**Multi-objective calibration of a hydrologic model using spatially distributed
remotely sensed/in-situ soil moisture**

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Abstract

The objective of this study is to evaluate the relative potential of spatially distributed surface and root zone soil moisture estimates in calibration of Soil and Water Assessment Tool (SWAT) towards improving its hydrologic predictability with reduced equifinality. The Upper Wabash and Cedar Creek, two agriculture-dominated watersheds in Indiana, USA are considered as test beds to implement this multi-objective SWAT calibration. The proposed calibration approach is performed using remotely sensed Advanced Microwave Scanning Radiometer-Earth Observing System surface soil moisture (~1 cm top soil) estimates (NASA's Aqua daily level-3 gridded land surface product-version 2) in sub-basin/HRU level together with observed streamflow data at the watershed's outlet. Although application of remote sensing data in calibration improves surface soil moisture simulation, other hydrologic components such as streamflow, evapotranspiration (ET) and deeper layer moisture content in SWAT remain less affected. An extension of this approach to apply root zone soil moisture estimates from limited field sensor data showed considerable improvement in the simulation of root zone moisture content and streamflow with corresponding observed data. Difference in relative sensitivity of parameters and reduced extent of uncertainty are also evident from the proposed method, especially for parameters related to the subsurface hydrologic processes. Regardless, precise representation of vertical soil moisture stratification at different layers is difficult with current SWAT ET depletion mechanism. While the results from this study show that root zone soil moisture can play a major role in SWAT calibration, more studies including various soil moisture data products are necessary to validate the proposed approach.

Keywords: AMSR-E, Calibration; Remote Sensing; Soil Moisture; SWAT; Uncertainty

1. INTRODUCTION

Parameter calibration is a necessary step in setting up a hydrologic model for any study. Regardless of the uncertainties in input weather data and imperfections in model physics, a calibrated model tends to provide an “acceptable” output. Simulation of surface and subsurface fluxes in a hydrologic model is strongly affected by the choice of objective variables in model calibration procedure and resultant parameter values adopted from therein (Abbaspour et al., 2007; Park et al., 2014). Similarly, several parameter combinations are possible during calibration, producing equally reasonable simulation results (equifinality; Beven, 1993). Therefore, parameters associated with subsurface fluxes get poorly optimized when models are typically calibrated against observed streamflow hydrograph (Immerzeel and Droogers, 2008; White and Chaubey, 2005).

Simultaneous use of multiple gauging stations in model calibration can help to reduce parameter uncertainty and improve streamflow simulations (e.g. Bekele and Nicklow, 2007; Chiang et al., 2014; Her and Chaubey, 2015; Zhang et al., 2008), but the outcomes are often region-specific (e.g. Gong et al., 2012) and are also affected by the spatial distribution of gauges included in the study (Migliaccio and Chaubey, 2007). Additionally, there is no literature which shows that use of multiple gauges can lead to better estimation of subsurface fluxes such as soil moisture and evapotranspiration (ET), including the reduction of uncertainty/equifinality of the associated parameters. Therefore, the traditional approach of model calibration using observed streamflow at one or more stations can still lead to a model where several components of the watershed's hydrologic system may remain virtually uncalibrated (Wanders et al., 2014). Considering these issues, good correspondence between observed and simulated streamflow is not sufficient to evaluate the simulation capability of physically based hydrologic models (Demarty et al., 2005;

1 Eckhardt, 2005; Gupta et al., 1998; Kuczera and Mroczkowski, 1998). Alternatively, the trade-
2 off between model fits constrained by multiple hydrologic variables observed at different spatial
3 scale of evolution might lead towards lower parameter uncertainty, improving model robustness
4 and predictability and implicitly encountering possible deficiencies in model structure. The
5 solution to this multi-objective calibration produces a parameter set that is optimal in a Pareto
6 efficiency sense (Xie et al., 2012). Among different surface/subsurface components, soil
7 moisture plays an important role in energy and water balance of hydrologic cycle (Brocca et al.,
8 2012), and hence, ensuring accurate soil moisture accounting in a hydrologic model can lead to
9 better simulation of hydrologic processes including ET, surface runoff generation, groundwater
10 recharge, and streamflow. While obtaining in-situ monitoring data of soil water fluxes/state
11 variables is a long-standing challenge, remotely sensed surface soil moisture estimates can be
12 obtained at high temporal resolution for the entire globe (Wanders et al., 2014).

13 Most studies that use surface soil moisture estimates to improve model simulation involves
14 assimilation of in-situ, synthetic or remotely sensed data (e.g. Alvarez-Garreton et al., 2015;
15 Bolten et al., 2010; Brocca et al., 2010; Chen et al., 2011; Draper et al., 2011; Han et al., 2012a,
16 b; Houser et al., 1998; Lei et al., 2014; Pauwels et al., 2001, 2002; Reichle et al., 2002; Sawada
17 et al., 2015; Scipal et al., 2008). Only few recent studies have applied remotely sensed surface
18 soil moisture information in model calibration process (e.g. Milzow et al., 2011; Poovakka et al.,
19 2013; Parajka et al., 2009; Sutanudjaja et al., 2014; Wanders et al., 2014). All these past studies
20 conclude that using surface soil moisture, either in data assimilation or model calibration,
21 improves model simulated surface soil moisture, without causing appreciable change in deeper
22 layer (root zone) soil moisture and streamflow/surface runoff outputs. The limited success in
23 modeling results from using remotely sensed soil moisture estimates is related to the shallow

depth of assimilation/calibration which is in fact dependent on the sensing depth of the satellite product being used (1-5 cm top soil), and the model conceptualizations related to coupling of surface and root zone soil layers (e.g. Brocca et al., 2012; Chen et al., 2011; Han et al., 2012a).

Considering the role of root zone soil moisture in regulating subsurface hydrology, Parajka et al. (2006) and Silvestro et al. (2015) showed the use of an empirically derived root zone soil moisture index for calibrating a hydrologic model. Brocca et al. (2012) and Chen et al. (2011) recommended model calibration using both streamflow and root zone soil moisture prior to assimilating soil moisture data into the model, which can potentially improve the efficiency of data assimilation techniques. Despite the limitation of sensing depth from space-borne satellites and the scarcity of field based information, recent advancements in multi-model land surface data assimilation projects such as National Astronomy and Space Administration (NASA)'s North American Land Data Assimilation Systems (NLDAS; Xia et al., 2015a, b) and Soil Moisture Active Passive (SMAP; Entekhabi et al., 2014; Reichle et al., 2014) mission can lead to high resolution root zone soil moisture estimations. These estimates can ultimately be used to improve the representation of subsurface processes in hydrologic models through multi-objective calibration.

Given the potential availability of root zone soil moisture, the overall goal of this study is to evaluate the performance of the Soil and Water Assessment Tool (SWAT) hydrologic while using both soil moisture information and streamflow for calibration. Specific objectives include: (i) use of remotely sensed sub-basin/HRU scale surface soil moisture estimates along with streamflow observations in a spatially distributed calibration scheme; and (ii) use of root zone soil moisture and streamflow in similar spatially distributed model calibration scheme. Accordingly, comparison of the outcomes from these two objectives are used to evaluate the

relative influence of surface and root zone soil moisture estimates in improving SWAT's soil moisture accounting, streamflow simulation and parameter equifinality.

The Soil and Water Assessment Tool (SWAT) is selected for this study because it is a semi-distributed, continuous-time, process-based hydrology and water quality model (Neitsch et al., 2011) that is widely used globally to simulate hydrologic processes under different conditions and scales (Arnold et al., 2012; Gassman et al., 2007). Even with the recent remarkable advancements in developing new optimization algorithms and automatic tools specifically designed for SWAT, hydrologic calibrations of SWAT models can still be "conditional" (Abbaspour et al., 2015) and "sub-optimal" (Chen et al., 2011). Application of remote sensing data and/or associated data products, as shown in this study, is expected to overcome these limitations and provide more realistic hydrologic simulations.

2. STUDY AREA AND DATA

The Upper Wabash and Cedar Creek watersheds in Indiana, USA (Figure 1) are selected as the test beds for this study. Both watersheds are well suited for creating a SWAT model at two different scales; Upper Wabash (18,500 km²) is suitable for the first objective because of its larger size to capture the variability in surface soil moisture from the coarse resolution satellite data, whereas field sensor-based profile/root zone soil moisture data are available for certain parts of Cedar Creek (700 km²) to accomplish the second objective of this study. In order to evaluate the "relative" role of surface soil moisture, satellite data are also used for Cedar Creek watershed. Both watersheds have United States Geological Survey's (USGS) streamflow gauge station at the respective outlet as shown in Figure 1. The landuse in both watersheds is mostly

1 agricultural, although significant difference exists in the forest and developed portion. Table 1
2 presents a summary of their geospatial and hydro-climatic characteristics.

3 SWAT models for both watersheds are created by the ArcSWAT GIS interface by using the
4 following data: (i) 30m digital elevation model (DEM) from the USGS National Elevation
5 Dataset (USGS-NED, 2013); (ii) 30m land cover data for year 2006 from the National Land
6 Cover Database (USGS-NLCD, 2013); and (iii) 1:250,000 scale State Soil Geographic Data
7 (STATSGO) that is included within SWAT 2012 database. Total daily precipitation, average
8 minimum and maximum daily temperature data covering the study period of 2004-2012 are
9 obtained from the National Climatic Data Center for the stations that fall within or adjacent the
10 watershed boundary. All other related climate variables, including solar radiation, wind speed
11 and relative humidity, are obtained from the internal weather generator within ArcSWAT.
12 Penman-Monteith equation is selected for computing potential evapotranspiration (PET).

13 For model evaluation, observed daily streamflow time series is obtained from respective USGS
14 station located at each watershed's outlet (Figure 1). Remotely sensed surface soil moisture data
15 (~1 cm top soil) is extracted from the Advanced Microwave Scanning Radiometer - Earth
16 Observing System (AMSR-E). It is noteworthy that several algorithms have been so far applied
17 to retrieve soil moisture information from AMSR-E, the most prominent of which have been
18 developed by Jones et al. (2009), Koike et al. (2004), Njoku et al. (2003) and Owe et al. (2001).
19 The data retrieved by the National Astronomy and Space Administration (NASA) following
20 Njoku et al. (2003) (Aqua daily level-3 gridded land surface product-version 2 (AE_Land_3),
21 Njoku, 2004) is used in this study. Metadata associated with this particular estimate, including
22 data format, projection system, spatio-temporal coverage and resolution, as well as the procedure
23 for accessing the data can be found at http://nsidc.org/data/ae_land3. In-situ soil moisture

estimates at 5, 20, 40 and 60 cm depths in the Cedar Creek watershed are obtained from <http://amarillo.nserl.purdue.edu/ceap/> for two of the permanent field sensors (AS1 and AME in Figure 1). These sensors are part of the National Soil Erosion Research Laboratory's (NSERL) environmental monitoring network (Flanagan et al., 2008; Han et al., 2012c; Heathman et al., 2012a,b). The STATSGO database is modified while preparing the ArcSWAT model for Cedar Creek so that a uniform stratification of soil profile depth all over the watershed can be maintained from 0-5 cm, 5-20 cm, 20-60 cm, and 60 – 150 cm. This modification makes SWAT simulated soil moisture values at different layers compatible with the placement of field sensors. Such modification is not necessary while using the AMSR-E data because SWAT model invariably considers a 1 cm surface layer for any watershed (Neitsch et al., 2011), which is identical to the approximate sensing depth of the satellite data being used for this watershed. Prior assumptions and processing are essential to make remotely sensed and field sensor-based soil moisture estimates comparable with SWAT simulations.

3. METHODOLOGY

3.1 Watershed spatial discretization and model setup

While creating a watershed model in the GIS interface of SWAT model (ArcSWAT), spatial heterogeneity is represented through a two-step discretization (Geza and McCray, 2008). A watershed can be first divided into sub-basins, and then each sub-basin is further divided into multiple Hydrologic Response Units (HRUs). Considering the coarse spatial resolution of NASA AMSR-E soil moisture data (25 km x 25 km), sub-basins in the Upper Wabash watershed are not divided into multiple HRUs. Instead only one HRU is created per sub-basin based on dominant landuse, soil type and slope class (Winchell et al., 2010), resulting into total 36 sub-basins (or 36 HRUs). Being a smaller watershed, boundary of Cedar Creek intersects with only four AMSR-E

grid cells (not shown here). In order to imitate a condition when fine resolution spatially distributed soil moisture estimates (remotely sensed or model assimilated such as NLDAS/SMAP) are available, Cedar Creek watershed is discretized into 106 sub-basins and 370 HRUs (Table 1). HRU level calibration is performed in the Cedar Creek watershed, using both remotely sensed and in-situ soil moisture data. Curve Number and Variable Storage methods (Neitsch et al., 2011) are selected for surface runoff generation and channel routing simulation respectively, invariably in all cases.

3.2 Calibration configurations

Evaluating the relative effect of remote sensing and field sensor-based soil moisture estimates in model calibration needs prior consideration of several consistency factors. For example, drainage areas of the two study watersheds are very different (700 and 18,500 km²); AMSR-E surface soil moisture estimates are available for the whole basin in both cases, but in-situ estimates are obtained at fixed depths across the root zone and limited only to the few locations of the Cedar Creek watershed. Furthermore, surface soil moisture obtained from remote sensing are “noisier” than in-situ root zone estimates (Draper et al., 2009). Most importantly, in contrast to the field data which are point measurements, remotely sensed data are spatial estimates where the value of a grid cell denotes the average surface moisture of the entire landscape of a cell, ignoring the effects of possible heterogeneity in climate and land use-land cover therein. Thus, the climatology (mean and variance) captured by the satellite-derived soil moisture estimates can be very different from those in the in-situ data and model simulations (Entekhabi et al., 2010; Koster et al., 2009; Reichle and Koster, 2004; Reichle et al., 2004). The differences, traditionally referred as the systematic bias, get enhanced by the physical conceptualizations in satellite's soil moisture retrieval algorithm (Draper et al., 2009); respective retrieval algorithms can generate

quite different soil moisture fields, with different degrees of realism (e.g. Tuttle and Salvucci, 2014). Persistence of systematic bias would be a considerable factor while applying other root zone soil moisture products as well including those from the NLDAS or SMAP. Hence, comparison of calibration results involving either remotely sensed, model assimilated or field measured soil moisture estimates should base upon the respective representativeness, scale and inherent uncertainty of these data sources.

The proposed multi-variable spatial calibration scheme is evaluated under two configurations (M1 and M2 in Table 2) for each of the study watersheds. The first configuration (M1) involves calibration with streamflow only, and the second configuration (M2) is for the spatial calibration involving both streamflow and soil moisture. As indicated in Table 2, M2 configuration for the Upper Wabash watershed includes only the remotely sensed surface soil moisture. To enable a fair evaluation considering the aforementioned consistency issues, M2 in case of Cedar Creek is executed in three separate settings including remotely sensed surface moisture (~1 cm, same as in Upper Wabash), in-situ surface moisture (5 cm) and in-situ total root zone moisture (60 cm) contents.

3.3 Spatial scaling of satellite data and creation of time-series

The AMSR-E data needs to be geo-referenced and processed to enable the comparison between surface soil moisture values in an individual/group of AMSR-E grid cell(s) with the average sub-basin/HRU level model estimates. The geo-processing task is accomplished by creating a python based automatic tool which can account for the heterogeneity in size, shape and location of the sub-basins/HRUs within any watershed. For a given temporal extent in the form of start and end date, and geographic extent in the form of shapefile, the python based tool creates an area averaged time series of AMSR-E soil moisture estimates for all the individual sub-basins (or

HRUs) by directly accessing http://nsidc.org/data/ae_land3. Once the time series is obtained, the data are rescaled using a statistical method in order to reduce its systematic bias relative to the SWAT model simulations.

3.4 Reducing systematic bias in satellite data

Systematic bias mostly arises from resampling the raw data into grid cells, continuously variable sensing depth of satellite instrument as a function of moisture content and the satellite's soil moisture retrieval algorithms (Draper et al., 2009; Reichle et al., 2004). Several approaches, including linear regression (Milzow et al., 2011), cumulative distribution function (CDF) matching (Reichle and Koster, 2004; Scipal et al., 2008; Brocca et al., 2011; Matgen et al., 2012), μ - σ linear rescaling (Brocca et al., 2012, 2010; Dharssi et al., 2011; Draper et al., 2009; Jackson et al., 2010), min-max correction (Albergel et al., 2010) and water holding capacity method (Bisselink et al., 2011; Wanders et al., 2014) can be applied for reducing the bias in remotely sensed soil moisture data. It is noteworthy that the temporally rescaled output might vary depending on the choice of scaling technique.

Sub-basin and HRU scale AMSR-E soil moisture values, respectively for Upper Wabash and Cedar Creek, are first transformed into plant-available water (PAW, in mm H₂O depth unit), because SWAT does not simulate residual water content of soil (DeLiberty and Legates, 2003; Milzow et al., 2011). Following the method used in SWAT source code (Neitsch et al., 2011), water content held at wilting point (WP) is calculated for the top 1 cm layer for a sub-basin/HRU as a function of percent clay content and bulk density, and then this calculated amount is deducted from the respective AMSR-E data, thereby producing sub-basin or HRU scale surface PAW values. These PAW values are then rescaled with the μ - σ linear technique using equation (1):

$$\theta'_{(RS)} = [\theta_{(RS)} - \mu(\theta_{(RS)})] \times \sigma(\theta_{(M)}) / \sigma(\theta_{(RS)}) + \mu(\theta_{(M)}) \dots (1)$$

Here, each AMSR-E PAW value ($\theta_{(RS)}$) in a sub-basin/HRU is normalized ($\theta'_{(RS)}$) to match the long-term mean (μ) and variance (σ^2) of the SWAT simulated PAW time-series ($\theta_{(M)}$), being limited by the period of model simulation. $\theta_{(M)}$ is obtained after the model parameters are adjusted against observed streamflow data with a small number of trial calibration iterations. This particular step is quite subjective, yet necessary to ensure a reasonable state of SWAT simulation. After the application of eq. (1), the resulting rescaled AMSR-E PAW product is used in SWAT calibration along with streamflow data.

3.5 Processing field sensor-based soil moisture data

SWAT simulated soil moisture cannot be directly compared with the estimates from field sensors because of two factors: (i) the sensors AS1 and AME (Cedar Creek watershed in Figure 1) measure the dielectric permittivity of soil to determine volumetric moisture content (m^3/m^3) for every 10 minutes using the frequency domain reflectometry method (Heathman et al., 2012a), whereas SWAT simulated soil moisture content represents the PAW content in the depth unit (mmH_2O) at the end of each simulation time-step (a day) (Deliberty and Legates, 2003); (ii) the sensors deliver point estimates at four different depths (5, 20, 40 and 60 cm) (Han et al., 2012c; Heathman et al., 2012a), but values obtained from SWAT are spatially averaged over particular HRUs. To overcome such limitations, sensor values are transformed into daily averages and then multiplied with the depth interval of sensor placement, producing soil moisture observations in the depth unit (mmH_2O) for those particular depth intervals (0-5, 5-20, 20-40 and 40-60 cm). Following the same method as discussed in section 3.4, water content held at wilting point is calculated for each layer and then this calculated amount is deducted from the sensor values, thereby producing observed PAW. Total PAW in the top 60 cm of the soil profile is obtained by

adding the PAW values in all the four constituent layers. The total PAW in top 5 cm and 60 cm profile from the AS1 and AME locations are employed in HRU-scale calibration of the Cedar Creek model (Table 2), assuming that the point estimates are representative of the average PAW in respective HRUs where these sensors are actually located. To keep the terminology simple, PAW will be referred to as soil moisture in the subsequent sections.

3.6 Multi-variable spatial calibration using streamflow and soil moisture

Following a split-sample approach (Klemes, 1986) over a continuous daily simulation period, all the six model setups for the Upper Wabash and Cedar Creek watersheds are calibrated for 2004-2008 and 2004-2010, using year 2004 as the warm-up period in each case. Total 14 parameters involving surface, subsurface and channel hydrologic responses are used for calibration (Table 3). The selection of parameters and their initial ranges are based on the review of existing literature and prior knowledge of the study area (e.g. Kumar and Merwade, 2009; Larose et al., 2007; Rajib and Merwade, 2016), as well as suggestions from SWAT developers (Abbaspour, 2015; Neitsch et al., 2011). Calibration is conducted by using the Sequential Uncertainty Fitting algorithm-version 2 (SUFI-2), which is a semi-automated inverse modeling procedure available inside SWAT-CUP. Kling-Gupta Efficiency (KGE) (Gupta et al., 2009; Kling et al., 2012) is used as an objective function to measure the agreement between simulated and observed variables. The KGE statistic decomposes Nash-Sutcliffe Efficiency (NSE) and Mean Squared Error (MSE) into a three-dimensional criteria space and finds out a Pareto front in terms of the shortest Euclidean distance (ED):

$$KGE = 1 - ED = 1 - \sqrt{\{ (r - 1)^2 + (\beta - 1)^2 + (\gamma - 1)^2 \}} \dots\dots\dots (2)$$

$$\beta = \mu_s / \mu_0$$

$$\gamma = \sigma_s / \sigma_o$$

where r represents the correlation, β and γ respectively represent bias and variability ratio between the simulated and observed variable. μ and σ are the mean and standard deviation of the variable; the indices s and o denote simulation and observation, respectively. KGE ranges from ∞ to 1, with a value closer to 1 produces a more accurate model. Soundness of KGE against the conventional application of NSE in hydrologic model calibration is discussed in detail by Gupta et al. (2009).

In the first set of iteration, SWAT models for both watersheds are calibrated against daily streamflow records at the watershed outlets. In the case of Upper Wabash watershed, sub-basin scale surface soil moisture output (top 1 cm layer) from this initial streamflow-based calibration is used in the temporal rescaling of corresponding AMSR-E data (eq. (1)). After each set of iterations, SUFI-2 produces an updated parameter range which is centered on their best value. Taking the updated parameter range from the initial streamflow-based iteration as input, successive iterations are performed where streamflow at the watershed outlet and rescaled AMSR-E surface soil moisture estimates from all the 36 sub-basins are set as target variables for calibration. A similar approach is followed in the case of Cedar Creek, where the first set of calibration iterations is run only with streamflow; from the second set and onwards, AMSR-E surface moisture (~1 cm), in-situ surface moisture (5 cm) and in-situ total root zone moisture (60 cm) contents at two particular HRUs are added into the calibration process along with streamflow data, in three separate settings. No prior rescaling (eq. (1)) of the field sensor-based soil moisture is necessary in this case, because of the relatively less uncertainty and systematic bias in these estimates compared to remote sensing data.

With the addition of soil moisture as objective variable from the second set of iteration and

onwards, the goal/objective function, KGE is modified to a weighted mean value, KGE' following the approach shown by Abbaspour et al. (2015):

$$KGE' = \sum_{i=1}^{n_f} w_{f_i} (KGE_{f_i}) + \sum_{j=1}^{n_s} w_{s_j} (KGE_{s_j}) \dots (3)$$

where n and w are the number of objective variables (observational datasets) involved and the weight assigned to each of them, respectively; the indices f and s stand for streamflow and soil moisture, respectively. Also, i denotes the streamflow gauge stations and j denotes sub-basins/HRUs with soil moisture estimates brought under calibration. Thus, KGE calculated for individual sets of observed and simulated values are aggregated into KGE' and it is maximized toward an optimal solution. The assignment of weights being subjective, it may affect the outcome of the optimization exercise by SUFI-2 (Abbaspour et al., 1997). On the basis of few test iterations, the weights in this study are set as $w_f = 0.5$ (since only one streamflow gauge station for both study areas) and $w_{s_j} = 0.5/n_s$ (n_s is the total number of sub-basins/HRUs in calibration with soil moisture estimates). On the contrary, assigning equal weights to both streamflow and soil moisture components ($w_f = w_{s_j} = 1/(n_f + n_s)$) is found to have improved the KGE for soil moisture in individual sub-basins/HRUs, compromising with the KGE of streamflow.

For an even comparison, M1 and M2 configurations are evaluated after equal number of iterations (1500). In each case, maximum three batches are executed each having 500 SUFI-2 iterations. For each of the six calibration setups (Table 2), coefficient of determination (R^2) and Percent Bias (PBIAS, Sorooshian et al., 1993) are also calculated to evaluate the goodness of fit between the observations/estimates and the best simulation having maximum objective function value (KGE or KGE' in this case).

3.7 Modification of SWAT source code

The default configuration of SWAT-CUP does not allow calibration with respect to estimates in a particular soil layer (e.g. top 1 cm in Upper Wabash and Cedar Creek) or in a portion of the whole soil profile (e.g. top 5 cm and 60 cm in Cedar Creek). To enable this layer-based calibration scheme, subroutine *hruday.f* from the SWAT 2012 version source code (revision 629) is modified such that the simulated soil moisture in top 1 cm layer, and the sum of soil moisture in all the layers up to 5 cm and 60 cm get exported as three new variables in the HRU-level output file (*output.hru*). The edited sub-routine is then compiled with the rest of the source code to get a new SWAT executable file, which can be run in SWAT-CUP.

3.8 Relative parameter sensitivity analysis

A relative sensitivity ranking of parameters is performed in order to ascertain the possible reasons behind the changes in simulation results caused from insertion of surface/root zone soil moisture estimates into model calibration process. The global sensitivity analysis technique in SWAT-CUP measures the average changes in objective function due to the changes in one parameter while all other parameters are also simultaneously changing (Abbaspour, 2015). Accordingly, the measure of relative sensitivity is translated in terms of p-values; where a smaller p-value represents more sensitive parameter. Relative sensitivity of parameters depends on the objective variables (soil moisture and/or streamflow) involved in the calibration process. Hence, to identify the effect of soil moisture by comparing the p-values between M1 and M2, this global sensitivity scheme is executed after the second set of 500 iterations for both model configurations.

3.9 Measure of parameter uncertainty

Equifinality means that that several parameter combinations from the optimized range can potentially produce behavioral solutions that are considered equally satisfactory in comparison with the observed data (Beven, 1993; Vrugt et al., 2008). In this study, all parameter values staying within their final optimized space and producing a value of the objective function higher than a specified threshold (KGE or $KGE' > 0.5$) are categorized as behavioral solutions. Then, in order to compare the extent of uncertainty associated with each parameter in the same scale, all these behavioral parameter values are normalized from 0 to 100 using equation (4):

$$P_n = \left[\frac{P_b - L_l}{U_l - L_l} \right] \times 100 \dots \dots \dots (4)$$

Where P_n is the normalized uncertainty score, P_b is the behavioral parameter value identified by SUFI-2, U_l and L_l are respectively the upper and lower limit of the corresponding parameter; P_b corresponds to the final batch of iterations producing optimized parameter set. Example application of this normalized uncertainty scoring technique can be found in Kumar and Merwade (2009) and Rajib and Merwade (2016).

3.10 Model Validation

The final optimized parameter ranges from the calibration scenarios are used in model validation, with respect to streamflow records and soil moisture estimates. SWAT models for Upper Wabash and Cedar Creek watersheds are validated for the period 2009-2010 and 2011-2012, respectively.

4. RESULTS AND DISCUSSION

This section presents the findings on the relative improvement in SWAT performance due to the simultaneous application of surface/root zone soil moisture and streamflow data in a spatial

calibration approach. Various flow components from the two model configurations (M1 and M2) are compared both at temporal and spatial scale, in terms of their simulated values as well as their goodness of fit statistics with estimates/observations. The possible reasoning behind the differences in simulation results is analyzed in terms of relative parameter sensitivity between M1 and M2. Furthermore, potential reduction in equifinality is evaluated with the corresponding reduction in parameter uncertainty range.

4.1 Fitness statistics for streamflow and soil moisture

Table 4 compares the goodness of fit scores (KGE, PBIAS and R^2) for the M1 and M2 configurations after equal number of SUFI-2 iterations. Overall, it is evident that high KGE and R^2 with low PBIAS for streamflow can be achieved from M1, without using any soil moisture information for data assimilation or model calibration (e.g. Immerzeel and Droogers, 2008; Park et al., 2014). Clearly the M1 configuration exhibit higher amount of bias, when the fit scores are compared for soil moisture. This validates the presence of sub-optimality of model calibration practices (Abbaspour et al., 2015) even with acceptable streamflow results. The scores for streamflow are slightly negatively impacted with M2 configuration for Upper Wabash, but this can be attributed to the optimization algorithm. The Upper Wabash has 37 objective functions (one for each sub-basin and the outlet), and optimization algorithm seeks a goal that is best for all the objectives and thereby implicitly imposing an "averaging effect" across scales and the variables involved (White and Chaubey, 2005; Wanders et al., 2014). Having lesser number of objective functions (only 3) compared to the Upper Wabash, streamflow fit scores remain virtually the same for Cedar Creek when calibrated either with satellite or field estimates of surface moisture. This is not the case for Cedar Creek when root zone moisture is employed in the M2 configuration; KGE and R^2 increase from 0.75 to 0.81 and 0.69 to 0.72, respectively,

1 PBIAS shows a substantial decrease from -12.2 to -0.9. Depending on how the relationship
2 between soil wetness and runoff generation within a particular model is conceptualized, it is
3 possible that the stronger influence of root zone moisture on regulating the parameters can
4 overrule the "averaging effect" of multi-objective calibration, thus improving the fitness scores
5 for streamflow simulation.

6 Improved agreement between simulated soil moisture and the field/satellite estimates is also
7 found in the M2 configuration (Table 4), especially in Cedar Creek, when total root zone
8 moisture in upper 60 cm of the soil profile is brought into calibration and compared with the
9 corresponding field estimates; PBIAS decreases from -19.1 to -8.7 with the increase in KGE and
10 R^2 from 0.13 to 0.35 and 0.18 to 0.23, respectively. Similar improvement is evident when
11 watershed-average simulated surface moisture in Upper Wabash is compared with the AMSR-E
12 estimates. These low fitness values may indicate that SWAT is still under-performing in soil
13 moisture simulation even with the multi-objective calibration scheme. From this aspect, it is
14 important to clarify that these fitness statistics are calculated for the entire duration of simulation
15 and are impacted by the differences in absolute values between the simulations and the
16 observations; hence, they do not represent the actual improvement in the temporal dynamics of
17 soil moisture simulation. However, using either AMSR-E or field sensor-based surface estimates
18 in calibrating the Cedar Creek model does not produce any noticeable difference in fit scores for
19 the 60 cm root zone moisture content, relative to those in the M1 configuration (Table 4).

20 In general, using surface estimates in model calibration can improve the simulation of surface
21 moisture itself, but that may not be influential over the deeper layer moisture content which
22 implicitly refers to the insensitivity of surface moisture to streamflow simulation. Assuming that
23 the available field/satellite soil moisture estimates are representative of actual wetness

conditions, calibration with root zone moisture is considered an effective approach as it makes the overall water budget more realistic in terms of the improvement in soil moisture and corresponding enhancement in streamflow prediction.

4.2 Enhancement in soil moisture simulation

In the case of Upper Wabash watershed, fitness scores for surface soil moisture listed in Table 4 actually represent watershed-average values. Figure 2, in contrast, helps to identify the actual extent of model performance improvement in terms of bias removal from individual sub-basins. A spatial comparison of sub-basin scale PBIAS, R^2 and KGE between the simulated daily surface soil moisture and the AMSR-E estimates over the entire simulation period (2005-2010) is presented in Figure 2. Clearly, the spatially distributed calibration approach improves model simulation all over the watershed, irrespective of scales. However, the soil and landuse characteristics of the sub-basins may have affected this particular spatial pattern of bias removal, but this is not explored further in the current study. Figure 3 shows the frequency distribution of the values being mapped in Figure 2. As seen from the results of M1 configuration in Figure 3, surface soil moisture in 12 out of 36 sub-basins is overestimated by more than 10% (PBIAS), while R^2 in all the sub-basins is less than 0.25. In the M2 configuration, maximum PBIAS in any of the sub-basins decreases to 8%, with almost half of the sub-basins showing much improved R^2 (0.25~0.5). Consequently, KGE in majority of the sub-basins also increases from 0.2 - 0.3 in M1 to 0.25 - 0.35 in M2.

Figure 4 shows the temporal comparison of simulated surface soil moisture with AMSR-E estimates in the Upper Wabash watershed. Regardless of M1 or M2, there is a resemblance in temporal dynamics of AMSR-E estimates with that of the model simulation which validates the ability of SWAT model in subsurface characterization. However, extensive disagreement in their

absolute values is visible in case of M1. Especially, SWAT simulated moisture for M1 is seen to have reached wilting point ($PAW \approx 0$) at numerous occasions both during calibration and validation. Calibration with M2 setting enhances model simulation, but disagreement between the absolute values of model simulation and AMSR-E estimates still persists. Literature supports similar findings in other modeling studies that used remotely sensed surface soil moisture in calibration (e.g. SWAT (Milzow et al., 2011), LISFLOOD (Wanders et al., 2014)). Considering that the surface layer is the most interactive and hence very "noisy", the improvement in the temporal dynamics of SWAT simulated daily surface soil moisture obtained in this study, as evident in Figure 2-4, is quite convincing.

In order to further ascertain the ability of surface moisture in regulating deeper layer soil moisture content through model calibration, the in-situ total root zone moisture (top 60cm soil profile) content in the AS1 location of Cedar Creek watershed is plotted with corresponding SWAT simulations resulted from the M2 configurations when the model was calibrated with AMSR-E (top 1 cm) and in-situ (top 5 cm) surface moisture estimates (Figure 5). In either case, there is no noticeable improvement in root zone soil moisture. On the contrary, considerable improvement in model simulation is observed when root zone moisture (60 cm) is employed in the multi-objective calibration (Figure 6). Parajka et al. (2006) and Silvestro et al. (2015) reported similar findings with more consistent root zone soil moisture simulation. Large offsets in M1 simulations from the field estimates are evident; the deviation, as seen from the error plots, can be more than 25 mm on a day which is quite significant considering the average daily precipitation in the watershed. In comparison, the M2 configuration matches well with the field estimates invariably during the calibration and validation phase, except during the summer months. The error plot clearly indicates minimal or even zero residual of M2 simulations in the

significant portion of the time-span being plotted, thereby attesting the greater utility of root zone soil moisture estimates toward improving model performance through calibration. The "summer deficiency" identified here is very much a model-specific issue and can be linked with the limitations in SWAT's ET depletion mechanism.

4.3 Potential model deficiency in ET mechanism

SWAT's ET mechanism uses an exponential depth distribution function for soil moisture depletion that tends to withdraw 95% of soil evaporative demand and 50% of plant transpiration uptake approximately from upper 6% (~10 cm) of the root zone (~150 cm in this case) (Neitsch et al., 2011). In reality, the upper portion of the root zone may not always hold enough moisture to satisfy this calculated demand. SWAT regulates ET depletion such that when the moisture depletes from one layer due to ET, moisture from another layer cannot be extracted to replenish the deficit. According to the availability of soil moisture in upper layers, the exponential depth distribution function can be adjusted through two empirical parameters 'ESCO' and 'EPCO' such that the lower layers can take part in meeting the actual evaporative demand. Either way, the upper layers tend to dry out ($PAW \approx 0$) even when sufficient moisture is still available in the deeper layers. This is a model structure issue rather than a parametric issue, hence cannot be resolved by model calibration even using soil moisture estimates. Therefore, regardless of the M1 or M2 configuration, significantly large error in model simulation is observed at the time of heavy ET demand during the peak of crop growing season in summer months (July-August). During this period, SWAT simulated soil moisture (PAW) in the top 60 cm stays around the wilting point over a persistently long period of time. This has caused the high negative PBIAS score in SWAT simulated root zone moisture (Table 4), even though M2 configuration produces substantial improvement in model performance by fairly imitating total amount of "observed"

1 moisture in the top 60 cm throughout the rest of the year (Figure 6).

2 Although M2 configuration tends to match total moisture in the top 60 cm profile (Figure 6),
3 SWAT may still be unable to replicate actual vertical distribution of moisture content in individual
4 soil layers. Figure 7 shows monthly model simulated and observed average soil moisture values
5 in the year 2009 at particular soil layers (0-20, 20-40 and 40-60 cm) at the AS1 sensor location
6 of Cedar Creek watershed. Relative to the model simulations, average sensor values in a summer
7 month (August 2009) are higher across the entire 60 cm depth being plotted here. Besides the
8 structural limitation in SWAT's ET mechanism, this can also be attributed with the actual
9 agricultural management operations (e.g. spatial/temporal information on specific crop plantation
10 and harvesting) which are not been considered in the model. Irrespective of that, relatively higher
11 field estimates at around 15-35 cm depth compared to the model simulations (both M1 and M2)
12 are persistent in other months along the year (e.g. May 2009 and November 2009), when
13 growing crops and relevant management operations are not considerable issues. That indicates
14 toward insufficient parameterization related to soil moisture and/or non-physical application of
15 'ESCO' and 'EPCO', as well as the lack of vertical coupling strength among soil layers in
16 SWAT's soil moisture accounting structure. From this standpoint, refurbishment of SWAT's ET
17 mechanism would make the soil moisture based calibration even more efficient.

18 *4.4 Effect on ET and profile soil moisture*

19 Use of soil moisture in model calibration can alter the volume of ET, and consequently total soil
20 moisture content in the entire root zone (~150 cm). Figure 8 shows the calculated differences in
21 simulated ET (M2-M1) and the temporal comparison of the two configurations for moisture
22 content in the entire 150 cm soil column for both study watersheds during their respective
23 calibration periods. Variation of ET resulting from the M2 configuration in Cedar Creek

watershed is quite analogous to the temporal changes of soil moisture shown in Figure 6. For example, M2 configuration elevates the amount of ET, but keeping it within the theoretically calculated PET limit whenever SWAT simulated moisture in the top ~60cm soil profile is overestimated by M1, and vice versa. For the case of Upper Wabash, calibration with surface soil moisture in the ~1 cm top soil improves the moisture content in that particular layer itself (Figure 4), but it seems to have minimal effect in changing the total moisture content across the entire root zone. On the contrary, noticeable changes can be observed in the case of Cedar Creek while attempting to match the total field estimate over a fairly large segment of the root zone (top 60 cm out of the 150 cm profile) through model calibration procedure; the difference (M2-M1) therein (Figure 8) can be as high as ± 30 mm in a day. These potential differences in ET and total root zone soil moisture storage can be significant in applications related to nutrient transport and crop yield.

4.5 Enhancement in streamflow simulation

Antecedent soil wetness condition is the major controlling factors for surface runoff generation. Therefore, it is expected that the extent of changes in the whole root zone moisture (Figure 8) caused by the model calibration scheme will lead to possible changes in streamflow hydrographs (Figure 9). Both runoff methods in SWAT (Curve Number and Green-Ampt) use moisture content (PAW) in the whole root zone for necessary parameterizations and subsequent calculations. Theoretically, the larger the change being imparted in the entire root zone moisture content, the higher will be the impact on SWAT simulated runoff volume and streamflow, following a storm event. In the case of Upper Wabash watershed, where only the surface soil moisture is improved, simulated hydrograph from M2 configuration does not suggest appreciable enhancement in streamflow prediction (Figure 9). This can be explained by the inability of

1 surface moisture estimates in producing big changes in the deeper layer moisture contents
2 through model calibration, as evident in the examples of Cedar Creek (Figure 6 and Table 4).
3 This is quite analogous to the findings by Parajka et al. (2009) and Wanders et al. (2014). On the
4 other hand, in the case of Cedar Creek, where the entire root zone moisture (60 cm) is included
5 in the M2 configuration, simulated streamflow matches well with the observed hydrograph
6 compared to M1. Brocca et al. (2012) assimilated a semi-empirical exponential filter-based root
7 zone soil moisture product into a hydrologic model and showed similar significant improvement
8 in streamflow simulation. Especially for high flow conditions in Cedar Creek, SWAT
9 simulations from M2 configuration are quite precise, thereby addressing the long-standing
10 limitation of SWAT in replicating watershed physics under extreme flow situations (e.g. Arnold
11 and Allen, 1996; Arnold et al., 2000; Chu and Shirmohammadi, 2004; Vazquez-Amábile and
12 Engel, 2005; Arabi et al., 2006; Bracmort et al., 2006; Larose et al., 2007; Wang et al., 2008;
13 Kumar and Merwade, 2009; Oeurng et al., 2011; Rahman et al., 2012; Qiu and Wang, 2013;
14 Rahman et al., 2014). Since a simple hydrograph comparison does not appear to be decisive
15 enough for the Upper Wabash watershed (Figure 9), Figure 10 provides supplementary
16 information in this regard. Figure 10 shows the Percentage Error (PE) in daily streamflow for all
17 the individual data points over the entire duration of model simulation along with the average
18 daily residual for specific flow regimes. Comparison of average daily residuals (observed *minus*
19 simulated streamflow) indicates that simulations for high and low flow regimes are improved
20 invariably for both watersheds, with slight exception for the moist flow condition. Considerable
21 degree of reduction in PE for Upper Wabash is evident as well, thereby validating the potential
22 of remotely sensed data in enhancing streamflow prediction through a model calibration
23 approach. In conjunction with the better fit between simulated and observed hydrographs for

Cedar Creek watershed (Figure 9), much pronounced reduction of PE in Figure 10 further proves the comparatively efficient role of root zone moisture in model calibration.

4.6 Evaluation of relative parameter sensitivity

During a model calibration, the parameter space gets optimized, and the outcome is heavily dependent on the choice of objective variable (observation). Hence, relative sensitivity of parameters in a calibration only with observed streamflow will be different from a calibration involving both streamflow and soil moisture. Figure 11 compares the relative ranking of sensitive parameters between the two configurations based on p-value measurements. Obtained from the global sensitivity analysis of parameters during a set of calibration iterations, p-value determines the significance of the sensitivity, where a value closer to zero indicates more significance. The important feature from Figure 11 is that some of the parameters related to subsurface processes such as GWQMN, ESCO, ALPHA_BF in Upper Wabash, and SOL_AWC, ESCO, EPCO, SOL_K in Cedar Creek become more sensitive in the M2 configuration. In streamflow based calibration (M1), these subsurface related parameters do not get an appropriate constraint in their own spatial scale of variation (observations/estimates on soil moisture and ET in HRU/sub-basin scale) based on which they can be optimized, as such they play a less effective role in the calibration process. This is likely to be the cause for which the M1 configuration in this study suffers from imprecise soil moisture accounting even having well-predicted streamflow results with high goodness of fit scores. This shows that streamflow based calibration leads to parameter equifinality (Beven, 1993) and higher degree of uncertainty.

4.7 Parameter uncertainty reduction

The calibrated parameter values for all the four modeling cases are listed in Table 5. Although

Table 5 denotes the best estimate on how the parameters should be changed in order to best fit the simulated outputs with the observations, it does not help measuring the reduction in parameter uncertainty that might have happened with the application of soil moisture in model calibration. Reduction in equifinality and associated degree of uncertainty can be evaluated in terms of the "behavioral range" of parameters. Hence, the narrower the behavioral range, the lower is the extent of equifinality or uncertainty (Price et al., 2014). In this section, the range of uncertainty in parameters produced by M1 and M2 is tested by applying equation (4), which converts each behavioral parameter value into a normalized uncertainty score (Figure 12). For Upper Wabash watershed, two major parameters related to subsurface hydrology, GWQMN and ESCO, show prominent decrease in their uncertainty range in the M2 configuration compared to M1. Applying remotely sensed surface soil moisture in calibration of LISFLOOD, Wanders et al. (2014) obtained similar results related to parameter uncertainty. However, the output from M2 in the case of Cedar Creek watershed is more remarkable as it is showing significant decrease in the uncertainty for all the parameters involved. This proves the stronger effect of root zone soil moisture in reducing equifinality when employed in model calibration.

4. CONCLUSIONS

Good correspondence of observed and simulated streamflow cannot be sufficient as a criterion for evaluating physically based hydrologic models. Being derived from such perception, this study employs remotely sensed AMSR-E surface soil moisture (~ 1 cm top soil) estimates in calibrating SWAT model simultaneously at individual sub-basins, along with observed streamflow data at particular stream location. In order to validate the stronger role of root zone moisture over the surface moisture estimates in model calibration, similar approach is followed involving AMSR-E surface moisture (~1 cm), in-situ surface moisture (5 cm) and in-situ total

1 root zone moisture (60 cm) contents in HRU scale calibration under three different settings.
2 These cases are tested over two different agriculture-dominated watersheds in Indiana, USA
3 (Upper Wabash and Cedar Creek, respectively) and compared with calibration results based on
4 streamflow only. Following conclusions are drawn:

5 1. Acceptable streamflow simulation can be obtained without using any soil moisture
6 information in model calibration. However, considerable amount of bias is still noticed in
7 soil moisture outputs, indicating significant room for model uncertainty/equifinality. Using
8 sub-basin scale AMSR-E data in calibration improves model simulated surface soil moisture
9 all over the Upper Wabash watershed.

10 2. Such improvement is more prominent when root zone soil moisture data are employed in the
11 calibration process as the PBIAS in root zone moisture (~60 cm) decreases from -19.1 to -8.7
12 with corresponding increase in KGE and R^2 from 0.13 to 0.35 and 0.18 to 0.23, respectively.
13 Regardless of these low performance scores which may give an impression that SWAT is
14 still under-performing even with the multi-objective calibration scheme, improvement
15 achieved in the temporal dynamics of root zone soil moisture simulation is quite
16 considerable.

17 3. Even though root zone moisture based calibration produces minimal or zero residual
18 (simulation *minus* observed) in fairly large portion of the simulation time-span invariably
19 during the calibration and validation periods, significant negative PBIAS (model
20 underestimation) is detected in the peak of summer growing season along with the inability
21 of the model to replicate vertical distribution of moisture content throughout the year. This is
22 likely to be influenced by SWAT's structural limitation regarding ET mechanism which
23 cannot be resolved by calibration even with soil moisture information.

4. Use of either AMSR-E or field sensor estimates of surface moisture in calibrating the Cedar Creek model does not change the total moisture content of the top 60 cm soil profile. Thus, using surface estimates in model calibration can improve the simulation of surface moisture itself but that may exert minimal effect on the deeper layer moisture contents. Whereas, calibration using total root zone field estimates (top 60 cm) has caused noticeable changes (± 30 mm in a day) in the moisture content of the entire soil profile (0-150 cm); accordingly, this gives way to large extent of changes in ET as well.

5. Greater effect of root zone soil moisture estimate in model calibration compared to that of surface layer is further validated in terms of enhancement in streamflow prediction. Especially for high flow conditions, SWAT simulation from the root zone moisture based calibration is found fairly matching with the observed data. In contrast, potential of surface estimates in improving streamflow simulation is still noticeable in terms of the reduced Percentage Error (PE) and residual of different flow conditions; however, those improvements may not be considered as substantial as in the earlier case.

6. Besides producing better water budget, the proposed approach shows reduced uncertainty of parameters. Also, the parameters specifically related to sub-surface hydrologic processes have been found more influential in this proposed scheme in contrast to the streamflow based calibration, thereby producing a less equifinal optimization.

Prior to the application of the distributed multi-objective calibration, this study also shows application of an automatic tool that helps to address the long-standing problem of extracting remotely sensed data in desired spatio-temporal resolution of SWAT model. While the tool is tested only on SWAT model framework through this study, it has a flexible design to be adopted for any hydrologic/land surface model's geo-spatial structure.

Although the results from this study are promising, vigorous experiments are necessary to endorse the proposed approach across different scales, geographic and hydro-climatic settings. Increasing the number of streamflow gauge stations in calibration along with the spatially distributed soil moisture estimates might result into improved watershed average streamflow simulations, however, that would complicate the optimization problem with too many objective variables involved. Another point of attention is the availability of remotely sensed ET data. ET, being a major driver of controlling the vadose zone and atmospheric interaction, inclusion of ET estimates in model calibration can also be considered as a potential avenue for increasing the efficiency of the proposed approach. The enhanced prediction skills and reduced equifinality from SWAT simulations, as shown here, can significantly contribute in studies related to long-term climate and land use impacts, flood forecasting, as well as nutrient transport, crop yield and agricultural management practices.

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Table 1. Watershed characteristics

	Upper Wabash	Cedar Creek
Drainage area, km ²	18,500	700
No. of Subbasins ^a	36	106
No. of HRUs ^b	36	370
Average Annual Rainfall during 2004-2012, mm	1050	993
Number of weather stations used in the model	6	5
Maximum daily streamflow at the watershed outlet till December 31, 2014, m ³ /s	350	163
Landuse as per NLCD 2006 (%)		
Agricultural	80	71
Developed	9	11
Forest	9	14
Wetland/Open Water	2	4

^a Flow accumulation area threshold: 5% (Upper Wabash), 0.5% (Cedar Creek)

^b Basis of HRU definition: Upper Wabash (one subbasin-one HRU with dominant landuse, soil type and slope class in a particular subbasin), Cedar Creek (one subbasin-multiple HRUs, 10% threshold to create a unique combination of landuse, soil type and slope class within each subbasin)

Table 2. SWAT calibration configurations

	M1	M2		Source and scale of soil moisture data in calibration
Upper Wabash ^a	Streamflow	Streamflow	Surface moisture (~1 cm)	AMSR-E, all sub-basins
Cedar Creek ^a	Streamflow	Streamflow	Surface moisture (~1 cm)	AMSR-E, two particular HRUs ^b
		Streamflow	Surface moisture (5 cm)	In-situ, two particular HRUs ^b
		Streamflow	Total root zone moisture (60 cm)	

M1: calibration only with streamflow

M2: Multi-objective calibration with streamflow and soil moisture

^a Streamflow observations are at the watershed outlet

^b Two HRUs within which AS1 and AME field sensors (Figure 1) are located (in all the three M2 setups for Cedar Creek)

Table 3. SWAT calibration parameters

No.	Parameter	Description ^a	Scale of Variation	Adjustment ^b	Initial Range
1	CN2	Curve Number, moisture condition II	HRU	x	-0.2 – 0.2
2	CH_K2	Channel Hydraulic Conductivity, mm/hr	Watershed	=	5.0 – 100.0
3	CH_N2	Main Channel Manning's n	Watershed	=	0.01 – 0.15
4	CANMX	Maximum Canopy Storage, mm	HRU	=	0.0 – 25.0
5	SURLAG	Surface Runoff Lag Coefficient, days	Watershed	=	0.05 – 24.0
6	ESCO	Soil Evaporation Compensation Factor	HRU	=	0.01 – 1.0
7	EPCO	Plant Uptake Compensation Factor	HRU	=	0.01 – 1.0
8	SOL_AWC	Available Soil Water Capacity, mmH ₂ O per mm of soil	HRU	x	-0.15 – 0.15
9	SOL_K	Saturated Hydraulic Conductivity, mm/hr	HRU	x	-0.15 – 0.15
10	ALPHA_BF	Baseflow Recession Constant, days	Watershed	=	0.01 – 1.0
11	REVAPMN	Re-evaporation (Upward Diffusion) Threshold, mm	Watershed	=	0.01 – 500.0
12	GW_DELAY	Groundwater Delay, days	Watershed	+	-10.0 – 10.0
13	GWQMN	Threshold Groundwater Depth for Return Flow, mm	Watershed	=	0.01 – 5000.0
14	GW_REVAP	Groundwater Re-evaporation Coefficient	Watershed	=	0.02 – 0.2

^a Source: Neitsch et al. (2011)

^b Type of change to be applied over the existing parameter value: 'x' means the original value is multiplied by the adjustment factor (1+a given value within the range), '=' means the original value is to be replaced by a value from the range, '+' means a value from the range is added to the original value

Table 4. Descriptive statistics of calibration and validation schemes ^a

Goodness of Fit criteria	Upper Wabash		Cedar Creek			
	M1	M2 (AMSR-E: ~ 1 cm)	M1	M2 (In-situ: 60 cm)	M2 (In-situ: 5 cm)	M2 (AMSR-E: ~ 1 cm)
Streamflow at watershed outlet						
KGE	0.74 (0.73)	0.72 (0.74)	0.75 (0.71)	0.81 (0.74)	0.75	0.75
PBIAS	- 4.2 (- 9.4)	- 8.6 (1.7)	- 12.2 (- 7.5)	- 0.9 (2.2)	-12	-12.7
R ²	0.68 (0.65)	0.65 (0.67)	0.69 (0.64)	0.72 (0.68)	0.69	0.69
Soil moisture ^{b, c}						
KGE	0.25 (0.2)	0.31 (0.24)	0.13 (0.11)	0.35 (0.25)	0.14	0.14
PBIAS	8 (12.2)	3.5 (5)	-19.1 (-25.6)	-8.7 (-11.7)	-18.8	-19.1
R ²	0.18 (0.2)	0.3 (0.25)	0.18 (0.19)	0.23 (0.21)	0.18	0.18

^a Within parentheses are the values from model validation

^b Upper Wabash: watershed-average statistics for surface soil moisture (~1 cm top soil). Rescaled AMSR-E surface estimates are used in calculation

^c Cedar Creek: Values are calculated with respect to the in-situ total root zone soil moisture estimates for top 60 cm of the soil profile. Averages of the two sensor locations (AS1 and AME) are reported here

Table 5. Calibrated parameter ranges ^{a, b}

Parameter	Initial range ^c	Best parameter value			
		Upper Wabash		Cedar Creek	
		M1	M2	M1	M2
CN2	-0.2 – 0.2	-0.002	0.009	0.09	0.04
CH_K2	5.0 – 100.0	64	60	38	74
CH_N2	0.01– 0.15	0.15	0.13	0.02	0.02
CANMX	0.0 – 25.0	21.4	25	18.5	7.7
SURLAG	0.05 – 24.0	14.8	14.5	1.1	3.45
ESCO	0.01 – 1.0	0.97	0.91	0.93	0.86
EPCO	0.01 – 1.0	0.54	0.32	0.77	0.31
SOL_AWC	-0.15 – 0.15	0.09	0.04	0.01	-0.08
SOL_K	-0.15 – 0.15	-0.01	0.03	0.14	0.11
ALPHA_BF	0.01 – 1.0	0.77	0.65	0.73	0.45
REVAPMN	0.01 – 500.0	500	391	500	361
GW_DELAY	-10.0 – 10.0	10	1.83	3.7	-1.9
GWQMN	0.01 – 5000.0	81	14.7	1222	1135
GW_REVAP	0.02 – 0.2	0.15	0.15	0.2	0.2

^a After equal number of iterations (1500) in all the cases^b M1: calibration only against streamflow; M2: calibration against both streamflow and soil moisture^c Basis of adjustment is shown in Table 2

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Figure 9. Comparison of streamflow hydrographs. Only a representative segment from the whole simulation period is shown here: (a) Upper Wabash, (b) Cedar Creek.

Figure 10. (Left) Percentage Error (PE) in simulated streamflow during the entire calibration-validation period. $PE = \frac{Abs[Model - Observed]}{Observed} \times 100\%$. (Right) Average daily residual for three different flow regimes: (exceedance probability 0.0-0.1: high flow, 0.1-0.6: moist and mid flow, 0.6-1.0: dry and low flow).

Figure 11. Relative sensitivity of parameters. The numbers on the vertical axis indicate sensitivity ranking based on p-value; within parentheses are the values corresponding to M1 configuration. Results shown here are based on the Global Sensitivity Analysis being run after the 2nd set of 500 iterations in all the cases.

Figure 12. Normalized uncertainty of parameters. Out of total 14 parameters, 10 most sensitive parameters are selected for this plot.