Combined Estimation of Hydrogeologic Scenario, Model, and Parameter Uncertainty with Application to Groundwater Reactive Transport Modeling

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1. Introduction

➢Groundwater contamination has been a serious health and environmental problem in many areas over the world nowadays. Groundwater reactive transport modeling is vital to make predictions of future contaminant reactive transport. However, these predictions are inherently uncertain, and uncertainty is one of the greatest obstacles in groundwater reactive transport.

➢We propose a Bayesian network approach for quantifying the uncertainty and implement the network for a groundwater reactive transport model for illustration. In the Bayesian network, different uncertainty sources are described as uncertain nodes. All the nodes are characterized by multiple states, representing their uncertainty, in the form of continuous or discrete probability distributions that are propagated to the model endpoint, which is the spatial distribution of contaminant concentrations.

➢After building the Bayesian network, uncertainty quantification is conducted through Monte Carlo simulations to obtain probability distributions of the variables of interest. In this study, uncertainty sources include scenario uncertainty, model uncertainty, parameter uncertainty. Variance decomposition is used to quantify relative contribution from the various sources to predictive uncertainty. While these new developments are illustrated using a relatively simple groundwater reactive transport model, our methods is applicable to a wide range of models. The results of uncertainty quantification are useful for environmental management and decision-makers to formulate policies and strategies.

2. Bayesian Network Model Description

2.1 Uncertainty Quantification Framework

The sources of the predictive uncertainty, from a system point of view, can be categorized into scenario uncertainty in system input, model uncertainty in model structure and parametric uncertainty in model parameters.

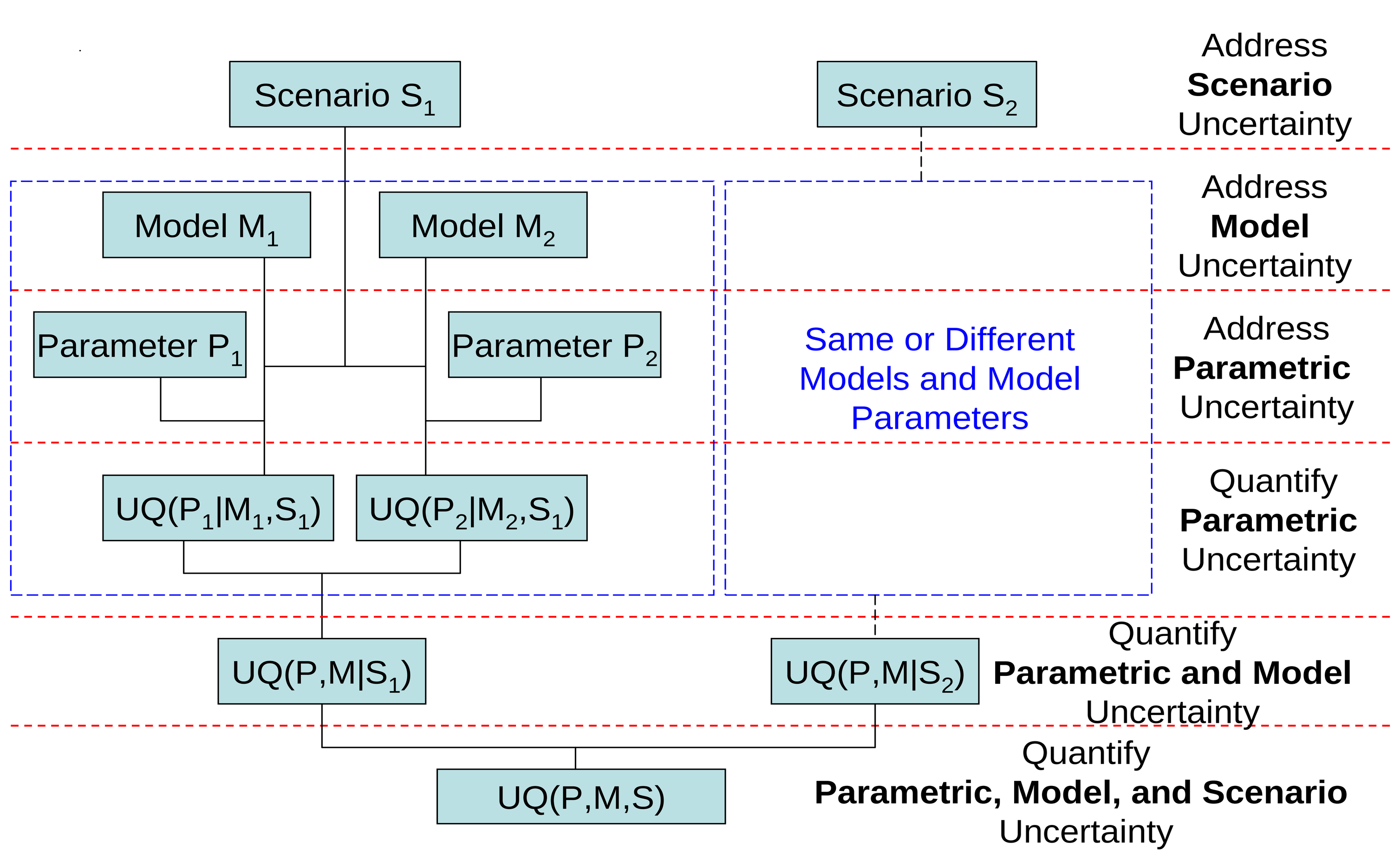

Figure 1. Hierarchical structure of characterization and quantification of scenario, model, and parametric uncertainties.

2.2 Bayesian Network Model Structure

Bayesian network represents a set of random variables and their conditional dependencies via a directed acyclic graph (DAG). It is suitable to be implemented into the groundwater reactive transport modeling for uncertainty quantifications considering multiple uncertainty sources simultaneously.

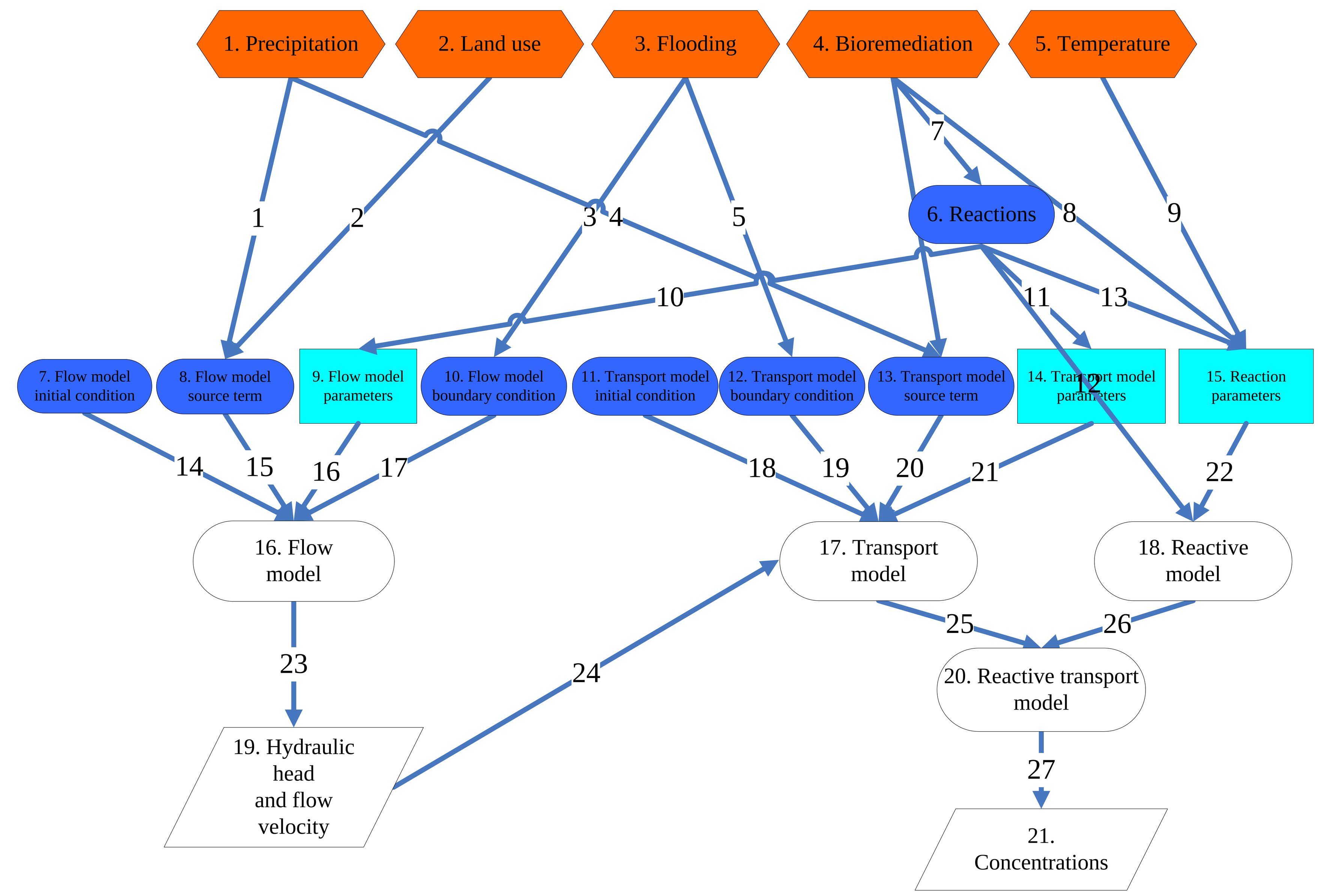

Figure 2. Bayesian network model structure.

As Fig. 2. shows, each node in the graph represents a random variable, while the edges between the nodes represent probabilistic dependencies among the corresponding random variables. Different colors indicate different uncertainty sources.

2.3 Bayesian Network Model Application

One synthetic test case is built to demonstrate the application of the Bayesian network model.

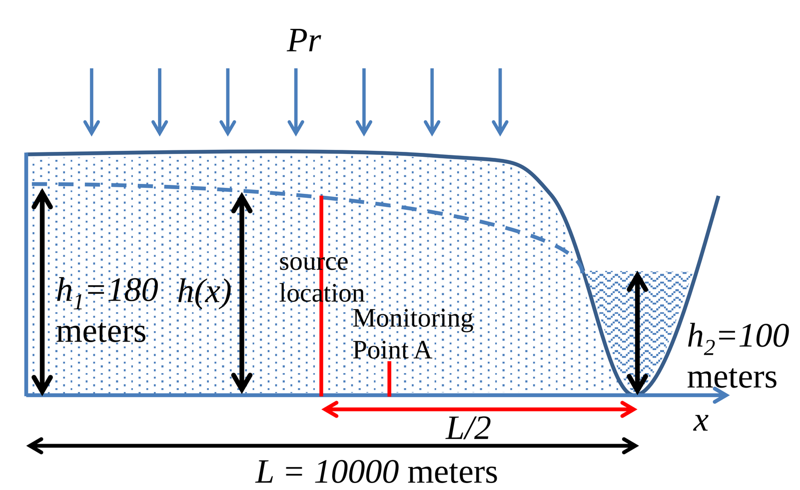

Figure 3. Test case domain profile.

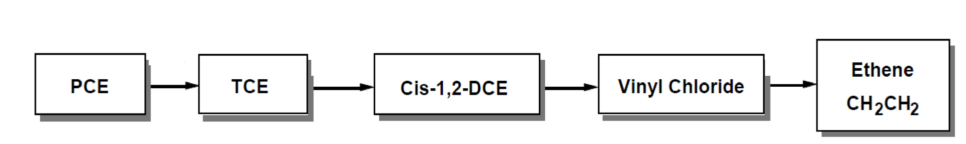

Figure 4. Chain reactions considered in the test case.

$$\frac{\partial}{\partial x}\left(K_x\frac{\partial h^2}{\partial x}\right)=-2w$$

$$R_1\frac{\partial c_1}{\partial t}=D_x\frac{\partial^2 c_1}{\partial x^2}-v_s\frac{\partial c_1}{\partial x}-k_1c_1$$

$$R_i\frac{\partial c_i}{\partial t}=D_x\frac{\partial^2 c_i}{\partial x^2}-v_s\frac{\partial c_i}{\partial x}+y_{i-1}k_{i-1}c_{i-1}-k_ic_i,\quad \text{for } i=2,3,\ldots,n$$

As shown above, the test case is built in one dimensional domain (L = 10000 meters) with a unconfined aquifer and precipitation recharge. A series of single direction chemical reactions include five reactants are considered in the reactive transport model.

3. Bayesian Network Model Results

The relative contributions of different uncertainty sources to the predictive uncertainties are studied in this research. Hydraulic head and Ethene concentration are two chosen interested model outputs. The results can be shown in Fig. 5 - 8.

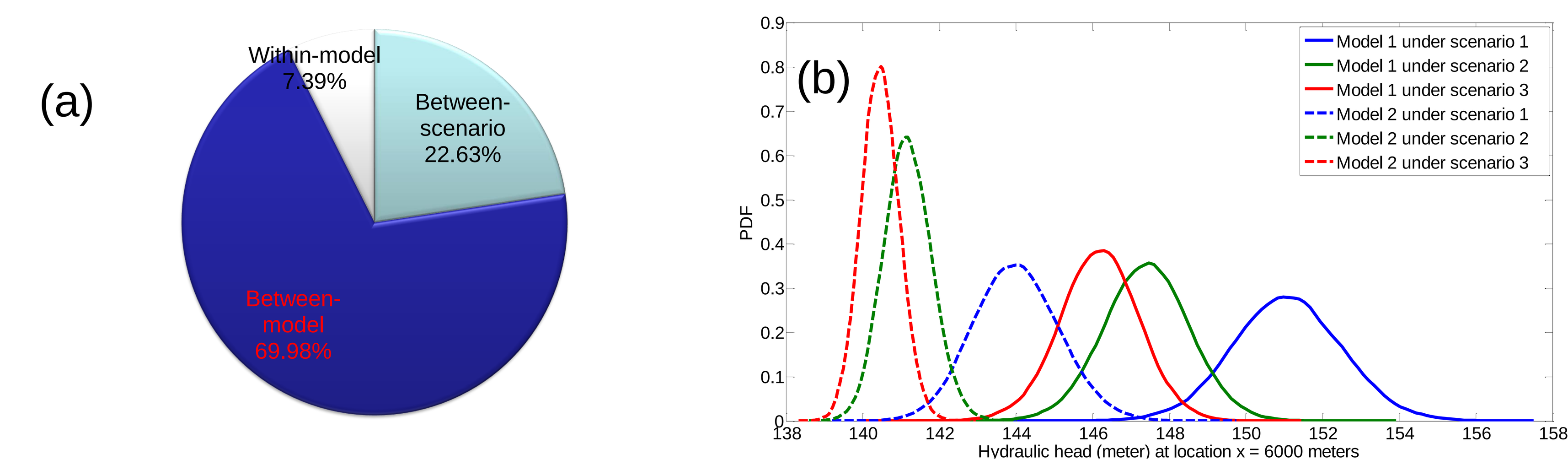

Figure 5. (a) Relative contributions of scenarios and model uncertainties to the hydraulic head predictions and (b) the PDF of hydraulic head predictions under different scenarios and models at location x = 6000 meters.

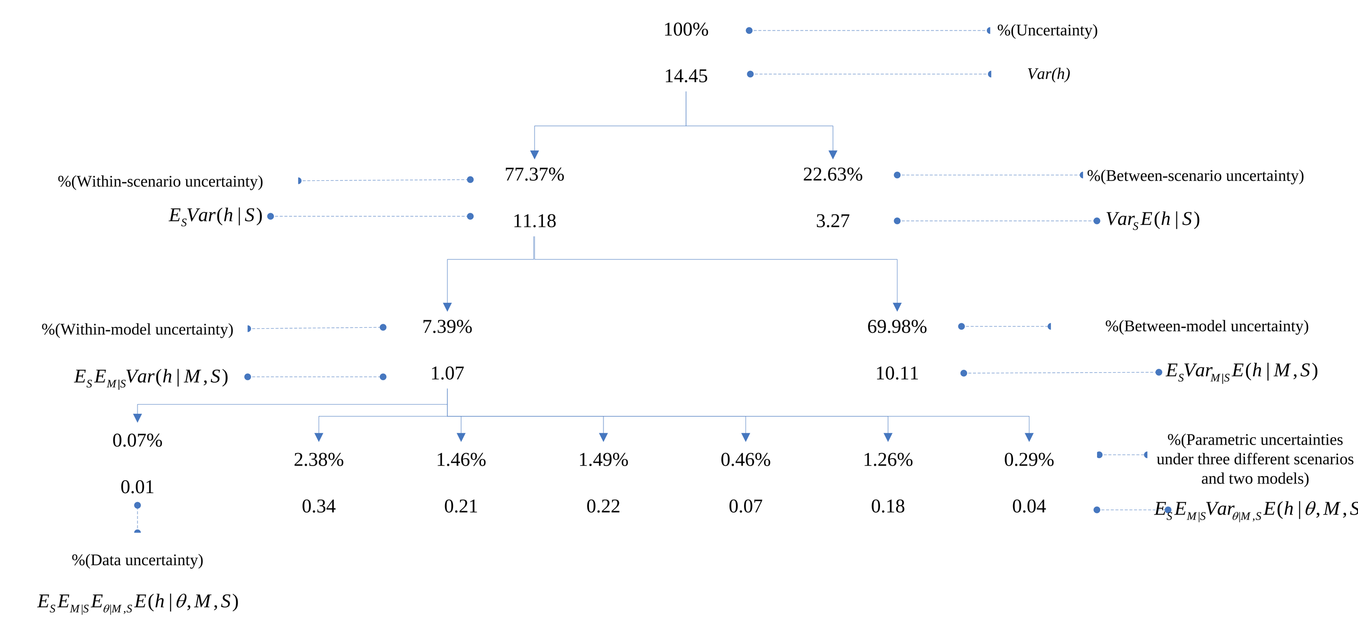

Figure 6. Relative contributions of different uncertainty sources to the hydraulic head at location x = 6000 meters represented using Bayesian uncertainty tree.

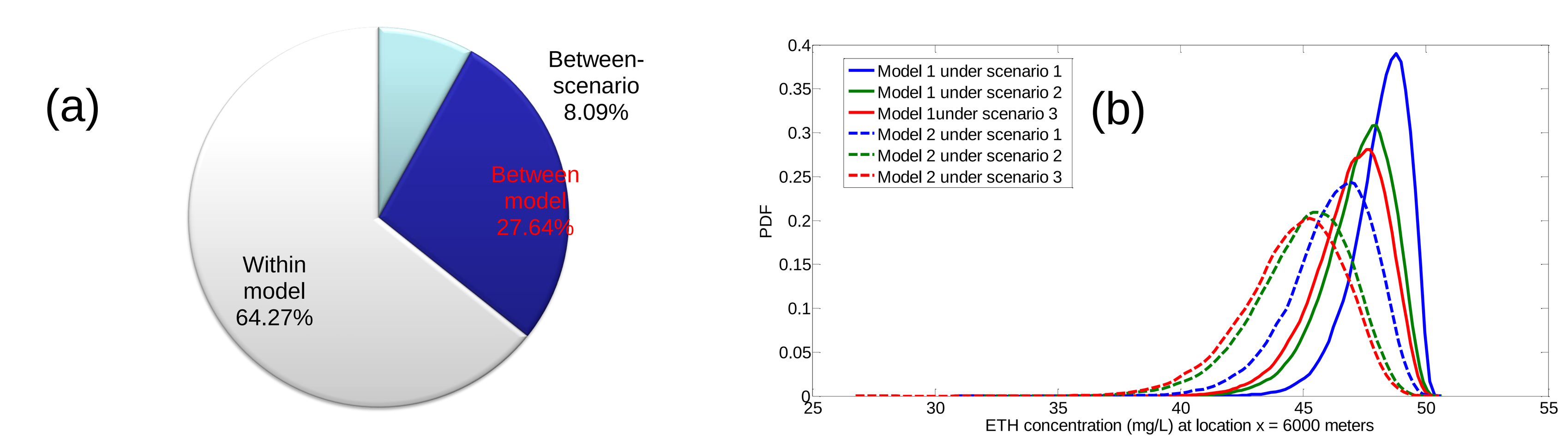

Figure 7. (a) Relative contributions of scenarios and model uncertainties to the Ethene concentration predictions and (b) the PDF of Ethene concentration predictions under different scenarios and models at location x = 6000 meters.

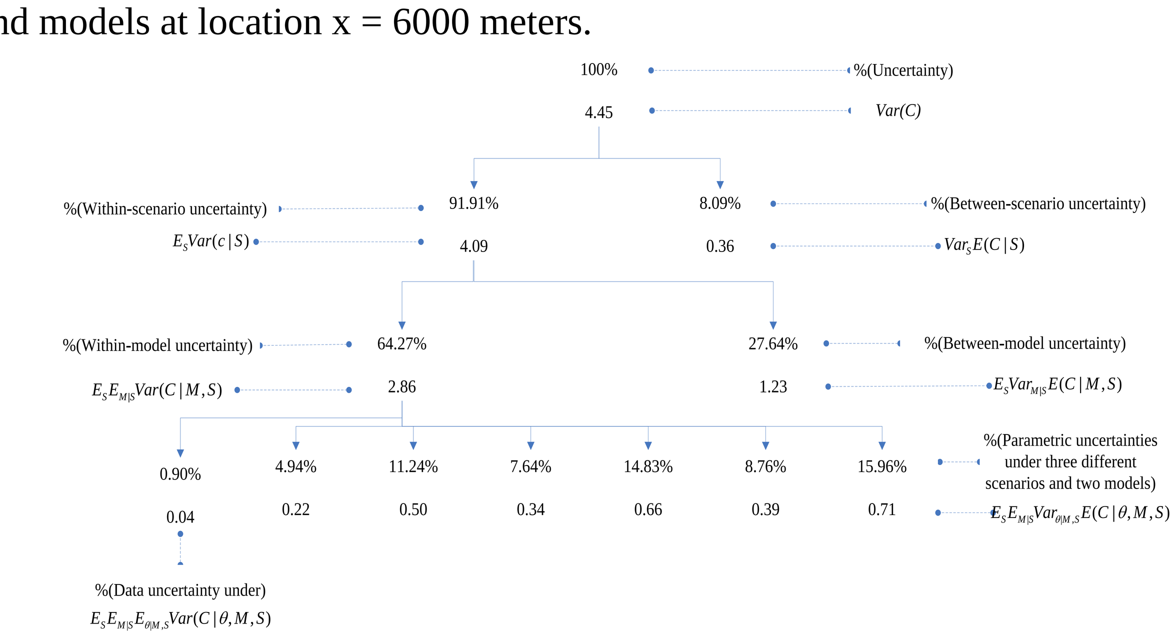

Figure 8. Relative contributions of different uncertainty sources to the hydraulic head at location x = 6000 meters represented using Bayesian tree.