Uncertainty Propagation in Puff-based Dispersion Models using Polynomial Chaos

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Abstract – *A simple three-dimensional Gaussian puff-based dispersion model is designed to study the effect of uncertainties in the model parameters on the solution. A polynomial chaos approach to solve stochastic systems with parametric and initial uncertainties is described. The solution of the dispersion model is investigated numerically using this approach. The polynomial chaos solution is found to be an accurate approximation to ground truth, established by Monte Carlo simulation, while offering an efficient computational approach for large nonlinear systems with a relatively small number of uncertainties.*

Keywords: Atmospheric dispersion, polynomial chaos, uncertainty propagation, sensitivity analysis, nonlinear, non-Gaussian distributions

I. Introduction

Real-time detection, tracking, backcasting and prediction of chemical, biological and radiological (CBR) releases is important for fast response to CBR leakages and attacks. Atmospheric dispersion models are used to track the evolution of the releases and assess the impact of the exposure to potentially harmful contaminants over space and time. They enable acquisition of useful knowledge about the hazardous releases due to chemical incidents like the Bhopal gas disaster in 1984 and radiological incidents like the Chernobyl nuclear accident in 1986 [1]. These are also used to estimate or predict the downwind concentration of air pollutants emitted from sources such as industrial plants and vehicular traffic.

Dispersion involves transport (advection) and diffusion of the target species released into the atmosphere. Dispersion modeling uses mathematical formulations to characterize the atmospheric processes that disperse a pollutant emitted by a source. Dispersion is a complex nonlinear physical process with numerous uncertainties in model parameters, inputs, source parameters, initial and boundary conditions. Accurate propagation of these uncertainties through the model is crucial for an robust prediction of the probability distribution of the states and assessment of risk. Uncertainty analysis is recommended as an integral part of any risk assessment to quantify the degree of confidence in the estimate of risk and is particularly significant in CBR applications [2], [3].

Uncertainty propagation in various kinds of dynamical models has been studied extensively in various fields. Most of the methods incorporate linear approximations to nonlinear system response, or involve propagating only a few moments (often, just the mean and the covariance) of the distribution. Adjoint models [4] and parametric differentiation belong to this class and are widely used in sensitivity analysis of the models. These work well if there is adequate local linearity. Another class of methods, often used with models involving nonlinearities, are the various sampling techniques [5]. The uncertainty distributions are taken into account by sampling values from known or approximated distributions and the model is run repeatedly for those values to obtain a distribution of the outputs. A Gaussian mixture based approach is proposed in [6] for accurate uncertainty propagation through nonlinear dynamical systems due to uncertain initial conditions. A survey of the various methods used for uncertainty analysis in dispersion and transport models can be found in [3], [7].

The present work applies generalized polynomial chaos theory [8] to efficiently approximate the solution of a nonlinear dynamical model with parametric uncertainties. Polynomial chaos is a term originated by Norbert Wiener in 1938 [9], to describe the members of the span of Hermite polynomial functionals of a Gaussian process. According to the Cameron-Martin Theorm [10], the Fourier-Hermite polynomial chaos expansion converges, in the L^2 sense, to any arbitrary process with finite variance (which applies to most physical processes). This approach is combined with the finite element method to model uncertainty in [11]. This has been generalized in [8] to efficiently use the orthogonal polynomials from the Askey-scheme to model various probability distributions. This approach has been to applied in modeling uncertainties in multibody dynamical systems [12], structural mechanics [13] and computational fluid dynamics [14], [15]. The present work involves the propagation of parametric uncertainty through a nonlinear puff-based Lagrangian dispersion model. Gaussian puff-based models [16], [17] of this sort are often used to make fast release concentration prediction, in which a series of Gaussian shaped puffs (pollutant atmospheric parcels with a Gaussian distribution of the concentration field for each puff)

are released at the sources and propagated in the atmosphere.

In this work, a representative three-dimensional nonlinear Gaussian puff based dispersion model is designed to study the effects of diffusion parametric uncertainties on the solution. The model is introduced and its dynamics are described in Section II. The polynomial chaos approach is described in Section III. Then, the uncertainty propagation is considered for uncertainties in diffusion parameters for two cases important in the target applications: normal and uniform distributions. The results of numerical trials are discussed in Section IV. The conclusions and further work are presented in Section V.

II. Dispersion Model

The atmospheric dispersion model used is based on the RIMPUFF [17] (Riso Mesoscale PUFF) model which was designed to calculate the concentration and doses resulting from the dispersion of airborne particles. It is a Lagrangian mesoscale atmospheric dispersion puff model, which applies both to homogeneous and inhomogeneous terrain with moderate topography on a horizontal scale of up to 50 km, and responds to changing (non-stationary) meteorological conditions. The model simulates the time varying release (emission) of airborne materials by sequentially releasing a series of Gaussian shaped puffs at a fixed rate on a specified grid. The amount of airborne materials allocated to individual puffs equals the release rate multiplied by the time elapsed between puff releases. At each time step, the model advects, diffuses and deposits the individual puffs according to local meteorological and physico-chemical parameter values. This model is used as a basis to design the present simple dispersion model to study the effects of parametric uncertainty on the solution.

A. Gaussian Puff Characteristics

The concentration distribution in each puff is Gaussian in three-dimensional location space. Its mean represents the location of the puff center, and the standard deviations scales the size of the puff in the three spatial directions. For convenience, the standard deviation σ_x in the downwind direction is made equal to the standard deviation σ_y in the crosswind direction and is denoted by σ_{xy}. The mass Q of the puff is assumed to be constant, that is, deposition and species conversion are not modeled.

Each Gaussian puff has five scalar parameters which vary with time: $[X, Y, Z, \sigma_{xy}, \sigma_z]$, where

$$\begin{aligned} \mathbf{X} &= [X, Y, Z]^T, \text{Centroid of the Gaussian puff} \\ \sigma_{xy} &= \text{Puff size in x and y directions (std. deviation)} \\ \sigma_z &= \text{Puff size in z direction} \end{aligned}$$

The concentration c at a grid point $\mathbf{x_g} = [x_g, y_g, z_g]^T$, at each time step, is calculated by summing the contributions of all the puffs at that instant.

$$c(\mathbf{x_g}) = \sum_{j=1}^{N} \frac{Q_j}{\sqrt{(2\pi)^3 \left|\Sigma_j\right|}} e^{\left[-\frac{(\mathbf{x}_j - \mathbf{x_g})^T \Sigma_j^{-1} (\mathbf{x}_j - \mathbf{x_g})}{2}\right]} \quad (1)$$

where N is the number of puffs and

$$\Sigma_j = \begin{bmatrix} {\sigma_{xy}}_j^2 & 0 & 0 \\ 0 & {\sigma_{xy}}_j^2 & 0 \\ 0 & 0 & {\sigma_z}_j^2 \end{bmatrix}$$

B. Puff Dynamics

The advection and diffusion of each puff takes place according to local meteorological parameter values. In this model, the advection of each puff is calculated according to the surface wind vector, $\mathbf{u}$ at the puff center and the time step, ΔT used to determine the next position of the puff center. Wind shear will cause the puff height to increase when the vertical diffusion σ_z increases. Plume rise due to heat content, buoyancy, release momentum and other effects is ignored for the present simple model.

$$\begin{aligned} X_{k+1} &= X_k + u_X \Delta T \\ Y_{k+1} &= Y_k + u_Y \Delta T \\ Z_{k+1} &= \sqrt{Z_k^2 + \frac{{\sigma_z}_{k+1}^2 - {\sigma_z}_k^2}{2\pi}} \\ \text{where, } \mathbf{u} &= [u_X, u_Y]^T \text{ at } [X_k, Y_k]^T \end{aligned} \quad (2)$$

Expansion with time of a single puff is fundamentally related to the relative diffusion process. It is computed from simultaneous measurements or specifications of the atmospheric turbulence intensity and/or stability in the dispersion area. For the current model, standard plume dispersion information is used. Pasquill parameterization, using a modified Karlsruhe-Jülich system [17], is employed. These parameters can be used to describe puff growth in a constant wind field scenario [18] which we consider in the present work. This parameterization is valid for limited cases of near ground level releases and dispersion over flat terrains. The growth of each puff is described by

$$\begin{aligned} {\sigma_{xy}}_{k+1} &= p_y s_{k+1}^{q_y} \\ {\sigma_z}_{k+1} &= p_z s_{k+1}^{q_z} \\ \text{where, } s &= \text{downwind distance given by,} \\ s_{k+1} &= s_k + \sqrt{u_X^2 + u_Y^2}\Delta T \\ &= \left(\frac{{\sigma_{xy}}_k}{p_y}\right)^{1/q_y} + \sqrt{u_X^2 + u_Y^2}\Delta T \\ p_y, q_y, p_z, q_z &= \text{stability dependent parameters} \\ &\quad \text{(Karlsruhe-Jülich diffusion coefficients)} \end{aligned} \quad (3)$$

Deposition and target species chemical reactivity are neglected for the present model and hence the mass of each puff remains constant during the dispersion process.

III. Polynomial Chaos

The polynomial chaos theory is applied to the solution of a system of stochastic differential equations. A dynamical system with uncertainties represented by a set of stochastic differential equations can be transformed into a deterministic system of equations in the coefficients of a series expansion using this approach. The development in this section largely follows [11] and [8]. The basic goal of the approach is to approximate the stochastic system states in terms of finite-dimensional series expansion in the infinite-dimensional stochastic space. The completeness of the space allows for the accurate representation of any random variable, with a given probability density function (*pdf*), by a suitable projection on a carefully selected basis. The bases can be chosen based on the given *pdf*, to represent the random variable with the fewest number of terms. For example, the Hermite polynomial basis can be used to represent random variables with Gaussian distribution using only two terms. For dynamical systems described by mathematical equations, the unknown coefficients are determined by minimizing an appropriate norm of the residual.

Let us consider a dynamical system of the form:

$$\dot{\mathbf{x}}(t;\mathbf{p}) \quad = \quad \mathbf{f}(\mathbf{x},\mathbf{u};\mathbf{p}) \tag{4}$$

where, $\mathbf{x}(t;\mathbf{p}) \in \mathbb{R}^n$ represents the stochastic system state vector, $\mathbf{u}$ represents the deterministic input and $\mathbf{p} \in \mathbb{R}^m$ represents the uncertain system parameters each of which is a function of random variable ξ with a known *pdf* $g(\xi)$. Now, each of the uncertain states and parameters can be expanded approximately by the finite dimensional Wiener-Askey polynomial chaos as:

$$x_i(t,\mathbf{p}) \quad = \sum_{r=0}^{P} x_{ir}(t)\phi_r(\boldsymbol{\xi}) = \quad \mathbf{x}_i^T(t)\Phi(\boldsymbol{\xi}) \tag{5}$$

$$p_j(\boldsymbol{\xi}) \quad = \sum_{r=0}^{P} p_{jr}\phi_r(\boldsymbol{\xi}) = \quad \mathbf{p}_j^T\Phi(\boldsymbol{\xi}) \tag{6}$$

The total number of terms in the expansion is $P+1$ and is determined by the chosen highest order (l) of the polynomials $\{\phi_r\}$ and the dimension (m) of uncertain variables $\mathbf{p}$.

$$P+1 \quad = \quad \frac{(l+m)!}{l!m!} \tag{7}$$

A. Example

For a dynamical system with two uncertain parameters, each of which is a Gaussian $\mathcal{N}(\mu_j,\sigma_j^2)$ for $j=1,2$, Hermite polynomials are chosen as the random orthogonal basis for expansion. The Hermite polynomials up to order $l=2$ can be written as (see [8], [12] for details on how to select and construct the basis functions):

$$\begin{aligned}
\phi_0(\xi_1,\xi_2) &= 1\\
\phi_1(\xi_1,\xi_2) &= \xi_1\\
\phi_2(\xi_1,\xi_2) &= \xi_2\\
\phi_3(\xi_1,\xi_2) &= \xi_1^2-1\\
\phi_4(\xi_1,\xi_2) &= \xi_1\xi_2\\
\phi_5(\xi_1,\xi_2) &= \xi_2^2-1
\end{aligned}$$

where each ξ_i is $\mathcal{N}(0,1)$. Note that there are six terms in the expansion as given by Eq. (7). The system states can be written as:

$$x_i(t;\xi_1,\xi_2) \quad = \quad \sum_{r=0}^{5} x_{ir}(t)\phi_r(\xi_1,\xi_2), \text{ for } i=1,\ldots,n \tag{8}$$

The two uncertain parameters can be expanded as:

$$p_j(\xi_1,\xi_2) \quad = \quad \mu_j+\sigma_j\xi_j, \text{ for } j=1,2 \tag{9}$$

Note that the coefficients for the other terms are all zero.

B. Solution

Substitution of the expressions for $\mathbf{x}$ and $\mathbf{p}$ in Eq. (5) and Eq. (6) in Eq. (4) leads to:

$$e_i(\boldsymbol{\xi}) = \dot{\mathbf{x}}_i^T(t)\Phi(\boldsymbol{\xi}) - f_i(\mathbf{x}_1,\ldots,\mathbf{x}_n,\mathbf{u},\mathbf{p}_1,\ldots,\mathbf{p}_m;\Phi(\boldsymbol{\xi})) \quad \text{for } i=1,2,\ldots,n \tag{10}$$

The $n(P+1)$ time-varying unknown coefficients x_{ir} can be obtained using the Galerkin projection method. Projecting the error onto the space of basis functions $\{\phi_r\}$ leads to $n(P+1)$ deterministic ordinary differential equations (ODEs):

$$\langle e_i(\boldsymbol{\xi}),\phi_r(\boldsymbol{\xi})\rangle = 0 \quad \text{for } i=1,2,\ldots,n \text{ and } r=0,1,\ldots,P \tag{11}$$

where $\langle u(\boldsymbol{\xi}),v(\boldsymbol{\xi})\rangle = \int_{\mathbb{R}^m} u(\boldsymbol{\xi})v(\boldsymbol{\xi})g(\boldsymbol{\xi})d\boldsymbol{\xi}$ represents the inner product introduced by *pdf* $g(\boldsymbol{\xi})$. For linear and polynomial functions, these integrals can be easily evaluated analytically [11] to obtain the differential equations. For non-polynomial nonlinearities, these integrals represent a challenge. Numerical quadrature methods are used to evaluate the multi-dimensional integrals in the present work. For instance, Gauss-Hermite quadrature formulae are used to evaluate the integrals for a Hermite polynomial basis. These quadrature methods fall under the broader sampling-based Non-Intrusive Spectral Projection (NISP) methods discussed in [19]. The differential equations can then be solved to obtain the time-history of the time-varying coefficients x_{ir}. The solution of the stochastic system in Eq. (4) can thus be obtained in terms of Hermite functionals of Gaussian random variables ξ_i:

$$x_i(t,\mathbf{p}) \quad = \quad \sum_{r=0}^{P} x_{ir}(t)\phi_r(\boldsymbol{\xi}),\ i=1,\ldots,n$$

This expression can be used to plot the *pdf* of the solution by Monte Carlo sampling of the random variables. Further, the first coefficient $x_{i0}(t)$ represents the mean of the solution $x_i(t,\mathbf{p})$ when $\phi_0(\boldsymbol{\xi})=1$. The other coefficients similarly represent the combinations of various moments of the *pdf*:

$$\begin{aligned}
x_{ir}(t) &= \frac{\langle x_i(t,\mathbf{p}),\phi_r(\boldsymbol{\xi})\rangle}{\langle \phi_r(\boldsymbol{\xi}),\phi_r(\boldsymbol{\xi})\rangle}\\
&= \frac{\int_{\mathbb{R}^m} x_i(t,\boldsymbol{\xi})\phi_r(\boldsymbol{\xi})g(\boldsymbol{\xi})d\boldsymbol{\xi}}{\int_{\mathbb{R}^m}\phi_r^2(\boldsymbol{\xi})g(\boldsymbol{\xi})d\boldsymbol{\xi}}
\end{aligned} \tag{12}$$

IV. Results and Discussion

In the present work, the effects of uncertainties in diffusion parameters p_y, q_y, p_z and q_z on the solution of the dispersion model are studied in a simulated CBR dispersion scenario. The simulation experiments are performed for a single puff release whose target species mass is $5e5$. The release occurs at the origin. The wind blows horizontally across the domain at $5m/s$ at an angle of 30° from the x-axis. The evolution of the 5 states of the puff is shown in Fig. 1, for the following diffusion parameters to determine the growth of a puff:

$$\begin{aligned} p_y &= 0.640, \quad q_y = 0.784 \\ p_z &= 0.215, \quad q_z = 0.885 \end{aligned} \tag{13}$$

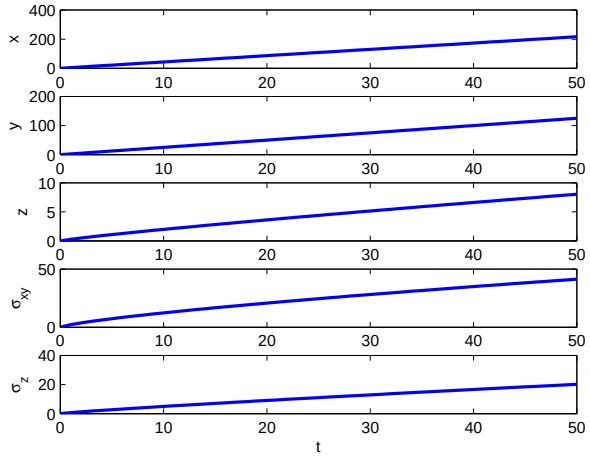

Figure 1. Evolution of puff states

The evolution of the surface concentration (concentration at $[x, y, 0]$) due to the release is shown in Fig. 2, where the concentration surface and contour plots are shown for two time instants $t = 10$ and $t = 20$.

The effects of parametric uncertainty are discussed for the cases of normal and uniform distribution of the four diffusion parameters p_y, q_y, p_z and q_z. Since these parameters do not effect the evolution of X_k and Y_k, they are deterministic.

A. Normal distribution

The diffusion parameters are assumed to be normally distributed around the values chosen in Eq. (13), with a standard deviation of 0.05. The three uncertain puff states are expanded, as described in Eq. (8), in terms of Hermite polynomial functionals of $\boldsymbol{\xi} \in \mathbb{R}^4$, each ξ_m being a random variable with distribution $\mathcal{N}(0, 1)$. The series expansion is done up to a maximum order 4. The diffusion parameters are similarly expanded, as described in Eq. (9). These polynomial chaos expansions are substituted in Eq. (2) and Eq. (3). Using Galerkin approximation as in Eq. (10), a set of deterministic ODEs are obtained which can be solved to obtain the solution of the stochastic system.

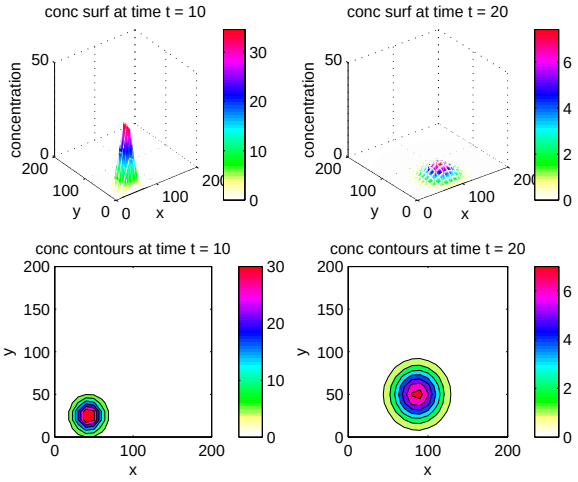

Figure 2. Evolution of concentration

The resulting *pdf*s of the states are plotted for each of the uncertain states in Fig. 3. These are compared with the *pdf*s obtained by the Monte Carlo solution, which involves solving the stochastic system several times, each time with a sample of the diffusion parameters drawn from their uncertainty distributions. 10000 sample draws are chosen in the current example. The polynomial chaos approach involves fewer computations than the standard Monte Carlo approach while it can be seen that the approach captures the distribution of all the states as well as the Monte Carlo approach.

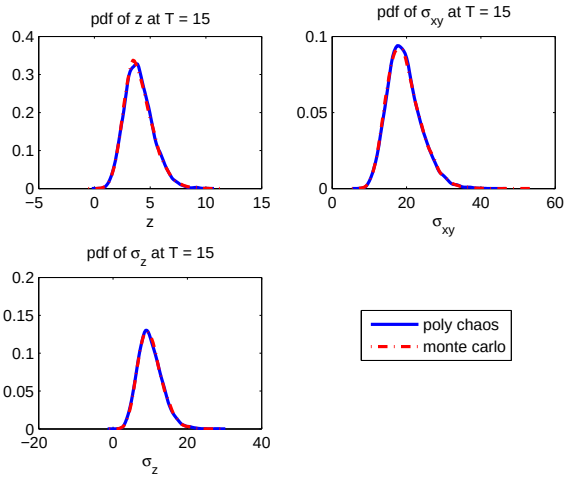

Figure 3. pdf of uncertain states for normally distributed uncertainties

The concentration can be obtained by substituting the solution in Eq. (1). The uncertain concentration at a grid point at various time instants can be obtained using a Hermite polynomial chaos expansion of the concentration. The coefficients can be similarly calculated using the Galerkin projection. The resulting *pdf* is compared with that obtained from Monte Carlo

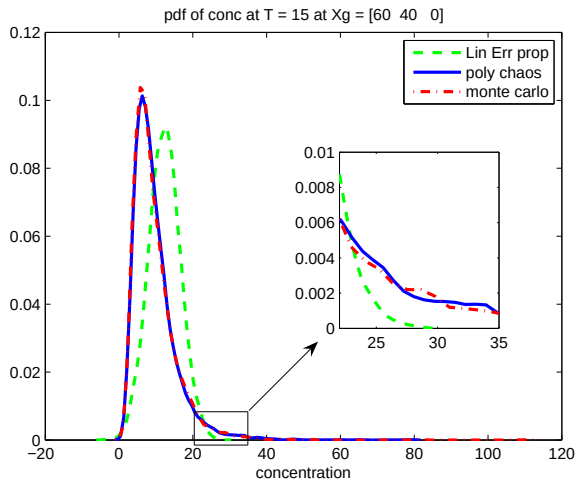

Figure 4. pdf of concentration for normally distributed uncertainties

p_j	a_j	b_j
p_y	0.64	0.84
q_y	0.75	0.85
p_z	0.16	0.26
p_z	0.75	1

Table I
UNIFORM DISTRIBUTION BOUNDS OF DIFFUSION PARAMETERS

solutions of the system in Fig. 4. It can be seen from the figure that the result agrees with the Monte Carlo solution. In the same Fig. 4, the *pdf* of the concentration, obtained using the mean and variance information propagated using a linearized error model of the system, is also plotted (see the green dashed line). Since this method propagates only the mean and covariance, the true distribution is approximated with a Gaussian. It can be seen that the nonlinearities in the model and concentration equation cause the true *pdf* to be very different from this result. For instance, it can be seen from the magnified section of Fig. 4, that this approximation gives a negligible probability for concentrations above 25, while the *pdf* obtained from Monte Carlo/polynomial chaos approach gives a significant probability to influence the risk assessment of a decision-maker. In a CBR scenario, a decision-maker might order an evacuation based on the more accurate risk assessment, while not doing so given the less accurate method propagating only low order moments. Or take other protective measures such as requiring first responders to wear protective coverings. This illustrates the limitations of the linearization approach.

B. Uniform distribution

The diffusion parameters are assumed to be uniformly distributed in this case. The bounds $[a_j, b_j]$ of the distribution of each of the parameters are as shown in Table I.

The three uncertain puff states are expanded, in terms of Legendre polynomial functionals of $\boldsymbol{\xi} \in \mathbb{R}^4$, each ξ_m being a random variable with distribution $\mathcal{U}(-1, 1)$. The series expansion is done up to a maximum order 4. The diffusion parameters are similarly expanded as follows:

$$p_j(\boldsymbol{\xi}) = \frac{b_j - a_j}{2} + \frac{b_j + a_j}{2}\xi_j, \text{ for } j = 1, \ldots, 4$$
$$\text{where, } p_j \in \mathcal{U}(a_j, b_j)$$

These polynomial chaos expansions are substituted in Eq. (2) and Eq. (3). Using Galerkin approximation as in Eq. (10), a set of deterministic ODEs are obtained which can be solved to obtain the solution of the stochastic system. The resulting *pdf*s of the states are plotted for each of the uncertain states in Fig. 5, and compared with the *pdf* of the Monte Carlo solutions. It can be seen that the polynomial chaos approach captures the distribution of all states as well as the Monte Carlo approach. The highly non-Gaussian nature of the *pdf*s is well captured. In addition to the mean and variance, the higher moments are also well captured.

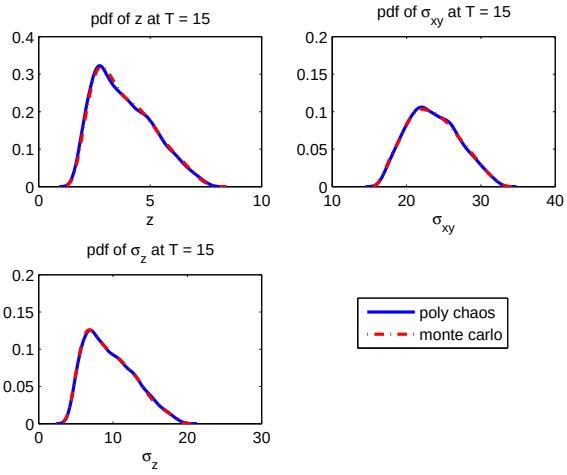

Figure 5. pdf of uncertain states for uniformly distributed uncertainties

The uncertain concentration at a grid point at various time instants can be similarly obtained using a Legendre polynomial chaos expansion of the concentration. The coefficients are calculated using the Galerkin projection. The resulting *pdf* is compared with that obtained from Monte Carlo solutions of the system in Fig. 6.

The results show the ability of the method to correctly propagate the *pdf* of the uncertain states through nonlinear dynamics, for a wide variety of uncertainty distributions in the model parameters. The same approach is similarly valid for the propagation of initial uncertainties in the states.

V. Conclusion

A three-dimensional puff-based model has been tested for the purpose of accurately estimating the uncertainty distribution of the solution, caused by the uncertainty in the diffusion parameters of the model. The polynomial chaos method has

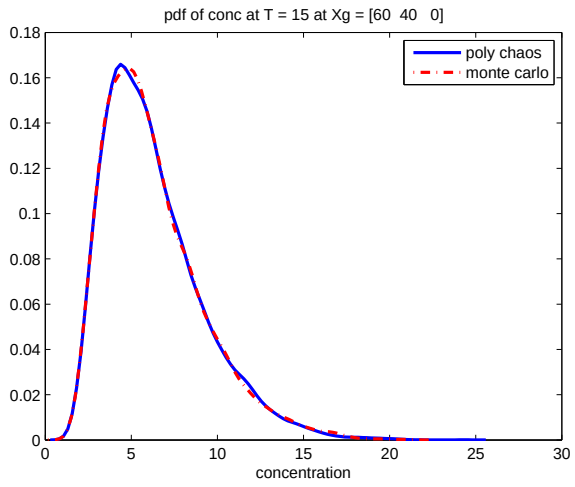

Figure 6. pdf of concentration for uniformly distributed uncertainties

been discussed in the context of uncertainty propagation and applied to the puff model. The approximate solution to the stochastic system is obtained as a linear combination of the selected orthogonal basis functionals, whose coefficients are functions of time.

Using the polynomial chaos approach, the solution to a stochastic nonlinear dynamical system is obtained in terms of functionals of random variables, using which the true distribution of the solution can be approximated. The solution is shown to compare well with the true Monte Carlo solution. The polynomial chaos approach involves fewer computations than the standard Monte Carlo solution approach which requires solving the dynamical model many times for many realizations of the uncertain parameters. When measurements are available, this information about the distribution of the solution can be used to make accurate predictions using data assimilation. This suggests an extension of this approach to filtering problems with dynamical models having known parametric uncertainty distributions, a task currently under investigation.

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