

## A Framework to Assess Model Structural Stability through a Single-Objective Global Optimization Method

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### Introduction

The problem of model structural uncertainty with advanced automatic calibration methods is an issue of increasing interest in recent researches (Yapo *et al.*, 1996; Gupta *et al.*, 1998; Boyle *et al.*, 2000, Vrugt *et al.*, 2003). Gupta *et al.* (1998) pointed out that a subjective selection of objective functions (e.g., SLS, RMSE, HMLE) for calibration of conceptual hydrologic models lead to an overemphasis on a certain aspect of the response (e.g., peak flows), while neglecting the model performance with regard to another aspect (e.g., low flows). In other words, different parameter combinations can exist according to various objective functions due to the presence of structural uncertainty. Structure error is unavoidable problem in hydrological modeling since hydrologic models are conversion and simplification of reality, thus no matter how sophisticated and accurate they may be, those models only represent aspects of conceptualization or empiricism of modelers. In consequence, output time series of hydrologic models are as reliable as hypothesis, structure of models, and quantity and quality of available forcing data, and parameter estimates (Gupta *et al.*, 1999).

Hydrologists have concentrated their effort on development of more powerful model calibration scheme to assess the suitability of model structure for representing the natural system and for identifying model structural inadequacy (Gupta *et al.*, 1998; Boyle *et al.*, 2000). Their new scheme well explains the inherent multi-objective nature of the problem and the role of model errors in rainfall-

runoff simulation. However, their research is limited to improve a classical calibration strategy, i.e., single-objective optimization algorithm coupled with their own conceptual models (e.g., SAC-SMA model). Hence, it is questionable that a physically based distributed model, which has a different model structure to reflect real rainfall-runoff processes from a conceptual model, results in the overemphasis on particular portion of predicted hydrographs or whether optimal parameter sets change or not according to objective functions. As reported in previous studies (Yapo *et al.*, 1996, 1998; Gupta *et al.*, 1998; Boyle *et al.*, 2000), the result of variation of optimal parameter combination calibrated by a single-objective optimization method can be employed as one of the well-founded indicators to account for model structural stability.

This study is conducted to investigate answers to the following questions: 1) What kinds of models are stable in terms of model structure for description of rainfall-runoff process? (i.e., Definition of model stability). 2) How can modelers or engineers identify model stability and suitability? (Methodology for identifying model stability and suitability). A framework is outlined as an attempt to assess the model structural stability using single-objective global optimization method. The Shuffled Complex Evolution (SCE-UA) algorithm is used to calibrate a conceptual lumped model, Storage Function Model (SFM) and a physically based distributed model, CDRMV3 using five historical flood events (see Table 1) from Kamishiiba catchment located in Kyushu area.

Parameters	Sept. 1997	June 1999	Aug. 1999	Sept. 1999	Sept. 2005
Peak discharge (m <sup>3</sup> /s)	1203	210	489	644	1840
Initial discharge (m <sup>3</sup> /s)	33	59	82	34	11
Total amount of rainfall (mm)	496	463	473	339	831
Total amount of discharge (mm)	415	238	237	256	780
Runoff ratio	0.84	0.51	0.50	0.77	0.94

Table 1 The characteristics of each year heavy rainfall and flood discharge at Kamishiiba catchment.

## Methodology for Model Structure Analysis

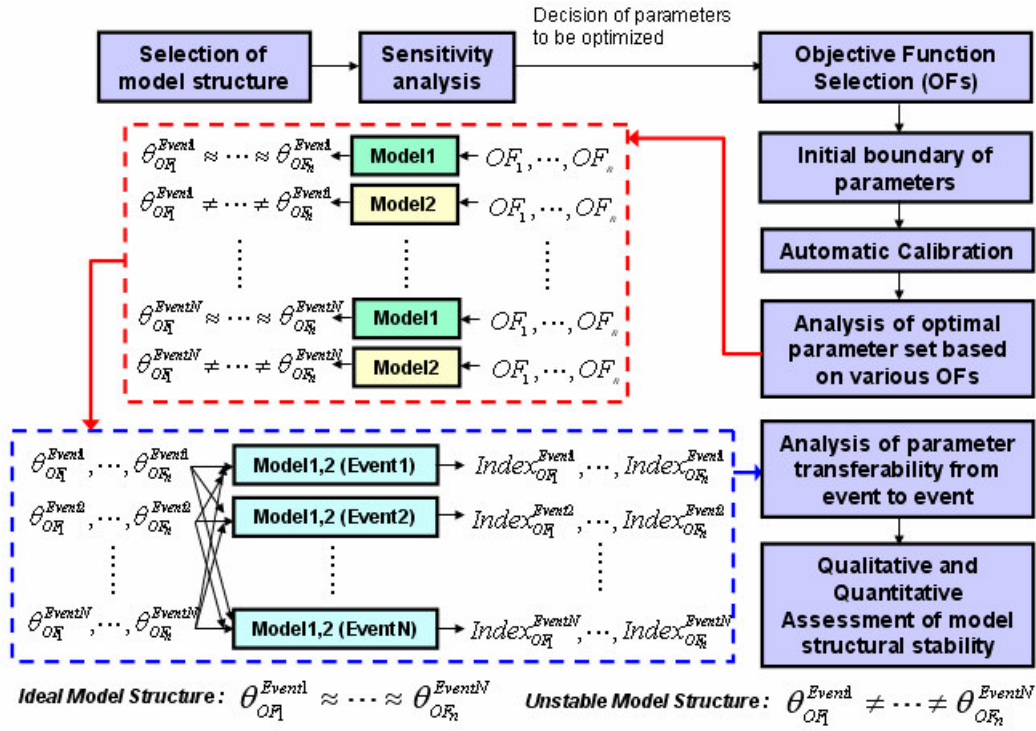


Fig. 1 Schematic illustration of a framework to assess model structural stability;  $\theta_i^j$  = optimal parameter set;  $Index_i^j$  = guideline index for assessment of model structural stability;  $i$  = objective Function;  $j$  = storm event.

Our purpose of this study is to establish a framework for how to assess the model structural stability. This work is summarized by two main procedures. The first step is a qualitative identification of model stability according to selection of objective functions. The second procedure is a quantitative assessment of model structural stability through the analysis of parameter transferability with a development of benchmarks or guideline indexes. Figure 1 illustrates the schematic process of the framework for assessment of model structural stability.

This assessment procedures are based on the following ideas:

1) If hydrologic forcing input data (e.g., rainfall, stream flow) for model calibration using efficient and robust optimization algorithm are not erroneous, calibrated parameter set can reflect explicitly the structural stability of hydrologic model.

2) An ideally-structured model can be regarded as a stable model which has the identical best parameter set regardless of objective functions and have high parameter transferability from

event to event, i.e.,  $\theta_{OF_1}^{Event1} \approx \dots \approx \theta_{OF_n}^{EventN}$ .

3) Therefore, variation of optimal parameters calibrated by using an appropriate single-objective optimization scheme can be one of the indicators for assessment of model structural stability.

After considering synthetically all concepts above mentioned, we conclude that a more reliable model structure leads to the constant optimal parameter set without regard of any objective func-

tions selected subjectively, i.e.,  $\theta_{OF_1}^{Event1} \approx \dots \approx \theta_{OF_n}^{Event1}$ . Moreover, such model structure maintains high degree of accuracy for predicted hydrographs when

applying parameter set for various type and magnitude of floods in the same study site, i.e.,

$\theta_{OF_1}^{Event1} \approx \dots \approx \theta_{OF_1}^{EventN}$ . As a result, model structural stability is evaluated by the ability enable to reduce the influence of objective functions and flood events. Two different types of model structures are applied to compare model structural stability for verification of our framework and each model is calibrated by SCE-UA optimization strategy with three objective functions. Applied models and optimization method, objective functions are introduced in following sub-sections.

## Hydrologic Models

### Conceptual lumped model, Storage Function Model (SFM)

This model is a lumped model with the reflection of nonlinear characteristics of hydrologic response behavior. SFM is used for the rainfall-runoff simulation in a small watershed usually less than five hundred square kilometers in Japan. The form of SFM is expressed as:

$$\frac{dS}{dt} = r_e(t - T_l) - q, \quad S = kq^p \quad (1)$$

$$r_e = \begin{cases} f \times r, & \text{if } \sum r \leq R_{SA} \\ r, & \text{if } \sum r > R_{SA} \end{cases} \quad (2)$$

where,  $S$  = water storage;  $r_e$  = effective rainfall intensity;  $r$  = rainfall intensity;  $q$  = runoff;  $t$  = time step;  $k$  = storage coefficient;  $p$  = coefficient of

nonlinearity;  $f$  = primary runoff ratio;  $T_l$  = lag

time; and  $R_{SA}$  = cumulative observed rainfall from the beginning of storm.

### Physically based distributed model, CDRMV3

CDRMV3 is a physically based distributed hydrologic model developed by Kojima *et al.* (2003) including discharge-stage relationship with saturated-unsaturated flow (Tachikawa *et al.*, 2004). The model solves the one-dimensional kinematic wave equation with the discharge-stage equation using the Lax-Wendroff finite difference scheme according to orderly nodes and edges, edge connection based on flow direction map (see Figure 2). All geomorphologic information are extracted from 250m based DEM data. Channel routing is also carried out by the kinematic routing scheme as well as calculation of slope elements reflecting contributing areas.

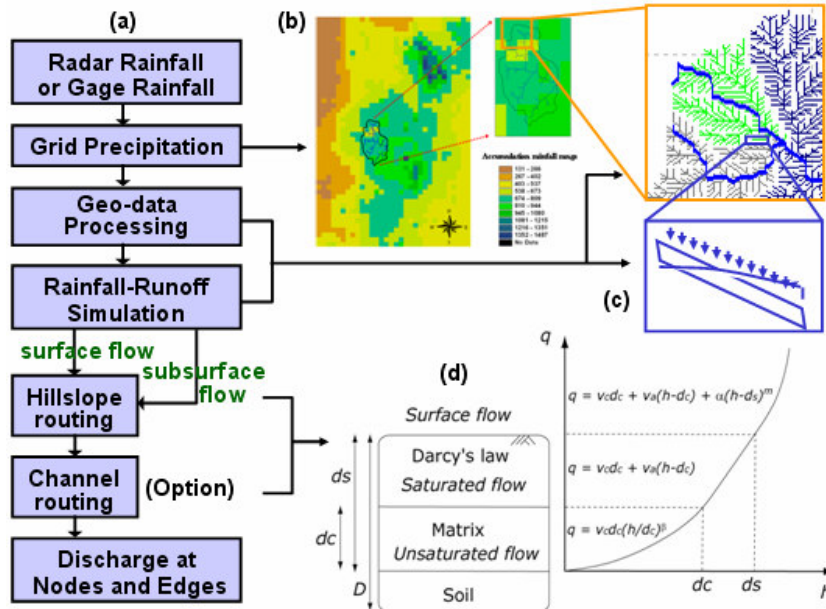


Fig. 2 Schematic representation of CDRMV3 (a) Modular structure of CDRMV3 (b) Distributed grid rainfall data (c) Close-up of edges and nodes extracted DEM (d) Model structure for the hillslope soil layer and discharge-stage relationship.

The model assumes that a permeable soil layer covers the hillslope as illustrated in Figure 2(d). The soil layer consists of a capillary layer which unsaturated flow occurs in and a non-capillary layer in which saturated flow occurs. According to this mechanism, if the depth of water is higher than the soil depth, then overland flow occurs. The discharge-stage relationship is expressed by equation (3) corresponding to water levels (see Figure 2(d)) defined as:

$$q = \begin{cases} v_c d_c (h/d_c)^\beta, & 0 \leq h \leq d_c \\ v_c d_c + v_a (h - d_c), & d_c \leq h \leq d_a \\ v_c d_c + v_a (h - d_c) + \alpha (h - d_s)^m, & d_s \leq h \end{cases} \quad (3)$$

$$\frac{\partial h}{\partial t} + \frac{\partial q}{\partial x} = r(t) \quad (4)$$

Flow rate of each slope segment are calculated by above governing equations combined with the continuity equation (4) where,

$v_c = k_c i$  ;  $v_a = k_a i$  ;  
 $k_c = k_a / \beta$  ;  $\alpha = \sqrt{i} / n$  ;  $i$  is slope gradient,  $k_c$  is saturated hydraulic conductivity of the capillary soil

layer,  $k_a$  is hydraulic conductivity of the non-capillary soil layer,  $n$  is roughness coefficient,

$d_c$  is the depth of the capillary soil layer and  $d_s$  is soil depth. Detailed explanations of model structure appear in Tachikawa *et al.* (2004).

### Shuffled Complex Evolution (SCE-UA) Algorithm

The reasons for difficulties in automatic calibration with respect to the response surface of parametric structures, i.e., existence of numerous local optima, non-smooth response surface, non-convex shape around global optimum, motivate a development of a global search algorithm in rainfall-runoff modeling (Sorooshian and Gupta, 1995). Evolutionary algorithms are probably the most commonly applied global optimization methods in rainfall-runoff simulation. The Shuffled Complex Evolution Algorithm (SCE, Duan *et al.*, 1992; 1993; 1994), one of the computer-based automatic optimization algorithms, is a single-objective optimization method designed to handle high-parameter dimensionality encountered in calibration of a nonlinear hydrologic simulation

models, apart from the Genetic Algorithm. This evolutionary approach method has been performed by a number of researchers on a variety of models with outstanding positive results (Gupta *et al.*, 1999) and has proved to be an efficient, powerful method for the automatic optimization (Gan and Bifu, 1996; Yu *et al.*, 2001). Basically, this scheme is synthesized by following three concepts: (1) combination of simplex procedure with the concepts of controlled random search approaches; (2) competitive evolution; and (3) complex shuffling. The integration of these steps above mentioned makes the SCE method effective, robust and flexible (Duan *et al.*, 1994).

### Objective Functions

The aim of computer-based automatic calibration is to find those values of the model parameters that minimize or maximize the numerical value of the objective function (Sorooshian and Gupta, 1995). Frequently, a number of statistics and techniques are utilized for evaluations of the model predictive abilities. In general, many objective functions contain a summation of the error term and to avoid the canceling of errors of opposite sign, the summation of the squared errors is often used for objective functions (Legates and McCabe, 1999). The most commonly utilized objective functions in hydrological modeling are variations of the Simple Least Squares (SLS) function defined as:

$$SLS = \sum_{t=1}^N (q_t^{obs} - q_t(\theta))^2 \quad (5)$$

where  $q_t^{obs}$  is observed stream flow value at time  $t$ ;  
 $q_t(\theta)$  is model simulated stream flow value at

time  $t$  using parameter set  $\theta$  ;  $N$  is the number of flow values available.

The main reason for the popularity of SLS has been its direct applicability to any model. The selection of SLS as an objective function implies assumptions concerning the probability distribution of the errors: 1) the residuals are independent and identically distributed; 2) the residual distribution has homogeneous variance; and 3) the residuals are normally distributed (Yapo *et al.*, 1996).

Moreover, the largest disadvantage of SLS is the fact that the differences between the observed and predicted values are calculated as squared values. This shortcoming results that larger values in a time series are overestimated

whereas lower values are neglected (Legates and McCabe, 1999). Krause *et al.* (2005) proposed the modified index of agreement (MIA, Willmott, 1984) to overcome the inefficiency of these measures with squared errors. This objective function is calculated as:

$$MIA = 1 - \frac{\sum_{t=1}^n \left( \frac{q_t^{obs} - q_t(\theta)}{q_t^{obs}} \right)^2}{\sum_{t=1}^n \left( \frac{|q_t(\theta) - q_t^{mean}| + |q_t^{obs} - q_t^{mean}|}{q_t^{mean}} \right)^2} \quad (6)$$

where  $q_t^{mean}$  is a mean value of observed time series.

Sorooshian and Dracup (1980) remarked that the problem often encountered in rainfall-runoff modeling is the fact that the residuals variance increases with increasing flow values, i.e., the assumption of homoscedascity cannot be justified. When we plot the residuals versus predicted runoff, we can easily find out whether the variance of the residuals increases with increasing flow values, i.e., the problem heteroscedascity. Generally, the commonly practiced methods of handling this heteroscedastic error cases in natural system have been through the application of Weighted Least Squares (WLS) function and transformation functions (Sorooshian and Dracup, 1980). They suggested the Heteroscedastic Maximum Likelihood Error (HMLE), which enables the estimation of the most likely weights through the use of the maximum estimation theory. This new procedure can eliminate some of the subjectivity involved in the selection of transformation and/or a weighting scheme and yields a more balanced performance over the entire hydrograph (Yapo *et al.*, 1996; Gupta *et al.*, 1998). It is calculated as:

$$\min_{\theta, \lambda} HMLE = \frac{1/N \sum_{t=1}^N w_t \varepsilon_t}{\prod_{t=1}^N w_t} \quad (7)$$

where  $\varepsilon_t = q_t^{obs} - q_t(\theta)$  is the model residual at time  $t$ ;  $w_t$  is the weight assigned to time  $t$ , computed as  $w_t = f_t^{2(\lambda-1)}$ . Where  $f_t = q_t^{true}$  is the expected true flow at time  $t$ ,  $\lambda$  is the unknown transformation parameter which stabilizes the variance. Fulton (1982) recommended using  $q_t^{obs}$  instead of  $q_t(\theta)$  to approximate  $f_t$ .

In this study, above mentioned three objective functions are used in the calibration trials and the analysis of hydrologic model stability.

## Result and Discussions

### The impact of objective functions to model performance

The plots of comparison between the simulated and the observed hydrographs according to the three objective functions (SLS, MIA and HMLE) are illustrated in Figure 3.

From Figure 3, we notice that:

- 1) In SFM cases, the simulated hydrographs based on the parameters calibrated by SLS are close to the observed ones while other parameters optimized by HMLE, MIA lead to less magnitude than the real measured stream flows under big flood events (e.g., Event 1, 4, 5).
- 2) The calibrated parameters based on MIA, HMLE result in underestimated outcomes in big flood but simulated results obtained from small floods reproduce closely to the observed (see Figure 3 (a)).
- 3) In CDRMV3 cases, all simulation results shown in Figure 3(b) are close to observed discharge for any objective functions. This result implies that the problem of subjectivity related with selection of objective functions for model calibration based on single-objective optimization algorithm can be ignored for distributed hydrological modeling used here.

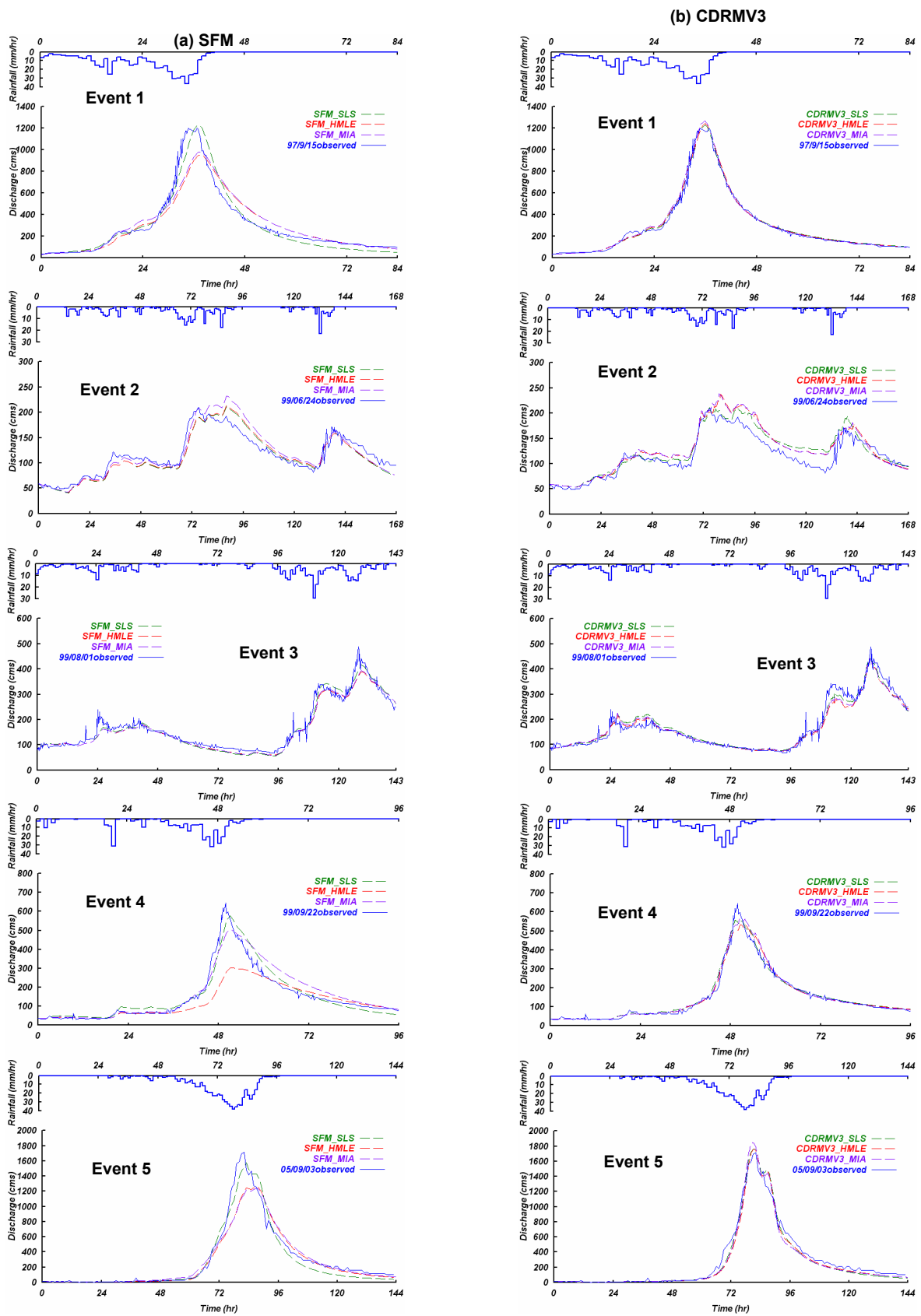


Fig. 3 Comparison between the simulated and the observed hydrographs according to three objective functions; (a) SFM cases, (b) CDRMV3 cases.

### The Assessment of Parameter Transferability from Event to Event

Despite of successfully calibration as shown in Figure 3, it is still questionable that best parameter set obtained from the event selected subjectively can be applicable to other arbitrary events in study site. If we expect good simulation results from transferred best parameter set, we can regard such model as a stable model structure, which has high parameter transferability. The each performance from transferred parameter sets are evaluated by peak discharge ratio (PDR) and Nash-Sutcliffe(NS) statistics of the residuals as guideline indexes for measurement of parameter transferability, defined as:

$$PDR = Peak_{sim} / Peak_{obs} \quad (8)$$

$$NS = 1 - \frac{\sum_{t=1}^N (q_t^{obs} - q_t(\theta))^2}{\sum_{t=1}^N (q_t^{obs} - q^{mean})^2} \quad (9)$$

where  $Peak_{sim}$  is the simulated peak discharge,

$Peak_{obs}$  is the observe peak discharge and  $q^{mean}$  is the mean observed discharge. PDR measures the tendency of the simulated peak discharge to be larger or smaller than the observed peak discharge; the optimal value is 1.0, larger values than 1.0 indicate an overestimation of the simulated peak discharge and smaller values than 1.0 indicate an underestimation of the simulated peak discharge. NS measures a relative magnitude of the residual variance to the variance of the observed stream flows; the optimal value is 1.0.

The quantified results of parameter transferability are plotted in Figure 4. As shown in Figure 4(a) and Table 2, the conceptual lumped model has low parameter transferability while the physically based model has high parameter transferability from event to event. Nevertheless, a successful transfer of parameters in CDRMV3 model, the results simulated by optimal parameters of Event 2 over entire cases are inaccurate; NS values

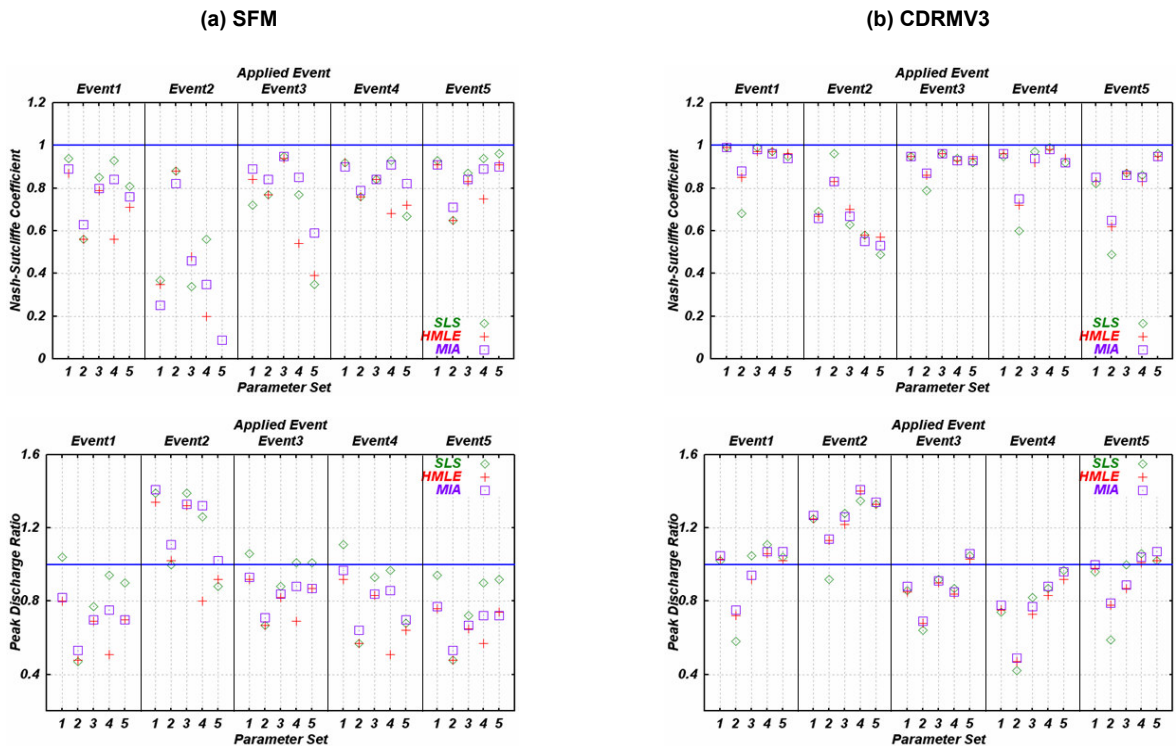


Fig. 4 Plots for assessment of parameter transferability from event to event; each point indicates the evaluated NS, PDR due to parameter transfer.

are usually less than 0.7 and PDR values are underestimated/overestimated irregularly. This result indicates that Event 2 input data during calibration has poor information. Moreover, this finding is allowable hydrologist or modelers to distinguish a high or low quality data. In CDRMV3, all of the measured points described in Figure 4 due to three objective functions converge into one position while points obtained from SFM are scattered very irregularly.

Unfortunately, the constant single optimal parameter set over all storm events is not observed

in the study site, i.e.,  $\theta_{OF_i}^{Event1} \neq \dots \neq \theta_{OF_i}^{EventN}$ . In the physically based distributed model, the different parameter combination also can lead to acceptable model performances with proper values of NS or

PDR, i.e.,  $I_{OF_i}^{Event1} \approx \dots \approx I_{OF_i}^{EventN}$ . This finding is strongly connected with “equifinality” (Beven, 2001). Therefore, the perfect framework of model structural stability still require analysis of uncertainty sources in hydrological processing and its effect on the predicted output variable.

## Conclusions

In this paper, we have demonstrated a framework for assessment of model structural stability through a single global optimization method (SCE-UA) and comparison of two hydrologic models (SFM, CDRMV3). The results under our framework lead to following conclusions that either conceptual lumped model or physically based model is suitable for rainfall-runoff simulation if based on available informative data during model calibration, and that the simulated results of CDRMV3 are not affected by objective functions while the computed results of SFM are fluctuated according to objective functions. Then, we test parameter transferability from event to event in the study site. The structural stability of CDRMV3 is superior to SFM in terms of parameter transfer. However, even though a physically based distributed model leads to high parameter transferability, problems of uncertainty still remain to be unsolved. The principal reason is that the identification of an appropriate model structure and the identification of appropriate parameter set within this structure are difficult due to a range of uncertainties involved in the modeling process, which are also unavoidably propagated into the model output. Therefore, the analysis of uncertainty in the modeling process must go side by side with identification of stable model structure.

Table 2 Evaluated NS and PDR for testing parameter transferability

Applied Event	Parameter Set	SFM						CDRMV3					
		NS_SLS	PDR_SLS	NS_HMLE	PDR_HMLE	NS_MIA	PDR_MIA	NS_SLS	PDR_SLS	NS_HMLE	PDR_HMLE	NS_MIA	PDR_MIA
Event1	Event1	0.94	1.04	0.87	0.80	0.89	0.82	0.99	1.02	0.99	1.03	0.99	1.05
	Event2	0.56	0.47	0.56	0.48	0.63	0.53	0.68	0.58	0.85	0.72	0.68	0.75
	Event3	0.85	0.77	0.79	0.69	0.80	0.70	0.99	1.05	0.97	0.92	0.98	0.94
	Event4	0.93	0.94	0.56	0.51	0.84	0.75	0.97	1.11	0.97	1.06	0.96	1.07
	Event5	0.81	0.90	0.71	0.70	0.76	0.70	0.95	1.04	0.96	1.02	0.94	1.07
Event2	Event1	0.37	1.39	0.35	1.34	0.25	1.41	0.69	1.25	0.67	1.25	0.66	1.27
	Event2	0.88	1.00	0.88	1.02	0.82	1.11	0.96	0.92	0.83	1.13	0.83	1.14
	Event3	0.34	1.39	0.48	1.32	0.46	1.33	0.63	1.28	0.70	1.22	0.67	1.26
	Event4	0.56	1.26	0.20	0.80	0.35	1.32	0.58	1.35	0.58	1.40	0.55	1.41
	Event5	-0.96	0.88	-0.57	0.92	0.09	1.02	0.49	1.33	0.57	1.33	0.53	1.34
Event3	Event1	0.72	1.06	0.84	0.92	0.89	0.93	0.95	0.86	0.95	0.85	0.95	0.88
	Event2	0.77	0.67	0.77	0.67	0.84	0.71	0.79	0.64	0.86	0.68	0.87	0.69
	Event3	0.95	0.88	0.94	0.82	0.95	0.84	0.96	0.92	0.96	0.90	0.96	0.91
	Event4	0.77	1.01	0.54	0.69	0.85	0.88	0.94	0.87	0.93	0.84	0.93	0.85
	Event5	0.35	1.01	0.39	0.87	0.59	0.87	0.92	1.05	0.94	1.03	0.93	1.05
Event4	Event1	0.92	1.11	0.92	0.92	0.90	0.97	0.95	0.74	0.96	0.75	0.96	0.78
	Event2	0.76	0.57	0.76	0.57	0.79	0.64	0.60	0.42	0.72	0.47	0.75	0.49
	Event3	0.84	0.93	0.84	0.83	0.84	0.84	0.97	0.82	0.92	0.73	0.94	0.77
	Event4	0.93	0.97	0.68	0.51	0.91	0.86	0.99	0.87	0.98	0.83	0.98	0.88
	Event5	0.67	0.68	0.72	0.64	0.82	0.70	0.92	0.97	0.94	0.92	0.92	0.96
Event5	Event1	0.93	0.94	0.91	0.76	0.91	0.77	0.82	0.96	0.83	0.98	0.85	1.00
	Event2	0.65	0.48	0.65	0.48	0.71	0.53	0.49	0.59	0.62	0.78	0.65	0.79
	Event3	0.87	0.72	0.83	0.65	0.84	0.67	0.87	1.00	0.87	0.87	0.86	0.89
	Event4	0.94	0.90	0.75	0.57	0.89	0.72	0.86	1.06	0.83	1.01	0.85	1.04
	Event5	0.96	0.92	0.91	0.74	0.90	0.72	0.96	1.02	0.95	1.02	0.95	1.07
AVE.		0.63	0.90	0.6	0.77	0.70	0.85	0.80	0.95	0.83	0.94	0.83	0.97



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