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Research paper

# A comparison of various uncertainty models: An example of subsurface contaminant transport

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**Abstract**

Groundwater resources are under increasing threat of contamination and wasteful use in many parts of the world. Groundwater flow and integrated contaminant transport models are commonly used to predict the fate of contaminants in the subsurface environment. However, the lack of reliable data and complexity of the natural environmental systems, the predictions are subjected to large uncertainties. For reliable decision-making, these contaminant transport models are required to explicitly consider associated uncertainties in their parameters. This paper aims to compare the results of four common uncertainty models using an example of contaminant transport in groundwater. The research employed an advection−dispersion equation (ADE) to describe the transport of a contaminant in groundwater. For simplicity, two parameters − dispersion coefficient and velocity − were considered in the uncertainty analysis. Fuzzy set theory, one- and two-dimensional (1-D and 2-D) Monte Carlo simulations, and Probability Box (P-Box) methods were investigated. The cumulative distribution functions generated from these analyses were compared to evaluate the capabilities of these methods. The comparison showed that P-Box method provides a more comprehensive analysis with lesser assumptions as compared to other methods, and also found to be more pragmatic way to describe and propagate uncertainties in complex environmental systems. Furthermore, execution time required to perform uncertainty analysis using P-Box method is comparatively much less than 2-D Monte Carlo simulations.


*Keywords:* Contaminant transport; Uncertainty analysis; Probability box; Monte Carlo simulations; Fuzzy set theory

## 1. Introduction

The level of uncertainty associated with a system is proportional to its complexity, which arises as a result of vaguely known relationships among various entities, and randomness in the mechanisms governing the domain. The complex systems like environmental, socio-political, engineering, or economic systems, which involve human interventions with vast arrays of inputs and outputs cannot all possibly be captured analytically or controlled in a conventional sense. Water systems are extremely complex and dynamic in nature. To understand the impacts of the physico-chemical, biological and socio-economical changes in the surrounding environment, tremendous efforts have been devoted to enhance the body of knowledge about various processes occurring in hydrosystems. However, the lack of reliable data due to resource constraints and complexities inherent in the natural environmental systems limits human ability to make correct predictions. Therefore, proper treatment of uncertainties is required for modeling hydrosystems.

### *1.1. Taxonomy of uncertainties*

Uncertainties can arise from various sources in water resources engineering. These include data uncertainty, structural uncertainty (raised from the imperfect description of physical reality by a limited number of mathematical relations), and parameters uncertainty (Mannina and Viviani, 2010; Freni

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et al., 2009; Willems, 2008). Data uncertainties may include (but are not limited to) measurement errors, inconsistency and non-homogeneity of data, data handling and transcription errors, and inadequate representation of data sample due to time and space limitations. Moreover, the uncertainty in the estimation of model parameters implicitly considers the error induced by incorrect model structure, data errors and climatic variation factors. Simonovic (1997) indicated randomness and lack of knowledge as the two major sources of uncertainty. As a result, uncertainty is either an objective fact of the phenomenon under consideration or a subjective impression of human perception (Zimmermann, 2001). Aleatory uncertainty (also known as stochastic or objective uncertainty) results from the fact that a system can behave in random ways. In general, the uncertainties due to inherent randomness of a physical process cannot be eliminated or reduced. An epistemic uncertainty (also known as subjective or ignorance) results from the lack of knowledge about a system. Due to stochastic nature of natural phenomena, an aleatory uncertainty is always associated with the natural systems. On the other hand, an epistemic uncertainty is reducible by data analysis, making additional monitoring, and deepening our understanding and knowledge of the phenomenon. The traditional approach to handle an aleatory uncertainty is probabilistic analysis based on historical data (a frequentist approach). An epistemic uncertainty, on the other hand, has traditionally been addressed through Bayesian approach even though the approach was limiting as it required priori assumptions (Sentz and Ferson, 2002).

### 1.2. Uncertainty analysis in water resources engineering

In water resources engineering, the design quantities and system outputs depend on several system parameters, and not all of them can be quantified with absolute accuracy. Thus, several techniques with different levels of mathematical complexity and data requirements have been reported in the literature for conducting uncertainty analysis in different areas of water resources engineering. Selection of an appropriate technique to be used in a particular problem depends strongly on the nature of the problem, availability of information, resources constraint, model complexity, and type and the desired level of the accuracy and/or reliability of the results. Overall, the uncertainty methods are generally classified into the two groups of analytical and approximation techniques. Table 1 provides a summary of this classification along with several recent applications in water resources engineering.

Analytical techniques: These techniques (e.g., first and second order reliability methods) are mathematically less demanding, and therefore can be implemented straightforwardly. Their applications, as indicated in Table 1, are fairly limited due to oversimplification and/or assumptions.

Approximation techniques: These techniques are mathematically more complex and have traditionally been applied to a broad range of water resources problems. The most common examples of approximation techniques are fuzzy set theory, one- and two-dimensional (1-D and 2-D) Monte Carlo simulations, Bayesian and Probability Box (P-Box) methods.

The fuzzy set theory, 1-D and 2-D Monte Carlo simulations, and P-Box method have been frequently applied to conduct an uncertainty analysis in water resources area. Although Guyoanet et al. (1999) reported more realistic results for the fuzzy set theory (in human health and environmental risk analyses where response values at the tails are important), there is still no clear and direct study comparing the performance and robustness of these techniques. Thus, the primary objective of this study is to compare the four common approximation techniques (i.e., fuzzy set theory, 1-D and 2-D Monte Carlo simulations, and P-Box method) with regards to their conservativeness, execution time, ease of formulation, and complexity in uncertainty analysis in water resources. The study advances by applying the techniques to a case of contaminant transport in a groundwater flow. Both numerical and analytical solutions of the governing advection−dispersion equation (ADE) are used to compute temporal and spatial variations of a contaminant concentration. Two parameters, namely, velocity and contaminant dispersion coefficient, are identified to perform uncertainty analyses using above four methods.

## 2. Contaminant transport in groundwater

Groundwater resources are vulnerable to a wide variety of hazards that could potentially limit their ability to perform satisfactorily. Groundwater pollution resulting from agriculture, industrial, and waste-disposal activities is a very serious problem that often requires extensive treatments. In case of groundwater pollution, remediation procedures are required to keep contaminant concentrations below threshold limits. Moreover, the remediation procedures are often cost-effective and require careful evaluations of the extent of the pollutions. On the other hand, such evaluations rely on the accuracy of the data for aquifer properties. Vague or imprecise information especially arises in the identification and determination of aquifer properties. Comprehensive collection of aquifer data is extremely expensive due to their large spatial and temporal variations of the effective parameters. The lack of field data and parameters variations may have impacts on the reliability of a model's results. The diversity of uncertainty sources presents a great challenge to groundwater systems' planning and management. Therefore, a comprehensive modeling approach is required to 1) consider parameters' uncertainties, 2) propagate uncertainties throughout the system, and 3) help authorities to wisely make informed decisions at planning, design, and management levels. This is particularly important because conventional deterministic techniques in practice are unable to account for possible variations of system responses.

### 2.1. Governing equation

Fig. 1 shows a typical one-dimensional contaminant transport in a uniform groundwater flow field. The aquifer is assumed to be homogeneous and isotropic. For simplicity, the contaminant is considered conservative; therefore no decay or growth process is considered. Assuming a steady uniform flow