Uncertainty Quantification Using Stochastic Response Surface Method Case Study – Transport of Chemical Contaminants through Groundwater

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Abstract

Transport of contaminants through groundwater is an important research component in the field of nuclear industry for designing the waste disposal facilities and remedial action plans. Randomness of the input parameters of the governing groundwater model necessitates the uncertainty quantification of the concentration of the contaminant at any specific spatial location for a fixed time or vice versa. Stochastic response surface method, i.e., response surface of the contaminant concentration with these random parameters is applied to estimate the associated uncertainty. Stochastic response surface is based on polynomial chaos theory. The method is illustrated with a case study in which flow of a tracer chemical is considered. The purpose of this study was to know the role of various hydro geologic parameters in the uncertainty assessment of the contaminant concentration. This study can also provide an environmental monitoring program in the nuclear industry.

Keywords: *groundwater model, uncertainty, polynomial chaos*

1. Introduction

Successive progress of computer simulation technology in science and engineering facilitates researcher in the respective domain to solve a large number of complex problems pertaining to various stochastic processes. However, uncertainties associated with the physical parameters of the processes originated due to lack of sufficiency of data or knowledge and error in the measurements makes difficult to provide objective confidence measures of the numerical predictions. Uncertainties are typically classified as aleatory and epistemic [1]. Aleatory uncertainty (also called probabilistic uncertainty) arises from randomness in the system. Uncertainty that is explicitly recognized by a stochastic model is also aleatory. The stages involved in the uncertainty quantification of a model include, (a) estimation of uncertainties of model inputs, (b) estimation of uncertainty of the model output, and (c) propagation of uncertainty in the model output. Monte Carlo methods are the most widely used techniques for statistical/probabilistic uncertainty analysis, with diverse applications [2]. Given input uncertainty distributions (frequency or probability density data) these methods involve repeated generation of pseudo-random instantiations (sampling) of inputs followed by application of the model to these instantiations to yield a set of model responses. These model outputs are then further analyzed statistically. As a starting point for the method of uncertainty propagation, it is assumed that the nonlinear system under investigation is broken down into interconnected components. The disadvantage of this traditional sampling based technique is the requirement of large number of model simulations

(for example ~10^6 or more) [2, 3] to achieve an acceptable level of confidence about model output uncertainty characterizations. So, obviously the basic target is to reduce the large number of simulations so that the algorithm involved in the computation scheme can be labelled as efficient [3].

Stochastic response surface method is adopted to achieve the goal in which the number of model simulations for adequate estimation of uncertainty is substantially reduced as compared to conventional simulation. The input uncertain random parameters are transformed into the space of corresponding standard normal random variables (srvs); Coefficients of the stochastic response surface is solved by standard regression analysis. Statistical behaviour of the response surface is evaluated by a large number of standard Monte Carlo simulations of the associated srvs corresponding to uncertain input parameters. This efficient simulation method presented in this paper is called as "Polynomial Chaos Expansion" (PCE) [4]. PCE is applied for quantification and propagation of the uncertainty of the model output with a limited number of model run.

Stochastic response surface method (SRSM) of uncertainty analysis for a non-linear problem is demonstrated with the groundwater model in which the injection of a tracer chemical and its corresponding concentration as a function of time and distance is presented. Advection, dispersion and retardation processes are considered for the flow of the solute through a confined aquifer.

2. Theory of SRSM

SRSM is based on polynomial chaos theory. So, explanation of SRSM is presented here through he Polynomial Chaos Expansion (PCE) approach. The PCE approach has its foundation in the work of Wiener (1938) [4], who represented a Gaussian process as an infinite series of Hermite polynomials that take a vector of random variables as arguments. Ghanem and Spanos (1991) [5] used this representation to develop the stochastic finite element method. Xiu and Karniadakis (2002) [6] extended the theoretical framework to non-Gaussian process by using different polynomial basis functions. This generalized polynomial chaos approach was used to address the problem of heat transfer with random material properties by Wan et al. 2004 [7].

The PCE is the representation of a random variable, more generally a stochastic process, with an infinite series of orthogonal polynomials that take a vector of independent and identically distributed (iid) random variables as arguments. The expansion uses a rescaled version of Hermite polynomials which correspond to a Gaussian or normal distribution when used in combination with Gaussian random variables. The expansion technique is based on independent random variable ξ which are associated with independent random event θ. In polynomial chaos every uncertain parameter or variable in the examined system is represented by a random variable ξ. Every variable in the examined system must be expanded along the entire multi-variable polynomial basis. The individual polynomials of the basis will be denoted by Γ. So, if the number of uncertain variables are 'n' and order of the basis polynomial is 'r', then in PCE, an uncertain variable Y(t) can be written in terms of a basis of a 'stochastic space' as

$$Y(t,\xi) = \sum_{i=0}^{N} y_i(t)\,\Gamma_i(\xi) \tag{1}$$

where, N represents the total number of terms (also number of simulations required to generate the response surface) in the expansion and is written as

$$N = \frac{(n+r)!}{n!\,r!} \tag{2}$$

The multi-variable polynomial basis can be mathematically described generally as a second order random process) by

$$y_j = a_{j,0} + \sum_{i_1=1}^{n} a_{j,i_1}\Gamma_1(\xi_{i_1}) + \sum_{i_1=1}^{n-1}\sum_{i_2>i_1}^{n} a_{j,i_1 i_2}\Gamma_2(\xi_{i_1},\xi_{i_2}) + \ldots\ldots \tag{3}$$

where $\{a_{j,k} \mid k = 0, 1,\ldots., n-1\}$ are unknown coefficients to be determined with respect to the specified model used for uncertainty analysis, n represents the number of uncertain model inputs and $\Gamma_p(\{\xi\})$'s are defined to be multivariate Hermite polynomials in the p – dimensional sequence of uncorrelated standard normal random variables, $\{\xi_i\}$. The multivariate Hermite polynomials can be written as,

$$\Gamma_p(\xi_{i_1},..,\xi_{i_p}) = (-1)^p e^{\frac{1}{2}\xi^T\xi}\frac{\partial^p}{\partial\xi_{i_1}.....\partial\xi_{i_p}} e^{-\frac{1}{2}\xi^T\xi} \tag{4}$$

The inputs are represented as functions of identically independently distributed (iid) normal random variables $\{\xi_i| i=1,n\}$ and each ξ_i has zero mean and unit variance. These random variables are referred to as "Standard Random Variables (srvs)". Once the inputs are expressed as functions of these srvs, the output metrics can be represented as functions of the same set of srvs [8]. The minimum number of srvs needed to represent the inputs is defined as the "number of degrees of freedom" in input uncertainty. In practice, in the theory of PCE, the minimum number of simulations required for generating the sample points of the uncertain inputs from the respective pdf depends on the order of the Hermite polynomial and the number of uncertain inputs. Since the model outputs are deterministic functions of model inputs, they have at most the same number of degrees of freedom in uncertainty. So, the number of unknown coefficients to be determined for the model output (fitted polynomial as stochastic response surface) can be explicitly written using eqn. (2) as

$$N_2 = 1 + 2n + \frac{n(n-1)}{2} \quad , \qquad \text{for } 2^{nd} \text{ order Hermite polynomial} \tag{5}$$

$$N_3 = 1 + 3n + \frac{3n(n-1)}{2} + \frac{n(n-1)(n-2)}{6} \text{ , for } 3^{rd} \text{ order Hermite polynomial} \tag{6}$$

So, an explicit representation of 2nd order polynomial chaos expansion for two and three uncertain inputs can be written using equations (1-5) as:

$$\begin{aligned} y_2 &= a_0 + a_1\xi_1 + a_2\xi_2 + a_3(\xi_1^2 - 1) + a_4(\xi_2^2 - 1) + a_5\xi_1\xi_2 \\ y_2 &= a_0 + a_1\xi_1 + a_2\xi_2 + a_3\xi_3 + a_4(\xi_1^2 - 1) + \\ &\quad a_5(\xi_2^2 - 1) + a_6(\xi_3^2 - 1) + a_7\xi_1\xi_2 + a_8\xi_1\xi_3 + a_9\xi_2\xi_3 \end{aligned} \tag{7}$$

According to the number of uncertain model inputs, n = 2, 3, and 4, the number of unknown coefficients to be determined in the polynomial chaos expansion can be obtained using equations (5) and (6) as {6, 10 and 15} and {10, 20 and 35} respectively. Note that, number of unknown coefficients is equal to the number of simulations required at least to generate the response surface. Thus for two uncertain model inputs, second order polynomial

chaos expansion needs six simulations to estimate the unknown coefficients. For reference, the first few Hermite polynomials are given by

$$H_0(\xi) = 1,\ H_1(\xi) = 2\xi,\ H_2(\xi) = 2(\xi^2 - 1) \tag{8}$$

and the higher order Hermite polynomials can be generated using the recurrence relation given by

$$H_{k+1}(\xi) = 2\xi\, H_k(\xi) - 2\, k\, H_{k-1}(\xi) \tag{9}$$

Polynomial chaos theory is not limited to the Hermite polynomials. Generalized polynomial chaos (otherwise known as Wiener-Askey Polynomial Chaos) expanded the theory to use all the polynomials from the Askey scheme of orthogonal polynomials [9]. In reference with the most common distribution we have: Hermite polynomials are associated with the Gaussian distribution, Legendre polynomials are associated with the uniform distribution, and Laguerre polynomials are associated with the exponential distribution [9]. The use of Hermite, Legendre, and Laguerre polynomials will from now on be referred to as Hermite-Chaos, Legendre-Chaos, and Laguerre-Chaos respectively [10]. When all of the variables in the examined system have been expanded onto the basis of choice, a Galerkin projection onto the basis is applied. The Galerkin projection is realized by the integration of each component of the examined system with the polynomial basis. The projection takes the form of an integral because the chosen polynomial bases are all continuous. The limits of the integral correspond to the region where the chosen polynomials are valid. The limits for Hermite-Chaos, Legendre-Chaos, and Laguerre-Chaos are $-\infty$ to ∞, -1 to 1, and 0 to ∞ respectively. This region is represented by the symbol Ω.

2.1. Chaotic Representation of Model Input Distributions

Number of sample values for the model outputs will have to be generated on the basis of number of unknown coefficients. Therefore, for six unknown coefficients, six model outputs are to be generated for the specified model. Sampling points for generation of these outputs will be obtained from the model uncertain inputs for which inputs are to be transformed into standard normal random variables (srvs) [10]. In PCE, approach for transforming model uncertain inputs is based on the principle that random variables with well-behaved (square-integrable) probability density functions (pdfs) can be represented as functions of a set of srvs [10, 11]. Standard transformation of the uniform, normal, lognormal and gamma pdfs of model inputs in terms of srvs can be written as

$$\textit{Uniform [a,b]}: \quad a + (b-a)\left\{\frac{1}{2} + \frac{1}{2} erf\left(\frac{\xi}{\sqrt{2}}\right)\right\} \tag{10}$$

$$\text{Normal } (\mu,\sigma): \quad \mu + \sigma\xi \tag{11}$$

$$\text{Lognormal } (\mu,\sigma): \quad \exp(\mu + \sigma\xi) \tag{12}$$

$$\text{Gamma (a, b)} = ab\left(\xi\sqrt{\frac{1}{9a}} + 1 - \frac{1}{9a}\right)^2 \tag{13}$$

Sample values of the output metrics (eqn. (7)) and the corresponding polynomial chaos expansion are finally arranged in the matrix form as $[\xi]\{a\} = y$, from which coefficient vector, $\{a\}$ can be solved using singular value decomposition.

3. Case Study: Transport of Chemical Contaminants Through Groundwater: One Dimensional Solute Transport Through Groundwater

The physical process involved in transport of chemical contaminants through groundwater is advection, dispersion and retardation. The governing equation representing the advection dispersion and retardation in one dimension form for chemical (solute) transport in groundwater is given by [12]

$$R_f \frac{\partial C}{\partial t} = D_L \frac{\partial^2 C}{\partial x^2} - V_w \frac{\partial C}{\partial x} \tag{14}$$

where,

C = concentration of the dissolved chemical species (contaminant) in gm/l

$D_L = Longitudinal\ dispersion coefficient = \alpha_L V_c + D^* / \theta_e$

V_w = pore water velocity in the x – direction = $-(K/\theta_e)(dh/dx)$ *in cm/s*

K = hydraulic conductivity (cm/s), dh/dx = hydraulic gradient (m/m),

R_f = retardation factor = $1 + (\rho K_d / \theta_e)$

$\rho = bulk\ density of\ the\ soil (g/cc), \theta = total\ porosity of\ the\ soil$

$\theta_e = \text{effective porosity of the soil}, K_d = \text{distribution coefficient of the soil} = K_{oc} f_{oc}$

$K_{oc} = \text{organic carbon partition coefficient (cc/g)},$

$f_{oc} = \text{fraction of organic carbon content}, V_c = V_w / R_f \ \ cm/s, T = period of\ injection$

Boundary and initial conditions for the above equations are:

$$C(x, t=0) = 0, \ \ \partial C(x=\infty, t=0)/\partial x = 0$$

$$C(x=0, 0 < t \le T) = C_0 \ \ , C(x=0, t > T) = 0 \tag{15}$$

Analytical solution to the governing equation with the given initial and boundary conditions can be written as per [12] as

$$C(x,t) = 0.5 * C_0 \left[erfc\left(\frac{x - V_c t}{\sqrt{4 D_L t}} \right) + \exp\left(\frac{V_c x}{D_L} \right) erfc\left(\frac{x + V_c t}{\sqrt{4 D_L t}} \right) \right], \quad 0 < t \le T$$

$$C(x,t) = 0.5 * C_0 \left[erfc\left(\frac{x - V_c (t-T)}{\sqrt{4 D_L (t-T)}} \right) + \exp\left(\frac{V_c x}{D_L} \right) erfc\left(\frac{x + V_c (t-T)}{\sqrt{4 D_L (t-T)}} \right) \right], \quad t > T \tag{16}$$

For the present problem, we have considered K_{oc} and hydraulic conductivity, K as random uncertain inputs and both the parameters are considered as uniformly distributed for the convenience of simplicity in computation. However, variability of both the random

parameters can be described by their realistic probability distribution. Total number of simulations chosen for sampling the random parameter is here based on the order of the polynomial to be fitted and the number of uncertain inputs. We have considered second order polynomial and accordingly as per the theory of PCE mentioned in the section 2.0, number of simulations required as six. Six values of respective srvs corresponding to K_{oc} and hydraulic conductivity, K are generated and six sample values of C(x, t) following equation (16) are generated. Finally the regression coefficients are solved using singular value decomposition. Statistics of the response surface thus constructed using a large number of Monte Carlo simulations.

4. Results and Discussions

Transport of chemical contaminant trichloroethylene through groundwater is considered for uncertainty analysis using stochastic response surface method. Basic aim is to generate a probabilistic response surface of concentration of trichloroethylene, so that at any spatial location and at any instant of time the response as the magnitude of the concentration can be predicted. In order to achieve this goal initially, we have computed the concentration profile of the solute concentration at various downstream distance for a fixed time, t = 1000 days for three different values of longitudinal dispersivity, viz., 1m, 5 m and 10 m. Profile of the computed concentration is as shown in figure.1. It can be easily mentioned from figure 1 that as the longitudinal dispersivity increases concentration of the contaminant decreases at a larger downstream distances; viz. concentration of the contaminant dies out at distance of 70 m downstream for alpha = 10 m compared to the same at 40 m for alpha = 1 m. So, longitudinal dispersivity is one of the controlling factor of the decreasing value of the concentration at smaller downstream distance. However, value of alpha is basically obtained experimentally and experimental value possesses a certain amount of error. In other words, alpha is an uncertain quantity and similarly flow of the contaminant through any specific geological media is guided by many other uncertain parameters. From this point uncertainty analysis is essential. Accordingly, uncertainty analysis of the concentration of the solute at any spatial distance from the point of discharge for a fixed time is carried out. In order to quantify the uncertainty of the solute concentration during its transport through porous media, initially, 10000 mg/l of trichloroethylene (C_0 = 10000 mg/L) as a chemical tracer is injected for a period of 1,000,000 days. Flow of the system is considered within a confined aquifer of length 100 m. The porous media through the transport of the chemical takes place is considered as soil of silty type. Concentration is evaluated at a time of 1000 days. The list of the required deterministic inputs is as shown in Table 1. The probability density function of the random inputs is as shown in Table 2.

Table 1 List of Deterministic Input Parameters of the Model

Parameters	ρ (g/cc)	dh/dx	D^*	K (cm/s)	K_{oc} (cc/g)	f_{oc} (%)	θ (%)	θ_s (%)
Values	1.6	-0.007	0	0.001	100	0.1	35	25

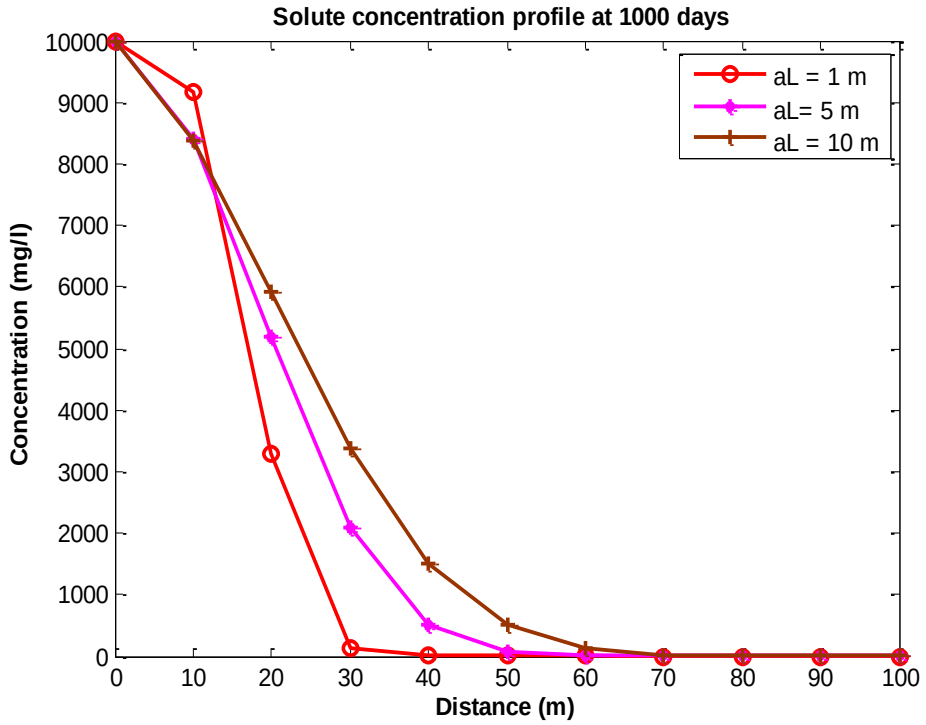

Figure 1. Profile of Deterministic Concentration for Different Longitudinal Dispersivity

Table 2 Specification of the Input Random Parameters

Parameters (unit)	Distribution	Lower limit	Upper limit
K (cm/s)	Uniform	1.0E-7	1.0E-3
K_{oc} (cc/g)	Uniform	20	500

Uncertainty analysis is carried out using stochastic response surface method and the stochastic response surface of the solute concentration is simulated for the longitudinal dispersivity α_L = 1 m. The values of the coefficients of the response surface for various downstream distances are given in Table 3. Time of observation used in the computation is kept as 1000 days only as per the requirement. Uncertainty of the contaminant concentration is quantified as the lower bound (5^{th} percentile) and the upper bound (95^{th} percentile), wherein 50^{th} percentiles represent the most probable value. All these percentiles are computed on the basis of its cumulative probability distribution. Cumulative probability distributions of the response surface for each downstream distance are plotted and presented in figure 2. Uncertainty plot of the 5^{th}, 50^{th} and 95^{th} percentiles of the concentration profile at different downstream distance is as shown in figure 3. Mean and standard deviation of the response surface of the concentration at any specific downstream distance provides the average value of the concentration and its error signifying the spread on either side of the mean value. Statistics such as skewness of the response surface being greater than 1 at downstream distance ranging from 1 to 15 m indicate that the probability density of the concentration at those downstream distances is not normally distributed. Kurtosis provides the peaked of the concentration profile.

Table 3 Coefficients of Response Polynomial for Downstream Distance x = 1, 5, 8, 10, 15 and 20 m

Downstream Distance, x (m)	$a_0 \times 10^3$	$a_1 \times 10^3$	$a_2 \times 10^3$	$a_3 \times 10^3$	$a_4 \times 10^3$	$a_5 \times 10^3$
1	9.6690	-0.1568	0.2826	-0.0385	-0.1053	0.1511
5	5.1359	-2.1373	3.8674	-0.4065	-1.2710	1.7415
8	1.6603	-2.9925	5.5336	-0.1593	-1.2134	1.3214
10	1.3846	-2.1840	4.2418	0.3625	-0.1961	-0.3743
15	1.7523	0.0007	0.3059	0.6074	1.1502	-1.8554
20	446.4897	54.8988	-89.6219	93.1672	353.3084	-367.9466

Table 4 Statistics of the Stochastic Response Surface of the Concentration at t = 1000 days

Downstream Distance, x (m)	Mean value x 10^3	Standard deviation x 10^3	Skewness x 10^3	Kurtosis x 10^3	5^{th} percentile x 10^3	95^{th} percentile x 10^4
1	9.6669	0.4797	2.1006	11.4369	9.1151	1.0596
5	5.1266	6.5402	2.1414	11.3496	-2.3147	1.7914
8	1.6553	9.1019	2.3738	13.0096	-8.0130	1.9697
10	1.4465	6.9840	2.4896	13.1412	-5.2991	1.5052
15	1.7566	1.5022	2.7871	15.0563	0.5732	0.4757
20	0.4555	0.4056	0.1792	8.8015	-0.1648	0.1114

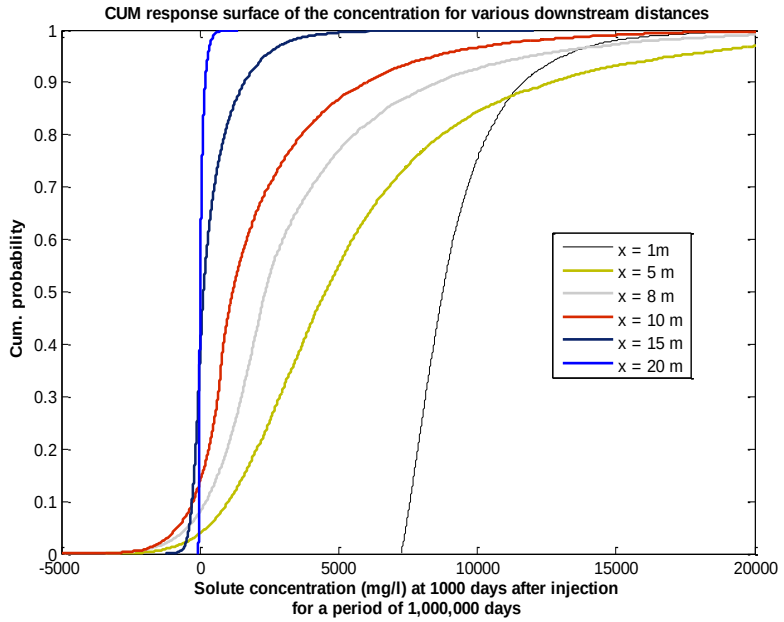

Figure 2 Cumulative Distribution of the Stochastic Response Surface of Solute Concentration at Different Downstream Distance

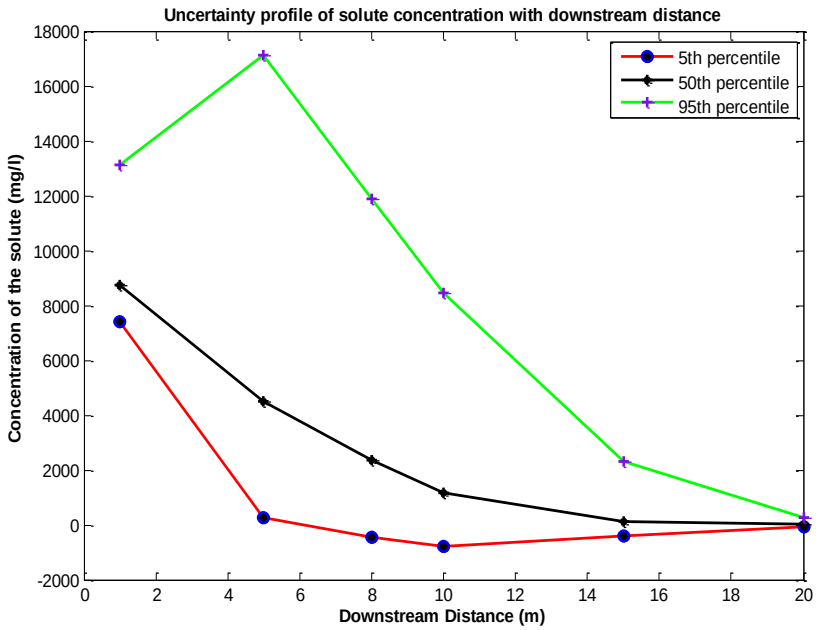

Figure 3 Uncertainty Plots of the Solute Concentration

Uncertainty plot of the solute concentration basically signifies that if the sample is collected at any downstream distance, say 10 m from the origin of the source, the concentration of the contaminant measured for that sample should be within 0 and 9000 mg/l with a 95% confidence. Therefore, uncertainty quantification provides guidance to the analyst that whether the measured value can be accepted or rejected.

5. Conclusions

In this work, uncertainty of concentration of contaminant at time, t = 1000 days for an injection period of 100000 days of trichloroethylene of initial concentration 10000 mg/l at various downstream distances such as x = 1, 5, 8, 10, 15 and 20 m is analyzed. The longitudinal dispersivity for stochastic simulation is taken as 1 m. It has been assessed from the deterministic computation that higher the longitudinal dispersivity larger the downstream distance for decaying the concentration. Stochastic simulation is carried out using Hermite polynomials as the basis polynomial and all the input uncertain parameters are transformed into space of standard normal random variable. Hermite polynomials being represented as Gaussian, the expansion scheme can be named as Hermite (polynomial) chaos. The selection of the basis polynomial will be based on the domain dependence of the input uncertain parameters. For example, if the uncertain input parameters are known to vary within the interval [-1, 1], one can select Lagrange polynomial as the basis polynomial. Whatever be the basis polynomial computation scheme will remain intact and always the number of simulations will be less compared to the traditional Monte Carlo simulation. Stochastic response surface method based uncertainty analysis concludes that, the method is efficient from the point of large number of simulations as often required in standard Monte Carlo method. Study also concludes that knowledge of the uncertainty of the concentration of the solute preambles the acceptability criteria of the systematic sampling. The cumulative probability of the concentration being zero is an indicator of the failure probability, the

cumulative response surface of the solute concentration also provides the knowledge of the reliability of the model adopted for study.

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