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Development of an automated procedure for estimation of the spatial variation of runoff in large river basins

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Summary The use of distributed parameter models to address water resource management problems has increased in recent years. Calibration is necessary to reduce the uncertainties associated with model input parameters. Manual calibration of a distributed parameter model is a very time consuming effort. Therefore, more attention is given to automated calibration procedures. This paper describes the development and demonstration of such an automated procedure developed for a national/continental scale assessment study called Conservation Effects Assessment Project (CEAP). The automated procedure is developed to calibrate spatial variation of annual average runoff components for each USGS eight-digit watershed of the United States. It uses nine parameters to calibrate water yield, surface runoff and sub-surface flow respectively. If necessary, the procedure uses a linear interpolation method to arrive at a better value of a model parameter. When tested for the Upper Mississippi river basin of the United States, the automated calibration procedure gave satisfactory results. Other test results from the procedure are very encouraging and show potential for its use in very large-scale hydrologic modeling studies.
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Introduction

In recent years, distributed parameter models are widely used to address watershed and large-scale water quality management problems. These models use many different

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parameters whose values vary widely in space and time. Some model parameters are physically based and can be measured while in some models parameters can only be estimated by a calibration procedure (Duan et al., 1994). Measurement uncertainties are associated with the measurable parameters. Uncertainty, access difficulties for measurement of parameters and budget constraints increase the difficulty of working with models (Lenhart et al., 2002). Therefore, to reduce uncertainties of both measurable and non-measurable parameters, a modeler relies heavily on calibration. Scientists and hydrologists also believe that certain level of calibration is necessary for successful application of models (Hogue et al., 2000). For models with several parameters (such as Soil and Water Assessment Tool (SWAT) (Arnold et al., 1993)), manual calibration is cumbersome for large-scale studies. A successful and efficient manual calibration requires a detailed understanding of the model (Van Liew et al., 2005) and significant amount of time and effort. Moreover, manual calibration involves subjective decisions and therefore it is difficult to assess the confidence of model simulations (Madsen et al., 2002). Therefore, development and use of automated calibration procedures are gaining importance.

In recent years, many automated calibration procedures have been developed and used for hydrological modeling (Duan et al., 1992, 1993; Gan and Biftu, 1996; Gupta et al., 1998; Yapo et al., 1998; Hogue et al., 2000; Madsen et al., 2002). The optimized parameter set derived from the automated calibration procedures depends on (1) the conceptual base and structure of the hydrologic model, (2) the power and robustness of the optimization algorithm, (3) the quality and amount of information present in the calibration dataset (4) calibration criteria or objective functions used (Gan and Biftu, 1996). In the context of this article some important items are briefly described.

Optimization algorithms can be classified into two categories (1) local search and (2) global search. Local search optimization methods are adequate provided the response to parameter adjustments is unimodal. The major limitation of local search optimizations is that they get trapped in local optima that are typically present in lumped rainfall—runoff models (Johnston and Pilgrim, 1976; Duan et al., 1992; Madsen, 2000). To address the limitations of local search optimization procedures, global search optimization procedures are developed. Some of the examples are Shuffled Complex Evolution—University of Arizona (SCE-UA) algorithm (Duan et al., 1992, 1993), the most popular global search algorithm and Multiple Start Simplex methods. Global search optimization procedures search the entire parameter space and do a controlled random search and a systematic evaluation of function in the direction of global optimum (Gan and Biftu, 1996). Most of the hydrologic studies conducted using SCE-UA approach reported improved results than the other methods (Duan et al., 1994; Eckhardt and Arnold, 2001; Van Griensven and Bauwens, 2003; Van Griensven et al., 2002). However, a few studies point out the problems with this method in reaching global optimum or maintaining a reasonable water balance (Madsen, 2000; Madsen et al., 2002; Van Liew et al., 2005).

Based on objective function, the automated calibration procedures can be classified as (i) single objective procedures and (ii) multiple objective procedures. Single objective procedures typically defines an objective function (a goodness of fit measure such as Mean Squared-Errors (MSE) estimator, Nash and Sutcliffe Efficiency, etc.) and try to maximize or minimize (depending on the case) in order to obtain a better fit between predicted and observed time series of flow. Most of the existing auto-calibration procedures are based on single objective function.

Calibration based on a single criterion may not be adequate to simulate all the important characteristics of the hydrologic system (Gupta et al., 1998; Madsen, 2000). Apart from getting a close match between the predicted and observed time series, modeling of low flow, peaks, and recessions of hydrograph are also important, which makes the hydrologic calibration a multi-objective task. Moreover, most of the present models are designed to simulate sediment, nutrients, pesticides, and pathogens and calibration of these are also regularly performed (Gupta et al., 1998). Therefore, for calibration of hydrologic models, multiple objective calibration procedures were developed. The generated output from this approach is a set of solutions (called pareto solutions) instead of a unique solution (Madsen et al., 2002). However, it should be noted that an improvement in one objective is possible only at the expense of the other (Yapo et al., 1998).

Some automated calibration procedures were exclusively designed for SWAT (Van Griensven and Bauwens, 2003; Van Griensven and Meixner, 2003; Van Griensven et al., 2002; Eckhardt and Arnold, 2001; Immerzeel and Droogers, 2008; Bekele and Nicklow, 2007; Muleta and Nicklow, 2005; Di Luzio and Arnold, 2004) and used successfully. Most of them are based on SCE-UA algorithm. They are: automated calibration procedure (1) for ESWAT (another version of SWAT model) described by Van Griensven and Bauwens (2003, 2005) for Dender river basin in Belgium, (2) for SWAT-G for simulation of watersheds in Germany described by Eckhardt and Arnold (2001), Eckhardt et al. (2005), (3) for SWAT model simulation of a watershed in Oklahoma, USA (Di Luzio and Arnold, 2004), (4) described by Van Liew et al. (2005, 2007) for SWAT simulations of some watersheds in Georgia, Oklahoma, Arizona, Idaho and Pennsylvania in USA. More information on the watersheds calibrated, parameters, quality of results obtained are described in detail in a review paper by Gassman et al. (2007). Apart from the above, there are some other versions of automated calibration procedures used with SWAT. They are (1) a calibration approach based on the non-linear parameterization estimation package PEST (Doherty, 2005) for SWAT model simulation of Upper Bhima watershed in Krishna river basin in southern India. Minimizing the sum of squared deviations between model generated values and observations was the objective function (Immerzeel and Droogers, 2008). (2) An automated calibration approach designed on three sequential techniques namely screening, parameterization and parameter sensitivity analysis (using Latin hypercube sampling). The calibration approach was applied to simulation of flow and sediment for a watershed in Southern Illinois in USA (Muleta and Nicklow, 2005). (3) An automatic calibration routine developed using the Non-dominated Sorting Genetic Algorithm II (NSGA-II) (Deb, 2001). The automatic routine is capable of incorporating multiple objectives into the calibration process and employs parameterization to help reduce the number of calibration parameters. In their

study, SWAT is calibrated for daily streamflow and sediment concentration for Big Creek watershed (sub-basin of lower Cache river basin) in USA (Bekele and Nicklow, 2007). Apart from the above-automated procedures, there exists a semi-automated calibration approach described by Kannan et al. (2007). It has a pre-designed framework for changing parameters at watershed, sub-watershed, and HRU levels. Parameter change based on land use is also possible. The parameter values have to be defined before calibration. After this, the parameter change can be done automatically. The program was exclusively developed for calibration of small watersheds using SWAT 2000 model without any optimization algorithm (Kannan et al., 2007). Most of the other calibration approaches attempted by SWAT users used manual procedures specifically catered to their project needs. Gassman et al. (2007) give a comprehensive review of all the manual calibration approaches attempted by different SWAT users worldwide. After a review of the existing auto-calibration procedures, their advantages and limitations, we agree with the views of Madsen et al. (2002), that automatic calibration is not an easy solution to calibration of rainfall—runoff models, although we realize that there is a significant saving in time and effort with automated calibration procedures. Selection of a particular calibration procedure (among different existing procedures) for a problem mostly depends on efficiency of the algorithm (Madsen et al., 2002) and the demands of the project.

There is an ongoing national scale assessment study called Conservation Effects Assessment Project (CEAP). CEAP project uses the revised HUMUS/SWAT (Hydrologic Unit Modeling for the United States) modeling framework (Srinivasan et al., 1998; Santhi et al., 2005). Under this framework each water resource region (or major river basin such as Missouri, Upper Mississippi) is treated as a watershed and each USGS (United States Geological Survey) delineated eight-digit watershed (more details are available in the section Modeling Framework) as a sub-watershed. The main objective of the CEAP study is to quantify the environmental and economic benefits obtained from conservation practices implemented in the United States. The benefits will be reported at the eight-digit watershed and river basin scales (major water resource regions). This requires a reasonably accurate estimation of runoff and material transfer via both surface and sub-surface for all the eight-digit watersheds. The leaching of chemicals through the soil profile depends on infiltration and percolation rates, which, thus, need to be well described. In addition to matching predicted and targeted runoff, it is therefore, essential to partition runoff correctly into different hydrological pathways. This, in turn requires a robust procedure that calibrates runoff/water yield as well as the partition of runoff into surface runoff and sub-surface flow. The specific expectation of CEAP is a calibration procedure to spatially calibrate long-term annual average runoff at sub-watershed level to capture the spatial variations in runoff across different parts of the river basin. In addition, the procedure is expected to provide good results (with little or no additional calibration) for annual and monthly stream flow addressing the seasonal variability in hydrological processes.

For the CEAP project, first the attention was focused to use one of the widely used automated calibration procedures outlined in this article. They use a proper optimization algorithm to narrow down the best possible value for a parameter. However, to do so, they divide the parameter range in many small discrete steps, search the entire parameter space and therefore make thousands of model runs. These many model runs are not affordable (in terms of time and computational requirements) for the calibration of a regional/national/continental scale hydrologic study such as CEAP. Our goal was to have a reasonably better result from calibration by limiting the procedure within 20 model iterations. As well, we wanted to have the right partition of water yield into surface runoff and sub-surface runoff. Therefore, a calibration procedure with a simple parameter interpolation method is proposed to calibrate the spatial variation of annual average runoff components for each sub-watershed (eight-digit watershed) of major river basins of the United States. This paper describes the development and a demonstration of the automated calibration procedure. Within the context of this paper, Hydrologic Unit Catalog (HUC), eight-digit watershed and sub-basin are the same. River basin and water resource region are used interchangeably. For this study, sub-surface flow is considered as the sum of base flow and lateral flow (or through flow).

Modeling framework

For this study, the revised HUMUS/SWAT (Hydrologic Unit Modeling for the United States) modeling framework (Srinivasan et al., 1998; Santhi et al., 2005) comprised of SWAT with updated databases for the 18 major river basins in the United States was used (Fig. 1). The United States is divided into four major levels of hydrologic units as regions, sub-regions, accounting units, and cataloging units. Each hydrologic unit is identified by a unique numerical hydrologic code. The hydrologic code is a two, four, six and eight-digit number for the first, second, third and fourth level of classification respectively. The first level of classification corresponds to the drainage area of a major river basin (such as Missouri river basin), and the second level corresponds to a river system or a reach of a river and its tributaries or a closed basin or a group of streams forming a coastal drainage area. The third level of classification corresponds to sub-division of sub-regions (second level) and the fourth level corresponds to a geographic area representing part of all of a surface drainage basin, a combination of drainage basins, or a distinct hydrologic feature (Seaber et al., 1987). HUMUS was designed for making assessments at national and river basin scale of water demands and land management practices affecting the pollution of rivers. In this study, every major river basin of United States is modeled as a separate watershed and each HUC within a river basin is modeled as a sub-watershed.

SWAT

The SWAT model was developed to quantify the impact of land management practices on surface water quality in large, complex catchments (Arnold et al., 1993; Gassman et al., 2007; Neitsch et al., 2002; http://www.brc.tamus.edu/swat/index.html). It provides a continuous simulation of hydrological processes (evapotranspiration, surface runoff, percolation, return flow, groundwater flow, channel trans-

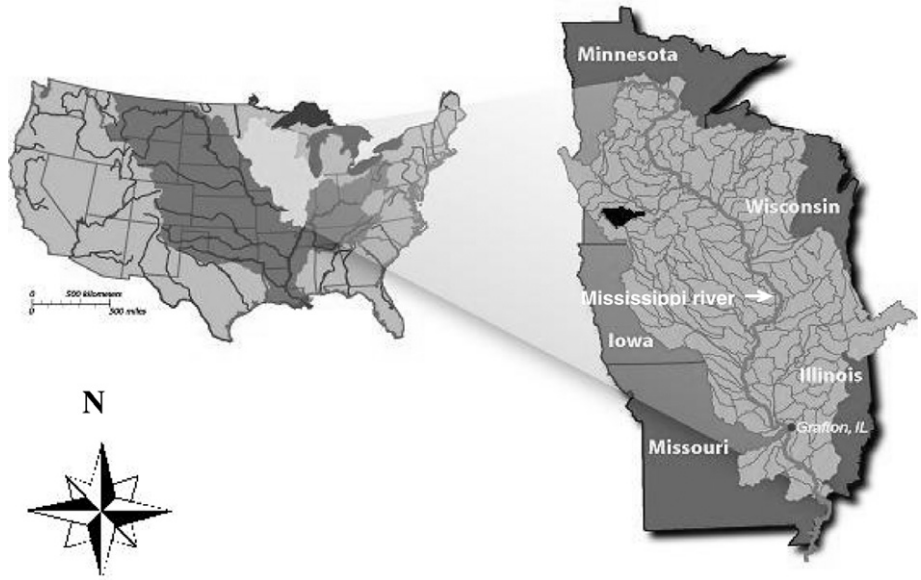

Figure 1 Location of study area — Upper Mississippi river basin (Source: Jha et al., 2006

mission losses, pond and reservoir storage, channel routing and field drainage), crop growth and material transfers (soil erosion, nutrient and organic chemical transport and fate). The model can be run with a daily time step, although sub-daily data can also be used. It incorporates the combined and interacting effects of weather and land management (e.g. irrigation, planting and harvesting operations and the application of fertilizers, pesticides or other inputs). SWAT divides the watershed into sub-watersheds using topography. Each sub-watershed is divided into hydrological response units (HRUs), which are unique combinations of soil and land cover. Although individual HRU's are simulated independently from one another, predicted water and material flows are routed within the channel network, which allows for large catchments with hundreds or even thousands of HRUs to be simulated.

Databases

The HUMUS/SWAT system requires several databases such as land use, soils, management practices and weather. For the present study, recently available data are processed to update the HUMUS/SWAT databases and prepare the SWAT input files for the river basins (Santhi et al., 2005).

Land use

The United States Geological Survey (USGS)—National Land Cover Data (NLCD) of 1992 is the spatial data currently available for land use at 30 m resolution for the United States (Vogelmann et al., 2001). For this study, the 1992 USGS—NLCD land cover data set is used as the base, which includes agriculture, urban, pasture, range, forest, wetland, barren and water.

Soils

Each land use within an eight-digit watershed is associated with soil data. Soil data required for SWAT were processed from the STATe Soil GeOgraphic (STATSGO) database (USDA—NRCS, 1994). Each STATSGO polygon contains multiple soil series and the areal percentage of each soil series. Within a STATSGO polygon, the soil series with the largest area was identified and the associated physical properties of the soil series were extracted for SWAT. This procedure was followed for all the eight-digit watersheds (Santhi et al., 2005).

Topography

Topographic information on accumulated drainage area, overland field slope, overland field length, channel dimensions and channel slope were derived from the DEM data of the previous HUMUS project (Srinivasan et al., 1998).

Management data

Management operations such as planting, harvesting, applications of fertilizers, manure and pesticides and irrigation water and tillage operations along with timings or potential heat units are specified for various land uses in the management files. Management operations/inputs vary across regions. These data are gathered from various sources such as Agricultural Census Data and USDA—National Agricultural Statistics Service (NASS)'s agricultural chemical use data (Santhi et al., 2005).

Weather

Measured daily precipitation and maximum and minimum temperature data sets from 1960 to 2001 are used in this study. The precipitation and temperature data sets are created from a combination of point measurements of daily precipitation and temperature (maximum and minimum) (Eischeid et al., 2000) and Parameter-elevation Regressions on Independent Slopes Model (PRISM) (Daly et al., 1994, 2002). The point measurements compose a serially complete (without missing values) data set processed from the

National Climatic Data Center (NCDC) station records. PRISM is an analytical model that uses point data and a digital elevation model (DEM) to generate gridded estimates of monthly climatic parameters. PRISM data are distributed at a resolution of approximately 4 km^2. A novel approach has been developed to combine the point measurements and the monthly PRISM grids to develop the distribution of the daily records with orographic adjustments over each USGS eight-digit watersheds (Di Luzio et al., 2008). Other data such as solar radiation, wind speed and relative humidity are simulated using the weather generator (Nicks, 1974; Sharpley and Williams, 1990) available within SWAT.

Target values for calibration

Sources of information

The target values for calibration are based on runoff contours for the entire United States prepared by Gebert et al. (1987). The preferred source of information for the runoff contours was stream flow recorded from 5951 United States Geological Survey (USGS) gauging stations during 1951—1980 with no diversions and an area of not more than a HUC. If records for the 30-year period were not fully available for a station, the records were extrapolated based on a correlation (method suggested by Matalas and Jacobs, 1964) with a nearby station. If data from stations without diversions were not available, then data from stations with diversions were used with correction for diversions. If the gauging station records indicated an amount for the diversions, it was used to adjust the flow otherwise the diversions were estimated based on other existing information. Irrigation diversions, commonly represented by number of acres irrigated were multiplied by the typical amount of water used for irrigation in that area less an allowance for return flows. These estimates of diversion were used to correct the measured stream flow, which in turn was used for computing runoff. If no information were available, estimates of runoff in adjacent areas, known variations of precipitation and elevation were used to compute runoff (Krug et al., 1989; Gebert et al., 1987). The data obtained as described above were used to produce runoff contours (lines joining equal runoff values) for the entire United States. More details on the procedure used for the preparation of runoff contours are available in Krug et al. (1989) and Gebert et al. (1987).

Estimating annual average runoff by HUC

The runoff contours (Fig. 2a) were discretized to points using a procedure developed by Di Luzio (Personal Communication, 2005). The discretized points were interpolated in order to obtain a runoff value for each cell (size 41.5 km × 41.5 km) in the map (Fig. 2b). This map was overlaid with HUC map and runoff values were averaged for each HUC in order to obtain one annual average runoff value per HUC.

Limitations of the target values obtained

Some HUCs form a closed basin with zero net runoff values. Estimating runoff using the procedure defined here produces runoff values slightly greater than zero, although no runoff leaves the unit. In regions with less-density of stream flow measurement gauges the interpolation procedure might introduce errors. A detailed discussion on the uncertainties of runoff estimates from runoff contours are described in Rochelle et al. (1989).

Despite the limitations cited above, the estimates of the procedure were used as target values of annual average runoff calibration because of the following reasons (1) Existence of no other similar dataset for calibration to

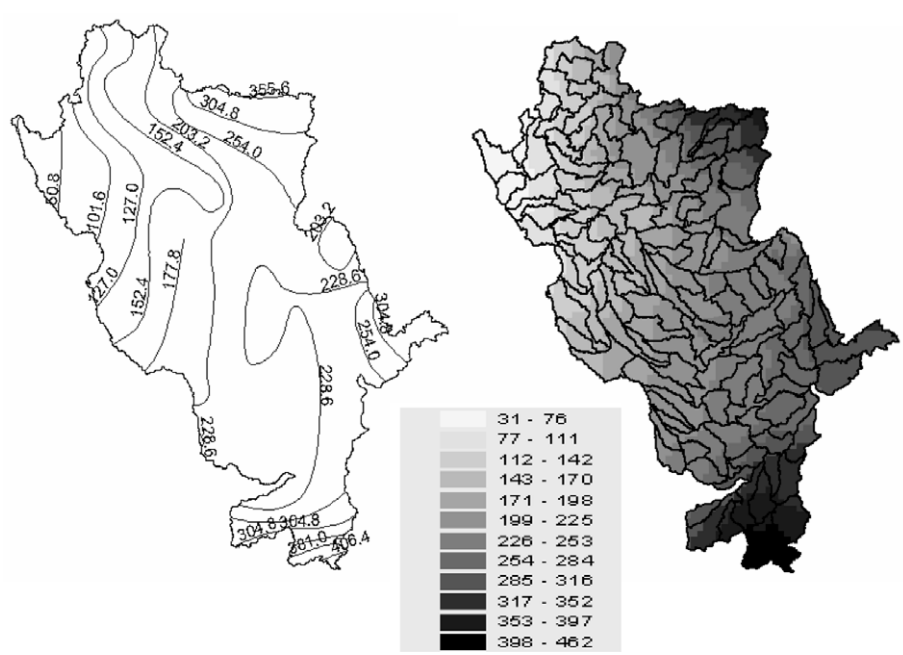

Figure 2 Annual average runoff (in mm) over Upper Mississippi river basin (a) runoff contours (b) runoff grids on eight-digit watersheds.

capture the spatial variation of runoff over region(s) or large river basins (2) Adequacy for the project (3) procedural simplicity and mathematical convenience.

A procedure similar to the above described is adopted for base flow (briefly described here). Base flow availability varies over space and time in a region due to climate, topography, landscape, and geological characteristics. Santhi et al. (2008a) have estimated the base flow index (BFI) or base flow ratio (ratio of base flow/total stream flow) from daily streamflow records of the USGS stream gages using a recursive digital filter method developed by Arnold et al. (1995). Nearly 8600 USGS stream gage locations distributed across the Conterminous United States were selected to estimate the base flow index. Gages were selected with drainage areas of 50—1000 km^2 to minimize the effects of flow routing, and limit the influence of reservoir releases. Each selected gage had a minimum of 10 years of daily streamflow observations. These base flow index values were used to develop a smooth grid map of the base flow index values using inverse distance weighting spatial interpolation method. To estimate the base flow, the base flow ratio map was multiplied by observed runoff map prepared by Gebert et al. (1987). The difference between runoff and sub-surface flow (or base flow) is assumed as surface runoff. The data obtained in this manner were used as targeted values for calibration of runoff, sub-surface flow and surface runoff.

Methods

This section describes the development of an automated procedure for calibration of spatial variation of annual average surface runoff, sub-surface flow and water yield over large river basins. In addition, the calibration procedure is expected to provide satisfactory results (with little or no additional calibration) for the predicted monthly mean stream flow when compared to observed time series at the flow gauging stations. Data from 1960 is used as a warm-up period for the model to make the state variables assume realistic initial values. Data from 1961—1990 is used for calibration and the remaining data from 1991—2001 is used for validation. Modeling was carried out at annual time step using Hargreaves method (Hargreaves and Samani, 1985) for estimation of ET and curve number method for rainfall—runoff modeling.

Introduction to model parameters

SWAT model has many parameters. Only the most sensitive (suggested in the user manual and other studies) nine parameters are used for the calibration procedure. They are (1) harg_petco (a coefficient used to adjust evapotranspiration (ET) estimated by Hargreaves method (Hargreaves and Samani, 1985) and water yield; (2) soil water depletion coefficient (a coefficient used to adjust surface runoff and sub-surface flow in accordance with soil water depletion) (Kannan et al., 2008); (3) curve number (CN) to adjust surface runoff; (4) groundwater re-evaporation coefficient (GWREVAP). It controls the upward movement of water from shallow aquifer to root zone in proportion to evaporative demand; (5) minimum depth of water in soil for base flow to occur (GWQMN). Groundwater flow is allowed only if the depth of water in the shallow aquifer is equal to or greater than the GWQMN parameter value; (6) soil available water holding capacity (AWC); (7) slope length (used to control lateral flow estimates-particularly from high-slope areas); (8) plant evaporation compensation coefficient (EPCO). This controls the depth distribution of water in soil layers to meet plant evaporative demand and (9) soil evaporation compensation coefficient (ESCO), which controls the depth distribution of water in soil layers to meet soil evaporative demand. Among the nine parameters harg_petco, depletion coefficient, GWREVAP, GWQMN are sub-basin level parameters and the other parameters operate at Hydrologic Response Unit (HRU) [sub-division of a sub-basin] level (Neitsch et al., 2002).

Development of the calibration procedure

The calibration procedure discussed here is somewhat different from other existing automated calibration procedures. The differences are (i) It is developed for calibration of spatial variation of runoff over large river basins, (ii) It calibrates different components of runoff such as surface runoff, sub-surface flow apart from water yield, (iii) Objective of calibration is different at different stages of the calibration procedure (obtaining close match between predicted and targeted values of water yield, surface runoff and sub-surface flow at steps 1—3, respectively), and (iv) the termination criterion is the percentage difference between prediction and targeted value (this is 20 %, 10 %, and 10 % for water yield, surface runoff and sub-surface flow, respectively). The development of the automated calibration procedure is discussed in two sections viz. (a) Separation of eight-digit watersheds (within a water resource region) that require calibration and (b) calibration procedure.

Separation of eight-digit watersheds requiring calibration

The preliminary requirements for using the calibration procedure are the arrangement of the necessary input files for running SWAT model for a particular river basin and obtaining the target values of annual average estimates of surface runoff, sub-surface flow and water yield for each eight-digit watershed in that river basin. As well, it requires a list of model parameters to be used in calibration along with their ranges as input. After having the two above-mentioned requirements, the next step involves running the SWAT model without any calibration. Then the procedure involves estimation of the percentage difference between annual average predictions and target values of surface runoff, sub-surface flow and water yield for each eight-digit watershed in the river basin. Based on the estimated percentage difference on the stipulated criteria (10%, 10% and 20% differences between predictions and target values), the eight-digit watersheds requiring calibration are identified and stored in a separate file (Fig. 3a).

Calibration procedure

The calibration process is carried out in three major steps viz. (1) calibration of water yield (parameterization of harg_petco), (2) surface runoff (parameterization of CN

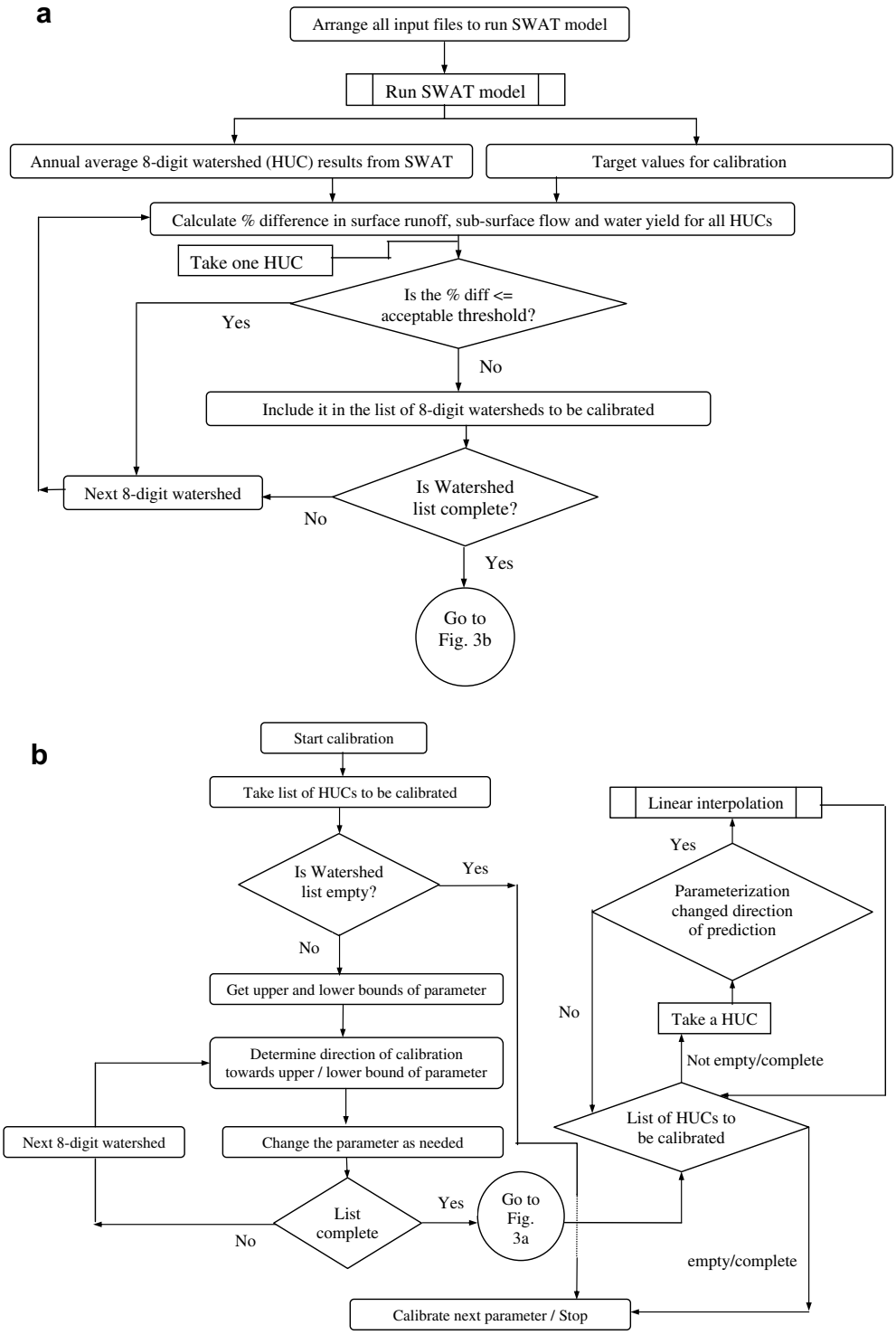

Figure 3 Automated calibration procedure (a) Determination of eight-digit watersheds to be calibrated (b) Adjustment and interpolation of parameters.

and soil water depletion coefficient), and (3) sub-surface flow (all the other parameters mentioned in Table 1), respectively. It should be noted that an adjustment in water yield (due to changes in model parameters) results in changes in surface runoff and/or sub-surface flow. Similarly, changes in surface runoff and sub-surface flow result in changes in water yield as well. Our experience indicates that calibration of spatial variation of sub-surface flow is relatively difficult for many water resource regions of United States. Therefore, more parameters are included for calibrating sub-surface flow than surface runoff.

The calibration procedure starts with the list of eight-digit watersheds that need calibration. Then it involves the identification of the model parameter and suitable value

Table 1 Parameters used in the auto-calibration procedure, their range and their effect on different components of runoff

Parameter	Spatial level of parameterization	Changes			Range used	
		Surface runoff	Sub-surface flow	Water yield	Minimum	Maximum
Harg_petco	Sub-watershed	x	x	x	0.0019	0.0027
Depletion Coefficient	Sub-watershed	x	x	x	0.5	1.50
Curve Number[a]	HRU	x		x	−5	+5
GWQMN	Sub-watershed		x	x	−3	+3
GWREVAP	Sub-watershed		x	x	0.02	0.20
AWC[b]	HRU		x	x	−0.04	+0.04
Slope Length	HRU		x	x	−40%	+40%
EPCO	HRU		x	x	0.01	0.99
ESCO[b]	HRU		x	x	0.73	0.99

[a] Curve Number changes with land use, soil and hydrologic condition.
[b] Under some situations changes in AWC and ESCO results in changes in surface runoff also.

for that parameter (Table 1), which is based on the percentage difference between predictions and target values. A positive difference indicates over-estimation and vice versa. Based on under/over-estimation, the new value of a parameter is selected as the upper/lower value (from the range assumed (see Table 1)). The next step is replacing the old parameter value with the new value. The above-processes are repeated for all the eight-digit watersheds that need calibration (result of section 1 of calibration procedure). Another SWAT run is made with the modified set of input parameters. Then section 1 of calibration procedure (Fig. 3a) is repeated to identify the eight-digit watersheds still requiring calibration.

Each eight-digit watershed needing calibration in the previous step is analyzed to check whether the parameter change (at the present step) has improved the estimation. If the estimation has improved and further calibration is not needed (% difference between predictions and target values of surface runoff, sub-surface flow and water yield are within or equal to the stipulated criteria), that particular eight-digit watershed is eliminated from the calibration procedure. If the estimation has improved and further calibration is needed and the direction of estimation has not changed (e.g. under-estimation of surface runoff before and after parameter change), the procedure proceeds to next parameter. If the estimation has improved and further calibration is needed and if the direction of estimation has changed (e.g. under-estimation before parameter change and over-estimation after parameter change), a new value for the same parameter is estimated based on a linear interpolation technique using the parameter values at the previous and present step and the percentage differences at previous and present step (Fig. 3b). The linear interpolation method is used in the calibration procedure for finding a better value for a particular parameter. It should be noted that linear interpolation may not work well for some parameters (e.g. GWQMN) that show very high sensitivity to surface or sub-surface flow within a short-range. However, linear interpolation is still used in the calibration procedure owing to its simplicity, convenience, unimodal nature of response for parameterization (a progressive increase/decrease in parameter will cause a progressive increase/decrease in model output, and the direction of response will not change) and the ability to find a better value. In the second iteration, the above procedure is repeated for all the HUCs that need estimation of a new value of parameter based on linear interpolation (Fig. 3b). The calibration procedure is carried out (in a similar fashion described in the previous sections 'Separation of eight-digit watersheds requiring calibration' and 'Calibration procedure') for all the other parameters included in the procedure, one by one. The parameterization proceeds in the following order: harg_petco, depletion coefficient, CN, GWREVAP, GWQMN, AWC, Slope length, EPCO and ESCO. The entire automated calibration procedure is written in FORTRAN.

Results

Effects of initial parameter values on calibration

Unless altered by the user, the calibration procedure uses default initial parameters written by the user interface. The parameter CN is a unique value obtained from a look up table (within the interface) for a particular combination of soil and land use. Therefore, the initial value for this parameter is also fixed. Available Water Capacity (AWC), the property of a particular soil layer is obtained from the soil database. Therefore, the initial value of AWC is also fixed. Slope length for a particular HRU is obtained from the DEM and hence the user for the initial condition may not alter its value. However, the other model parameters (harg_petco, depletion coefficient, GWREVAP, GWQMN, EPCO, and ESCO) can have any initial value within the allowed range. Therefore, an analysis is done to ascertain whether there are differences in results by having initial values other than the default. The initial value of only one model parameter is changed at a time; all the other parameters are kept at their default initial values (Table 2a). For this analysis, the lower and upper limits of a parameter are chosen, and the calibration procedure is used in each trial independently (starting from a no calibration scenario). Only one experiment was possible for the parameter GWQMN. This is because the default initial value of this parameter was 0.0 (range of adjustment ± 3) for the HUC 7020008 and the parameter cannot take negative values.

Table 2a Effects of initial parameter values on calibration: demonstration of results using an eight-digit watershed (7020008) from Upper Mississippi river basin

Parameter	Initial Values	Predicted values after calibration (mm)		
		Surface runoff	Sub-Surface flow	Water Yield
All parameters	Default[a]	45.1	37.14	82.24
Harg_petco	0.0019	46.12	39.49	85.61
Harg_petco	0.0027	46.12	39.49	85.61
Depletion coefficient	0.5	46.12	39.49	85.61
Depletion coefficient	1.5	46.12	39.49	85.61
GWREVAP	0.02	46.12	42.17	88.29
GWREVAP	0.2	46.12	39.25	85.36
GWQMN	3	47.46	34.9	82.36
EPCO	0.01	44.03	42.15	86.17
EPCO	0.99	41.6	34.95	76.54
ESCO	0.73	48.05	44.92	92.97
ESCO	0.99	48.31	42.79	91.1
Target values	Not applicable	44.3	40.1	84.4

[a] The initial parameter values were 0.0023, 0.75, 0.10, 0.0, 0.0, and 0.95 for harg_petco, depletion coefficient, GWREVAP, GWQMN, EPCO, and ESCO, respectively.

The predicted results of surface runoff, sub-surface flow and water yield for different initial values of parameters are shown in Table 2a. Considering the stipulated criteria for calibration (10%, 10%, and 20% differences between predictions and target values), the results from the experiments using different initial parameters are very similar to the results of default initial parameters although there exists some marginal numerical differences. On an average, the differences exhibited by the different initial parameter combination to that of default initial values are 0.9 mm, 2.8 mm and 3.7 mm, respectively, for surface runoff, sub-surface flow, and water yield. The maximum differences observed are 3.5 mm in surface runoff, 7.8 mm in sub-surface flow and 10.7 mm in water yield. Experiments with initial EPCO value of 0.99 and initial ESCO value of 0.73 bring slightly different results than that of default initial values. All the other experiments bring very similar results. This shows that the calibration procedure brings similar results irrespective of the initial parameter values.

Demonstration of auto-calibration procedure

A demonstration of the auto-calibration procedure is given in Table 2b using the eight-digit watershed 07020008 of the Upper Mississippi river basin (shaded area in black near the left river basin boundary in Fig. 1). From Table 2b it can be seen that the percentage difference between predicted and targeted water yield at the beginning is within the stipulated value (4.2% existing vs. 20% target). Therefore, harg_petco was not parameterized to adjust the water yield (Table 2b). However, the percentage difference between predicted and targeted annual average surface runoff is beyond the threshold (−54% existing vs. 10% threshold) indicating under-estimation of surface runoff. Therefore, depletion coefficient is adjusted to bring predicted surface runoff within 10% of targeted value. In doing so, the under-estimation (before depletion coefficient parameterization) has changed to over-estimation after depletion coefficient parameterization. Hence, a linear interpolation was performed to identify the suitable value for depletion coefficient that keeps the predicted surface runoff within 10% of targeted value. After the adjustment of depletion coefficient, the percentage difference between predictions and target values of annual average surface runoff is 1.9% (within the target) eliminating the need for further adjustment of surface runoff using CN (Table 2b). Although the predicted water yield is still within 20% of target value (after adjustment of depletion coefficient), the sub-surface flow is not within the target value of 10%. Therefore, sub-surface flow was adjusted using the suitable parameters (Table 2b). After the parameterization of GWREVAP, GWQMN, slope length, EPCO, and ESCO, respectively, the predicted annual average sub-surface flow for the HUC 07020008 is brought within 10% (Table 2b). In Table 2b, the predicted values of surface runoff, sub-surface flow and water yield and the percentage difference between predictions and target values are shown at every step of calibration for better understanding of the calibration procedure.

Demonstration of parameterization

In the previous section, a demonstration of the entire procedure used for calibration is discussed. In this section, a detailed discussion of calibration of one parameter is presented to show how the parameterization is carried out. Parameterization of the depletion coefficient is used for this demonstration.

Nature of the depletion coefficient parameter

An increase in depletion coefficient causes an increase in surface runoff and a decrease in sub-surface flow without appreciably affecting the water yield (Kannan et al., 2008). Although a change in depletion coefficient affects both surface runoff and sub-surface flow, in this calibration

Table 2b Demonstration of auto-calibration procedure using an eight-digit watershed (7020008) from Upper Mississippi river basin

Parameter	Adjustment/ interpolation	% difference between predictions and target values			Predicted values (mm)		
		Surface runoff	Sub-surface flow	Water yield	Surface runoff	Sub-surface flow	Water yield
No calibration	None	−54.0	68.4	4.2	20.39	67.52	87.92
Harg_petco	None	−54.0	68.4	4.2	20.39	67.52	87.92
Depletion coefficient	Adjusted	17.5	8.2	13.1	52.03	43.38	95.41
Depletion coefficient	Interpolated	1.9	20.6	10.8	45.13	48.37	93.51
Curve number	None	1.9	20.6	10.8	45.13	48.37	93.51
GWREVAP	Adjusted	1.9	19.6	10.3	45.13	47.95	93.08
GWQMN	Adjusted	1.9	−79.9	−37.0	45.13	8.05	53.18
GWQMN	Interpolated	1.9	13.3	7.3	45.13	45.42	90.55
AWC	Adjusted	1.9	13.3	7.3	45.13	45.42	90.55
Slope length	Adjusted	1.9	13.2	7.3	45.13	45.39	90.53
EPCO	Adjusted	1.9	13.3	7.3	45.13	45.43	90.56
ESCO	Adjusted	1.1	−58.4	−27.2	44.78	16.7	61.48
ESCO	Interpolated	1.8	−7.4	−2.6	45.1	37.14	82.24
Target values	Not applicable	Not applicable	Not applicable	Not applicable	44.3	40.1	84.4

Adjusted: better value of parameter obtained in the first iteration.
Interpolated: better value of parameter obtained in the second iteration.

procedure, the depletion coefficient is adjusted to obtain a good match between predictions and target values of surface runoff rather than sub-surface flow because the sub-surface flow calibration is performed after the surface runoff calibration using the depletion coefficient (Table 1).

Parameterization of depletion coefficient

With the initial value of depletion coefficient (0.75) (and without any adjustment of the other parameters used in the calibration procedure), surface runoff is under-estimated and sub-surface flow is over-estimated (row 1 of Table 3) with respect to the target values. Therefore, to address under-estimation of surface runoff and over-estimation of sub-surface flow, the depletion coefficient is increased from 0.75 (initial value) to 1.5 (the upper limit assumed for calibration). This results in over-estimation of surface runoff. On the other hand, the severe over-estimation of sub-surface flow at the beginning is controlled because of the change in depletion coefficient (row 2 of Table 3). This shows that a depletion coefficient value of 0.75 is too low and 1.5 is too high to get a reasonable match of predicted and targeted surface runoff. Therefore, an interpolation of depletion coefficient is carried out between 0.75 and 1.5 based on the percentage difference between predicted and targeted value of surface runoff at the previous (row 1 of Table 3) and present calibration steps (row 2 of Table 3). Using the interpolated value of 1.32 for depletion coefficient, the predicted surface runoff (45.13 mm) is close to the target value (44.3 mm).

Evaluation of the performance of the automated calibration procedure

In this section, the performance of the automated calibration procedure is analyzed for the calibration period (1961—1990) considering the entire Upper Mississippi river basin (Fig. 1). There are 131 HUCs in the river basin. A comparison of predicted (average values for 1961—1990) and targeted annual average surface runoff, sub-surface flow and water yield for all the eight-digit watersheds in the Upper Mississippi river basin are shown in Figs. 4—6,

Table 3 Demonstration of parameterization — example of surface runoff calibration using depletion coefficient

Depletion coefficient	Adjustment/ interpolation	Objective	% difference between predictions and target values			Predicted values (mm)		
		Adjust surface runoff	Surface runoff	Sub-surface flow	Water yield	Surface runoff	Sub-surface flow	Water yield
0.75	None (initial value)		−54.0	68.4	4.2	20.39	67.52	87.92
1.5	Adjusted (increased)	Increase	17.5	8.2	13.1	52.03	43.38	95.41
1.32	Interpolated (decreased)	Decrease	1.9	20.6	10.8	45.13	48.37	93.51
						44.30[a]	40.10[a]	84.40[a]

[a] Target values.

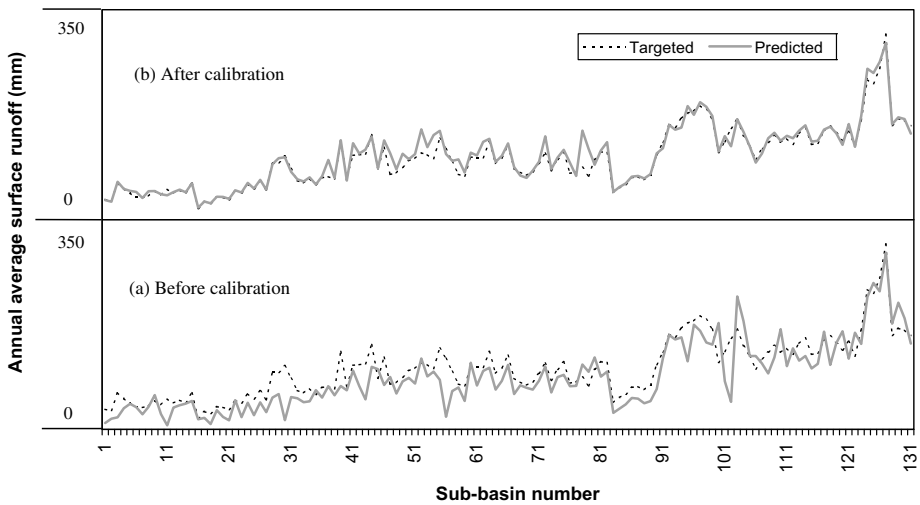

Figure 4 Annual average surface runoff for all the eight-digit watersheds in the Upper Mississippi river basin.

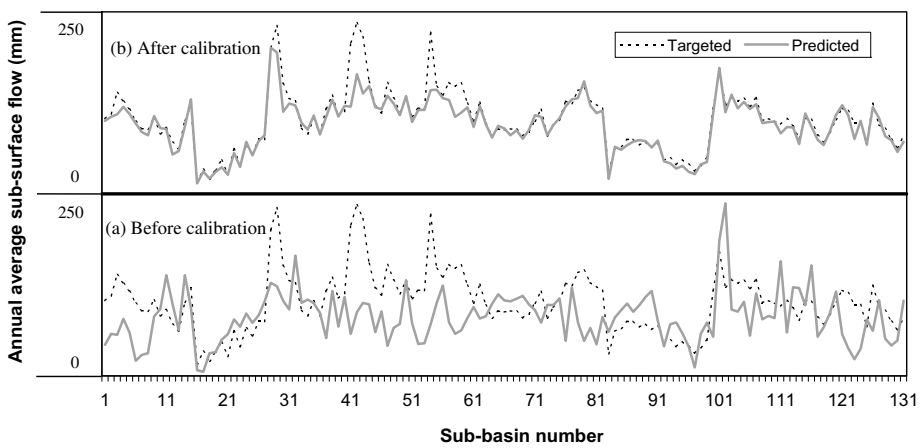

Figure 5 Annual average sub-surface flow for all the eight-digit watersheds in the Upper Mississippi river basin.

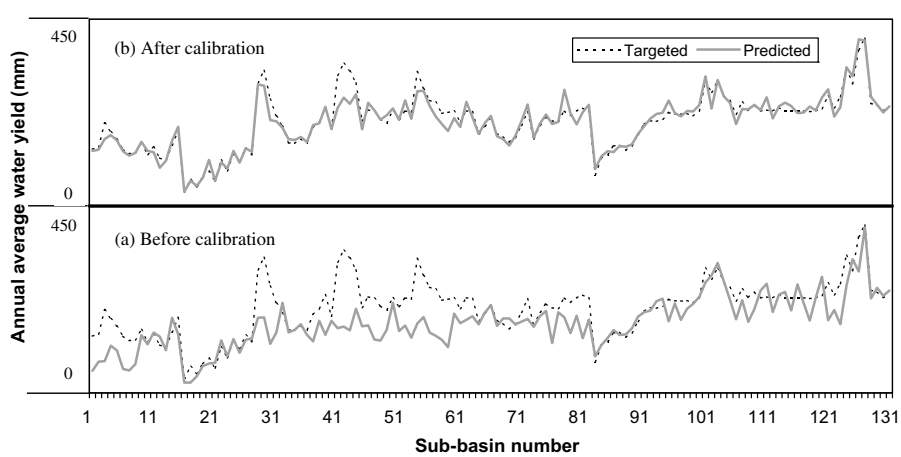

Figure 6 Annual average water yield for all the eight-digit watersheds in the Upper Mississippi river basin.

respectively. It can be observed that calibration has made significant improvement in surface runoff (Fig. 4), sub-surface flow (Fig. 5) and water yield (Fig. 6) when compared to uncalibrated values. Predicted and targeted annual average (of all the HUCs in the river basin) means and standard deviations of surface runoff, sub-surface flow and water yield values before and after calibration, also supports the conclusion (Table 4).

Table 4 Comparison of basin-average predicted and target runoff components

	Model performance evaluation criteria	Surface runoff	Sub-surface flow	Water yield
Before calibration	Mean (mm)	87.8	81.3	169.1
	Standard deviation (mm)	55.3	34.8	61.5
After calibration	Mean (mm)	106.3	94.5	200.8
	Standard deviation (mm)	50.7	35.0	64.9
Target values	Mean (mm)	101.9	101.2	203.1
	Standard deviation (mm)	49.7	41.7	66.4

Table 5 Model performance evaluation criteria for the river basin

Calibration	Model performance evaluation criteria	Surface runoff	Sub-surface flow	Water yield
Before calibration	Nash and Sutcliffe efficiency (%)	65.8	−47.5	21.2
	R^2	0.67	−0.43	0.38
	Eight-digit watersheds needing calibration	97	112	52
After calibration	Nash and Sutcliffe efficiency (%)	93.9	83	93.3
	R^2	0.95	0.86	0.93
	Eight-digit watersheds needing calibration	18	26	5

Performance evaluation of model before and after calibration using Nash and Sutcliffe prediction efficiency and R^2 are given in Table 5. From Table 5, it can be seen that the prediction efficiency has improved significantly after calibration (in particular for sub-surface flow and water yield) when compared to prediction efficiency before calibration. In addition, the number of HUCs requiring calibration (out of 131 HUCs in the Upper Mississippi river basin) has decreased appreciably after calibration (Fig. 7, Table 5).

Analysis of eight-digit watersheds with inadequate calibration

The automated calibration procedure developed in this study, carried out surface runoff calibration satisfactorily (Fig. 4). However, a visual inspection of the predicted and targeted values of water yield (Fig. 6) reveals that a few HUCs were not adequately calibrated. For detailed examination, three HUCs 7050001, 7050002, and 7050003 (Sub watershed numbers 41—43) were chosen. These HUCs show the

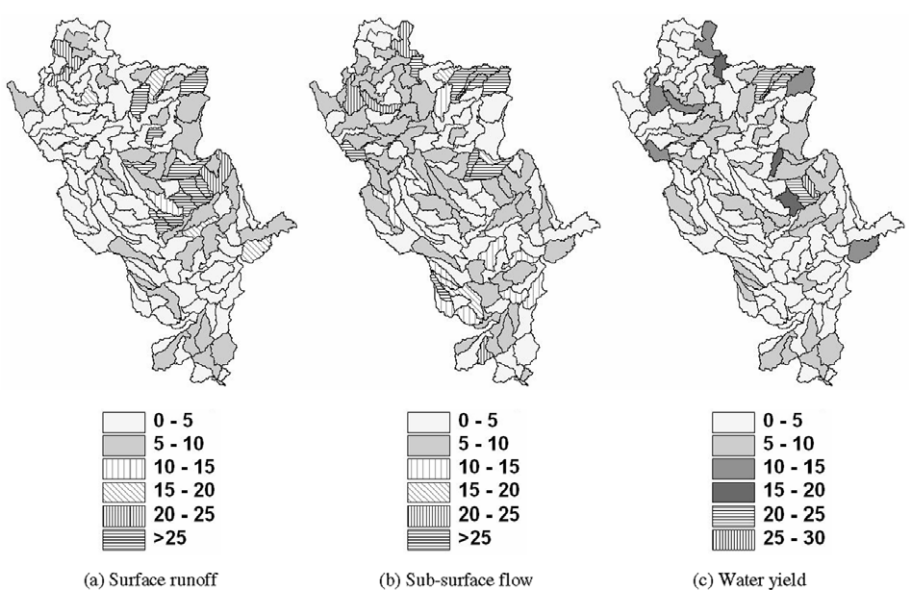

Figure 7 Percentage difference between predictions and target values after calibration (hatched areas are not within target values).

maximum difference between predicted and targeted water yield. The differences are mainly due to the under-estimation of sub-surface flow (Fig. 5) which in turn is due to over-estimation of ET by Hargreaves method in forest and forested wetlands which account for 55–65 % of the area of the sub-watersheds analysed. Changing harg_petco parameter to the lower bound (using the calibration procedure) in order to reduce ET values was not adequate for these HUCs, although this is not the case for other HUCs calibrated.

Application of the calibration procedure

In connection with the CEAP study, the calibration procedure described in this article is used for calibration of Ohio river basin and Arkansas–White–Red river basins covering two different hydrological conditions (high flow and low flow) (Santhi et al., 2008b). Spatial variation of runoff across the two river basins was calibrated using the automated procedure and satisfactory results were obtained (R^2 values of 0.78 and 0.99 were obtained between predicted and targeted annual average runoff for Ohio and Arkansas–White–Red river basins, respectively). When validated at gauging stations, for annual and monthly stream flow, good results were obtained for both the river basins. For the Ohio basin, 86% and 72% Nash and Sutcliffe efficiency values were obtained at the annual and monthly time steps. For the same region, R^2 values (predictions vs. observations) of 0.94 and 0.83 were obtained at the annual and monthly time steps. For the Arkansas–White–Red river basins basin, 79% and 64% Nash and Sutcliffe efficiency values were obtained for annual and monthly stream flow. For the same region, R^2 values (predictions vs. observations) of 0.86 and 0.66 were obtained for annual and monthly stream flow. More details on the study area, range of values for different parameters and results can be found in Santhi et al. (2008b). The study by Santhi et al. (2008b), has shown that the calibration procedure outlined in this article is capable of calibrating river basins with a range of hydrological conditions.

Limitations of the procedure

Unlike the standard automated calibration procedures, the procedure described here does not cover all the possible combinations of parameters. It does not use multiple objectives for carrying out calibration. It uses a simple linear interpolation technique for finding a better value of a parameter instead of search procedure as used in the other auto-calibration procedures. Some fine-tuning of model parameters may be required for HUCs with inadequate calibration.

Summary and conclusions

United States Department of Agriculture has implemented many conservation practices throughout the country to reduce the pollution of soil and water. A national assessment study called ''Conservation Effects Assessment Project'' is ongoing with the objective of quantifying the environmental and economic benefits obtained from those conservation practices. The study considers major water resource regions (or river basins) as watershed boundaries and hydrologic modelling of the river basins with reasonable accuracy is a pre-requisite to achieve the objectives of the project. For hydrologic modelling of the entire United States with reasonable accuracy, a simple, methodical automated procedure is developed to calibrate the spatial variation of runoff and the partitioning of runoff into surface runoff and sub-surface flow for each eight-digit watershed. The developed calibration procedure is described and demonstrated with example results from Upper Mississippi river basin. Based on the results obtained from the study the following conclusions can be drawn.

1. A simple methodical automated procedure is developed to calibrate the spatial variation of annual average runoff components for large-scale hydrologic modeling studies.
2. The simple linear interpolation algorithm is performing satisfactorily in identifying better parameter values for most of the parameters included in the calibration procedure.
3. Test results from Upper Mississippi river basin suggest that the annual average surface runoff, sub-surface flow and water yield values are calibrated satisfactorily using the calibration procedure developed
4. Selection of the suitable range of parameter values is crucial for getting desired results from the calibration procedure.
5. Test results from the calibration procedure are promising and show great potential for its use to all the 18 major river basins of the United States and similar large-scale studies using SWAT.

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