}
α_{ice}	3.45	2.90	3.64	3.53
K_l (m/day)	$0.305 - 105.07(26.96, 34.99)$	$0.249 - 62.86(17.41, 13.58)$	4.660-80.34(24.3,24.84)	$0.097 - 75.05(19.15, 18.27)$
K_2 (m/day)	$0.019 - 5.05(1.61, 1.38)$	$0.017 - 6.18(0.947, 1.30)$	$0.018 - 6.07(1.86, 3.74)$	$0.004 - 1.96(0.10, 0.16)$
K_s (mm/hour)	$1.25 - 263.72(73.18, 78.83)$	$0.58 - 205.84(54.26, 24.59)$	$0.38 - 275.15(113.53,98.64)$	$0.69 - 246.02(67.73,70.49)$
\boldsymbol{N}	$1.05 - 2.26(1.30, 1.31)$	$0.99 - 2.13(1.19, 1.16)$	$1.06 - 1.93(1.31, 1.31)$	$1.25 - 2.81(1.51, 1.53)$
A(1/m)	$0.032 - 6.48(4.06, 4.21)$	$0.038 - 6.37(3.01, 3.22)$	$0.041 - 6.22(4.35, 4.90)$	$0.051 - 6.99(4.68, 5.06)$
l(m)	365	394	346	356
$h_o(m)$	4.24×10^{-2}	4.45×10^{-2}	4.38×10^{-2}	3.98×10^{-2}
K_r (m/day)	$0.011 - 0.206(0.109, 0.110)$	$7.1 \times 10^{-3} - 0.113(0.059, 0.058)$	$0.077 - 0.318(0.174, 0.177)$	$0.014 - 0.385(0.190, 0.190)$
$h_r(m)$	246.23-348.54 (289.84, 287.56)	247.12-287.05 (267.06, 266.69)	232.71-285.50 (232.71, 258.65)	172.56-285.44 (211.90, 212.56)

3 **Table 2.** Calibrated parameter values for MLT methods. For spatially heterogeneous parameters we listed the minimum (min), the maximum 4 (max), the mean and the median values within the specific simulated domain.

5

Table 4. Water Budgets.

Table 5. The fitted ω values and the R² for the curve fitting using Equation (9)

	direct ET		inferred ET		effective precipitation	
	ω	\mathbb{R}^2	ω	\mathbb{R}^2	ω	R^2
SW ₁	2.45	0.76	2.55	0.45	2.47	0.73
SW ₂	2.44	0.73	2.48	0.81	2.44	0.70
SW3	2.27	0.74	2.26	0.68	2.27	0.72
SW ₄	2.85	0.8	2.98	0.63	2.84	0.80
whole KRW	2.44	0.8	2.54	(147)	2.46	0.72

	SW1	SW ₂	SW ₃	SW ₄	whole KRW
Area (km^2)	1395.81	726.41	1154.08	1983.92	5260.22
Elevation (m)	303.46	278.39	272.12	225.59	266.15
Average slope $(\%)$	0.92	0.96	1.30	1.09	1.06
Basin Center Latitude	42.20	42.43	42.36	42.59	42.39
Compound Topographic Index (CTI)	9.18	9.09	8.82	9.19	9.14
Average NDVI	0.39	0.41	0.40	0.42	0.41
Forest $(\%)$	21.32	20.93	22.46	22.82	21.47
Agricultural (%)	53.32	54.80	43.08	47.38	47.32
Urban area $(\%)$	4.97	4.72	10.41	4.58	6.60
Mahalanobis distance	2.23	3.47	4.37	5.49	----
PET, Ep (mm/year)	807.19	848.71	887.35	857.81	846.52
Average K_S (mm hr ⁻¹)	73.18	54.26	113.53	67.73	80.83
Mean precip intensity i_r (mm hr ⁻¹)	12.69	9.3	13.83	19.17	11.25
S_{max} (mm)	48.56	48.46	51.77	50.98	50.09
θ_f - θ_w	0.35	0.34	0.36	0.35	0.35
$d_{root}(mm)$	140.34	142.10	144.74	147.38	144.73
ω based on simulation	2.47	2.44	2.27	2.84	2.46
ω calculated with Eq.(12)	2.30	2.26	2.12	2.51	2.16
ω calculated with Eq.(13)	2.81	2.8	2.78	2.86	2.95

Table 6. Paramters invloved in plotting the Budyko pairs and for calculating the ω value in Equations (12) and (13)

