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Uncertainty modelling of atmospheric dispersion by stochastic response surface method under aleatory and epistemic uncertainties

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Abstract. The parameters associated to a environmental dispersion model may include different kinds of variability, imprecision and uncertainty. More often, it is seen that available information is interpreted in probabilistic sense. Probability theory is a well-established theory to measure such kind of variability. However, not all available information, data or model parameters affected by variability, imprecision and uncertainty, can be handled by traditional probability theory. Uncertainty or imprecision may occur due to incomplete information or data, measurement error or data obtained from expert judgement or subjective interpretation of available data or information. Thus for model parameters, data may be affected by subjective uncertainty. Traditional probability theory is inappropriate to represent subjective uncertainty. Possibility theory is used as a tool to describe parameters with insufficient knowledge. Based on the polynomial chaos expansion, stochastic response surface method has been utilized in this article for the uncertainty propagation of atmospheric dispersion model under consideration of both probabilistic and possibility information. The proposed method has been demonstrated through a hypothetical case study of atmospheric dispersion.

Keywords. Uncertainty; polynomial chaos expansion; fuzzy set theory; cumulative distribution function; uniform distribution; membership function.

1. Introduction

Atmospheric dispersion models are mathematical expressions relating the emission of material into the atmosphere to the downwind ambient concentration of the material. The main aim of

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dispersion modelling is to estimate the concentration of a pollutant at a particular receptor point by calculating the basic information about the source of the pollutant and the meteorological conditions. Concentration of an air pollutant at a given place is a function of a large number of variables such as rate of emission, distance of the receptor from the source and atmospheric conditions. The important atmospheric conditions are wind speed, wind direction and vertical temperature structure of local atmosphere. Air pollution dispersion models are subject to scientific uncertainty, but the way this is handled, for air quality management policy differs depending on the scale of modelling and the impact under consideration (Colvile *et al* 2002). Information about parameters in dispersion models can be gained through measurement, calibration, expert judgement, etc. However, value of these parameters may be subject to uncertainty due to lack of measurement point and over-calibration or inaccurate expert judgement. Inherent uncertainty of the input parameters is one of the main cause of uncertainty in model output. Parameter uncertainty is present because a single value of a parameter cannot completely characterize a modelling platform (Saeedi *et al* 2008).

A large number of mathematical methods have been developed for handling those uncertainties. Probabilistic and statistical methods available are usually preferred for analysis of aleatory uncertainty. Some of the methods for uncertainty propagation are available in Du & Chen (2001), Hessian *et al* (1996), Hoybe (1998), Isukapalli & Georgopoulos (1998), Mahadevan & Raghothamachar (2000), Wang (1999). The most popular existing method of aleatory uncertainty analysis is Monte–Carlo Simulation (Mahadevan & Raghothamachar 2000) where large number of parameters are generated based on the distribution functions of the parameters and propagated to draw distribution function for model output. Most important methods of handling epistemic uncertainties consist of interval analysis (Sengupta & Pal 2000), possibility theory (Dubois & Parde 1988) and fuzzy set theory (Zadeh 1978). On the other hand, several competing approaches have been suggested when both aleatory and epistemic uncertainties are present (Baudrit *et al* 2007; Ferson *et al* 1999; Guyonnet *et al* 2003; Kentel & Aral 2005).

With advances in fuzzy mathematics, researchers have applied this theory into different fields. Some of the literature describing the application of fuzzy mathematics and fuzzy logic in the field of atmospheric dispersion are Fakhraee *et al* (2007) and Saeedi *et al* (2008), where the authors used direct fuzzy modelling to construct fuzzy-rule-base considering the Gaussian plume function. An approach to non-probabilistic sensitivity analysis of dispersion model RIMPUFF using the Hartley-like measure is explained explicitly by Chutia *et al* (2013). Also, a non-probabilistic sensitivity and uncertainty of atmospheric dispersion using fuzzy set theory can be found in Chutia *et al* (2013). Further, a hybrid method of uncertainty analysis of atmospheric dispersion under the presence of fuzzy numbers and imprecise probability as input uncertainties is discussed by Chutia *et al* (2013).

The objective of this paper is to present a theory of the stochastic response surface method (SRSM) under both the probability and the possibility theories and its application through a hypothetical case study of atmospheric dispersion. The previous uncertainty modelling of atmospheric dispersion was mostly based on either stochastic or fuzzy approaches. But only a few of previous studies on atmospheric dispersion admits integration of both aleatory and epistemic uncertainties into a single modelling platform. So, an attempt has been made to combine these types of uncertainty into a single modelling platform. Also the SRSM is a purely probabilistic method where the input parameters have probability density functions. Here an attempt has been made to incorporate possibility information into it. The primary purpose is to promote a methodology for uncertainty modelling when information about model parameters are both probabilistic and fuzzy. The proposed method is rather an extension of the SRSM to a Hybrid SRSM. The proposed method has been successfully applied to a hypothetical atmospheric dispersion model and the results are interpreted in terms of percentile.

The structure of the paper is as follows. In section 2, general concept of different types of uncertainty and a brief concept of fuzzy set theory are laid down. Also the different uncertainty modelling method under probabilistic, possibility and hybrid (probabilistic-possibility) are discussed. In section 3, the SRSM under both the probabilistic and the possibility environment is discussed. In section 4, a hypothetical atmospheric dispersion model is considered as a case study. The concerned model and the input data are taken from Abrahamsson (2002). Finally, in section 5, the conclusions have been provided.

2. Types of uncertainty and approaches of analysis

2.1 *Uncertainty representation*

Two types of uncertainty exist in the real world, namely aleatory and epistemic. Uncertainty which results from the fact that a system behaves in random ways is aleatory and uncertainty that results due to lack of knowledge about fundamental phenomena, system and property of analysis performing the analysis is epistemic. If sufficient amount of information are available, stochastic simulations with parameters generated by probability density functions can be used to assess aleatory uncertainty. This type of uncertainty is also referred to as irreducible, stochastic, or random uncertainty. On the other hand, reasons for epistemic uncertainty is lack of reliable experimental data, which can be ambiguous, conflicting, insufficient, or not in agreement with existing conceptual models used for predictions and quantifying uncertainty (Faybishenko 2010).

Uncertainties can be represented in many ways. The literature describes many types of uncertainty representation. Among the most encountered uncertainty representations are probability distributions, interval, probability bounds and fuzzy numbers. Aleatory uncertainties are represented by probability distributions and fuzzy is the representation of epistemic uncertainty. Probability bounds and interval are used to represent both aleatory and epistemic uncertainties. Probability bounds are constructed from parametric probability distributions where the parameters are uncertain. Probability bounds can also be constructed without making any assumption about the shape of the distribution (Ferson *et al* 1999). Uncertainty may not always be due to randomness, and if available information is not much informative or subjective or in the form of expert judgement or with imprecise boundaries, fuzzy set introduced by Zadeh (1965) is the best tool to represent it.

2.2 *Fuzzy set theory*

The application of fuzzy set theory has been evident in different fields of study. The concept of fuzzy numbers arise from the experiences of everyday life when many phenomena which can be quantified but cannot be characterised in terms of absolutely precise numbers. Fuzzy numbers are convex and normalised fuzzy sets which are defined on the set of real numbers. The membership function of a fuzzy number assigns degree of 1 to the most probable value, also called the mean value and lower degrees to other numbers which reflect their proximity to the most probable value according to the used membership function. Thus, the membership function decreases from 1 to 0 on both sides of the most probable value.

As an illustration, let $\eta = (a, b, c)$ be triangular fuzzy number defined in a real line R. The membership function $\mu_\eta(x)$ of η is defined as

$$\mu_\eta(x) = \begin{cases} \frac{x-a}{b-a}, & \text{if } a \le x \le b; \\ \frac{c-x}{c-b}, & \text{if } b \le x \le c; \\ 0, & \text{otherwise.} \end{cases} \tag{1}$$

The membership function of a trapezoidal fuzzy number $\beta = (a, b, c, d)$ is defined as

$$\mu_\beta(x) = \begin{cases} \frac{x-a}{b-a}, & \text{if } a \le x \le b; \\ 1, & \text{if } b \le x \le c; \\ \frac{d-x}{d-c}, & \text{if } c \le x \le d; \\ 0, & \text{otherwise.} \end{cases} \tag{2}$$

The most important concept of fuzzy set is α-level set or α-cuts. The α-cut of a fuzzy number is a interval defined for a specific value of the membership function. The α-cut of the triangular fuzzy number η is defined as $[a + \alpha(b - a), c + \alpha(b - c)]$, where $\alpha = [0, \frac{1}{p}, \frac{2}{p}, \cdots, 1]$, p is any natural number and for a trapezoidal fuzzy number defined by the membership function 2 the α-cut is defined as $[a + \alpha(b - a), d + \alpha(c - d)]$, where $\alpha = [0, \frac{1}{p}, \frac{2}{p}, \cdots, 1]$, p is any natural number. The *core* of a membership function for some fuzzy set is defined as that region of the universe that is characterized by complete and full membership in the set. The *support* of a membership function for some fuzzy set is defined as that region of the universe that is characterized by non-zero membership in the set.

2.3 *Uncertainty analysis*

Most commonly used approach for propagating uncertainty in model input parameters are the analytical and the Monte Carlo (MC) Methods. In analytical methods, (Adomian 1980; Isukapalli 1999), output uncertainties are represented explicitly as functions of input uncertainties. These methods cannot be applied to complex non-linear models with large number of uncertainties, but are useful when only small range of uncertainty is considered. Monte Carlo Methods (Frey & Bammi 2003; Ibrahim 1998; Isukapalli 1999; Mahadevan & Raghothamachar 2000), involve the estimation of probability density functions for selected model outputs by performing a sufficiently large number of model runs with randomly sampled inputs. First-order second-moment analysis (Hoybe 1998), stochastic response surface methods (Isukapalli & Georgopoulos 1998), Polynomial Chaos Expansion Method (Wang 1999) and Reliability Analysis based approaches (Du & Chen 2001) are some of the methods that are applicable to aleatory uncertainty analysis.

The growing trend of uncertainty analysis and uncertainty representation need studies in coupling various types of uncertainty existing in a system. Extensive studies are made by coupling probabilistic and fuzzy knowledge in a single platform. The Hybrid Method (Guyonnet *et al* 2003) is a method that combines aleatory and epistemic uncertainties. In fact this is a method for combining the model parameter uncertainty which combines Monte–Carlo technique with extension principle of fuzzy set theory. The Two-phase Monte–Carlo simulation approach can be used to treat both probabilistic and possibility uncertainties. The Two-phase Monte–Carlo approach allows the evaluation and propagation of natural stochastic variability and knowledge uncertainty separately (Hessian *et al* 1996). The probability box (p-box) approach combines intervals and probability density functions, by imposing bounds on a cumulative distribution function (CDF) used to express different sources of uncertainty. This method provides an envelope of distribution functions, which bounds all possible estimations (Ferson *et al* 1999; Ferson & Ginzburg 1995; Tucker & Ferson 2003). The Probabilistic-Fuzzy approach (Kentel & Aral 2004) is also a hybrid method which combines probabilistic and fuzzy parameters and the combined utilization of fuzzy and random variables produces membership functions of model output at different fractiles of model output as well as probability distributions of model output for various α-cut levels of the membership function. The 2D Fuzzy Monte Carlo Analysis (2D FMCA) (Kentel & Aral 2005) is a modification of 2D Monte Carlo Method (2D MCM). The main difference between them is that the former uses fuzzy numbers as input where as the latter uses probability density functions as inputs. Kentel & Aral (2005) proved that the 2D FMCA is more realistic than the pure 2D MCM in health risk assessment applications where probabilistic and possibility information may exist. A joint-propagation method (Baudrit *et al* 2007) is discussed for groundwater contamination risk assessment and compared to interval analysis and MC method. Integrated fuzzy-stochastic modelling (IFSM) (Heng *et al* 2008) approach is developed for assessing air pollution impacts towards asthma susceptibility. This approach also quantifies uncertainties associated with both source/medium conditions and evaluation criteria and thus assesses air pollution risk. Chen *et al* (2010) integrated fuzzy set theory with Monte Carlo method to study the uncertainties associated with produced water discharges and related regulated pollution criteria for the marine environment. An Integrated Simulation-Assessment Approach (ISAA) (Yang *et al* 2010) is developed to systematically tackle multiple uncertainties associated with hydrocarbon contaminant transport in subsurface and assessment of carcinogenic health risk by integrating Fuzzy Latin Hypercube Sampling (FLHS) and Fuzzy-rule-based Risk Assessment (FRRA) within a general risk assessment framework. Fuzzy Parametrized Probabilistic Analysis (FPPA) (Qin 2012) is a method for assessing risk associated with environmental pollution-control problems.

The above literature review admits that with the advancement of different types of uncertainty it has became a trend in coupling them into a single modelling platform . These types of modelling are often termed as Hybrid methods. The article proposes a hybrid method of uncertainty analysis. The SRSM is a purely probabilistic method of uncertainty analysis. Here an attempt is made to combine probability theory and fuzzy theory through the SRSM and to show its application in uncertainty analysis of atmospheric dispersion model as an hypothetical case study.

3. The stochastic response surface method (SRSM)

The SRSM is an extension of the classical deterministic response surface method (RSM), on which extensive discussion are made in Box & Draper (1987) and Box *et al* (1978). The basic difference between the SRSM and the RSM is that in the former the inputs are random variables, whereas in the latter the inputs are deterministic variables. The SRSM is based on Polynomial Chaos Expansion (PCE) approach. The PCE approach has its foundation in the work by Wiener (1938), who represented a Gaussian process as an infinite series of the Hermite polynomial that takes a vector of random variables as arguments. The explanation of the SRSM is presented here through the PCE approach.

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 random variables, each with zero mean and unit variance, as arguments (Datta & Kushwaha 2011). These random variables are referred as Standard Random Variables (*srvs*). The expansion uses a rescaled version of Hermite polynomials which correspond to a Gaussian or normal distribution. In SRSM, inputs are represented as functions of normal random variables, each having zero mean and unit variance. The same set of random variables that is used to represent input stochasticity can then be used for representation of outputs. The model output in terms of the *srvs* as multidimensional Hermite polynomial with unknown coefficients, as follows:

$$y_j = a_{j,0} + \sum_{i_1=1}^{n} a_{j,i_1}\Gamma_1(\zeta_{i_1}) + \sum_{i_1=1}^{n}\sum_{i_2=1}^{i_1} a_{j,i_1 i_2}\Gamma_2(\zeta_{i_1}, \zeta_{i_2}) + \sum_{i_1=1}^{n}\sum_{i_2=1}^{i_1}\sum_{i_3=1}^{i_2} a_{j,i_1 i_2 i_3}\Gamma_3(\zeta_{i_1}, \zeta_{i_2}, \zeta_{i_3}) + ..., \quad (3)$$

where $a_{j,i_1}, a_{j,i_2}, \cdots$ are unknown coefficients to be determined with respect to the specified model used for uncertainty analysis, and $\Gamma_p(\zeta_{i_1}, \cdots, \zeta_{i_p})$ are defined to be multivariate Hermite polynomials in the p-dimensional sequence of uncorrelated standard normal random variables. The multivariate Hermite polynomial can be written as,

$$\Gamma_p(\zeta_{i_1}, \cdots, \zeta_{i_p}) = (-1)^p e^{\frac{1}{2}\zeta^T\zeta} \frac{\partial^p}{\partial\zeta_{i_1}\cdots\partial\zeta_{i_p}} e^{-\frac{1}{2}\zeta^T\zeta}, \quad (4)$$

where ζ is the vector of p identically independently distributed random normal variables $\{\zeta_{i_k}\}_{k=1}^{p}$.

The stochastic response surface described by Eq. (3) must be limited to a more reasonable size to allow for the evaluation of the model required. The limiting factor is the number of the uncertain parameter present in the system along with the chosen limit on the single variable representation of the polynomial basis. The space is limited to a finite number of terms N given by

$$N = \frac{(p+n)!}{p!n!}, \quad (5)$$

where p is the order of the polynomial and n is the number of *srvs* used to represent the uncertainty in model inputs. Thus for simplicity, the Eq. (3) may be written as

$$y_i = \sum_{i=0}^{N} \beta_i \Phi_i(\zeta), \quad (6)$$

in which β_i and $\Phi_i(\zeta)$ are identical to $a_{j,i_1}, a_{j,i_2}, \cdots$ and $\Gamma_p(\zeta_{i_1}, \cdots, \zeta_{i_p})$, respectively.

The minimum numbers 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 probability density functions depend 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 degree of freedom in uncertainty. So, the number of unknown coefficients to be determined for the model output can be explicitly written using Eq. (5) as

$$N_2 = 1 + 2n + \frac{n(n-1)}{2}, \quad \text{for } 2^{\text{nd}} \text{ order Hermite polynomial}, \quad (7)$$

$$N_3 = 1 + 3n + \frac{3n(n-1)}{2} + \frac{n(n-1)(n-2)}{6}, \quad \text{for } 3^{\text{rd}} \text{ order Hermite polynomial.} \tag{8}$$

So, an explicit representation of 2nd order polynomial chaos expansion for two and three uncertain inputs can be written using Eqs. (6–7) as

$$y_2 = a_0 + a_1\zeta_1 + a_2\zeta_2 + a_3(\zeta_1^2 - 1) + a_4(\zeta_2^2 - 1) + a_5\zeta_1\zeta_2, \tag{9}$$

$$y_3 = a_0 + a_1\zeta_1 + a_2\zeta_2 + a_3\zeta_3 + a_4(\zeta_1^2 - 1) + a_5(\zeta_2^2 - 1) + a_6(\zeta_3^2 - 1) + a_7\zeta_1\zeta_2 + a_8\zeta_1\zeta_3 + a_9\zeta_2\zeta_3. \tag{10}$$

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 Eqs. (7) and (8) as {6, 10 and 15} and {10, 20 and 35}, respectively. Thus for two uncertain model inputs the second order polynomial needs six simulations to estimate the unknown coefficients. The estimation of coefficients of series expansions model inputs are sampled in terms of *srvs* and the model outputs at these sample points are used in Equation (3) to obtain a linear system of equation as $[\zeta]\{a\} = y$, from which coefficient vector $\{a\}$ can be solved using singular value decomposition.

For reference, the first few Hermite polynomials are given by

$$H_0(\zeta) = 1, \; H_1(\zeta) = \zeta, \; H_2(\zeta) = \zeta^2 - 1, \tag{11}$$

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

$$H_{k+1}(\zeta) = \zeta H_k(\zeta) - k H_{k-1}(\zeta). \tag{12}$$

3.1 *Representation of input distribution in terms of srvs*

Normal random variables are selected as *srvs* as they have been extensively studied and their functions are typically well-behaved. Here, the *srvs* are selected from a set of independent, identically distributed normal random variables. Each ζ_i has zero mean and unit variance. With the advent of newer uncertainty theories such as fuzzy set theory, evidence theory, possibility theory, random set theory and others, it is necessary to revisit the different kinds of uncertainty inherent in different kinds of modelling. When some uncertain parameters are represented as probability distributions while others are represented as possibility distributions, a transformation method will then be used to propagate these hybrid uncertainties through different models. The SRSM is accomplished to incorporate fuzzy uncertainties as model inputs. This is performed by discretizing the fuzzy parameter into α-cuts, say $\alpha = [0, 1/m, 2/m, \cdots, 1]$, m is any natural number and each of these α-cuts represent an interval. Without loss of generality the underlying uncertainty can be very well expressed by a uniform distribution. Suppose that only thing known about a variable X is that it can take values between 0 and 1. Apparently, a uniform distribution $U(0, 1)$ is an obvious choice (Brandimarte 2011; Nguyen 2012). The α-cut of a fuzzy number gives the possible information of a variable with some degree of membership and its distribution is often unknown. In such a situation uniform distribution around the bounds of the α-cut is obvious choice. Thus each α-cut of the fuzzy number is finally transformed into *srvs*. Rather than discussing about the common univariate distribution following a univariate continuous probability density function, the following are the relationship between transformed and univariate probability density function for different distribution.

Uniform distribution (a, b): $X = a + (b - a)\left(\frac{1}{2} + \frac{1}{2}erf(\zeta/\sqrt{2})\right)$.

Normal distribution (μ, σ): $X = \mu + \sigma\zeta$.

Lognormal distribution (μ, σ): $X = exp(\mu + \sigma\zeta)$.

Gamma distribution (a, b): $X = ab\left(\zeta\sqrt{\frac{1}{9a}} + 1 - \frac{1}{9a}\right)$.

Exponential distribution λ: $X = -\frac{1}{\lambda}\left(\frac{1}{2} + \frac{1}{2}erf(\zeta/\sqrt{2})\right)$.

Triangular fuzzy number (a, b, c): $X_\alpha = p + (q - p)\left(\frac{1}{2} + \frac{1}{2}erf(\zeta/\sqrt{2})\right)$,

where, $p = a + \alpha(b - a)$, $q = c + \alpha(b - c)$ and $\alpha = [0, \frac{1}{p}, \frac{2}{p}, \cdots, 1]$, p being a natural number.

Trapezoidal fuzzy number (a, b, c, d): $X_\alpha = p + (q - p)\left(\frac{1}{2} + \frac{1}{2}erf(\zeta/\sqrt{2})\right)$,

where, $p = a + \alpha(b - a)$, $q = d + \alpha(c - d)$ and $\alpha = [0, \frac{1}{p}, \frac{2}{p}, \cdots, 1]$, p being a natural number.

3.2 *An illustration of the application of the SRSM under aleatory and epistemic uncertainties*

As an illustration, consider a computational model with two independent uncertain inputs X_1 and X_2, and output $Y_{\alpha,2}$, where the inputs are given by

$$X_1 = \text{Normal}(\mu, \sigma), \; X_2 = \text{Triangular fuzzy number}(a, b, c).$$

The input uncertain variables can be represented by *srvs* ζ_1 and ζ_2 as follows:

$$X_1 = \mu + \sigma\zeta_1, \; X_{\alpha,2} = p + (q - p)\left(\frac{1}{2} + \frac{1}{2}erf(\zeta_2/\sqrt{2})\right), \text{ where } p = a + \alpha(b - a),$$
$$q = c + \alpha(b - c) \text{ and } \alpha = [0, \frac{1}{m}, \frac{2}{m}, \cdots, 1], \; m \text{ being a natural number,}$$

where $X_{\alpha,2}$ is transformed input variable in terms of *srvs*, ζ_2 at a particular α level. A second order polynomial approximation for $Y_{\alpha,2}$ in terms of ζ_1 and ζ_2 is given by

$$y_{\alpha,2} = a_{\alpha,0} + a_1\zeta_1 + a_{\alpha,2}\zeta_2 + a_{\alpha,3}(\zeta_1^2 - 1) + a_{\alpha,4}(\zeta_2^2 - 1) + a_{\alpha,5}\zeta_1\zeta_2. \quad (13)$$

In order to estimate the 6 unknown coefficients, for response output, the inputs are sampled as $(x_{1,1}, x_{1,2}, \cdots, x_{1,6})$ and $(x_{\alpha,2,1}, x_{\alpha,2,2}, \cdots, x_{\alpha,2,6})$. Then the outputs at these sample points are obtained as $y_{\alpha,1,1}, y_{\alpha,1,2}, \cdots, y_{\alpha,1,6}$ and used to calculate the coefficients $a_{\alpha,0}, a_{\alpha,1}, \cdots, a_{\alpha,5}$ by solving the following linear equations through singular value decomposition. Let

$$M = \begin{bmatrix} 1 & \zeta_{1,1} & \zeta_{2,1} & \zeta_{1,1}^2 - 1 & \zeta_{2,1}^2 - 1 & \zeta_{1,1}\zeta_{2,1} \\ 1 & \zeta_{1,2} & \zeta_{2,2} & \zeta_{1,2}^2 - 1 & \zeta_{2,2}^2 - 1 & \zeta_{1,2}\zeta_{2,2} \\ 1 & \zeta_{1,3} & \zeta_{2,3} & \zeta_{1,3}^2 - 1 & \zeta_{2,3}^2 - 1 & \zeta_{1,3}\zeta_{2,3} \\ 1 & \zeta_{1,4} & \zeta_{2,4} & \zeta_{1,4}^2 - 1 & \zeta_{2,4}^2 - 1 & \zeta_{1,4}\zeta_{2,4} \\ 1 & \zeta_{1,5} & \zeta_{2,5} & \zeta_{1,5}^2 - 1 & \zeta_{2,5}^2 - 1 & \zeta_{1,5}\zeta_{2,5} \\ 1 & \zeta_{1,6} & \zeta_{2,6} & \zeta_{1,6}^2 - 1 & \zeta_{2,6}^2 - 1 & \zeta_{1,6}\zeta_{2,6} \end{bmatrix}$$

which can be calculated from the values of ζ's at each sample point whereas $y_{\alpha,1,i}$ are the corresponding model outputs obtained from the linear system

$$M \times [a_{\alpha,0}, a_{\alpha,1}, \cdots, a_{\alpha,5}]^T = [y_{\alpha,1,1}, y_{\alpha,1,2}, \cdots, y_{\alpha,1,6}]^T.$$

Now, the coefficients are estimated, the distribution of $Y_{\alpha,2}$ is fully described by polynomial chaos expansion as shown in Eq. (13). The whole process is repeated for all the α-cut taken. Statistical properties from response can be obtained by performing a large number of Monte–Carlo simulation at each level of α's.

4. A case study

4.1 *Problem statement*

A case study is made by considering the example cited in Abrahamsson (2002), the problem involves a simplified pressurized ammonia storage facility, consisting of a pressurized tank and 3 meters of pipeline. The assessment will consider the release of pressurized ammonia to the surroundings, and the assessment end-points are to determine concentration of ammonia at a geographical location. A dispersion model is used for estimating the concentration of ammonia at a specific geographic point. The average concentration of ammonia at a particular location, following a discharge is given by the following expression.

$$C = \frac{Q}{\pi \sigma_y \sigma_z U}, \tag{14}$$

where,

C Concentration of ammonia (kg/m^3).
Q Mass discharge/release rate (kg/sec).
σ_y, σ_z Dispersion coefficients (m).
U Wind speed (m/sec).

The equation of mass discharge rate is given by

$$Q = C_d A \sqrt{\frac{2(P_o - P_a)}{V_f}}, \tag{15}$$

where,

C_d Discharge coefficient.
A Area of the hole (m^2).
P_o Pressure in the tank (N/m^2) $= 5 \times 10^5$.
P_a Atmospheric pressure (N/m^2) $= 1 \times 10^5$.
V_f Specific volume of liquid (m^3/kg) $= 1/617$.

The state of art models related to atmospheric dispersion is deterministic in nature. The Eq. (14) describing the average concentration of ammonia, as a case study to support our approach of combining aleatory and epistemic uncertainty, presents the simplified version of Gaussian plume model under the conditions of plume centerline (coordinate, $y = 0$), ground level (vertical coordinate, $z = 0$) and ground release. Average concentration as depicted in Eq. (14) is a function of the release quantity, the horizontal dispersion coefficient, the vertical dispersion coefficient and the wind speed. In a deterministic model, all these input parameters of the model are crisp, but in real practice, one can never have deterministic value of all these parameters. For example, wind speed is obviously a probabilistic parameter due to its random variation over a certain cycle. On the other hand, the horizontal dispersion and the vertical dispersion coefficients are dependent on the stability class of the wind, which further depends on solar radiation, wind speed, etc. The measured value of the solar radiation and the wind speed averaged over a certain cycle by any instrument is obtained in the form of a range value, and these range value can be possibly tackled by using the theory of fuzzy set. Therefore, if a realistic situation is considered the output cannot be a crisp value, and it is also a fact that, one cannot take any decision if only crisp value of the output as well as the input are optioned. Decision making in the field of atmospheric dispersion modelling has to be taken in presence of uncertainty which is a combination of both the aleatory (probabilistic) and epistemic (lack of knowledge or incomplete information).

In view of this reality, the present model in which the approach of handling both the uncertainties have been presented, will facilitate the decision makers in the said field to take a decision on the quality of the air if pollutants get released in the event of the failure of a system or mal operation during normal practice. For reader's information, it is worth to mention that the atmospheric dispersion models in practice always dictate about the health status of the atmosphere with the help of computed air concentration, without quantifying its uncertainty. But uncertainty of the air concentration is always desired to have a safety measure of any nuclear or industrial facility.

4.2 *Input parameters and the methodology*

Randomness behaviour of uncertain input variable is described by a probability density function and this is basically constructed by adopting a statistical fitting technique. Very often, in practice, parameters of the probability distribution are estimated using available or given experimental data by maximum likelihood method. Implementation of this procedure results the specific probability density function of the input random uncertain variable. On the other hand, imprecise uncertain variables are expressed in terms of a triangular fuzzy numbers, 'in the sense that linguistic phrase of this kind of' uncertainty is very often practised by saying that 'the value of the area of hole is around A m^2'. Now this 'around A' is further expressed by giving a lower and a upper bounds, and accordingly then one have, $\langle$lower bound of A, crisp value of A, upper bound of $A\rangle$ and this comprises a triangular fuzzy number which express the epistemic uncertainty of the uncertain variable A.

Wind speed, discharge coefficient and area of hole are considered to be uncertain variables. Table 1 depicts the uncertainty of the input parameters at different stability categories B, D, E and F. The wind speed U under different stability category constitute of probability distributions similarly the discharge coefficient C_d is taken to be uniformly distributed and the parameter area of hole A is considered uncertain in the sense of fuzzy theory and is considered as triangular fuzzy number. The average ammonia concentration is evaluated at downwind distance $x = 300$ m and the crosswind distance $y = 0$ m. The dispersion coefficient in the horizontal and the crosswind direction are calculated from the Eimutis & Konicek table in Eimutis & Konicek (1972). The fuzzy parameter area of hole A is discretized into 6 number of α-cuts that is $p = 5$ which is chosen arbitrarily. Then each of these α-cuts are expressed as *srvs*, that is, uniformly distributed *srvs*. Total number of simulations chosen for sampling the random parameters here based on the order of the polynomial to be fitted and the number of uncertain inputs. The number of uncertain parameters are 3 and the considered order of Hermite polynomial is 2, so the numbers of unknown coefficients to be determined in the polynomial chaos expansion is 10. Number of repeations of the whole computation depends on the numbers of α-cuts chosen for the fuzzy inputs. Since, the number of α-cuts chosen is 6, the computation repeats for 6 times. At each repeation, that is, for a particular α-cut level, of the computation 10 numbers of coefficients of the response are solved using singular value decomposition. Finally, for all the α-cut levels 6×10 coefficients are solved by using single value decomposition. Statistics of the response surface at the various α-cut levels are thus constructed using a large number of Monte–Carlo simulations.

4.3 *Results and discussions*

The conventional SRSM is a probabilistic process where the inputs are always aleatory. However, the present methodology tries to address the uncertainty due aleatory and epistemic uncertainties. This methodology is applicable, whether the inputs are aleatory or epistemic, however the conventional SRSM is only applicable when the information about the inputs are aleatory. As mentioned earlier, all the information about input parameters may not be always probabilistic or may have uncertainties due to lack of measurement point and over calibration or inaccurate expert judgement. In such case the conventional SRSM is not applicable. But the present methodology can be very well applied to such situation where fuzzy numbers exist as epistemic uncertainties.

Uncertainty analysis is carried out using the SRSM and the stochastic response surface of ammonia concentration is simulated at different α-cuts. The values of the coefficients of the response surface for various α-cuts and for stability categories B, C, D and E are given in tables 2, 3, 4 and 5, respectively. A second order polynomial chaos expansion of ammonia concentration is generated at each α-cut. For the stability category F in the table 5 the first column

Table 1. Information for uncertain parameters.

Parameters	Values
Wind speed U, (Stability B)	Normal [4, 0.4] (m/sec)
Wind speed U, (Stability D)	Normal [5, 1.5] (m/sec)
Wind speed U, (Stability E)	Normal [4, 0.4] (m/sec)
Wind speed U, (Stability F)	Uniform [1, 2] (m/sec)
Discharge coefficient C_d	Uniform [0.7, 0.9]
Area of hole A	tfn $\langle 0.0012, 0.00185, 0.0025 \rangle$ (m^2).

tfn - Triangular fuzzy number

Table 2. Coefficients of response polynomial for the various α-cuts level under the stability category B.

	$\alpha = 0.0$	$\alpha = 0.2$	$\alpha = 0.4$	$\alpha = 0.6$	$\alpha = 0.8$	$\alpha = 1.0$
a_0	01849.0376	01844.3953	01839.7529	01835.1106	01830.4683	01825.8260
a_1	00380.7306	00305.1876	00229.6447	00154.1017	00078.5588	00003.0159
a_2	−0121.3199	−0131.4698	−0141.61972	−0151.7696	−0161.9194	−0172.0693
a_3	00018.3564	00042.0024	00065.6484	00089.2944	00112.9404	00136.5864
a_4	00058.5818	00049.0799	00039.5779	00030.0759	00020.5740	00011.0720
a_5	00119.4595	00101.3484	00083.2372	00065.1260	00047.0149	00028.9037
a_6	−0062.5325	−0049.9506	−0037.3687	−0024.7868	−0012.2049	00000.3770
a_7	−0134.9909	−0109.4779	−0083.9649	−0058.4519	−0032.9389	−0007.4260
a_8	−0091.9802	−0081.4068	−0070.8334	−0060.2601	−0049.6867	−0039.1133
a_9	−0025.2772	−0019.7766	−0014.2761	−0008.7754	−0003.2749	00002.2256

Table 3. Coefficients of response polynomial for the various α-cuts level under the stability category D.

	$\alpha = 0.0$	$\alpha = 0.2$	$\alpha = 0.4$	$\alpha = 0.6$	$\alpha = 0.8$	$\alpha = 1.0$
a_0	07207.3914	07161.9173	07116.4431	07070.9690	07025.4948	06980.0207
a_1	01653.9969	01353.6105	01053.2240	00752.8376	00452.4512	00152.0648
a_2	−1629.0261	−1744.7611	−01860.4961	−01976.2312	−02091.9663	−2207.7013
a_3	00630.9017	00572.8878	00514.8739	00456.8599	00398.8460	00340.8321
a_4	00351.3703	00243.8312	00136.2922	00028.7532	−0078.7858	−0186.3249
a_5	00249.1773	00265.6040	00282.0306	00298.4572	00314.8838	00331.3105
a_6	−0060.7011	−0069.7562	−0078.81130	−0087.8664	−0096.9215	−0105.9766
a_7	00387.8209	00262.1281	00136.4353	00010.7425	−0114.9502	−0240.6430
a_8	00443.4241	00373.8080	00304.1920	00234.5760	00164.9599	00095.3439
a_9	00681.3018	00520.7143	00360.1268	00199.5393	00038.9518	−0121.6356

Table 4. Coefficients of response polynomial for the various α-cuts level under the stability category E.

	$\alpha = 0.0$	$\alpha = 0.2$	$\alpha = 0.4$	$\alpha = 0.6$	$\alpha = 0.8$	$\alpha = 1.0$
a_0	16359.4832	16423.5991	16487.7149	16551.8307	16615.9466	16680.0624
a_1	03879.1608	03190.5227	02501.8847	01813.2466	01124.6086	00435.9705
a_2	−1432.5703	−01384.1971	−1335.8240	−1287.4509	−1239.0778	−1190.7047
a_3	00967.9851	01104.9898	01241.9945	01378.9992	01516.0039	01653.0086
a_4	00590.4612	00487.5045	00384.5477	00281.5909	00178.6341	00075.6773
a_5	00123.4928	00089.9591	00056.4254	00022.8917	−0010.6419	−0044.1756
a_6	−0318.5054	−0148.2563	00021.9927	00192.2419	00362.4910	00532.7401
a_7	00364.6954	00460.3804	00556.0653	00651.7503	00747.4352	00843.1202
a_8	00329.1031	00393.3888	00457.6746	00521.9604	00586.2461	00650.5319
a_9	−0313.3557	−0225.5448	−0137.7341	−0049.9232	00037.8875	00125.6983

Table 5. Coefficients of response polynomial for the various α-cuts level under the stability category F.

	$\alpha = 0.0$	$\alpha = 0.2$	$\alpha = 0.4$	$\alpha = 0.6$	$\alpha = 0.8$	$\alpha = 1.0$
a_0	107518.359	107027.361	106536.363	106045.365	105554.366	105063.368
a_1	20202.4339	16353.9881	12505.5422	08657.0963	04808.6504	00960.2046
a_2	−19178.428	−19396.338	−19614.247	−19832.157	−20050.066	−20267.976
a_3	06115.3554	06604.8067	07094.2580	07583.7093	08073.1607	08562.6120
a_4	−4396.1782	−3630.9806	−2865.7830	−2100.5853	−1335.3877	−0570.1901
a_5	05754.0893	05441.0179	05127.9464	04814.8750	04501.8035	04188.7321
a_6	04139.9984	03764.6865	03389.3747	03014.0629	02638.7511	02263.4392
a_7	−8007.0406	−6779.9990	−5552.9574	−4325.9158	−3098.8742	−1871.8326
a_8	−0154.8431	−0802.9014	−1450.9596	−2099.0179	−2747.0761	−3395.1344
a_9	05616.7170	04105.1052	02593.4933	01081.8815	−0429.7302	−1941.3420

and the last column gives the response polynomial of ammonia concentration at the α-cut level 0 and 1, respectively as follows:

$$\begin{aligned} y_{0,3} = {} & 107518.359 + 20202.4339\zeta_1 - 19178.428\zeta_2 \\ & + 6115.3554\zeta_3 - 4396.1782(\zeta_1^2 - 1) + 5754.0893(\zeta_2^2 - 1) \\ & + 4139.9984(\zeta_3^2 - 1) - 8007.0406\zeta_1\zeta_2 - 154.8431\zeta_1\zeta_3 + 5616.717\zeta_2\zeta_3, \end{aligned} \tag{16}$$

$$\begin{aligned} y_{1,3} = {} & 105063.368 + 960.2046\zeta_1 - 20267.976\zeta_2 \\ & + 8562.612\zeta_3 - 570.1901(\zeta_1^2 - 1) + 4188.7321(\zeta_2^2 - 1) \\ & + 2263.4392(\zeta_3^2 - 1) - 1871.8326\zeta_1\zeta_2 - 3395.1344\zeta_1\zeta_3 - 1941.342\zeta_2\zeta_3. \end{aligned} \tag{17}$$

Eventually, response surface can be obtained at other α-cuts and for other stability categories.

Now the response surface are generated for all the stability categories and at different level of α-cuts, statistical properties of ammonia concentration are evaluated from these response surfaces. A large number of simulations, say 1500, is used to generate the cumulative distribution functions. These distribution functions of ammonia concentration at all the 6 α-cuts for the stability categories B, D, E and F are shown in figures 1, 2, 3 and 4, respectively. Percentiles are best representation of uncertainty; hence 5^{th} and 95^{th} percentiles of the cumulative distribution function of ammonia concentration are obtained and depicted in tables 6, 7, 8 and 9. The basic aim of the problem is to generate a response surface in terms of cumulative distribution functions of the ammonia concentration (mg/m^3) at different α-cuts. So, that different statistical properties can be obtained from the cumulative distribution functions at various α-cuts. Accordingly, uncertainty analyses of ammonia concentration at downwind distance 300 m are obtained. In order to quantify these uncertainties, the 5^{th} and the 95^{th} percentiles are obtained from the cumulative distribution functions at various α-cuts for the different stability categories.

As per regulatory practice under safe design it is always essential to consider a conservative estimate and conservative estimate generally addresses a maximum value, therefore it is mandatory to know that for which weather category maximum uncertainty of air pollutant concentration results. The 5^{th} and the 95^{th} percentiles in tables 6, 7, 8 and 9, indicate that uncertainty

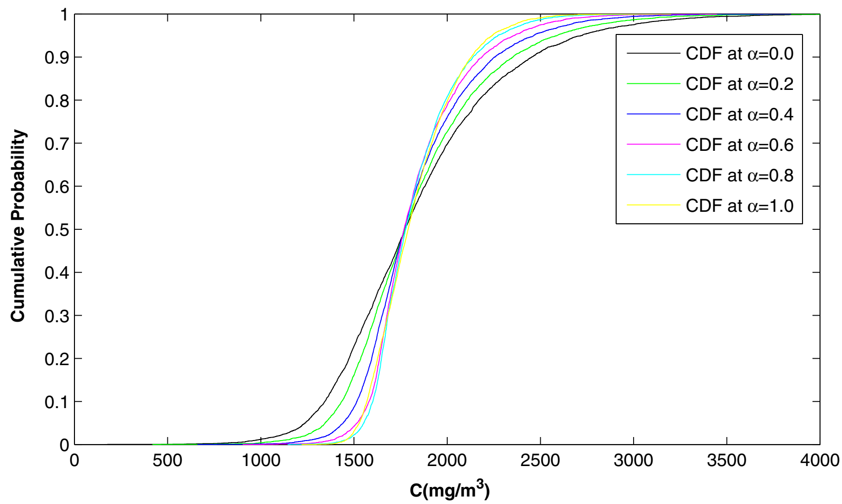

Figure 1. Cumulative distribution functions of ammonia concentration (mg/m^3) at different level of α-cuts by SRSM for stability B.

increases through B (moderately unstable) to F (very stable) for all the chosen α-cuts. Accordingly, the present methodology of uncertainty modelling of atmospheric dispersion indicates that safe design of the specific facility (either nuclear or chemical) should be with respect to extremely stable category of weather. Hence, utmost care should be taken for discharge of toxic or radioactive effluent under the stability category F.

Uncertainty in the domain of probability theory is expressed in terms of confidence interval and is always expressed as $\langle x \rangle \pm k\sigma$, where, $\langle x \rangle$ presents the average (crisp) value, k signifies the critical value (area under the curve representing the probability distribution, in case of a normal distribution, for 95% confidence interval, $k = 1.96$) and σ represents the standard deviation.

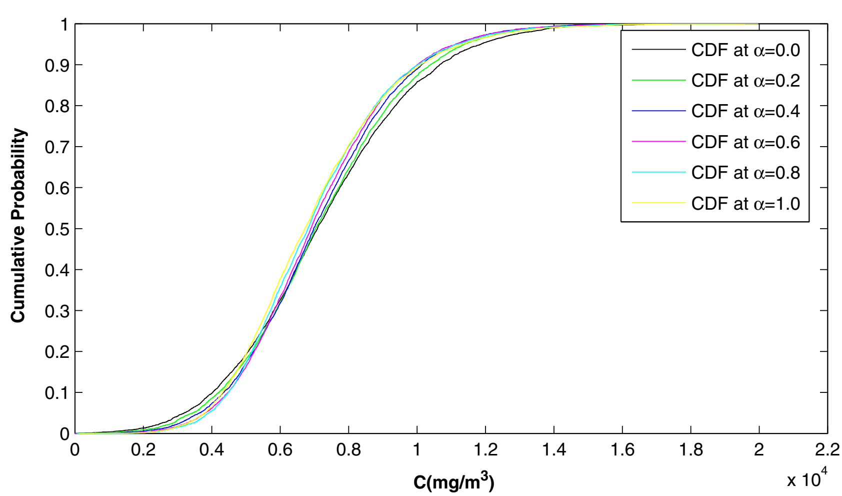

Figure 2. Cumulative distribution functions of ammonia concentration (mg/m^3) at different level of α-cuts by SRSM for stability D.

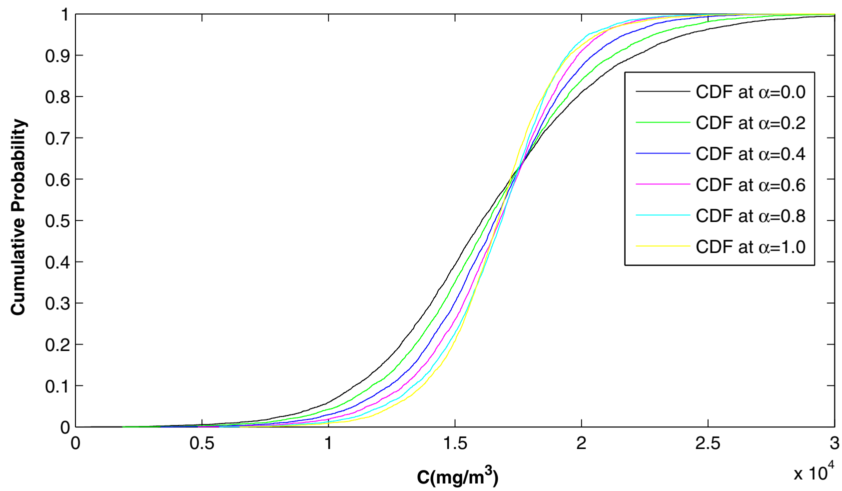

Figure 3. Cumulative distribution functions of ammonia concentration (mg/m^3) at different level of α-cuts by SRSM for stability E.

But the uncertainty in case of lack of information of an input parameter of a model is handled by using fuzzy set, since fuzzy set describes the vagueness or lack of information. Now, following the definition of a fuzzy set, practice is to construct α-cut of the system and since α-cut represents an interval in the real axis, uncertainty of the system is presented in terms of an interval that is nothing but a specific α-cut value. Maximum uncertainty of the system is obviously corresponds to zero α-cut value. According to practice in the field of fuzzy mathematics, uncertainty is expressed for zero α-cut value of the system, but one can also take any α-cut value to express

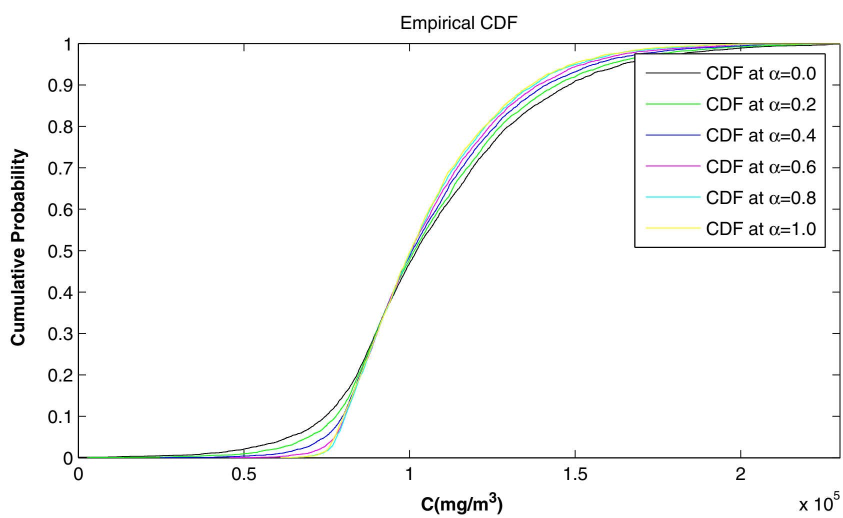

Figure 4. Cumulative distribution functions of ammonia concentration (mg/m^3) at different level of α-cuts by SRSM for stability F.

Table 6. 5^{th} and 95^{th} percentiles of the ammonia concentration (mg/m^3) at downwind distance 300 m under the stability category B by SRSM at different α-cut levels from 0.0 to 1.0.

	5^{th}	95^{th}
SRSM $\alpha = 0.0$	1237.0497	2721.6446
SRSM $\alpha = 0.2$	1344.5268	2590.4037
SRSM $\alpha = 0.4$	1441.6850	2464.5767
SRSM $\alpha = 0.6$	1516.1281	2359.3792
SRSM $\alpha = 0.8$	1551.8207	2272.0581
SRSM $\alpha = 1.0$	1528.1062	2240.7093

Table 7. 5^{th} and 95^{th} percentiles of the ammonia concentration (mg/m^3) at downwind distance 300 m under the stability category D by SRSM at different α-cut levels from 0.0 to 1.0.

	5^{th}	95^{th}
SRSM $\alpha = 0.0$	3195.9334	11872.0682
SRSM $\alpha = 0.2$	3438.0222	11389.3320
SRSM $\alpha = 0.4$	3643.6253	11132.1479
SRSM $\alpha = 0.6$	3814.7037	11171.6992
SRSM $\alpha = 0.8$	3908.6255	11194.8591
SRSM $\alpha = 1.0$	3799.8296	11312.6081

Table 8. 5^{th} and 95^{th} percentiles of the ammonia concentration (mg/m^3) at downwind distance 300 m under the stability category E by SRSM at different α-cut levels from 0.0 to 1.0.

	5^{th}	95^{th}
SRSM $\alpha = 0.0$	9613.7179	24111.5851
SRSM $\alpha = 0.2$	10374.7193	22872.7412
SRSM $\alpha = 0.4$	11002.5842	21715.0012
SRSM $\alpha = 0.6$	11527.2709	20805.7029
SRSM $\alpha = 0.8$	12137.4413	20267.9323
SRSM $\alpha = 1.0$	12530.3296	20638.9835

Table 9. 5^{th} and 95^{th} percentiles of the ammonia concentration (mg/m^3) at downwind distance 300 m under the stability category F by SRSM at different α-cut levels from 0.0 to 1.0.

	5^{th}	95^{th}
SRSM $\alpha = 0.0$	63720.4562	164217.2205
SRSM $\alpha = 0.2$	69559.2123	160201.9260
SRSM $\alpha = 0.4$	74467.4913	156083.3177
SRSM $\alpha = 0.6$	77420.9970	152954.7499
SRSM $\alpha = 0.8$	77990.1796	150527.4844
SRSM $\alpha = 1.0$	77386.7157	149179.9540

it, which can be agreed as an arbitrary. That is why one always tries to look for a method of quantification of uncertainty in which this arbitrariness can be avoided.

As the model is implemented under the presence of fuzzy uncertainty and random uncertainty under the SRSM, it is seen that cumulative distribution functions are generated at each level of α-cuts. Statistical inference such as parametric estimation can be made about the parameters at each level of α. The estimation to be made depends on consideration of the α-cuts which ultimately depends on the decision-maker. A pessimistic decision-maker would choose the estimations at $\alpha = 0$, whereas a optimistic decision-maker would choose the estimation at $\alpha = 1$. For the stable category F a pessimistic decision-maker concludes that 5th and 95th percentiles of pollutant concentration are at 63720.4562 mg/m^3 and 164217.2205 mg/m^3, respectively. Whereas a optimistic decision-maker concludes that 5th and 95th percentiles of pollutant concentration are at 77386.7157 mg/m^3 and 149179.9540 mg/m^3, respectively. Also a pessimistic decision-maker would interprete that 95% of the ammonia concentration scored 164217.2205 mg/m^3 or below and 5% of the ammonia concentration scored 63720.4562 mg/m^3 or below. Further, a optimistic decision-maker would interprete that 95% of the ammonia concentration scored 149179.9540 mg/m^3 or below and 5% of the ammonia concentration scored 77386.7157 mg/m^3 or below.

5. Conclusion

The conventional SRSM is a probabilistic method where the inputs are aleatory uncertainties. However, in the present methodology the SRSM is modified to incorporate aleatory and epistemic uncertainties. The aleatory uncertainties are probability density functions and epistemic uncertainties are fuzzy numbers. The inputs to the SRSM are always *srvs*, hence the fuzzy numbers are discretized into α-cuts and each α-cut is transformed into *srvs*. Hence a methodology of uncertainty analysis of a system under aleatory and epistemic uncertainties has been developed. The methodology is being demonstrated with the help of atmospheric dispersion model at the ground level for the atmospheric conditions B, D, E and F. It has been evident that ammonia concentration at the stability category F is higher than the other categories. Hence utmost care should be taken in modelling a situation under this category. The model output are demonstrated with the help of polynomial chaos expansions at different level of α-cuts. Also, it has been evident that one can take different decision at different level of α-cut. Any statistical properties could be generated from these response surface at different level of α-cuts. In another sense, statistical properties could be generated at different level of possibility.

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