Stochastic simulation of Advection-Diffusion equation considering uncertainty in input variables

Hossein Khorshidi, Gholamreza Rakhshandehroo, Nasser Talebbeydokhti

Abstract—Due to the lack of understanding of the flow parameters including roughness coefficient, bed slope, and initial conditions, governing equations may be considered in the stochastic form. Karhunen–Loeve expansion (KLE) approach as a perturbative expansion method is applied to explore uncertainty and its propagation based on the Advection-Diffusion equation (ADE). To assess the uncertainty in the present work, input variables (including initial condition, boundary condition, and diffusion coefficient), as source of uncertainty, is imposed in the framework of one-dimensional open channel flow. Our investigation is aimed at obtaining higher-order solutions to the statistical moments of the flow depth as random field. KLE approach is adopted to decompose the uncertain parameter in terms of infinite series containing a set of orthogonal Gaussian random variables. Eigenvalues and eigenfunctions of the covariance function associated with the random initial condition play a key role in computing the coefficients of the series and extracted from Fredholm's equation. The flow depth, as random dependent variable, is also represented as an infinite series which are obtained through decomposing by polynomial expansions in terms of the products of Gaussian random variables. The coefficients of the last series are governed by a set of recursive equations that are derived from the ADE. Monte Carlo simulation (MCS), as a reliable approach, is carried out for about 1000 realizations and compared with the KLE. The present results highlight statistical properties of input variables including initial condition, boundary condition and diffusion coefficient, then, flow depth variance is achieved based on the variance of the input random variable. It was found that when higher-order approximations are used to represent initial condition, KLE results (mean flow depth and the flow depth variance) would be as accurate as MCS, however, with much less computational time and effort.

Keywords— Stochastic Simulation, Advection-Diffusion equation, Karhunen–Loeve expansion, Polynomial expansion.

I. Introduction

GIVEN the heterogeneous nature of many fluid flows and difficulties associated with understanding this heterogeneity accurately, flow characteristics are often treated as random functions, leading to governing equations of stochastic types.

In environmental fluid mechanics, such as wave transformation, transport occurs in fluids through the combination of advection and diffusion. Due to the complexity of measurements for flow parameters (such as roughness coefficient, bed slope, initial and boundary conditions), therefore, these terms consider as source of uncertainty. Stochastic approaches to flow in open channels have been generally studied in the last two decades, and many stochastic models have been developed.

A conventional method to solve partial differential equations (PDEs) stochastically is Polynomial Chaos Expansion (PCE). It was put forward by Ghanem and Spanos [1], with application to transport in heterogeneous media [2], [3] and diffusion problems [4]. PCE is applied to model the uncertainty propagation from the beginning of a waterhammer with random system parameters and internal boundary conditions [5]. This technique includes representing the random variables in terms of polynomial chaos basis and deriving appropriate discretized equations for the expansion coefficients via Galerkin technique. PCE allows high order approximation of random variables and possesses fast convergence under certain conditions. However, the deterministic coefficients of PCE are governed by a set of coupled equations, which are difficult to solve when the number of coefficients is large. PCE is based on the expansion of variables by products of polynomial coefficients and orthogonal chaos bases. It is needed to treat a system of equations numerically. PCE applications to stochastic shallow water flows were reported by Ge *et al.* [6] and Liu [7]. A comprehensive review of PCE approach is discussed by Debusschere *et al.* [8].

Karhunen-Loeve Expansion (KLE) is a flexible approach to solve PDEs stochastically, leading to high order moments with relatively small computational efforts. PCE [9], [10], probabilistic collocation method [11], [12] and KLE [9], [13] have been utilized to illustrate random processes in porous media. This method is applied to decompose the solution of Boussinesq equations for the velocity, density and pressure fields [14].

KLE approach has been proven efficient for uncertainty analysis in groundwater hydraulics [9], [13], and [15].

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Contrary to PCE, the coefficients associated with KLE appear in uncoupled equations, from which required statistical moments can be extracted. However, this method has received little attention in open channel applications.

A reliable tool usually used as a reference for solving stochastic PDEs is Monte Carlo Simulation (MCS) which consists of three steps; 1) generating several realizations of the uncertain parameter based on its distribution function, 2) solving the governing equation by means of an appropriate deterministic scheme for the generated parameter, and 3) taking statistical moments on the entire realizations obtained in previous steps. MCS is simple to implement, however, it introduces considerable computational effort due to large number of realizations needed. Application of MCS in open channel flow has been reported by Gates and Alzahrani [16], [17] for Colombia River in US. The uncertainty in geometrical properties and bed slope are investigated via their distribution functions, and consequently, statistical moments are evaluated for the flow field. A virtual sampling MCS was proposed to address uncertainty quantification in flood modeling on a real test case for Tous dam break in Spain [18]. Dutykh *et al.* [19] adopted MCS to quantify the effect of bottom roughness on maximum run-up height by resorting to nonlinear shallow water equations. Multilevel MCS is applied to uncertainty quantification for porous media flow [20].

In the present work, KLE approach is applied to 1-D Advection-Diffusion equation considering uncertainty in initial condition for a synthetic case in open channel flow. Consequently, flow field parameter has appeared as a random variable, too. Validity of the proposed model has been ensured through comparing with MCS results for various spatial variability.

II. Governing Equation

One dimensional Advection Diffusion-equation (ADE) could be written for an incompressible fluid as

$$\frac{\partial H}{\partial t}+U\,\frac{\partial H}{\partial x}-D\,\frac{\partial^2 H}{\partial x^2}=0 \tag{1}$$

in which $H(x,t)$ is flow depth, U is flow velocity and D is diffusive coefficient, subject to the initial and boundary conditions given by

$$H(x,0)=h_0+a\,\mathrm{sech}^2\left[\sqrt{\frac{3a}{4h_0^3}}\left(x-\frac{L}{2}\right)\right],\ \ x\in D \tag{2}$$

$$H(0,t)=H(L,t)=h_0,\ \ t>0 \tag{3}$$

where L is channel length, $H(x,0)$ or $h(x)$ is initial water depth, h_0 is undisturbed uniform water depth, a is initial wave height and D is spatial domain in x direction. The initial condition corresponds to a first-order solitary wave propagating in the positive x-direction [21]. The random nature of $h(x)$ converts deterministic equations, (1)-(3), in to stochastic ones, the solution of which is sought in the form of statistical moments. The length of the channel is assumed sufficiently large compared to the characteristic length of solitary wave [22]. This justifies the validity of (3), implying that the boundary values remains unaffected by the initial wave form.

III. Karhunen-Loeve Expansion

In KLE approach, initial water depth $h(x)$ is considered a random variable due to many factors including uncertainty inherent in measurements. It may be decomposed to the mean term $\langle h\rangle$ and the fluctuation term h'. KLE expresses $h'(x)$ in terms of eigenstructure for covariance function $C_h(x_1,x_2)$ of the random field as follows [1]

$$h'(x,\omega)=\sum_{n=1}^{\infty}\xi_n(\omega)\sqrt{\lambda_n}f_n(x), \tag{4}$$

where x and ω are indices of real and probability spaces, respectively. $\xi_n(\omega)$ is an orthogonal Gaussian random variable with zero mean and λ_n and $f_n(x)$ are eigenvalues and eigenfunctions associated with the given covariance function, respectively. With a covariance function for the exponential distribution as

$$C_h(x_1,x_2)=\sigma_h^2\exp\left(-\frac{|x_1-x_2|}{\eta}\right), \tag{5}$$

The eigenstructures are obtained analytically from Fredholm's equation [13] as

$$\lambda_n=\frac{2\eta\sigma_h^2}{\eta^2 w_n^2},\qquad f_n(x)=\frac{\left[\eta w_n\cos(w_n x)+\sin(w_n x)\right]}{\sqrt{0.5L\left(\eta^2 w_n^2+1\right)+\eta}} \tag{6}$$

where σ_h^2 and η are variance and correlation length of the random variable $h(x,\omega)$, respectively. It is worth mentioning that a similar problem has been treated by Zhang and Lu [13] when modeling groundwater flow in a random porous medium. In the above expression, w_n refers to positive roots of the characteristic equation $\left(\eta^2 w^2-1\right)\sin(wL)=2\eta w\cos(wL)$. For notational convenience, the function $\sqrt{\lambda_n}f_n(x)$ is replaced with $f_n^*(x)$, hereafter.

IV. Moment Equations in KLE

Initial condition, $h(x)$ is considered as a random variable and other terms as deterministic ones. KLE, as a perturbative expansion technique, expand the dependent variable $H(x,t)$ as the following series

$$H(x,t)=H^{(0)}+H^{(1)}+H^{(2)}+\ldots \tag{7}$$

Substituting the above expansion and $h(x)=\langle h\rangle+h'$ in (1)-(3) and considering only the zero order terms, the governing equation and related conditions will take the form of

$$\frac{\partial H^{(0)}}{\partial t}+U\frac{\partial H^{(0)}}{\partial x}-D\frac{\partial^2 H^{(0)}}{\partial x^2}=0 \tag{8}$$

$$H^{(0)}(x,0)=h_0+\bar{a}\,\mathrm{sech}^2\left[\sqrt{\frac{3a}{4h_0^3}}\left(x-\frac{L}{2}\right)\right],\ \ x\in D \tag{9}$$

$$H^{(0)}(0,t)=H^{(0)}(L,t)=h_0,\ \ t>0 \tag{10}$$

in which $\bar{a}$ is mean value of a. Similarly, one may obtain the following expression for any higher order term m [13]

$$\begin{aligned}&U\frac{\partial}{\partial x}\left(H^{(m)}\right)-D\frac{\partial^2}{\partial x^2}\left(H^{(m)}\right)\\&+\sum_{k=0}^{m}\frac{(-1)^k}{k!}\left[h'(x)\right]^k\frac{\partial H^{(m-k)}}{\partial t}=0\end{aligned} \tag{11}$$

$$H^{(m)}(x,0)=0,\ \ x\in D \tag{12}$$

$$H^{(m)}(0,t)=H^{(m)}(L,t)=0, \tag{13}$$

Various components of (7) can now be expanded by suitable polynomial expansions in terms of the orthogonal Gaussian random variable ξ as illustrated in Table I.

Where $H_i^{(1)}$, $H_{ij}^{(2)}$ and $H_{ijk}^{(3)}$ (for $i,j,k=1,2,\dots$) are deterministic coefficients obtained from the associated governing equation, numerically. Note that, above governing equations are derived via substituting the expansions of $h'(x)$ and $H^{(m)}(x,t)$ with $m=1,2,3$ in (11)-(13) and simplifying the resulting expressions in view of orthogonality of the random variable ξ. Index $\sum_{P_{ijk}}(.)$ is found by a substitution manner, i.e., $\sum_{P_{ijk}}\nabla f_i^*.\nabla H_{jk}^{(2)}=\nabla f_i^*.\nabla H_{jk}^{(2)}+\nabla f_j^*.\nabla H_{ik}^{(2)}+\nabla f_k^*.\nabla H_{ij}^{(2)}$. For the trivial solutions to exist, $H^{(3)}(x,t)$ should be expanded in terms of ξ_n and $\xi_i\xi_j\xi_k$ simultaneously [13]. Manipulating the third order approximation of $H(x,t)$ (Eq. 7) mathematically, one may compute higher moments of the flow depth as shown in Table II. It is important to note that, the same approach is chosen to solve the governing equation of $H^{(0)}$ to $H_{ijk}^{(3)}$ because of the diversity in homogeneity property. Despite of analytical solution for (8)-(10) (i.e., convolution integral), QUICKEST (Quadratic Upstream Interpolation for Convective Kinematics with Estimated Streaming Terms) approach is utilized to treat all of the governing equation to have the same solution process as follow [23], [24]

$$\begin{aligned}H_i^{j+1}=H_i^j&+\left[C_d\left(1-C_a\right)-\frac{C_a}{6}\left(C_a^2-3C_a+2\right)\right]H_{i+1}^j\\&-\left[C_d\left(2-3C_a\right)-\frac{C_a}{2}\left(C_a^2-2C_a-1\right)\right]H_i^j\\&+\left[C_d\left(1-3C_a\right)-\frac{C_a}{2}\left(C_a^2-C_a-2\right)\right]H_{i-1}^j\\&+\left[C_d.C_a+\frac{C_a}{6}\left(C_a^2-1\right)\right]H_{i-2}^j\end{aligned} \tag{14}$$

in which H_i^j is flow depth at $i^{th}\,\Delta t$ (spatial step) and $j^{th}\,\Delta t$ (time step), and C_a and C_d are advective and diffusive Courant numbers, respectively

$$C_a=\frac{U.\Delta t}{\Delta x},\quad C_d=\frac{D.\Delta t}{\Delta x^2}, \tag{15}$$

Regions of stability for the QUICKEST scheme may be written as [25]:

$$\begin{cases}C_d\le\dfrac{\left(3-2C_a\right)\left(1-C_a^2\right)}{6\left(1-2C_a\right)} & if\ \ C_a<\dfrac{1}{2}\\[2ex] C_d\ge\dfrac{\left(3-2C_a\right)\left(C_a^2-1\right)}{6\left(2C_a-1\right)} & if\ \ C_a>\dfrac{1}{2}\end{cases}\quad and\ \ C_d\ge 0 \tag{16}$$

Table I Expansion and the governing equations of $H^{(m)}(x,t)$ in terms of the orthogonal Gaussian random variables

Term	Governing equation
$H^{(1)}(x,t)=\sum_{i=1}^{\infty}\xi_i H_i^{(1)}(x,t)$	$\frac{\partial H_i^{(1)}}{\partial t}-f_n^*(x)\frac{\partial H^{(0)}}{\partial t}+\mathrm{U}\frac{\partial}{\partial x}\left(H_i^{(1)}\right)-\mathrm{D}\frac{\partial^2}{\partial x^2}\left(H_i^{(1)}\right)=0$
$H^{(2)}(x,t)=\sum_{i,j=1}^{\infty}\xi_i\xi_j H_{ij}^{(2)}(x,t)$	$\frac{\partial H_{ij}^{(2)}}{\partial t}-\frac{1}{2}f_i^*(x)\frac{\partial H_j^{(1)}}{\partial t}-\frac{1}{2}f_j^*(x)\frac{\partial H_i^{(1)}}{\partial t}+\frac{1}{2}f_i^*(x)f_j^*(x)\frac{\partial H^{(0)}}{\partial t}+U\frac{\partial H_{ij}^{(2)}}{\partial x}-D\frac{\partial^2 H_{ij}^{(2)}}{\partial x^2}=0$
$H^{(3)}(x,t)=\sum_{n=1}^{\infty}\xi_n H_n^{(3)}(x,t)+\sum_{i,j,k=1}^{\infty}\xi_i\xi_j\xi_k H_{ijk}^{(3)}(x,t)$	$\frac{\partial H_{ijk}^{(3)}}{\partial t}-\frac{1}{3}\sum_{P_{ijk}}f_i^*(x)\frac{\partial H_{jk}^{(2)}}{\partial t}+\frac{1}{6}\sum_{P_{ijk}}f_i^*(x)f_j^*(x)\frac{\partial H_k^{(1)}}{\partial t}-\frac{1}{6}\sum_{P_{ijk}}f_i^*(x)f_j^*(x)f_k^*(x)\frac{\partial H^{(0)}}{\partial t}+U\frac{\partial H_{ijk}^{(3)}}{\partial x}-D\frac{\partial^2 H_{ijk}^{(3)}}{\partial x^2}=0$

Table II Statistical moments of the flow depth

Flow depth	$H(x,t) \approx \sum_{i=0}^{3} H^{(i)}(x,t)$
Mean value	$\langle H(x,t)\rangle \approx \sum_{i=0}^{3} \langle H^{(i)}(x,t)\rangle = H^{(0)}(x,t) + \sum_{i=1}^{\infty} H_{ii}^{(2)}(x,t)$
Perturbation term	$H'(x,t) = H(x,t) - \langle H(x,t)\rangle \approx \sum_{i=1}^{3} H^{(i)}(x,t) - \sum_{i=1}^{\infty} H_{ii}^{(2)}(x,t)$
Cross-covariance between initial water depth and flow depth	$C_{hH}(x;y,\tau) = \sqrt{\lambda_n} f_n(x) H'(x,\omega) = f_n^*(x) H'(x,\omega) = \sum_{n=1}^{\infty} f_n^*(x) H_n^{(1)}(y,\tau) + 3\sum_{i,j=1}^{\infty} f_i^*(x) H_{ijj}^{(3)}(y,\tau)$
Flow depth covariance	$C_H(x,t;y,\tau) = \sum_{i=1}^{\infty} H_i^{(1)}(x,t) H_i^{(1)}(y,\tau) + 2\sum_{i,j=1}^{\infty} H_{ij}^{(2)}(x,t) H_{ij}^{(2)}(y,\tau) + 3\sum_{i,j=1}^{\infty} H_i^{(1)}(x,t) H_{ijj}^{(3)}(y,\tau) + 3\sum_{i,j=1}^{\infty} H_i^{(1)}(y,\tau) H_{ijj}^{(3)}(x,t)$
Flow depth variance	$\sigma_H^2(x,t) = \sum_{i=1}^{\infty}\left[H_i^{(1)}(x,t)\right]^2 + 2\sum_{i,j=1}^{\infty}\left[H_{ij}^{(2)}(x,t)\right]^2 + 6\sum_{i,j=1}^{\infty} H_i^{(1)}(x,t) H_{ijj}^{(3)}(x,t)$

V. Illustrative Example

KLE approach is applied to a hypothetical channel to compute higher-order flow depth moments, and verified by comparing its results with those of MCS. A hypothetical channel of length $L = 100m$ is considered with a first-order solitary wave with maximum height of a within normal distribution and mean value of $\bar{a} = 0.05m$, centered at $x = L/2$. Moreover, the water depth is kept constant at $h_0 = 1m$ over the channel ends, advective velocity $U = 2.5m/s$, and diffusion coefficient f. Schematic of the initial condition over the channel and wave propagation sketch at different times are shown in Fig.1. Effects of different various degrees of spatial variability, σ_h^2 , on flow depth variance, σ_H^2 , were investigated. MCS was examined for about 1000 realizations and the moments of the flow depth were computed for different correlation lengths and variances of the input random variable.

VI. Results and Discussion

The effects of input random variables including diffusion coefficient, initial, and boundary conditions on flow depth variance were investigated using MCS. Then, KLE approach is applied to quantify uncertainty of initial condition. The sufficient number of terms to be incorporated in $H(x,t)$ and the effects of spatial variability of the random initial condition on flow depth variance were discussed.

A. *Investigation of diffusion coefficient on flow depth*

In this section, the effect the variance of diffusion coefficient, σ_D^2 , is investigated on flow depth variance σ_H^2 . Boundary and initial conditions are considered without any uncertainty. As shown in Fig.1, flow depth variances were solved via MCS for some time levels from the beginning of wave propagating. σ_H^2 is gained up to $6\times10^{-7} m^2$ on the peak wave which is due to the role of the random field D in (1). The maximum values are declined as σ_H^2 decreased. Due to the diffusion properties of flow, the maximum depth variances are flattened over the time.

B. *Investigation of boundary conditions on flow depth*

In the following, σ_H^2 is computed for random boundary conditions, $H(0,t) = H(L,t) = H_0$. Same as before, other parameters were considered without uncertainty. As shown in Fig.2, flow depth variances were computed for different $\sigma_{H_0}^2$. For $\sigma_{H_0}^2 = 0.25m^2$, the flow depth covariance is computed approximately $0.24m^2$ at the upstream end, but it is equal to zero at the downstream one. Due to the flow direction, the support domain of the propagating wave is reached to the downstream end for various $\sigma_{H_0}^2$. As $\sigma_{H_0}^2$ is decreased, the flow depth covariance is attenuated, however, one could be seen an identical trend for all $\sigma_{H_0}^2$. It seems necessary to note that for a certain time level, the domain of changes in σ_H^2 is covered a certain range of the channel length. This means that because of the flow velocity direction, the results are affected only according to the upstream boundary condition at first. Then, with respect to time *t*, downstream condition is played an important role to calculating σ_H^2 .

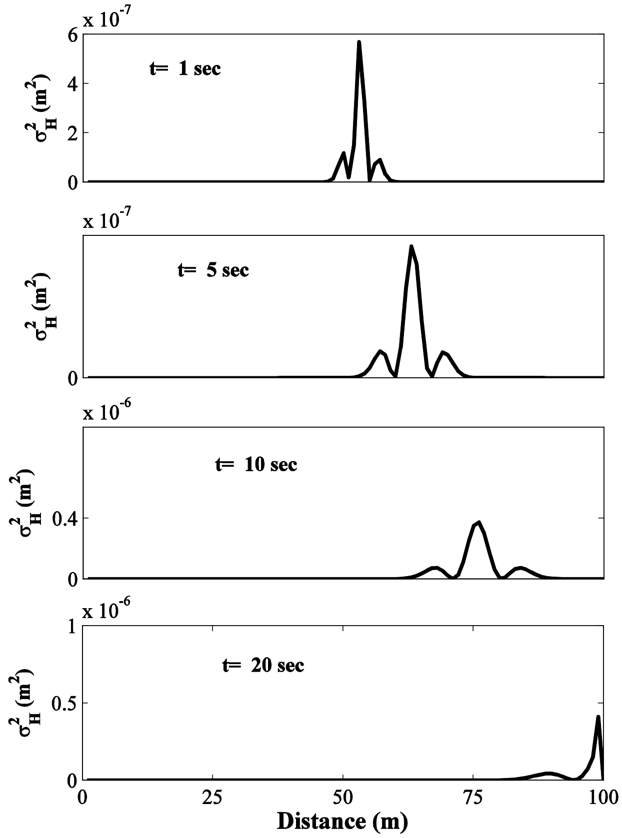


Fig. 1 Flow depth variances for diffusion coefficient variance, $\sigma_D^2 = 0.01m^2$ using 1000 MCS under different times

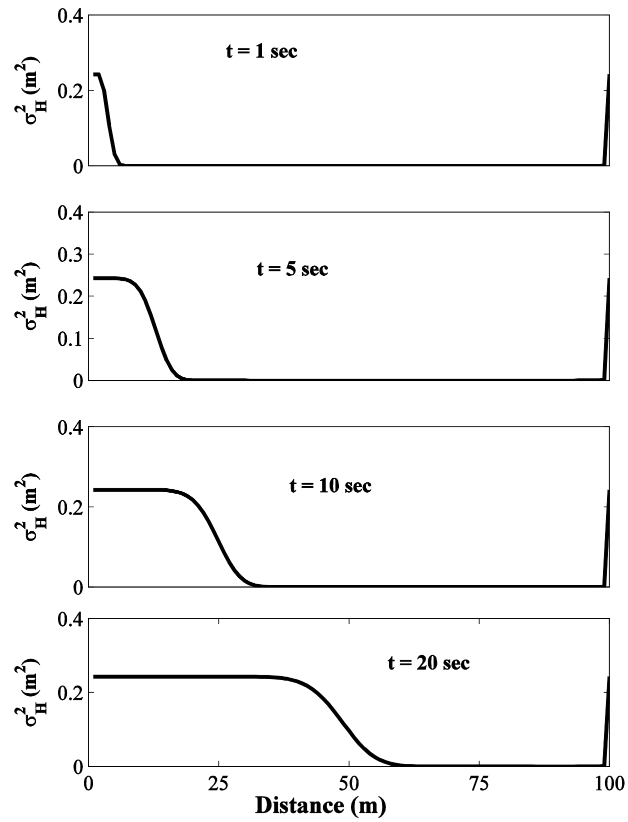


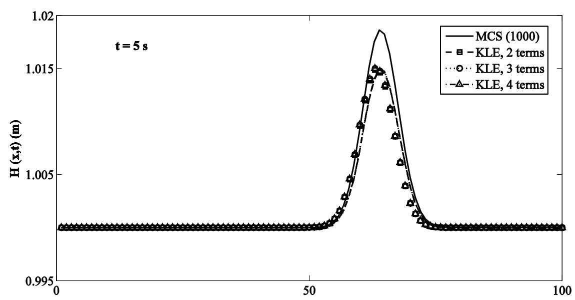
Fig. 2 Flow depth variances for variance of boundary conditions, $\sigma_{H_0}^2 = 0.25m^2$ using 1000 MCS under different times

C. Number of terms to be incorporated in $H(x,t)$

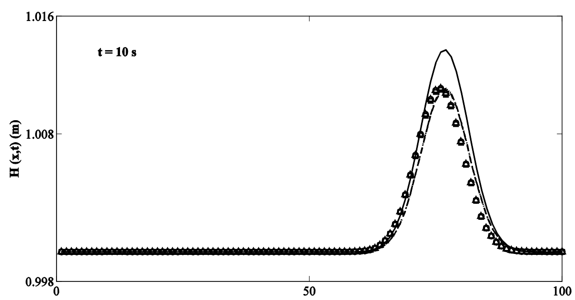
KLE approach was applied to compute mean flow depth profile at different times, and compared with results from MCS ones, as shown in Fig. 3. Incorporation of the first two terms in (7) makes the results in a good agreement with those of MCS (Fig. 3a). Incorporating two more terms, i.e., $H^{(2)}$ and $H^{(3)}$, only slightly improves $H(x,t)$ (Figs. 3b and 3c). Indeed, numerical values of subsequent terms decrease one order of magnitude. For example, $H^{(1)}(x,t)$ (with a certain number of terms considered in its expansion as illustrated in the next section) takes the value of $0.01m$, however, values in order of $0.001m$ was obtained in estimation of $H^{(2)}(x,t)$ with sufficient number of terms considered in its expansion. Moreover, $H^{(3)}(x,t)$ was gained at the order of $0.0001m$; two orders of magnitude smaller than $H^{(1)}(x,t)$. One may conclude that the more number of terms incorporated in $H(x,t)$, the more accurate the results, however, incorporation of four terms ($H^{(0)}$ to $H^{(3)}$) are doomed sufficient to expand $H(x,t)$, because of the size of the disturbance, $0.05m$, caused by the solitary wave.

D. Effects of water depth variances on σ_H^2

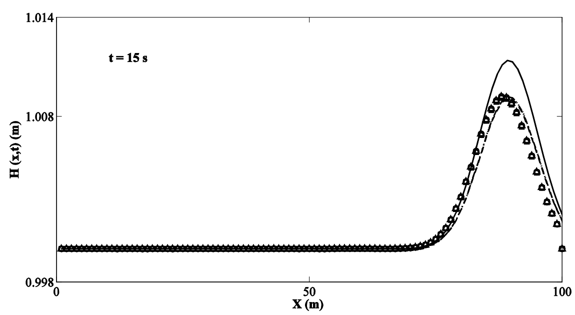
Fig. 4 compares flow depth variances from1st and 2nd order KLE approaches with those from MCS for different input water depth variances of 0.0025, 0.0064, and 0.0121 m^2, and correlation length of 4 at $t = 5s$. As shown, for $\sigma_h^2 = 0.0025m^2$, flow depth variances computed by 1st and 2nd order KLE were close to MCS ones with 1st order mainly overestimating MCS with a maximum error of 9% (Fig. 4a). As the variance increased, 1st order KLE results overestimated MCS again with a maximum error of 9%, however, 2nd order KLE underestimated MCS with a maximum error of 23% (Fig. 4b). Finally, for $\sigma_h^2 = 0.0121m^2$, flow depth variances calculated by the 1st order KLE remained unchanged (with errors similar to those in previous cases), but high errors of up to 52% were observed for the underestimating 2nd order KLE (Fig. 4c). It may be concluded that as the input variance, σ_h^2, increases, 1st order KLE mainly overestimating results remain unchanged, however, 2nd order KLE results increasingly underestimate MCS results. It is concluded that for higher input variances, unlike our expectations, flow depth variance will not improve considerably by incorporation of higher order.



a)



b)

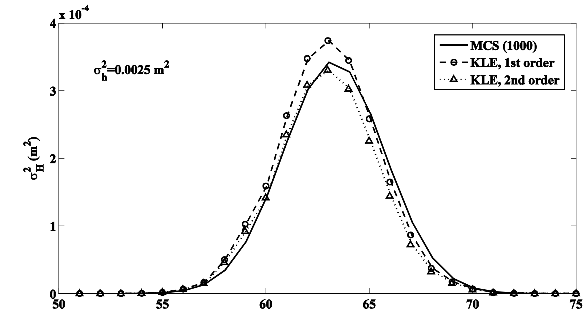


c)

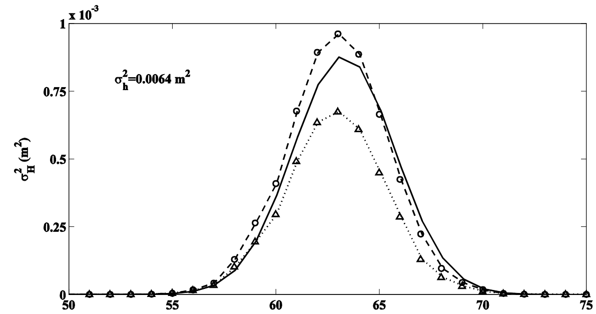
Fig. 3 Comparisons of mean flow depth profiles computed by KLE method (incorporating 2, 3, and 4 terms) with those derived by MCS (for 1000 realizations) at (a) $t = 5\ s$, (b) $t = 10\ s$, and (c) $t = 15\ s$.

E. Investigation of probability distribution of flow depth

As a conclusion, the probability distribution of the random flow depth is examined. The results of flow modeling for single mode standing wave were subjected to the Klomogorov-Smirnof test and the probability distribution of the random variable is determined. Given the normal distribution for input random variable, the normal distribution for the random flow depth was expected. In this regard, the Klomogorov-Smirnof test was applied to compare cumulative distribution function (CDF) of the present work with standard normal CDF. As shown in Fig. 5, KLE results would be as accurate as standard normal CDF, therefore, the values of flow depth have normal distribution.



a)



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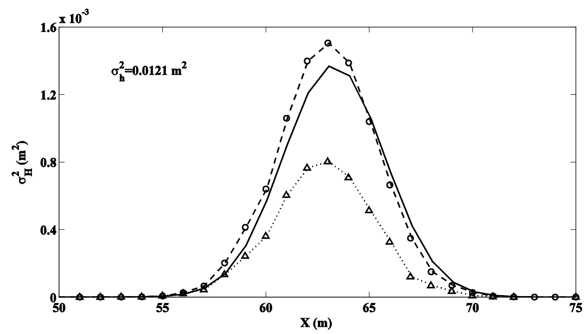

c)

Fig. 4 Comparison of flow depth variances computed by1st and 2nd order KLE with MCS, when a) $\sigma_h^2 = 0.0025 m^2$, b) $\sigma_h^2 = 0.0064 m^2$, and c) $\sigma_h^2 = 0.0121 m^2$ ($\eta_h = 4\ m$, for all the cases).

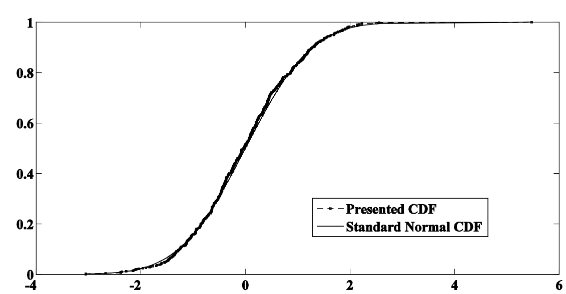

Fig. 5 Comparison of cumulative distribution function of the present work with standard normal CDF

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