# Estimating Return-Flow Fractions at the River Basin Scale Using Automatic Calibration of MODSIM

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**Abstract:** Estimating the return-flow fractions of different consumptive water uses for the effective management of water resource allocation and operation in a river basin is an essential issue. The purpose of this study was to estimate the return-flow fractions of domestic, industrial, and agricultural water demands, as well as to determine the contributed inflow from the return flows into surface and groundwater resources. This was done through the automatic calibration of a river basin software program, in conjunction with a genetic meta-search calibration algorithm. In this study, the calibration of parameters was made possible by using the customization features of the model. Calibration was done for three combinations of the objective functions. The results of the study demonstrated that the best and most logical results occurred in the third condition, which was a calibration by the objective function, including the root-mean-square error (RMSE) of the river basin's outflow and the RMSE of the aquifer's level. The fractions of the return flow from domestic, industrial, and agricultural demands in the case study of the Shian Basin in western Iran, were obtained as 87, 76, and 18%, respectively. **DOI: 10.1061/(ASCE)IR.1943-4774.0001033.** © 2016 American Society of Civil Engineers.

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#### Introduction

Return flow (RF) is defined as water that reaches a groundwater or surface-water source after release from the point of use and thus becomes available for further uses (Hayes and Horn 2009). One of the most complicated problems in the modeling of a water resource and demand system in a basin is the determination of the volume/ fraction of return flows. Return flows, or waters that have not been consumed by various upstream users in a basin, are a source of water for downstream users (Grafton and Hussey 2007; Qureshi et al. 2010) and have attracted marginal attention from managers and decision makers (Simons et al. 2015). Fig. 1 shows the relation between water withdrawal, water consumption, and return flows.

Some water resource planning studies have shown that the real amount of return-flow fractions differs from the assumed fractions (Gosian et al. 2005; Iran Ministry of Energy 2010). Water economy studies have also divided used water into two parts, consumed and return flow. The estimation of return flow is also important from economic aspect/view (MacDonald et al. 2005). Return flows contribute up to a few percent to the total value of water withdrawal (Hoekstra et al. 2001) because they have indirect benefits (Schiffler 1998) and can have positive externalities that must be considered in water economics (Taylor et al. 2014). The difference between water withdrawal and return flow is known as water consumption, and this plays an important role in the assessment of renewable water resources (Talebi Hossein Abad et al. 2014). In aquifers with overexploited water use, the proper estimation of the water balance is based on the amount of return flow into the aquifers (Pongkijvorasin and Roumasasset 2007).

The use of simulation models in the management of the allocation and utilization of water resources in a basin is a common issue and the coefficients of return flows are among the main parameters of these models that should be considered.

River basin simulation models, depending on the hydrological processes that should be modeled, include various parameters. For a confident use and estimation of the best value of the model parameters, the models should be calibrated (MacLean 2009). The calibration of a model may be treated as an optimization problem. The objective function of the optimization model is to minimize the differences between observed and estimated values (Fig. 2, Moradkhani and Sorooshian 2008).

No comprehensive studies have been conducted based on the calibration of return-flow fractions in which all coefficients are estimated for an area or river basin, although a few studies exist in the field of estimating return-flow fractions to surface water or groundwater flow in a specific region and for a specific sector (often agriculture) (Dewandel et al. 2008; Kim et al. 2009). Gosain et al. (2005) computed 50% for irrigation return flow. One of the early studies by Ilich (1993) assessed return flows from a water resource management viewpoint. Tiddalik is a model that was developed by Hornbuckle et al. (2005) to study a range of management options related to irrigation return flow. Various studies in the fields of water resource management and river basin simulation have shown that the need for coefficients has resulted in the use of assumed values for return-flow fractions. Alimohammadi et al. (2009) assumed that 10% of total water delivered for irrigation percolated into aquifers and 10% returned to the river. This implied that the irrigation return-flow fraction is equal to 20% in a conjunctive surface water and groundwater optimization model as a cyclic storage system. Qureshi et al. (2010) assumed that 25% of irrigation water withdrawal formed useful return flows in the Murray-Darling Basin, Australia. Karimi and Ardakanian (2006) used a 25% coefficient for agricultural demand and 50% coefficient for

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**GW**:Groundwater; **SW**: Surface Water; **CU**: Consumptive Use; **SWW**: Surface Water Withdrawal; **GWW**: GroundWater Withdrawal; **RF**: Total Return Flow; **RFG**: Return Flow Infiltrating to Groundwater; **RFS**: Return Flow Reaching Surface water





**Fig. 2.** Concept of calibration model as an optimization issue (reprinted from *Hydrological Modelling and the Water Cycle*, "General Review of Rainfall-Runoff Modeling: Model Calibration, Data Assimilation, and Uncertainty Analysis," 2008, pp. 1–24, Hamid Moradkhani and Soroosh Sorooshian, © Springer Science+Business Media B. V. 2009, with permission of Springer)

domestic and industrial demand to develop a simulation model based on finite elements and compared it with *MODSIM*. Liu et al. 2010)) concluded that the irrigation return-flow fraction was approximately 25–30% in Taiwan. Karimi (2011) assumed coefficients of return flow of domestic, industrial, and agricultural demand of, respectively, 60, 12, and 15% in order to compare the mechanism of water allocation in *MODSIM* and *WEAP* (water evaluation and planning model) software. A global estimation for return-flow fractions was carried out by Gassert et al. (2013). In this working paper, in the Aqueduct Global Risk Atlas of the World Resources Institute, the term return-flow ratio was used to refer to a catchment, a user, or a location.

It is obvious that many factors can influence the amount of return water, as illustrated by Liu et al. (2010) and Qureshi et al. (2010)). The complexity of the connections and interactions between flows in a river basin, in terms of both location and time, is one of the reasons for the lack of rigorous studies on the estimation of return-flow fractions (Shiklomanov 2000). Also, from a software design perspective, the calibration of river basin simulation models capable of considering return-flow coefficients represents a challenging and time-consuming issue. The customization capability of *MODSIM* facilitates the calibration of these parameters.

In this study, the return-flow coefficients/fractions for different demand activities and the fraction of water that returns to surface and groundwater sources are estimated by integrating the *MODSIM* river basin simulation model and a genetic algorithm (GA) (Goldberg 1989) in the Shian Basin in western Iran as a case study. This was done by coding the GA algorithm into *MODSIM*, so that the GA acts as a calibration engine for *MODSIM* to estimate return-flow fractions.

#### **Methods and Materials**

#### MODSIM

MODSIM is a river basin simulation and decision support model developed by Colorado State University in 1978 (Labadie 2010). The purpose in developing this model was to introduce a powerful tool capable of simulating physical operation and water allocation in a river basin (Wurbs 1994). This model utilizes network flow programming to optimize water allocation in each simulation time step. The objective function of the flow network at each time step is to minimize the cost of the flow network in order to optimally allocate water among users. MODSIM simulates water allocation mechanisms in a river basin through the sequential solution of a network flow optimization problem for each time period. Fig. 3 shows a fully circulating network of user-defined and artificial nodes and links (automatically created) in MODSIM. These artificial nodes and links are essential in insuring that mass balance is satisfied throughout the network (Labadie 2010). One unique feature of MODSIM is Visual Basic or C# coding, also known as customization (Assata et al. 2008). Customization provides a powerful environment in MODSIM for users to prepare customized code in the Visual Basic.NET or C#.NET languages, which are compiled with MODSIM through the Microsoft.NET framework. Users are provided access to all key variables and object classes in MODSIM, thereby allowing customization for any complex river basin operational and modeling constructs without the need for reprogramming and recompiling of the MODSIM source code (Labadie 2010).

*MODSIM* was not provided with automatic calibration/ parameter estimation capabilities. In the present study, through the use of the customization feature of *MODSIM* and coding the GA in a custom run environment of the model, a calibration capability is added to *MODSIM* and estimation of return-flow parameters are made possible.

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Fig. 3. Illustration of MODSIM network structure with artificial nodes and links (reprinted from Labadie 2010, with permission from John Labadie)

#### Calibration Components

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Automatic calibration of parameters in a model is based on three main components: the type of optimization algorithm, the objective function, and convergence criteria. GAs have been the most commonly applied type of evolutionary algorithm (EA) within water resource planning and management (Nicklow et al. 2010). The present study utilized a GA as the optimization algorithm. A GA is an EA that works with selection, crossover, and mutation operators (Gen and Cheng 2000). Briefly, a GA commences with a population of random feasible solutions (chromosomes), and then the value of the objective function or other performance function (usually called the fitness function) is computed for these solutions, then, using crossover and mutation and random selection (such as roulette wheel selection), a new population is generated based on the chance (probability) of new or previous chromosomes. There are two common types of chromosomes or strings in GAs, binary (0,1) and real coded strings. In this research, a real coded type was employed.

The values of GA parameters/operators are usually obtained by sensitivity analysis, i.e., several values for parameters are considered, and the model convergence and running time recorded in each model run. In this problem (presented as follows), the final values of the GA parameters were also obtained by sensitivity analysis and are summarized in Table 1. The final mutation rate (0.6) in proportion to other studies is a high value and prevents the algorithm from stopping at the local optimum points. The selection rate is also relatively high, as shown in Table 1. A high selection rate value results in the consideration of a large percentage of the previous search space (previous generation) by the GA (Razali and Geraghty 2011). The maximum number of iterations by the GA was obtained as 200. Also, no change in the objective function after 20 iterations stopped the algorithm after the 120th iteration. This is another criterion for algorithm stopping.

Table 1. Genetic Algorithm Parameters and Operators

Parameter/operator name	Value/type
Maximum number of generations	200
Mutation rate	0.6
Selection rate	0.7
Population size	100
Type of coupling operator	Two pointed
Type of selection operator	Roulette wheel

The most common objective function in the automatic calibration of models is the root-mean-square error (RMSE) between observed and simulated values [Eq. (1)]. Gosain et al. (2005) only considered the RMSE of surface flow discharge in the assessment of irrigation return flow. This research aimed to minimize the three different combinations of surface-flow RMSE and groundwaterlevel RMSE:

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (x_o^i - x_s^i)^2}$$
(1)

where n = number of periods;  $x_o^i =$  observed value in period I; and  $x_s^i =$  simulated value in period i.

#### Study Area, Modeling Assumptions

The Shian Basin, which is one of the subbasins of the Karkheh River in western Iran, serves as a case study for this research. Fig. 4 shows the location of the Shian Basin. The area of the basin is approximately 689 km<sup>2</sup>. The population of the study area was 21,659 people in 2006. Also, the mean annual precipitation in the area is around 460 mm. The mean annual levels of agriculture, urban/ domestic, and industrial demand for Shian Basin water are 45.8,



0.66, and 0.05 MCM, repectively. The area of cultivated lands (rain fed and irrigated) is approximately 20,000 ha and irrigates from surface water (53%) and groundwater (47%) resources (Iran Ministry of Energy 2010). The simulation was conducted for the period September 1991 to September 2000. While the time step of the simulation was 1 month, in the estimation of the lag time of the return flows, it was assumed that the return waters reached surface water and groundwater resources in the same period. Fig. 5 shows the relation between flows and demands, which is a basis for modeling the Shian River Basin.

Fig. 6 shows the Shian Basin model in *MODSIM*. In this figure, environmental, domestic, industrial, and agricultural demands are modeled based on the fact that the environmental demand has the highest priority and agriculture demand the lowest. According to Fig. 1, if X is the percentage of return flow (RF) that joins the surface water (RFS: return flow reaching the surface flow), then 100-X percent of the return flow infiltrates into the groundwater (RFG:

return flow infiltrating to groundwater) (obviously, RF = RFS + RFG). Therefore, for each level of demand, two parameters must be calibrated-RFF (return flow fraction) and RFFS (RFF that reaches the surface flow), and consequently, for three users, six parameters are needed. It should be noted that losses, such as from evaporation, were treated as part of the water consumption (based on Fig. 1).

In the modeling of groundwater flow, aquifers are modeled as reservoirs (i.e., lumped). In this regard, the safe yield (useful volume) of an aquifer equals the capacity of the reservoir. Since *MODSIM* does not allow for modeling precipitation, the flows of rivers and aquifer recharge were entered into the model as time series. The amount of drained flows and evaporation were also modeled as consumption demands. In addition, the only parameters affecting the output for calibration was the return-flow fraction; this means that no other parameters affected the model outputs. The mean values of the inflows and demands in the basin are presented in Table 2.



Fig. 5. Schematic of flow and water demands in basin

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Fig. 6. Shian Basin modeling in MODSIM

Table 2. Mean Monthly Flow and Water Demand of Shian Basin (Thousands of Cubic Meters)

Month	October	November	December	January	February	March	April	May	June	July	August	September
Basin inflow	1,375	1,310	2,167	1,880	2,824	6,919	10,490	8,755	6,779	4,845	3,428	2,304
Agricultural demand	1,755	706	165	45	35	1,576	5,242	7,542	10,548	8,151	6,144	3,991
domestic water demand	60	52	41	38	43	47	54	65	80	89	94	75
Aquifer inflow	337	272	418	350	445	974	1,840	1,618	1,399	1,015	752	522



Calibration Procedure

As shown in Fig. 7, in running the simulation model of the Shian Basin, the return-flow fractions were calibrated by coding the GA in *MODSIM*. As presented in the flowchart, in each iteration of the GA, *MODSIM* is run as population size and the return-flow fraction

equals the values obtained from the previous iteration in the GA; this cycle continues until convergence occurs in the GA, which results in a minimum RMSE between the simulated and observed values. Simulated data are *MODSIM* outputs (including surface flow and groundwater level) for each series of return-flow fractions (chromosomes of the GA).

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*MODSIM* should be runed to the count of GA iterations in its population. In each calibration, assuming an average population of 100, and 120 iterations, *MODSIM* was run 12,000 times, and the process requires about 12–17 h on a personal computer. There are six variables in the basin with three demand nodes: coefficients of return flow from the three nodes of domestic (*RFF<sub>d</sub>*: domestic return-flow fraction), industrial (RFF<sub>i</sub>: industrial return-flow fraction), and agricultural (RFF<sub>a</sub>: agriculture return-flow fraction) and also a ratio of the return flow from these nodes into the surface water [respectively RFFS<sub>d</sub> (fraction of RFF<sub>d</sub> reaching the surface flow), RFFS<sub>i</sub> (fraction of RFF<sub>i</sub> reaching the surface flow)]. These ratios in the GA equals the number of genes per population member. The range of variables is selected between 0 and 1.

Calibration was done for three different combinations of objective function: calibration by RMSE of surface flow, calibration by RMSE of groundwater level, and calibration by RMSE of surface flow and groundwater level. The objective functions for calibration are as follows.

First, the objective function includes only that of surface-flow RMSE:

$$\min\left[\sqrt{\frac{1}{n}\sum_{i=1}^{n}\left(\mathcal{Q}_{o}^{i}-\mathcal{Q}_{s}^{i}\right)^{2}}\right] \tag{2}$$

Second, the objective function includes only the groundwater-level RMSE:

$$\min\left[\sqrt{\frac{1}{n}\sum_{i=}^{n}\left(H_{o}^{i}-H_{s}^{i}\right)^{2}}\right]$$
(3)

Third, the objective function includes both surface-flow RMSE and groundwater-level RMSE:

$$\min\left[w_1\sqrt{\frac{1}{n}\sum_{i=1}^{n}\left(Q_o^i - Q_s^i\right)^2} + w_2\sqrt{\frac{1}{n}\sum_{i=1}^{n}\left(H_o^i - H_s^i\right)^2}\right] \quad (4)$$

In these objective functions, n = number of time periods;  $Q_o^i =$  observed flow in time period i (L<sup>3</sup>/T);  $Q_s^i =$  simulated discharge in time period i (L<sup>3</sup>/T);  $H_o^i =$  observed groundwater level in time period i (L);  $H_s^i =$  simulated groundwater level in time period i (L);  $H_s^i =$  simulated groundwater level in time period i (L);  $H_s^i =$  simulated groundwater level in time period i (L); and  $w_1$  (T/L<sup>3</sup>) and  $w_2$  (1/L) = weighting parameters for integrating discharge and groundwater-level values into one equation. The purpose of considering these three different cases for the objective functions is to determine the best case for the calibration, to determine the sensitivity of the model and objective function to the return-flow fractions, and, finally, to determine the effects of changing the surface flow and groundwater level in these fractions.

The difference in the dimensions in the RMSE of the surface flow (1,000 m<sup>3</sup>/month) from the RMSE of the groundwater table (m) resulted in the selection of the dimension of  $w_1$  and  $w_2$ , giving rise to a dimensionless objective function. The values of  $w_2$ were computed by trial and error for four values: 1, 10, 100, and 1,000. A greater value of the RMSE of surface flow than the RMSE of groundwater level resulted in the consideration of 1 as  $w_1$ , while only  $w_2$  was estimated by trial and error.

In the third case of calibration, two parts of the RMSE (RMSE of surface flows and RMSE of groundwater level) were integrated via the coefficients of  $w_1$  and  $w_2$ . Since the absolute values of surface flow were much larger than the groundwater level, the RMSE

value of the surface flow was estimated to be more than the RMSE value of the groundwater level in the objective function. In considering values of  $w_1$  and  $w_2$  equal to 1, the GA reduces the final value of the objective function through various iterations. However, if the groundwater-level RMSE increases, it has no effect on the trend of the total value of the objective function in the GA's different iterations because of its absolute low value. Increasing the value of the groundwater-level RMSE causes an improper calibration of the groundwater hydrograph. To overcome this problem, the RMSE term of the surface flow and groundwater level needs to be balanced in the objective function. In this study, as mentioned earlier,  $w_2$  was calculated, by trial and error, to be 100, and, because of the large amount of  $w_1$  was selected as 1.

#### Results

The obtained values of return-flow fractions and the share of surface water and groundwater of return flows are presented in Table 3. As shown in this table, in the first and third cases of the objective function, the domestic return-flow fraction showed better values in comparison to those in other studies, e.g., Simons et al. (2015), Perry (2007), and Shiklomanov (2000). In two cases of calibration, the return-flow fraction of domestic demand was obtained as 52.4%. The return-flow fraction of industrial demand varied in the third case from the first and two other cases; in this regard, it could be asserted that the third case demonstrated a reasonable value. For irrigation, the return-flow fraction was equal to 17.5% and was similar to the recommended (Shiklomanov 2000; Simons et al. 2015) and assumed values (Alimohammadi et al. 2009; Qureshi et al. 2010; Liu et al. 2010).

Figs. 8 and 9 present the hydrographs of the surface flow and groundwater level before and after calibration for different formulations of the calibration function. Since the weighting coefficient was different, it was not necessary to compare the final values of the objective functions to evaluate these three conditions. The scatter plots of the data are provided in Figs. 10 and 11. "First," "second," and "third" in these figures refer to different calibration functions. The  $R^2$  performance criterion is also shown in these figures. The value of  $R^2$  in the third case is higher than in the other cases, and in the first case the  $R^2$  value is zero. The results of the first and third cases demonstrated that the model's sensitivity was greater than the aquifer's hydrograph because the values of the aquifer level were less than the values of the surface flow and the variation in the groundwater level was more sensible to the return flow in the model. This result can be derived from Fig. 3 and Table 3 by comparing RFFGs (fraction of RFF infiltrating into groundwater) for three demand nodes. Ignoring the groundwater term from the

Table 3. Estimated Return-Flow Fractions in Three States of Calibration

	Value of fractions (%)					
Fraction	First condition	Second condition	Third condition			
RFF <sub>d</sub>	92.1	52.4	87.3			
RFF <sub>i</sub>	31.7	23.8	75.7			
RFF <sub>a</sub>	87.3	82.5	17.5			
$\operatorname{RFFS}_d [\operatorname{RFFG}_d]^a$	69.8 [30.2]	98.4 [1.6]	73 [27]			
RFFS <sub>i</sub> [RFFG <sub>i</sub> ] <sup>b</sup>	33.3 [66.7]	95.2 [4.8]	17.5 [82.5]			
$\operatorname{RFFS}_a[\operatorname{RFFG}_a]^c$	0 [100]	41.3 [58.7]	22.2 [77.8]			

<sup>a</sup>Fraction of  $RFF_d$  that infiltrates to groundwater.

<sup>b</sup>Fraction of RFF<sub>i</sub> that infiltrates to groundwater.

<sup>c</sup>Fraction of RFF<sub>a</sub> that infiltrates to groundwater.







calibration (first case of calibration) resulted in unsatisfactory values of  $R^2$  and return-flow fractions (Table 3). This resulted from the second and third cases, which were related to the volume of groundwater in proportion to surface water in the Shian Basin.

### **Summary and Conclusions**

Assessment of return flows is one of the most sophisticated and important components of water resource planning in a river basin. دائلو دکننده مقالات علمی FREE freepaper.me paper



The purpose of this study was to estimate the return-flow fractions of demand from different sectors of society by the calibration of the *MODSIM* simulation model. Three objective functions were considered for model calibration: surface water flow RMSE, ground-water table RMSE, and a combination of both. A GA was used as an optimization model solver. The calibration results for the second and third cases were very close. In the first case, where the RMSE value of the surface water flow was used for the optimization of the parameters of the objective function, the groundwater hydrograph was not well calibrated, and the GA performance was inferior. Furthermore, the contribution of the surface water from the return flow was zero (an illogical value).

The difference between observed and simulated surface flow hydrographs was negligible in the three cases. The fluctuation of the simulated groundwater hydrograph was related to the type of modeling in all cases; it was assumed that the aquifer had a specific heterogeneous medium, which contradicted reality. This limitation was specific not only to *MODSIM* but also for many river basin management models. The fluctuation of the simulated hydrograph resulted in a decrease in the correlation coefficient (Fig. 11).

In a basin having a high potential of runoff, the objective function was more sensitive to the groundwater-level RMSE because the effects of the return flow on the surface outflow were negligible. It is impossible to make a general remark because the values of the various demands were significant. The coefficients varied for different basins in different locations and climates (Shiklomanov 2000; Gassert et al. 2013), and the best method of estimating these coefficients is the calibration of the related models.

The values of the return flow in different basins differed from each other based on the climate, vegetation, location of different needs, consumption patterns, and the geology of the basin. In this study, the coefficients of the return flow of three types of demand, for domestic, industrial, and agricultural water, were approximately 87, 76, and 18% (rounded values). Return-flow fractions (return water divided by water withdrawal) depended on the nature of the user (Simons et al. 2015). The most typical values for agriculture (irrigation) return flow were between 30 and 70% (Simons et al. 2015), and the industrial return-flow fraction was usually insignificant. However, it varied greatly depending on the type of industry, the nature of the water supply, the technological process, and climatic conditions, reaching 30–40% in some industries, while in



most industries it was 5–20% (Shiklomanov 2000). Perry (2007) stated that the domestic return-flow fraction was 95%. The domestic return-flow fraction for modern and large cities ranged from 90 to 95% and for small cities from 40 to 60% (Shiklomanov 2000).

The most thorough calibration case was the third one, and it was recommended that it be used for other basins. Since the return flow was dependent on many aspects, for example soil characteristics and method of irrigation, it was not appropriate to set down a ruleof-thumb value on such quantities. Through modeling, the return flow was assessed and validated (Gosain et al. 2005). It was not possible to systematically measure and compare withdrawals and return flows anywhere in the region in order to calibrate the estimates used. It was also concluded that the portion of surface water and groundwater of the total water resources in a river basin was significant in estimating return-flow fractions. It should be mentioned that, apart from the amount (the goal of this study), the quality, reuse, economics, return location, and lag time of the returning flow were also important factors that should be the subject of future and separate studies. The use of Pareto optimal solutions (Caramia and Dell'Olmo 2008; Confesor and Whittaker 2007), instead of weighting coefficients  $[w_1 \text{ and } w_2 \text{ in Eq. (4)}]$ , is another way to find the optimal solutions of a multiobjective optimization problem [Eq. (4)].

This paper offers a new and innovative approach—the calibration of water resource planning models—to estimating return-flow fractions, which are important and complicated components of river basins, for all users.

#### Notation

The following symbols are used in this paper:

- $H_o^i$  = observed groundwater level at time step i (L);
- $H_s^i$  = simulated groundwater level at time step i (L);
- n = number of time periods;
- $Q_o^i$  = observed discharge at time step i (L<sup>3</sup>/T);
- $Q_s^i$  = simulated discharge at time step i (L<sup>3</sup>/T);
- $W_1$  = discharge weight coefficient (T/L<sup>3</sup>);
- $W_2$  = groundwater weight coefficient (1/T);
- $x_{o}^{i}$  = observed value in period i; and
- $x_s^i$  = simulated value in period i.

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