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Key Points:

- A new process sensitivity index is defined to identify important system processes when multiple competing process models are available
- The new index is derived by integrating the concept of model averaging into the framework of variance-based global sensitivity analysis
- The new index allows for interactions between process models and/or between process model parameters in the global sensitivity analysis

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A new process sensitivity index to identify important system processes under process model and parametric uncertainty

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Abstract A hydrological model consists of multiple process level submodels, and each submodel represents a process key to the operation of the simulated system. Global sensitivity analysis methods have been widely used to identify important processes for system model development and improvement. The existing methods of global sensitivity analysis only consider parametric uncertainty, and are not capable of handling model uncertainty caused by multiple process models that arise from competing hypotheses about one or more processes. To address this problem, this study develops a new method to probe model output sensitivity to competing process models by integrating model averaging methods with variance-based global sensitivity analysis. A process sensitivity index is derived as a single summary measure of relative process importance, and the index includes variance in model outputs caused by uncertainty in both process models and their parameters. For demonstration, the new index is used to assign importance to the processes of recharge and geology in a synthetic study of groundwater reactive transport modeling. The recharge process is simulated by two models that convert precipitation to recharge, and the geology process is simulated by two models of hydraulic conductivity. Each process model has its own random parameters. The new process sensitivity index is mathematically general, and can be applied to a wide range of problems in hydrology and beyond.

Plain Language Summary If we have only one model, we always know how to identify the important factors of the models. However, if there are multiple models, it is not always clear how to identify the important factors. The factors important to one model may not be important to another model. It is necessary to develop a method that can identify important factors not for a single model but for multiple models. This study aims at resolving this problem by developing a mathematically rigorous method to provide a single summary measure for identifying important factors in the face of competing models. This is called multi-model process sensitivity analysis, and the mathematical measure is called process sensitivity index. The new index is demonstrated using a numerical example of groundwater reactive transport modeling with two recharge models and two geology models. The multimodel process sensitivity analysis has a wide range of applications in hydrologic and environmental modeling.

1. Introduction

In hydrologic modeling, the need to identify important processes for model development and improvement has long been recognized [e.g., Grayson and Blöschl, 2000; Blöschl, 2001; Beven, 2002], prompting the development of many identification methods (see the review articles of Sivakumar [2004, 2008]). Most of the methods are model driven, starting from developing a system model that is composed of multiple process level submodels. Each submodel represents a process key to the operation of the simulated system. The relations between a system and its processes and between a system model and its process models are shown in Figure 1. In the conventional procedure of system model development, a system process is represented by a single process model, and the process models are integrated to form a single system model. Based on this conceptualization, to identify the important processes, sensitivity analysis is conducted for the parameters of the process models; a process is considered to be important if the parameters of the process model are important to system model outputs of interest [e.g., Saltelli et al., 2004, 2005; Hill et al., 2016;

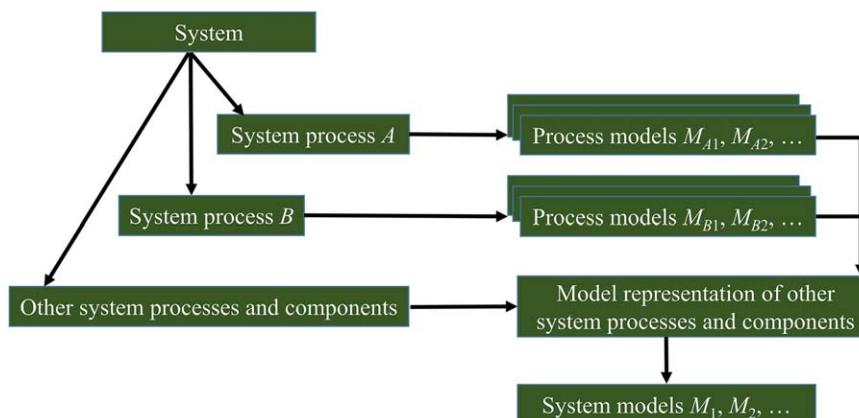


Figure 1. Relation between system and its processes as well as relation between process models and system models. This diagram does not consider process model uncertainty.

Markstrom et al., 2016]. However, using a single process model is questionable, when available data and knowledge support use of multiple process models [Beven, 2002; Bredehoeft, 2003; Neuman, 2003; Gupta and Nearing, 2014; Clark et al., 2016]. For example, Ye et al. [2010] showed that, for the Death Valley regional flow system, its recharge process can be simulated by five different models, and its hydrogeology can be described by five hydrostratigraphic frameworks. Similar examples for groundwater flow and reactive transport modeling and biogeochemical modeling have been constantly reported in the literature [e.g., Foglia et al., 2013, Zhang et al., 2014; Lu et al. 2015; Walker et al., 2015]. Figure 1 illustrates the procedure of developing multiple system models based on competing process models. A thorough discussion on development of process-based hydrologic models with consideration of process model uncertainty is referred to Clark et al. [2015a, 2015b] and Coon et al. [2016].

Since the modeled system behaviors presumably depend to some extent on the particular choice of process models that comprise the system model, the importance of a system process is likely to be different when the process is simulated by different process models. As a result, process identification without considering model uncertainty may lead to biased selection of important processes. A common drawback of the existing methods of important process identification is that they generally only consider parametric uncertainty but ignore process model uncertainty. This study aims at resolving this problem by developing a mathematically rigorous method to provide a single summary measure of process importance for identifying important processes in the face of competing process models. If a system process can be simulated by multiple process models and the parameters of the process models are random, the method derived in this study is designed to answer the following question: *how can we identify important processes for the explicitly proposed process models and the probabilistically defined random parameters?* Instead of using single process models, our method considers multiple models that are plausible for simulating system processes. This method is thus referred to as multimodel process sensitivity analysis, or just process sensitivity analysis for brevity.

The multimodel process sensitivity analysis is built upon integrating model averaging with variance-based global sensitivity analysis. The general procedure of model averaging is as follows [e.g., Ye et al., 2008a; Poeter and Hill, 2007; Burnham and Anderson, 2002; Hoeting et al., 1999; Draper, 1995]: (1) postulate multiple models and use the models to simulate the quantities of interest and their uncertainty, (2) evaluate model averaging weights (also known as model probabilities) as a measure of relative plausibility of the models, and (3) calculate weighted average of the simulated quantities and their associated uncertainties given by the multiple models. The model averaging methods are used for deriving process sensitivity index, because they provide a general purpose, statistical tool to quantify between-model uncertainty (i.e., variance of mean model output between competing process models) and within-model uncertainty (i.e., mean of model output variance caused by parametric uncertainty within each competing process model). In other words, the model averaging methods make it possible to combine model output variance caused by parametric uncertainty within each process model, together with the model output variance caused by the competing

process models. Mathematically rigorous definitions of between-model and within-model uncertainty are referred to *Draper* [1995].

Explained in detail in section 2, model averaging can be seamlessly integrated into the framework of variance-based global sensitivity analysis that has been widely used in hydrologic modeling [*Wainwright et al.*, 2014; *Razavi and Gupta*, 2015; *Song et al.*, 2015; *Hill et al.*, 2016]. Within the framework of sensitivity analysis, a process sensitivity index is derived as a metric of process importance in the context of competing process models for multiple processes. Analogous to the Sobol' parameter sensitivity index, the process sensitivity index ranks the importance of multiple processes. Deriving the index is a theoretical advance, because the index considers uncertainty of model outputs between different process models, which is unprecedented. With the process sensitivity index, quantitative and coherent conclusions on process importance can be drawn. Such conclusions cannot be reached by applying parametric sensitivity analysis to individual models. In other words, conducting parametric sensitivity analysis for individual models [e.g., *Graeff et al.*, 2009; *Herman et al.*, 2013] can only reveal importance of model parameters between process models, but cannot lead to definitive conclusions on process importance when multiple competing process models are available. Therefore, integrating model averaging methods into the variance-based global sensitivity analysis is necessary to account for variability of model outputs caused by not only parametric uncertainty but also process model uncertainty.

The rest of the paper is organized as follows. The mathematical derivation of the process sensitivity index is given in section 2. For the purpose of illustration, the new index is applied in section 3 for a synthetic study of groundwater reactive transport modeling to select the process that is more important to hydraulic head and solute concentration. Two processes are considered in the synthetic study: a recharge process that is simulated by two models and a geology process that is also simulated by two models. Each of the four process models has its own uncertain parameters. Section 4 discusses several ways for reducing the computational cost of evaluating process sensitivity index, and implements a binning method for the synthetic study of groundwater modeling. Several issues related to theoretical and practical aspects of the process sensitivity index are discussed in section 5, followed by the conclusions of this study presented in section 6.

2. Methodology

This section starts with a discussion of formulating process-based system model and process model uncertainty in section 2.1. The process sensitivity index is derived in section 2.2, and the way of evaluating the index is discussed in section 2.3.

2.1. Process-Based System Model and Process Model Uncertainty

Denote the quantity of interest as Δ . Without process model uncertainty, Δ is simulated by a single system model, M , i.e., $\Delta = M(\theta) = M(\theta_1, \dots, \theta_d)$, where $\theta = \{\theta_1, \dots, \theta_d\}$ is the vector of system model parameters. Note that we here use θ to denote a set of deterministic parameter values and reserve Θ to denote a set of random parameter values (θ can be viewed as a realization of Θ). If the system of interest consist of multiple processes (denoted as A, B, \dots) and each process has its own process model (denoted as M_A, M_B, \dots) and associated parameters (denoted as $\theta_A, \theta_B, \dots$), the system model, $M(\theta)$, may be viewed as an integration of the process models, i.e., $M(\theta) = \cup(M_A(\theta_A), M_B(\theta_B), \dots)$, together with other system model components common to the processes (e.g., domain discretization, system initial conditions, and driving forces). The process model integration (denoted by the union symbol above) may need to consider nonlinear interactions between the process models. An example of such integration is the development of a system model of groundwater reactive transport, as it integrates processes of groundwater flow, thermal transport, solute transport, and biogeochemical reactions. In addition, a process may have its subprocesses. For example, a groundwater flow process may consist of subprocesses such as recharge, geology, and evapotranspiration. Examples of building a system model using process models can be found in *Clark et al.* [2008], and an in-depth discussion on developing process-based hydrologic models is referred to *Clark et al.* [2015a, 2015b] and *Coon et al.* [2016].

With the presence of process model uncertainty, one or more process may be simulated by several alternative process models. Taking process A as an example, it may be represented by multiple process models that form a set, $\mathbf{M}_A(\theta_A) = \{M_{A_1}(\theta_{A_1}), M_{A_2}(\theta_{A_2}), \dots\}$; each process model may have its own parameters or

have parameters in common with other process models. The integration of the alternative process models leads to alternative system models, i.e., $\mathbf{M}(\theta) = \cup(\mathbf{M}_A(\theta_A), \mathbf{M}_B(\theta_B), \dots)$. In this configuration, the process model parameters, θ , are deterministic. If the process model parameters are random, they are denoted as Θ to be differentiated from θ , which now can be viewed as a realization of Θ . In this case, $\mathbf{M}(\theta) = \cup(\mathbf{M}_A(\theta_A), \mathbf{M}_B(\theta_B), \dots)$ becomes $\mathbf{M}(\Theta) = \cup(\mathbf{M}_A(\Theta_A), \mathbf{M}_B(\Theta_B), \dots)$.

An example of multiple possible system models is for the Death Valley regional flow system. As shown in Ye *et al.* [2008b], the system's recharge process can be simulated by five recharge process models, and the system's geological process can be represented by five hydrogeologic frameworks. Integrating the five process models of recharge and the five process models of geology into the modeling framework of Belcher and Sweetkind [2010] leads to a total of 25 alternative system models. Although the geology process appears to be more important than the recharge process to hydraulic head simulations [Ye *et al.*, 2010, 2016], there has been no quantitative statistical measure to evaluate the relative importance of the two processes.

2.2. Process Sensitivity Index

Given the above manner of system model formulation, this study derives the new process sensitivity index within the framework of variance-based global sensitivity analysis. For the uncertain model output, Δ , use its variance, $V(\Delta)$, to quantify its variability. According to the law of total variance, $V(\Delta)$ can be decomposed into the variance caused by process K and other processes (denoted as $\sim K$), i.e.,

$$V(\Delta) = E_K(V_{\sim K}[\Delta|K]) + V_K(E_{\sim K}[\Delta|K]) = E_{\mathbf{M}_K}(V_{\sim \mathbf{M}_K}[\Delta|M_K]) + V_{\mathbf{M}_K}(E_{\sim \mathbf{M}_K}[\Delta|M_K]), \tag{1}$$

where \mathbf{M}_K is the set of alternative models used to simulate process K , M_K is a single model in the set, and $\sim \mathbf{M}_K$ denotes the set of alternative models for other processes than process K . If there is only one process model M_K for process K (i.e., no uncertainty in the process model), the $V_{\mathbf{M}_K}(E_{\sim \mathbf{M}_K}[\Delta|M_K])$ term disappears and the $E_{\mathbf{M}_K}(V_{\sim \mathbf{M}_K}[\Delta|M_K])$ term becomes $V_{\sim \mathbf{M}_K}[\Delta|M_K]$. If multiple process models, \mathbf{M}_K , are available for simulating process K , the average, $E_{\mathbf{M}_K}(V_{\sim \mathbf{M}_K}[\Delta|M_K])$, over all the process models is used to measure the variability of Δ . The most important process is the one that gives the smallest value of $E_{\mathbf{M}_K}(V_{\sim \mathbf{M}_K}[\Delta|M_K])$, which corresponds to the largest value of $V_{\mathbf{M}_K}(E_{\sim \mathbf{M}_K}[\Delta|M_K])$ by virtue of equation (1). Therefore, the first-order process sensitivity index is defined as

$$PS_K = \frac{V_{\mathbf{M}_K}(E_{\sim \mathbf{M}_K}[\Delta|M_K])}{V(\Delta)}. \tag{2}$$

The process sensitivity index does not assume process independence, and allows interactions between processes, which is reflected in the $\sim \mathbf{M}_K$ term. This definition is symbolically similar to the first-order sensitivity index for parameters (or parameter sensitivity index for brevity),

$$S_j = \frac{V_{\theta_j}(E_{\sim \theta_j}(\Delta|\theta_j))}{V(\Delta)}, \tag{3}$$

used in the Sobol's method, where θ_j and $\sim \theta_j$ denote the j th parameter and other parameters, respectively. The derivation of equation (2) is similar to the derivation of equation (3) given in Saltelli *et al.* [2004]. However, it should be noted that the two indices are entirely different. The parameter sensitivity index (equation (3)) is used to select the important parameters, when parameter values are uncertain. Equations (2) and (3) show the relation between sensitivity and uncertainty (measured by variance here). The sensitivity analysis of this study is not for uncertainty quantification, but for uncertainty apportionment [Razavi and Gupta, 2015] to evaluate quantitative attribution of the variability in model outputs to the variability in process models.

If the parameters of process models are deterministically known, equation (2) alone is adequate for selecting important processes. However, when the process model parameters are also random, it is necessary to further develop the process sensitivity index to handle both random process models and random process model parameters for process sensitivity analysis. This is done by further expanding the $V_{\mathbf{M}_K}(E_{\sim \mathbf{M}_K}[\Delta|M_K])$ term in equation (2) to consider uncertainty in the parameters of the process models. First, evaluate $V_{\mathbf{M}_K}(E_{\sim \mathbf{M}_K}[\Delta|M_K])$ using the definition of variance via

$$V_{\mathbf{M}_K}(E_{\sim \mathbf{M}_K}[\Delta|M_K]) = E_{\mathbf{M}_K}(E_{\sim \mathbf{M}_K}[\Delta|M_K])^2 - (E_{\mathbf{M}_K}E_{\sim \mathbf{M}_K}[\Delta|M_K])^2. \quad (4)$$

Subsequently, applying the law of total expectation (or the posterior mean of model averaging) to the two expectations with respect to process model \mathbf{M}_K at the right-hand side of equation (4), equation (4) is expanded at the parameter level as

$$V_{\mathbf{M}_K}(E_{\sim \mathbf{M}_K}[\Delta|M_K]) = E_{\mathbf{M}_K}E_{\theta_K|M_K}(E_{\sim \mathbf{M}_K}[\Delta|\theta_K, M_K])^2 - (E_{\mathbf{M}_K}E_{\theta_K|M_K}E_{\sim \mathbf{M}_K}[\Delta|\theta_K, M_K])^2, \quad (5)$$

where subscript $\theta_K|M_K$ of $E_{\theta_K|M_K}$ indicates that the expectation is with respect to random parameter θ_K specific to model M_K , and $\Delta|\theta_K, M_K$ indicates that the model simulation Δ is for the single process model, M_K , and for a single realization θ_K of θ_K . Similarly, applying the law of total expectation again to other process models $\sim \mathbf{M}_K$ leads to

$$V_{\mathbf{M}_K}(E_{\sim \mathbf{M}_K}[\Delta|M_K]) = E_{\mathbf{M}_K}E_{\theta_K|M_K}(E_{\sim \mathbf{M}_K}E_{\sim \theta_K|\sim M_K}[\Delta|\theta_K, M_K, \sim \theta_K, \sim M_K])^2 - (E_{\mathbf{M}_K}E_{\theta_K|M_K}E_{\sim \mathbf{M}_K}E_{\sim \theta_K|\sim M_K}[\Delta|\theta_K, M_K, \sim \theta_K, \sim M_K])^2. \quad (6)$$

This equation allows considering uncertainty in both process models and their parameters for identifying important processes. In addition, since the $\Delta|\theta_K, M_K, \sim \theta_K, \sim M_K$ term indicates that the system model output (Δ) is simulated jointly by both process models M_K and $\sim M_K$ and their corresponding parameters θ_K and $\sim \theta_K$, equation (6) explicitly considers the interactions between process models, between process model parameters, and between process models and model parameters in the sensitivity analysis. For example, if θ_K and $\sim \theta_K$ are correlated, the impacts of the correlation on the sensitivity analysis is reflected in equation (6) through the integration of process models and their parameters. The interactions are explicitly accounted for when evaluating the process sensitivity index, and shown in the numerical example of groundwater modeling below.

2.3. Evaluation of Process Sensitivity Index

The mean (e.g., $E_{\theta_K|M_K}$) in equation (6) with respect to model parameters can be evaluated using either Monte Carlo (MC) or other stochastic methods. The mean (e.g., $E_{\mathbf{M}_K}$) in equation (6) with respect to models can be evaluated using the model averaging method. For example, $E_{\mathbf{M}_K}E_{\theta_K|M_K}$ is calculated via

$$E_{\mathbf{M}_K}E_{\theta_K|M_K}(\bullet) = \sum_{M_K} E_{\theta_K|M_K}(\bullet)P(M_K), \quad (7)$$

where $E_{\theta_K|M_K}$ is the mean with respect to model parameters, the dot (\bullet) denotes the two terms $((E_{\sim \mathbf{M}_K}E_{\sim \theta_K|\sim M_K}[\Delta|\theta_K, M_K, \sim \theta_K, \sim M_K])^2$ or $E_{\sim \mathbf{M}_K}E_{\sim \theta_K|\sim M_K}[\Delta|\theta_K, M_K, \sim \theta_K, \sim M_K])$ at the right-hand sides of equation (6), and $P(M_K)$ satisfying $\sum P(M_K) = 1$ is the model averaging weight that is used to evaluate plausibility of the model relative to other models. The weights can be evaluated with or without data (e.g., observations of system states). When the data are unavailable, the weights can be obtained through expert elicitation, which may give unequal weights by incorporating engineering judgement on alternative process models [e.g., Ye *et al.*, 2008b]. Such weights are equivalent to prior model probability from the Bayesian perspective. When field data (denoted as \mathbf{D}) are available, posterior model probability, $P(M_K|\mathbf{D})$ can be evaluated and used in equation (7). Evaluating $P(M_K|\mathbf{D})$ can be done by using the Bayes' theorem via [Ye *et al.*, 2008a]

$$P(M_k|\mathbf{D}) = \frac{p(\mathbf{D}|M_k)P(M_k)}{p(\mathbf{D})}, \quad (8)$$

where $P(M_k)$ is the prior model probability used in equation (7) above, and $p(\mathbf{D}|M_k)$ is the marginal likelihood function to measure how well data, \mathbf{D} , is simulated by model M_k . A comprehensive review and comparison of the methods for the Bayesian evaluation are referred to Schoniger *et al.* [2014], Knuth *et al.* [2015], and Liu *et al.* [2016]. It should be noted that the multimodel process identification method of this study is general, and equations (2) and (6) are compatible with model probability evaluated by any methods. It happens often that the model probability change dramatically after being conditioned on \mathbf{D} .

The data, \mathbf{D} , can significantly change not only model probability (from the prior to the posterior) but also the mean and variance values used for evaluating the process sensitivity index. This may lead to changes of the values of process sensitivity index, and thus to changes of important process identification. It is thus

necessary to calculate all the mean and variance terms involved in the process sensitivity index after data \mathbf{D} become available. Starting from equation (1), it becomes

$$V(\Delta|\mathbf{D}) = E_{\mathbf{M}_K}(V_{\sim\mathbf{M}_K}[\Delta|M_K, \mathbf{D}]) + V_{\mathbf{M}_K}(E_{\sim\mathbf{M}_K}[\Delta|M_K, \mathbf{D}]), \quad (9)$$

and the process sensitivity index becomes

$$PS_K = \frac{V_{\mathbf{M}_K}(E_{\sim\mathbf{M}_K}[\Delta|M_K, \mathbf{D}])}{V(\Delta|\mathbf{D})}. \quad (10)$$

Expanding equations (4–6) in the same manner is theoretically straightforward, and thus not presented. Although process identification can be completed by sensitivity analysis without using data, equations (9) and (10) provide a mean of data and model integration. For example, the equations can be used for model-enabled design of experiments and data collection campaigns so that important processes can be identified for a site of interest using the least amount of data.

When the MC method is used to evaluate equation (6), the implementation is computationally straightforward. Taking two processes, A and B , as an example, equation (6) for process A is

$$V_{\mathbf{M}_A}(E_{\mathbf{M}_B}[\Delta|M_A]) = E_{\mathbf{M}_A}E_{\theta_A|M_A}(E_{\mathbf{M}_B}E_{\theta_B|M_B}[\Delta|\theta_A, M_A, \theta_B, M_B])^2 - (E_{\mathbf{M}_A}E_{\theta_A|M_A}E_{\mathbf{M}_B}E_{\theta_B|M_B}[\Delta|\theta_A, M_A, \theta_B, M_B])^2. \quad (11)$$

The pseudo code for evaluating the two terms at the right-hand side of equation (11) is given in Figure 2a. The pseudo code handles the nested structures of the process models and model parameters. Taking the $E_{\mathbf{M}_A}E_{\theta_A|M_A}E_{\mathbf{M}_B}E_{\theta_B|M_B}[\Delta|\theta_A, M_A, \theta_B, M_B]$ term as an example, the inner expectation, $E_{\theta_B|M_B}[\Delta|\theta_A, M_A, \theta_B, M_B]$ is evaluated for all samples of parameter θ_B specific to M_B , with the conditioning on (1) a single model, M_A , of process A , (2) a single sample of θ_A specific to M_A , and (3) a single model, M_B , of process B . Similarly, although $E_{\mathbf{M}_B}E_{\theta_B|M_B}[\Delta|\theta_A, M_A, \theta_B, M_B]$ is evaluated for the model set, \mathbf{M}_B , of process B , the expectation is conditioned on the single sample θ_A of the single model M_A . This procedure expands to all samples of parameter θ_A of M_A and then to the model set, \mathbf{M}_A , of process A until the $E_{\mathbf{M}_A}E_{\theta_A|M_A}E_{\mathbf{M}_B}E_{\theta_B|M_B}[\Delta|\theta_A, M_A, \theta_B, M_B]$ term is evaluated.

For the pseudo code shown in Figure 2a, regardless of the number of processes, the number of loops needed for calculating the process sensitivity index is fixed as four. The first two loops are for the process for which the index is calculated, and the third and the fourth loops are for the combination of the process models corresponding to the rest of the processes. For example, if another process, say process C , is involved in the calculation, the third loop is for the combination of the process models of processes B and C , and the fourth loop is for the parameters of the model combinations. Therefore, applying the MC procedure given in Figure 2a to a general case with P processes, the total number of model executions needed for calculating the process sensitivity index of the i th process is $(m_i \times n_i) \times (m_{\sim i} \times n_{\sim i})$, where m_i is the number of models of the i th process, n_i is the number of model executions for a single model of the process, $m_{\sim i}$ is the number of process model combinations for the processes other than the i th process, and $n_{\sim i}$ is the number of model executions corresponding to the process model combinations. With certain assumptions (e.g., random samples of a process model are independent to other process models), the $(m_i \times n_i) \times (m_{\sim i} \times n_{\sim i})$ term may be rearranged as $(m_i \times m_{\sim i}) \times (n_i \times n_{\sim i})$. The $m_i \times m_{\sim i}$ term is the number of possible combinations of process models (i.e., the number of system models), and the $n_i \times n_{\sim i}$ term is the number of model executions needed for traditional parameter sensitivity analysis (e.g., the evaluation of the first-order sensitivity index defined in equation (3)) of a single system model. This connection between the process sensitivity index and traditional parameter sensitivity index with respect to the number of model executions may be useful for developing an algorithm that can evaluate the two kinds of sensitivity index simultaneously. We will pursue such an algorithm in future studies. Due to the nested structures of process models and model parameters, the computational cost of implementing the pseudo code shown in Figure 2a is still high. The reason is that the $n_i \times n_{\sim i}$ number of model executions is computationally demanding, although only four loops are needed in the MC procedure. Section 4 discusses a number of ways of reducing the computational cost.

3. Synthetic Example

The process sensitivity index is evaluated for a synthetic study of groundwater reactive transport modeling revised after *Dai and Ye* [2015]. Only built for the purposes of demonstration, the synthetic study is relatively

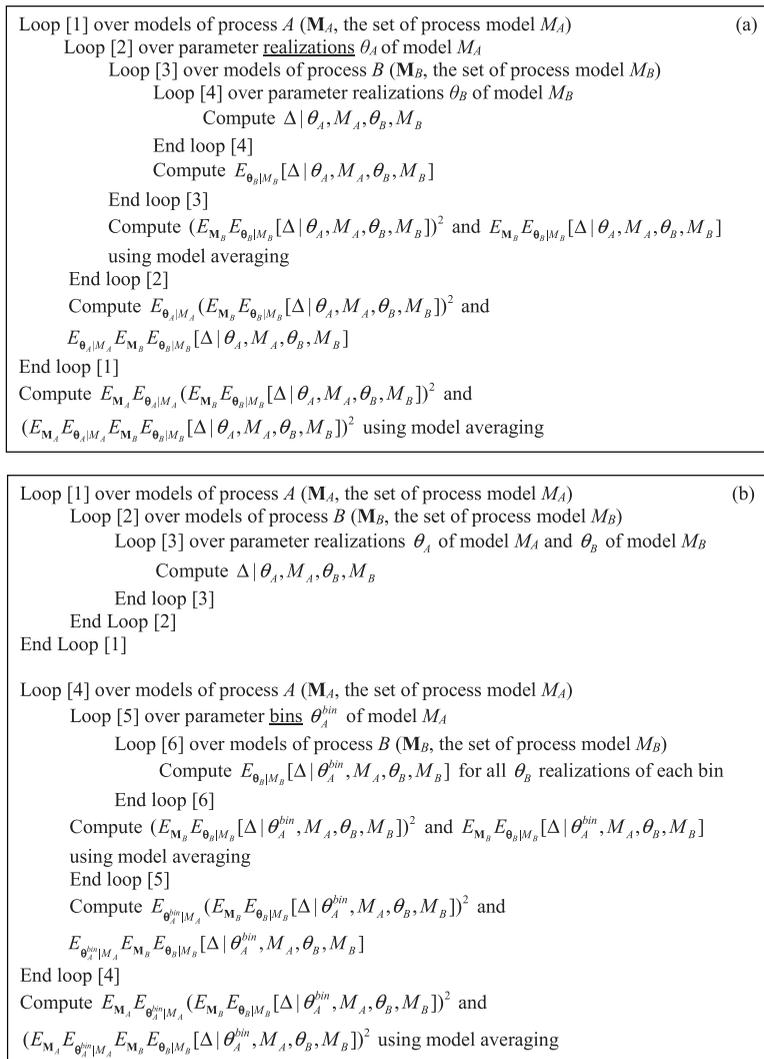


Figure 2. Pseudo codes for evaluating all the terms of equation (11) for the sensitivity index of process A using the Monte Carlo method and the model averaging method (a) without and (b) with the binning implementation. If more processes are involved more than processes A and B , the number of loops remains to be four, but loops [3] and [4] in Figure 2a and loops [2] and [3] in Figure 2b should include the process models of the new processes and corresponding model parameters. The posterior mean, $E_{\mathbf{M}_A}$ and $E_{\mathbf{M}_B}$, of the modeling averaging can be evaluated using equation (7).

simple so that it is computationally affordable for the MC simulation describe above. In the domain of groundwater flow shown in Figure 3, the unconfined groundwater aquifer of length L is under a steady state condition, and has a uniform precipitation, $P = 1524$ mm per year, over the entire domain. Two models (R_1 and R_2) are used to simulate the recharge process that converts precipitation to recharge, and they are

$$\begin{aligned}
 R_1 : w &= a(P - 355.6)^{0.50} \\
 R_2 : w &= b(P - 399.80)^{\quad} \quad ,
 \end{aligned}
 \tag{12}$$

Parameter a of model R_1 and parameter b of model R_2 are assumed to follow the normal distribution, $N(16.88, 25.4)$, and the uniform distribution, $U(0.1, 0.2)$, respectively. Similar to Wellmann et al. [2014], hydraulic conductivity (K) of the domain is parameterized by two geology process models (G_1 and G_2) that represent the following two ways of parameterization:

$$G_1 : K \text{ for any } x$$

$$G_2 : K = \begin{cases} K_1 & \text{for } x < 7000 \\ K_2 & \text{for } x \geq 7000 \end{cases} \quad (13)$$

In model G_1 , hydraulic conductivity is homogeneous, and follows the normal distribution, $N(15,1)$. Model G_2 has two zones with the zone boundary at the location of $x = 7000$. K_1 of zone 1 ($x < 7000$ m) and K_2 of zone 2 ($x > 7000$ m) are assumed to follow the normal distributions, $N(20,1)$ and $N(10,1)$, respectively. For model G_1 , the analytical solution of hydraulic head is available from hydrogeology textbooks; for model G_2 , numerical solution using the finite difference method is used. The distributions above are selected arbitrarily for the purpose of method demonstration. A combination of the recharge process models and the geology process models lead to a total of four system models, R_1G_1 , R_1G_2 , R_2G_1 , and R_2G_2 . For the transport process, a continuous contaminant source is placed at the center of the domain ($x = 5000$ m). A total of five chemical species are involved in the reactive transport modeling, and they are PCE (perchloroethene), TCE (trichloroethene), DCE (dichloroethene), VC (vinyl chloride), and ETH (ethene). The single chain reactions described in the user's manual of BIOCHLOR [Aziz *et al.*, 2000] are used in this study. The analytical solutions of the advection-dispersion-reaction model and their numerical implementation given by Sun *et al.* [1999] are used in this study. The transport model does not include competing process representation and random parameters.

When evaluating the process sensitivity index using the MC approach, 3000 parameter samples are generated for each of the two processes to ensure convergence of the terms in equations (6) and (11). The total number of model executions is $36,000,000 = (2 \text{ recharge models} \times 3000 \text{ simulations for each model}) \times (2 \text{ geology models} \times 3000 \text{ simulations for each model})$. It should be noted that the large number of model executions is unnecessary. Figure 4 is the convergence diagnosis for the sample means (over MC realizations) of hydraulic head and ethene concentration (the end production of the chain reaction of PCE degradation) at the location of $x = 6000$ m simulated by model R_1G_1 with recharge parameter varying (hydraulic conductivity is fixed at the mean value). The figure shows that the sample means converge after about 300 realizations. When 300 realizations are used, the number of model execution decreases to 360,000, and the corresponding values of the process sensitivity index are similar to those obtained using 36,000,000 model executions with the maximum absolute difference less than 3% (remembering that the sensitivity index is expressed in percentage). For simplicity but without loss of generality, equal weights are used for the models, i.e., $P(R_1) = P(R_2) = 0.5$ and $P(G_1) = P(G_2) = 0.5$. These are prior model probability; posterior model probability can be evaluated when field data are available, which, however, is not pursued in this study.

Table 1 lists the values of the first-order sensitivity index (S_i) evaluated for the parameters of the four models (R_1G_1 , R_1G_2 , R_2G_1 , and R_2G_2) evaluated for hydraulic head and ethene concentration at $x = 6000$ m. Taking model R_1G_1 as an example, the index values are for parameter a of model R_1 (equation (12)) and parameter

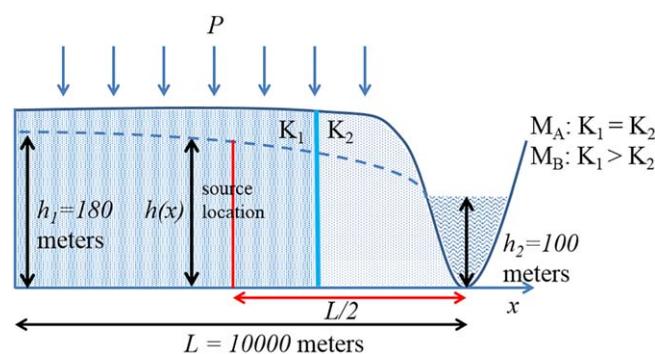


Figure 3. Diagram of the modeling domain of the synthetic study. $L = 10,000$ m is the domain length. Precipitation is uniform for the entire domain. Constant head (h) boundary conditions are $h_1 = 180$ m and $h_2 = 100$ m. The continuous contaminant source (marked in red) is located in the middle of the domain. The divide of the two zones of hydraulic conductivity at $x = 7000$ m is marked in blue.

K of model G_1 (equation (13)). For models R_1G_2 and R_2G_2 associated with the two-zone model (G_2), the values listed in Table 1 are for parameters K_1 and K_2 together. In other words, the parameter sensitivity index is calculated for the two parameters. Specifically speaking, the θ_i term in $V_{\theta_i}(E_{\theta_i})(\Delta|\theta_i)$ of equation (3) includes the two parameters. Since the first-order sensitivity index of a single model does not consider the interaction between model parameters, the summation of the index values of all model parameters is less than 100%. For example, for model R_1G_1 , the summation of the first-order sensitivity index for parameters a

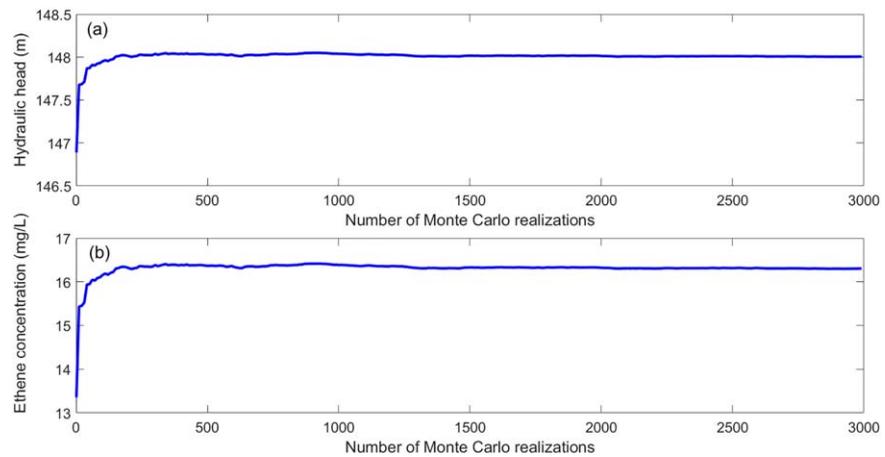


Figure 4. Convergence of sample mean of (a) hydraulic head and (b) ethene concentration for 3000 MC realizations. The sample means are stabilized after about 300 realizations.

and K is 99.63%, slightly smaller than 100%. This is true for all the four models, suggesting negligible parameter interaction for the individual models.

Without considering the process model uncertainty, important process would be identified using the parameter sensitivity index, S_i . Table 1 shows that the S_i values change dramatically between the individual models. As a result, if a single model is used and process identification is based solely on parameter sensitivity index, biased identification of important process may be resulted. Taking the hydraulic head as an example, Table 1 shows that the parameter sensitivity index of recharge parameters (a and b) decreases from 94.85% for model R_1G_1 to 6.51% for model R_2G_2 . It indicates that, to the head simulations, recharge is overwhelmingly more important than geology for model R_1G_1 , whereas geology is overwhelmingly more important than recharge for model R_2G_2 . The conflicting conclusions for the individual models in this example problem manifest the need of considering process model uncertainty for identifying important processes. The example modeling provides a general guideline that one should first start with parameter sensitivity analysis for individual models and then use the results to determine whether it is necessary to conduct processes sensitivity analysis for multiple models.

The problem of biased process identification may be resolved by considering the process model uncertainty. Table 1 lists the process sensitivity index (PS_K) of the two processes (recharge and geology) evaluated with considering the process models and their parameters. The PS_K values suggest that the geology process is significantly more important than the recharge process to the head simulation, and that the geology process is overwhelmingly more important than the recharge process to the ethene concentration simulation. The importance of geology process relative to the recharge process is physically meaningful, and it can be understood by examining Figure 5 that plots the probability density functions of hydraulic head and ethene

Table 1. Parameter and Process Importance to Simulated Head and Ethene Concentration at $x = 6000$ m Measured Using Parameter Sensitivity Index (S_i , %) of the Individual Models and Process Sensitivity Index (PS_K , %) of the Recharge and Geology Processes

Not considering process model uncertainty								
S_i (equation (3))	R_1G_1		R_1G_2		R_2G_1		R_2G_2	
	a	K	a	K_1 and K_2	b	K	b	K_1 and K_2
Head	94.85	4.78	61.5	37.83	88.70	10.62	6.51	93.24
Concentration	21.25	78.47	67.66	5.53	1.48	98.49	16.53	81.04
Considering process model uncertainty								
PS_K (equation (2))	Recharge				Geology			
Head	28.43				67.94			
Concentration	0.11				80.99			

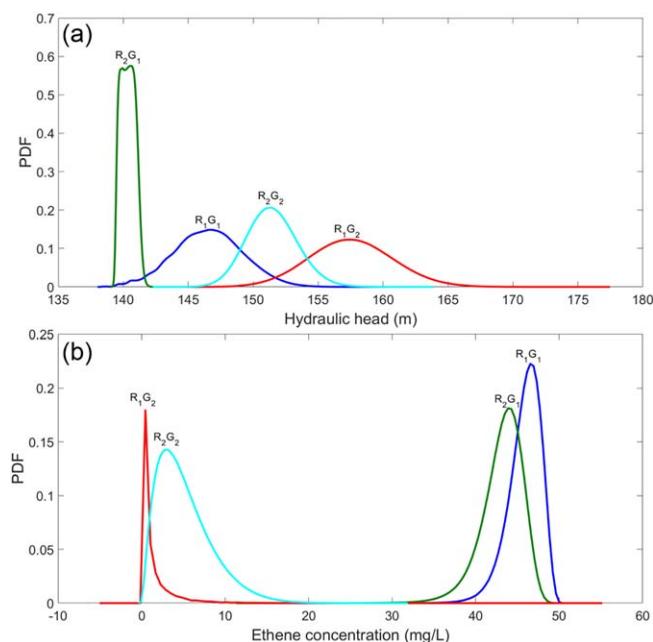


Figure 5. Probability density functions (PDFs) of (a) hydraulic head and (b) ethene concentration at $x = 6000$ m simulated by the four individual process models.

concentration simulated by the individual models. In Figure 5a, taking the right most three PDFs of models R_1G_2 , R_2G_2 , and R_1G_1 as an example, when the geological model is fixed at G_2 but the recharge model changes from R_1 to R_2 , the PDF of R_2G_2 deviates substantially from that of R_1G_2 . When the recharge model is fixed at R_1 but the geological model changes from G_2 to G_1 , the PDF of R_1G_1 deviates more substantially from that of R_1G_2 . The same is observed for the three PDFs of models R_2G_1 , R_1G_1 , and R_2G_2 . Therefore, the geology process should be more important than the recharge process for the head simulations. The same conclusion can be drawn for the PDFs of the concentration simulation plotted in Figure 5b. For both R_1 and R_2 , when the geological model changes from G_1 to G_2 , the corresponding PDFs change dramatically. The change is significantly larger than

that occurs when the recharge model changes from R_1 to R_2 for a geological model. These results indicate that the process sensitivity index is able to quantify the degree of relative importance for the recharge and geology processes.

The sensitivity index values listed in Table 1 and the PDFs plotted in Figure 5 for the individual models indicate the interactions between the process models and between the model parameters, because the index values and PDFs change dramatically between the models. The interactions are included in the process sensitivity index (equation (6)), because it considers all the process models and their parameters. It may be possible to use the process sensitivity index to quantitatively measure the degree of process interaction, which however is beyond the scope of this study. It should be noted that the parameter sensitivity index values of different models are not directly comparable, because the values are based on the simulation variance (i.e., $V(\Delta)$ used in equation (3)) that is different for different models. By the same token, the process sensitivity index values are not directly comparable with the parameter sensitivity index values, considering that the process sensitivity index is based on $V(\Delta)$ used in equation (2) that considers both parametric and model uncertainties. Taking the head simulated at $x = 6000$ m as an example, its variance values are 3.90, 6.21, 1.16, and 10.77 for models R_1G_1 , R_1G_2 , R_2G_1 , and R_2G_2 , respectively. After considering model uncertainty, the variance value increases to 446.48. As a result, it is not surprising that the process sensitivity index is not within the range of parameter sensitivity index.

Figure 6 plots the spatial variation of the processes sensitivity index of hydraulic head evaluated for the entire domain. The figure shows that, at the left end of the domain, the recharge process is significantly more important than the geology process. The recharge process gradually becomes less important, while the importance of the geology process gradually increases. After the location of $x = 3700$ m, the geology process becomes more important than the recharge process. At the location of $x = 7000$ m (the boundary of the two zones of hydraulic conductivity), the geology process index reaches its maximum, and the recharge process index reaches its minimum. After $x = 7000$ m, the geology process index decreases, and the recharge process index increases. This variation pattern is physically reasonable. At the left end of the domain near the constant-head boundary (Figure 3), hydraulic head is determined mainly by recharge. Since hydraulic conductivity of zone 1 ($x < 7000$ m) is larger than that of zone 2 ($x > 7000$ m) and zone 2 acts as a barrier to the flow from left to right, from the left boundary to the divide of the two zones, the influence of hydraulic conductivity on head becomes more and more important than recharge. After the

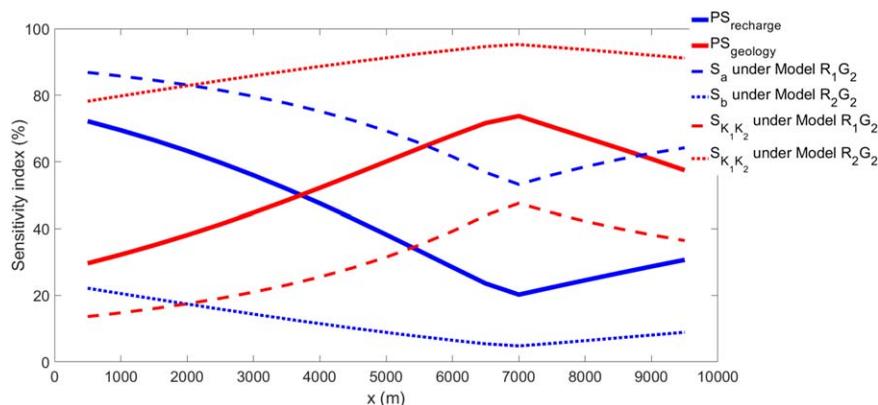


Figure 6. Parameter sensitivity index (S , %) (the recharge and geology process parameters under models R_1G_2 and R_2G_2) and process sensitivity index (PS , %) of hydraulic head estimated for the entire model domain.

zone boundary, since groundwater flows freely to the constant-head boundary at the right boundary, the influence of hydraulic conductivity reduces and that of recharge increases.

The profiles (along the x coordinate of the model domain shown in Figure 3) of the process sensitivity index and the parameter sensitivity index shown in Figure 6 suggest that there is a relation between the two kinds of sensitivity index. This is based on two observations. The first observation is that the profiles of process sensitivity index and the profiles of parameter sensitivity index have similar spatial variation patterns. For example, from the left to the right end of the modeling domain, the three profiles (the blue lines) of recharge sensitivity decrease within zone 1 ($x < 7000$ m) of hydraulic conductivity and then increases within zone 2 ($x > 7000$ m) of hydraulic conductivity. The other observation is that the profiles of the process sensitivity index are located between the profiles of the parameter sensitivity index. Since the profiles of the process sensitivity index are not located in the exact middle of the profiles of the parameter sensitivity index, the processes sensitivity index is not a simple average of the parameter sensitivity index of the individual models, recalling that the prior model probabilities are $P(R_1) = P(R_2) = 0.5$ and $P(G_1) = P(G_2) = 0.5$. Investigating the quantitative relation between the process and parameter sensitivity indices is warranted in future studies.

4. Reduction of Computational Cost

As discussed in section 2 and shown in Figure 2a, to evaluate the process sensitivity index for each process needs four loops, and the corresponding number of model executions is $(m_i \times n_i) \times (m_{\sim i} \times n_{\sim i})$, where m_i is the number of models of the i th process, n_i is the number of model executions for a single model of the process, $m_{\sim i}$ is the number of process model combinations for the processes other than the i th process, and $n_{\sim i}$ is the number of model executions corresponding to the process model combinations. The $n_i \times n_{\sim i}$ number of model executions is computationally demanding, which renders the evaluation of process sensitivity index practically unaffordable for models with moderate computational cost. This section discusses several ways of reducing the computational cost.

The computational cost can be reduced by using computationally frugal methods (rather than MC methods) to evaluate the mean and variance terms involved in the process sensitivity index. Example computationally frugal methods include Newton-type optimization methods and first-order sensitivity analysis and uncertainty intervals, and they take only 10–100 s model runs for evaluating mean simulations and corresponding variance [Hill et al., 2015]. An example application of the computationally frugal methods for global sensitivity analysis was given by Rakovec et al. [2014], who used the results of first-order sensitivity analysis to evaluate the variance term of the Sobol' first-order sensitivity index for model parameters. However, applying the computationally frugal methods to the evaluation of process sensitivity index is not straightforward, due to the nested structures of process models and process model parameters discussed in section 2.

The computational cost of evaluating the process sensitivity index can also be reduced by using computationally efficient methods of numerical integration (rather than MC methods) to evaluate the mean and

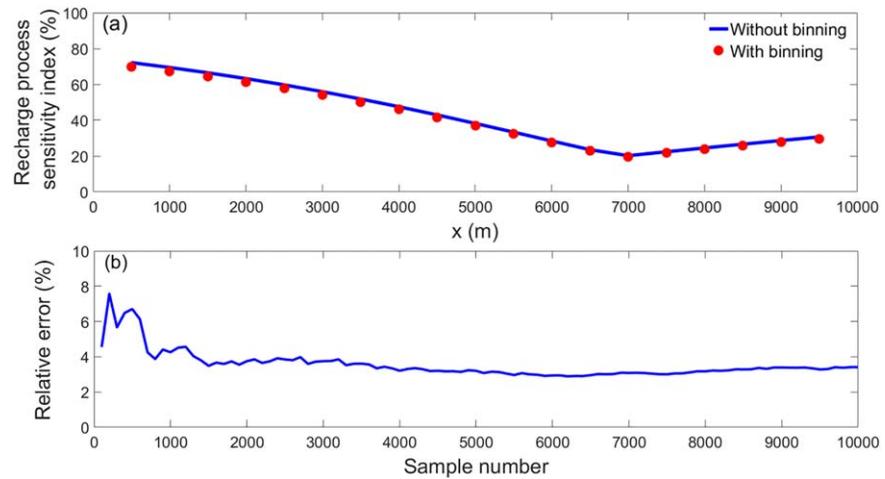


Figure 7. (a) Recharge process sensitivity index (%) for simulated head at different locations of the model domain using the MC methods with and without binning implementation. (b) Absolute relative error of the recharge process sensitivity index obtained using the binning implementation for simulated hydraulic head at the location of $x = 6000$ m; the recharge process sensitivity index obtained without using the binning implementation is used as the reference.

variance terms involved in the process sensitivity index. One promising method of numerical integration is the sparse-grid collocation methods, which have been used for evaluating mean and variance of hydraulic head and solute concentration [e.g., Lin and Tartakovsky, 2009]. Dai and Ye [2015] recently used the sparse-grid collocation methods for evaluating the mean and variance terms involved in the Sobol' first-order and total-effect sensitivity indices, and their numerical examples showed that a substantial amount of computational cost was saved by replacing the quasi-MC method [Saltelli et al., 2010] by the sparse-grid collocation methods. Applying the sparse-grid collocation methods to the evaluation of process sensitivity index is conceptually straightforward, and it can be done by evaluating $E_{\theta_B|M_B}[\Delta|\theta_A, M_A, \theta_B, M_B]$ directly without using the fourth loop of evaluating $\Delta|\theta_A, M_A, \theta_B, M_B$ shown in Figure 2a. This implementation requires developing computer codes for sparse-grid integration, which however is not trial and thus not attempted in this study.

This study implements a binning method to reduce the computational cost of evaluating the process sensitivity index by approximating the mean for a single parameter value by the mean for a bin of parameter values. Taking the $E_{M_A}E_{\theta_A|M_A}E_{M_B}E_{\theta_B|M_B}[\Delta|\theta_A, M_A, \theta_B, M_B]$ term in equation (11) as an example, since $E_{\theta_A|M_A}$ can be computed as $E_{\theta_A|M_A} = \sum E_{\theta_A^{bin}|M_A}$ for the binning method, the same accuracy can be achieved by replacing $E_{\theta_B|M_B}[\Delta|\theta_A, M_A, \theta_B, M_B]$ with $E_{\theta_B|M_B}[\Delta|\theta_A^{bin}, M_A, \theta_B, M_B]$. This makes it possible to break the nested structure of process model parameters in the following procedure: (1) generate multiple realizations (θ_A and θ_B) for random parameters θ_A and θ_B , (2) simulated Δ for the parameter realizations, (3) separate the θ_A realizations into bins, (4) for each θ_A bin, evaluate $E_{\theta_B|M_B}[\Delta|\theta_A^{bin}, M_A, \theta_B, M_B]$ using the θ_B realizations belonging to the θ_A bin. After $E_{\theta_B|M_B}[\Delta|\theta_A^{bin}, M_A, \theta_B, M_B]$ is evaluated for each θ_A bin, $E_{\theta_A|M_A}$ is evaluated by taking the average of the bin-based values. The pseudo code for evaluating all the terms in equation (11) of the process sensitivity index is given in Figure 2b. The number of model executions thus becomes from $(m_i \times n_i) \times (m_{\sim i} \times n_{\sim i})$ to $m_i \times m_{\sim i} \times n$, where n is the number of θ_A and θ_B realizations. The binning method can save significant amount of computational cost, because n can be significantly smaller than $n_i \times n_{\sim i}$. A test for the calculation of the means involved in the process sensitivity index.

Figure 7 compares the recharge process sensitivity index for hydraulic head evaluated with and without the binning method. Without the binning method, the number of model executions is 36,000,000 as explained in section 4, and the corresponding results are used as a reference to evaluate the accuracy of the binning method. Figure 7a shows that, except at the left boundary, the binning results are almost identical to the results without binning. The number of model executions for obtaining the binning results is only 40,000 (10,000 parameter realizations are generated for each of the four process model combinations). The computational cost can be further reduced, because Figure 7b shows the relative error of the binning results (for hydraulic head at the location of $x = 6000$ m) is stabilized at 3.8% after about 4000 parameter realizations. In other words, the binning results based on 16,000 model runs are of similar accuracy to those based

36,000,000 model runs without the binning method. The accuracy of the binning method can be improved by replacing the random sampling method used in this study by Sobol sequence or Latin hypercube sampling methods. More research to improve the computational efficiency and accuracy is warranted in future studies.

5. Discussion

The multimodel sensitivity analysis presented in this paper is the first step for identifying important system processes under the uncertainty in process models and process model parameters. It is necessary to further evaluate the derivation and calculation of process sensitivity index for complex and real-world processes models, e.g., those of *Ye et al.* [2010, 2016] and *Lu et al.* [2015] for groundwater systems and those of *Clark et al.* [2015a, 2015b] for hydrology and earth systems. Such process models may pose new challenges (theoretical and computational) to the current process sensitivity index presented in this paper. For example, for complex groundwater reactive transport models with nonlinear biogeochemical reactions, parameters and outputs can be non-Gaussian [*Zhang et al.*, 2013; *Shi et al.*, 2014]. In this case, entropy or other statistics of information theory may better quantify variability of model parameters and outputs [*Nearing and Gupta*, 2015].

The current derivation of the process sensitivity index relies on using the model averaging methods for quantifying model uncertainty (in competing process models) and parametric uncertainty (in process model parameters). This is based on the assumption that, given available data and information, one cannot either postulate any new models or discard any existing models. In other words, the models considered in the multimodel process sensitivity analysis reflect one's best understanding of the system of interest and its processes. While this assumption is reasonable in practice, the model averaging methods can only quantify the uncertainty reflected in the considered alternative models, but cannot quantify model uncertainty in an absolute sense for the following two reasons: (1) other plausible models are not included in the sensitivity analysis and (2) none of the considered models can adequately represent system processes [*Beven*, 2016; *Nearing et al.*, 2016]. To address these problems requires gathering data and information for in-depth understanding and characterization of system processes. New data and information may invalidate prevailing models and/or lead to new models [*Bredehoeft*, 2005]. In addition, new data can also be used to better rank existing models [e.g., *Dai et al.*, 2012; *Massoudieh et al.*, 2013] and/or to calculate the process sensitivity index conditioned on the data via equations (8)–(10). This may lead to model-enabled design of experiments and data collection campaigns so that important processes can be identified for a site of interest using the least amount of data. This may be done in the framework of data-worth analysis under model uncertainty [*Neuman et al.*, 2012; *Lu et al.*, 2012; *Xue et al.*, 2014].

6. Conclusions

This study derives for the first time a process sensitivity index to tackle the problem of identifying important processes of a hydrologic system when system processes can be simulated by multiple competing models. The process sensitivity index can be used a single summary measure to rank process importance in the situation that both process models and parameter values are uncertain. This situation is more complex than the situation of conventional sensitivity analysis that only quantifies parametric uncertainty. The process sensitivity index is built on the integration of model averaging and global sensitivity analysis methods, and explicitly breaks a system model into process models for analysis including uncertainty in both process models and model parameters. The synthetic example of groundwater reactive transport modeling illustrates that the important process can change when different process models are used. If process model uncertainty is not considered, biased process identification may result.

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Erratum

The originally published version of this article incorrectly stated that the parameter a of model R1 follows the normal distribution of $N(3.35,1)$, and the calculated sensitivity indices of models R1G2 and R2G1 in Table 1 were placed in wrong columns. The distribution has been corrected to $N(16.88,25.4)$; because the correct normal distribution was used in the numerical calculation, the numerical results were not impacted. Table 1 has also been corrected, and Figure 2 has been updated to improve readability. This updated version may be considered the official version of record.