CHEMICAL ENGINEERING TRANSACTIONS

VOL. 35, 2013

A publication of
AIDIC
The Italian Association of Chemical Engineering
www.aidic.it/cet

Guest Editors: Petar Varbanov, Jiří Klemeš, Panos Seferlis, Athanasios I. Papadopoulos, Spyros Voutetakis

ISBN 978-88-95608-26-6; **ISSN** 1974-9791

DOI: 10.3303/CET1335237

Uncertainty analysis of industrial fire effects simulation

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Smoke dispersion prediction systems are becoming increasingly valuable tools in smoke management. Numerical models for dispersion and chemical transport, also known as air quality models, can be used to investigate the fire plume evolution and the smoke impacts (e.g. concentration, temperature). However, all prediction systems include some level of uncertainty, which may occur from the meteorological inputs, diffusion assumptions, plume dynamics, or emission production.
Uncertainty analysis enables to avoid as much as possible bad decisions that may have a large impact in a field such as safety. In this study, we are interested in the uncertainty propagation related to NO_2 atmospheric dispersion resulting from a crude oil tank fire. Uncertainties were defined a priori in each of the following input parameters: wind speed, pollutant emission rate and its diffusivity coefficient. For that purpose, a Monte Carlo approach has been used.

1. Introduction

Due to the complex nature of fire, mathematical prediction models used in fire safety engineering are often simplified and based on a number of assumptions. Even when very sophisticated models are available, a trade-off is often necessary between accuracy, cost and time for design engineers (Lundin, 1999). Many years of research have made it possible to model a wide range of fire phenomena with fire and smoke transport models.
Accuracy of results from mathematical models is often complicated by the presence of uncertainties in their inputs data. Therefore, to be used in effective decision making process, the uncertainty in model predictions must be quantified (Refsgaard, 2007). Uncertainty analysis investigates the effects of lack of knowledge and other potential sources of error in the model (e.g., the uncertainty associated with model parameter values) (EPA, 2009). When carried out, uncertainty analysis allows model users to be more informed about the confidence that can be placed in model results and hence becomes a quality insurance factor.
Within the framework of industrial fire effects, uncertainties in fuel loads, fuel consumption, and emission factors limit our ability to provide the models with accurate emissions inputs. There are also various other uncertainties in meteorological inputs, and parameters related to modelling of smoke transport and dispersion. In addition, there are uncertainties in chemical reactions and phase transformations (gas to particle and vice versa) during the modelling of ozone and secondary particulate matter formation.
In this paper, we study the uncertainty propagation of input parameters of NO_2 atmospheric dispersion model on the variation of its output (NO_2 concentration). In particular, three input parameters are considered as variables: wind speed, pollutant emission rate and its diffusivity coefficient. Each of them is modeled through a probability density function (pdf). The uncertainty propagation has been conducted using the Monte Carlo sampling. All the results are presented in terms of mean values and confidence interval (lower and upper) bounds.
The remainder of this paper is organized as follow. Section 2 is devoted to the presentation of the developed numeric dispersion model. Section 3 gives the general scheme of uncertainty analysis process. Also, therein are given the different probability distributions with respect to the considered uncertain input parameters. Section 4 provides the study results in terms of NO_2 plume dispersion and its concentration at a given threshold distance (defined with regard to target elements). Finally, section 5 summarizes our concluding remarks.

Please cite this article as: Chettouh S., Hamzi R., Innal F., Haddad D., 2013, Uncertainty analysis of industrial fire effects simulation, Chemical Engineering Transactions, 35, 1423-1428 DOI:10.3303/CET1335237

2. Numerical Dispersion Model (NDM) for prediction of fire emissions

Smoke dispersion prediction systems are becoming increasingly valuable tools in smoke management. There are a variety of potential applications that can help current management issues (Ferguson, 2001). These include screening, where methods and models are used to develop "worst-case" scenarios that help determine if alternative burn plans are warranted or if more in-depth modelling is required. Such tools also help in planning, where dispersion predictions aid in visualizing what fuel and weather conditions are best suited for burning or when supporting data are needed to report potential environmental impacts (Ferguson, 2001).

The plume is described in terms of unsteady state convective transport by a uniform ambient wind of heated gas and particulates matter introduced into a stably stratified atmosphere by a continuously burning fire. The mathematical model of a smoke plume consists of the conservation equations of mass, momentum and energy which govern the temperature T, pressure P, density ρ and velocity (u,v) in the direction (x,y), in connection with the k-ε turbulence model (Mcgrattan, 1996).

The induced flow, mass fraction and temperature field can be described by a set of equations derived from the conservation laws for mean flow quantities, the model used in this paper is simplified and described below:

Table1: Numerical dispersion model equations

Transport equation	$\frac{\partial \Phi}{\partial t}+\frac{\partial U\Phi}{\partial x}+\frac{\partial V\Phi}{\partial y}=\Gamma\left(\frac{\partial^2\Phi}{\partial x^2}+\frac{\partial^2\Phi}{\partial y^2}\right)+S$	(1)
Numerical Dispersion Model (NDM)	Continuity equation: $\frac{\partial U}{\partial x}+\frac{\partial V}{\partial y}=0$ Movement equation: $\frac{\partial U}{\partial t}+\frac{\partial U.U}{\partial x}+\frac{\partial V.U}{\partial y}=\frac{1}{\mathrm{Re}}\left(\frac{\partial^2 U}{\partial x^2}+\frac{\partial^2 U}{\partial y^2}\right)-\frac{\partial P}{\partial x}$ $\frac{\partial V}{\partial t}+\frac{\partial U.V}{\partial x}+\frac{\partial V.V}{\partial y}=\frac{1}{\mathrm{Re}}\left(\frac{\partial^2 V}{\partial x^2}+\frac{\partial^2 V}{\partial y^2}\right)-\frac{\partial P}{\partial y}+(Gr_m.C+Gr_T.T)/\mathrm{Re}^2$ Equation of energy: $\frac{\partial T}{\partial t}+\frac{\partial U.T}{\partial x}+\frac{\partial V.T}{\partial y}=\frac{1}{\mathrm{Re}.\mathrm{Pr}}\left(\frac{\partial^2 T}{\partial x^2}+\frac{\partial^2 T}{\partial y^2}\right)$ Equation of conservation of mass: $\frac{\partial C}{\partial t}+\frac{\partial U.C}{\partial x}+\frac{\partial V.C}{\partial y}=\frac{1}{\mathrm{Re}.Sc}\left(\frac{\partial^2 C}{\partial x^2}+\frac{\partial^2 C}{\partial y^2}\right)$	(2)
Adimensional numbers	Reynolds Number $\mathrm{Re}=\frac{U_{jet}.L}{\nu}$ Grashof thermique Number $Gr_T=\frac{\beta_T.g.\Delta T_{\max}.L^3}{\nu^2}$ Grashof massique Number $Gr_m=\frac{\beta_m.g.\Delta C_{\max}.L^3}{\nu^2}$ Schmidt Number $Sc=\frac{\nu}{D_m}$ Prandtl Number $\mathrm{Pr}=\frac{\nu}{D_T}$	(3)

U_{jet} : Rate of pollutant

ν : Viscosity

D_T : Coefficient of thermal diffusion

D_m : Coefficient of mass diffusion

β_T : Coefficient of thermal expansion

β_m : Coefficient of mass expansion

$\Delta T_{\max}$: Maximum thermal gradient

$\Delta C_{\max}$: Maximum concentration gradient

The Dispersion model allows to follow-up of the plume by determining the quantities of the pollutants at each position and at every moment along the life cycle of the plume, which will make it to determine the residence time of the pollutant. That shows the importance of modelling as tool for decision making aid, especially to the experience feedback.

3. Uncertainty analysis in the NDM

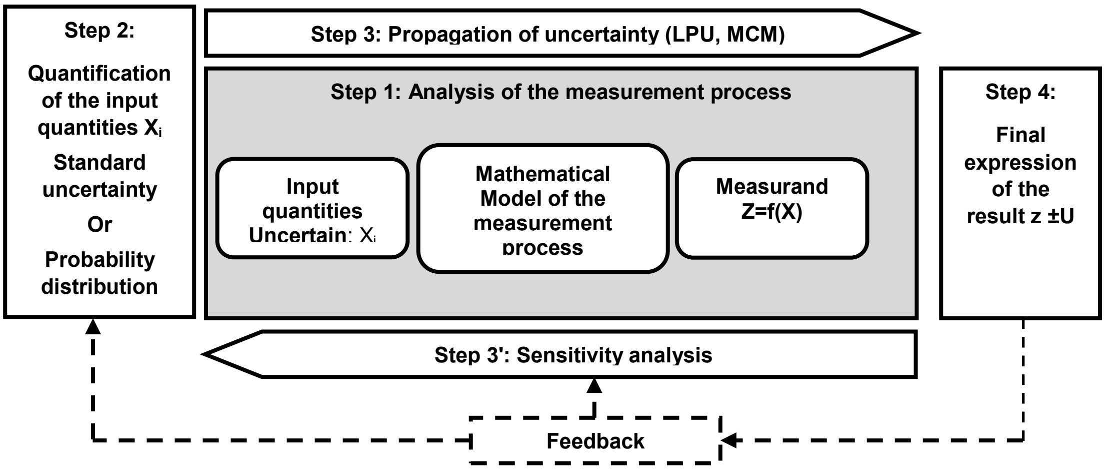


Figure 1: Uncertainty propagation framework

Uncertainty analysis may be achieved by means of different approaches depending on the level of uncertainty associated to the considered parameters. Monte Carlo sampling, fuzzy sets based-approach, intervals analysis are among these approaches (Buratti et al, 2012). Monte Carlo sampling method has become the industry standard for propagating uncertainties (NASA, 2002).

The general scheme of that method is depicted in Figure 1. We give hereafter, in connection with NMD, the main steps of Monte Carlo approach.

Construct a probability density function (pdf) for each input parameter (pdf reflects state of knowledge about the value of the parameter). In our case, the pdfs related to the previously mentioned uncertain parameters are defined in Table 2.

- Generate one set of input parameters by using random numbers (uniformly distributed between 0 and 1) according to pdfs assigned to those parameters.
- Quantify the output function (NO_2 concentration) using the above set of random values and according to the developed NDM. The obtained values are a realization of a random variable (X).
- Repeat steps 2 to 3 *N* times (until a sufficient number, e.g. 1000) producing *N* independent output values. These *N* output values represent a random sample from the probability distribution (empirical distribution) of the output function.
- Generate statistics from the obtained sample for the output result: Mean, standard deviation, confidence interval (percentiles), etc.

The precision in the generated statistics is improved by increasing the number of iterations. It is therefore important to run enough iteration so that the statistics are stable. We note that sensitivity analysis, i.e. the study of how a model's response can be apportioned to changes in model inputs (Saltelli et al, 2000), is out the scope of this paper.

Table 2: Probability distribution functions

Inputs parameters	Type of distribution	Parameters range		
		Min	Mod	Max
Wind speed ($m.s^{-1}$)	Triangular	2	4.5	7
NO_2 initial concentration (% in the smoke)	Continuous uniform	0.1		0.8
NO_2 diffusivity coefficient characterized via the Prandtl number	Continuous uniform	0.7		1

4. Analysis results and discussion

The solution of the partial differential equation described by the general Eq(1) and Table 1, using de finite volumes method which has been implemented on a FORTRAN environment, led to the establishment of curves depicted on Figures 2, 3, 4 and 5. These figures present, the NO_2 atmospheric dispersion (plume) at time t = 100 s and 1200 s from the beginning of the tank fire, NO_2 concentration profile for cloud height y = 50 m and y = 500 m against the Down wind distance (x) and NO_2 concentration profile for a fixed Downwind distances x= 500 m and x= 1.5 Km meters against the cloud height (y). For each figure, the Lower bound, Mean and Upper bound are reported. The achieved iterations number is 1000. The output of each iteration is stored in a matrix which gives the NO_2 concentration for all coordinates (*x*, *y*): c_{xy} .

On the basis of the resulted matrixes (1000 in total), one can compute the mean matrix (c_{xy}^{Mean}), the lower bound matrix (c_{xy}^{Lower}) and the upper bound matrix (c_{xy}^{Upper}) as follows:

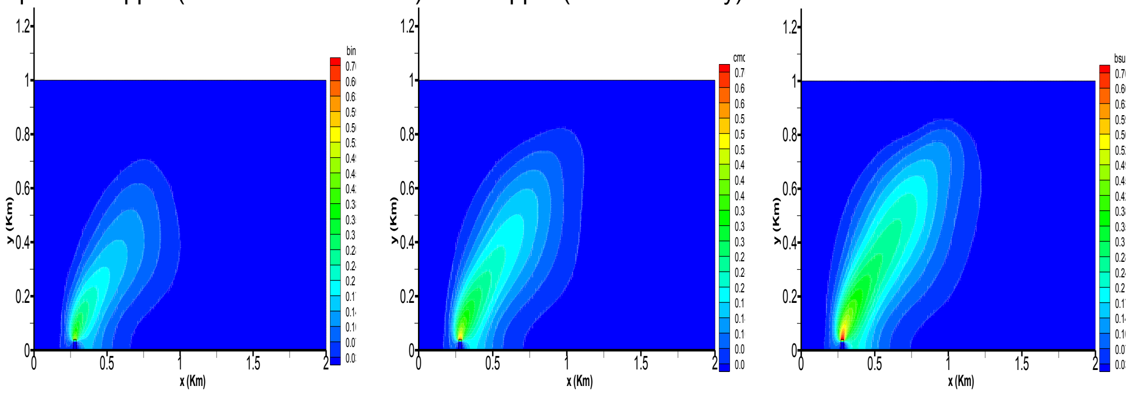
$$c_{xy}^{Mean} = \frac{\sum_N c_{xy}}{N} \; ; \; c_{xy}^{Lower} = c_{xy}^{Mean} - E \cdot \frac{\sqrt{\sum_N (c_{xy}^{Mean} - c_{xy})^2 / N}}{\sqrt{N}}) \; ; \; c_{xy}^{Upper} = c_{xy}^{Mean} + E \cdot \frac{\sqrt{\sum_N (c_{xy}^{Mean} - c_{xy})^2 / N}}{\sqrt{N}})$$

For 90% confidence interval, E equals to 1.64. This being the case, the NO_2 cloud dispersion related to Figures 2(a) and 2(c) (resp. 3(a) and 3(c)) shows respectively the 5th and 95th percentiles of that dispersion for t = 100 s (resp. for t= 1200 s). This means that the true plume dispersion is encompassed between these tow percentiles with a confidence of 90 %. Therefore, decision-makers should not base their judgment solely on the mean values, but they should, in particular, consider the upper bound plume concentration.
To investigate the NO_2 impact on the local population, Figure 4 has been drawn. In fact, NO_2 is a very toxic gas which leads, through inhalation, to pulmonary oedema because of its low solubility in water. Some NO_2 concentration threshold values are given in Table 3 (INERIS, 2004).

Table 3: Some NO_2 concentration threshold values

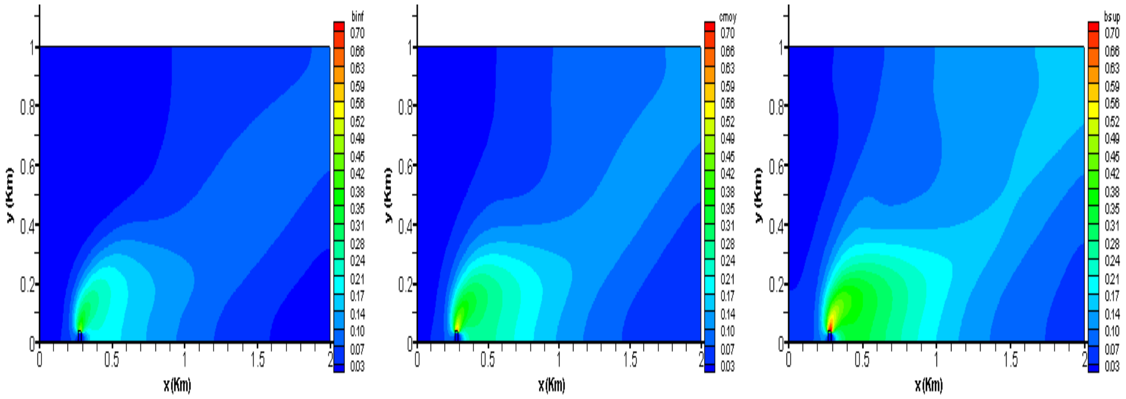
Exposure time (min)	Threshold for irreversible effects (ppm)	Threshold for 1 % lethality (ppm)
1	105	170
10	60	100
20	55	90
30	50	80
60	40	70

According to Table 3 and for 1200 s; (20 min) of release duration, the reference threshold values are taken equal to 55 ppm (for irreversible effects) and 90 ppm (for 1 % lethality).



(a) Lower bound (5th percentile) *(b) Mean* *(c) Upper bound (95th percentile)*

Figure 2: NO_2 plume dispersion for t = 100 s



(a) Lower bound (5th percentile) *(b) Mean* *(c) Upper bound (95th percentile*

Figure 3: NO_2 plume dispersion for t= 1200 s

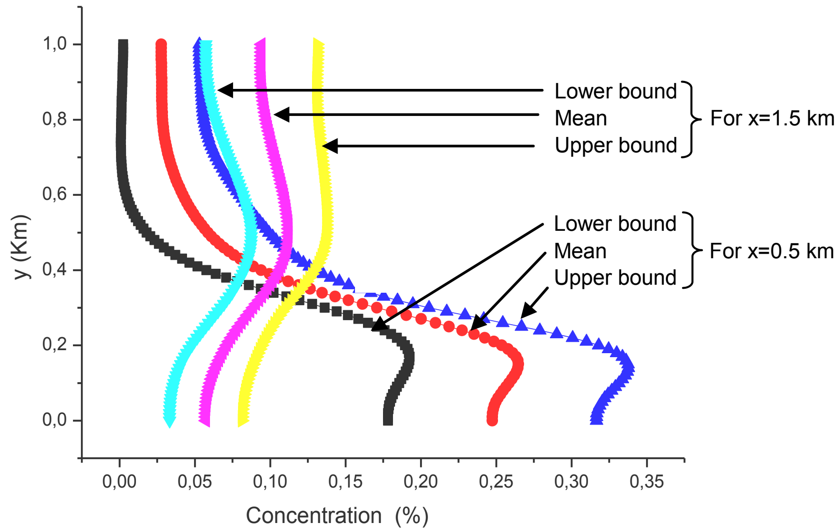


Figure 4: NO_2 plume dispersion at t= 1200 s, for (a) fixed x

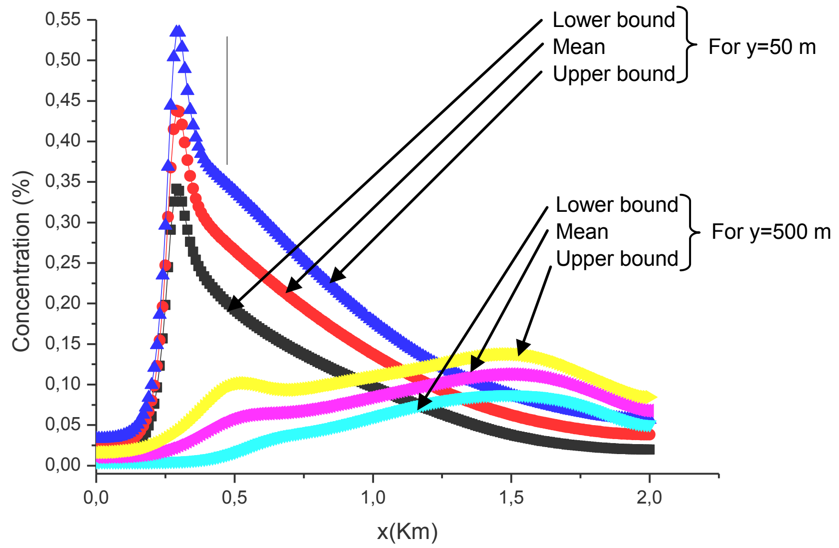


Figure 5: NO_2 plume dispersion at t= 1200 s, for fixed y

Figures 3, 4 and 5 show that the obtained concentrations (mean (1400 ppm), lower (1000 ppm) and upper bounds (1800 ppm)) at the fixed downwind distance (x=500 m) and for (y=50 m) are by far very high compared to threshold values. This means that in case of a similar accident, all the population would be exposed to an intolerable NO_2 concentration.
Hence, the population must be relocated to a safe area. For this purpose, concentration profiles, using upper bounds to be pessimistic, indicate that the threshold concentrations of 55 and 90 ppm remain exceeded even for the downwind distance of 2 km.

5. Conclusion

In this study, we have studied the relative influence of uncertainty in input parameters of an atmospheric dispersion model (wind speed, NO_x initial concentration and NO_x diffusivity coefficient) on the variation of the outputs. Knowing the uncertainty of a prediction is critical for the decision making process. While the uncertainties in various elements of the modelling process are being determined, it is also important to investigate how those uncertainties interact with each other and contribute to the uncertainty in the final result (e.g. NO_x concentration predictions).
Therefore, decision-makers should not base their judgment solely on the mean values, but they should, in particular, consider the upper bound plume concentration.
In further work, we will include all parameters and also consider the parametric sensitivity analysis of the numerical dispersion model.

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