Global and local sensitivity analysis of the Emission Dispersion Model input parameters

Samia Chettouh
Laboratory of Research in Industrial Prevention, Institute of Health and Industrial Safety, University of Batna 2, Batna, Algeria

Received 15 December 2020
Revised 9 April 2021
Accepted 14 April 2021

Abstract

Purpose – The objectives of this paper are the application of sensitivity analysis (SA) methods in atmospheric dispersion modeling to the emission dispersion model (EDM) to study the prediction of atmospheric dispersion of NO_2 generated by an industrial fire, whose results are useful for fire safety applications. The EDM is used to predict the level concentration of nitrogen dioxide (NO_2) emitted by an industrial fire in a plant located in an industrial region site in Algeria.

Design/methodology/approach – The SA was defined for the following input parameters: wind speed, NO_2 emission rate and viscosity and diffusivity coefficients by simulating the air quality impacts of fire on an industrial area. Two SA methods are used: a local SA by using a one at a time technique and a global SA, for which correlation analysis was conducted on the EDM using the standardized regression coefficient.

Findings – The study demonstrates that, under ordinary weather conditions and for the fields near to the fire, the NO_2 initial concentration has the most influence on the predicted NO_2 levels than any other model input. Whereas, for the far field, the initial concentration and the wind speed have the most impact on the NO_2 concentration estimation.

Originality/value – The study shows that an effective decision-making process should not be only based on the mean values, but it should, in particular, consider the upper bound plume concentration.

Keywords Sensitivity analysis, Emission dispersion model, Correlation analysis, Standardized regression coefficient, Monte Carlo simulation

Paper type Research paper

1. Introduction

Because of fires and related accidents, large amounts of carbon monoxide, nitrogen oxides (NOx), volatile organic compounds (VOCs) and other pollutants are produced. The effects of these pollutants have increased significantly and can be short- and long-term with high concentrations significantly affecting human health and air quality (Dadashzadeh *et al.*, 2014; Poudyal *et al.*, 2012; Srinivas *et al.*, 2016). To assess these effects, the so-called emission dispersion model (EDM) was developed by (Chettouh *et al.*, 2014; Hamzi, 2008). The EDM is a deterministic model that takes into account all the phenomena associated with a pollutant in an atmosphere during fire, including diffusion, transport and chemical kinetics in order to estimate its concentration over a given area (Chettouh *et al.*, 2014). The results are deterministic estimates and the analysis does not provide accurate information about the modeled event due to the non-consideration of the associated uncertainty and the sensitivity analysis (SA) to the various involved parameters. Therefore, the main objective of this paper is the estimation of several sensitivity measures related to the EDM to evaluate its sensitivity to its input parameters variation by determining their impact on the concentration of the NO_2 plume at given threshold distances (defined in relation to the target elements). This analysis is an important contribution to the identification of sensitive urban areas in terms of air quality

Funding: This study was not funded.
Conflict of interests: The authors declare that they have no conflict of interest.

World Journal of Science, Technology and Sustainable Development
Vol. 18 No. 4, 2021
pp. 513-532

2042-5945
DOI 10.1108/WJSTSD-12-2020-0102

and evaluation of human exposure to pollutants. The application of the sensibility analysis is also important in accidents management and in the definition of strategies for air quality management in urban areas, through the prevention of future industrial accidents scenarios, which is relevant for safety reports and to prevent wrong decisions that could have a significant impact on the field of industrial safety (Ali and Bruen, 2016).

SA in atmospheric dispersion and fire modeling has been carried out by various studies in different applications and based on some case studies. We cite for example the studies of (Salvador *et al.*, 2001; Ramroth *et al.*, 2006; Clark *et al.*, 2008; Hasofer, 2009; Suard *et al.*, 2013; Alzbutas *et al.*, 2014; Hopkin *et al.*, 2018; Tondini *et al.*, 2019; Gernay *et al.*, 2019) that have oriented toward SA of fire propagation and heat transfer models. While the work of (LIU *et al.*, 2007; Bubbico and Mazzarotta, 2008; García-Díaz and Gozálvez-Zafrilla, 2012; Pandya *et al.*, 2012; Gant *et al.*, 2013; Zhan and Zhang, 2013; Girard *et al.*, 2014; Srinivas *et al.*, 2016; Li *et al.*, 2018; Dhyani and Sharma, 2018; Cao *et al.*, 2020) aimed at the SA of atmospheric dispersion models to study the chemical effects and ecological risks generated by the dispersion of pollutants. These studies were based on different approaches of SA, which varied from local to global with the use of different techniques and sensitivity indices.

In our study, we will perform local and global SA. The obtained result is a hierarchization of the input parameters depending on their contribution to the overall uncertainty. The SA, then allows model users to be more informed about the confidence that can be placed in model results and hence becomes a quality insurance factor (Chettouh *et al.*, 2014).

This study is structured into six main sections: the second section gives the basics ideas of fire modeling and the EDM. The third section presents a general methodology for uncertainty and SA based on Monte Carlo simulation, the included input parameters in the SA and a case study. The fourth section presents the different techniques used to perform the SA. An industrial case study is analyzed, the fifth section shows numerical results and, the sixth section completes the study with conclusions.

2. Fire modeling

Fire models can be categorized into three principal classes (Perry, 1998):

(1) Empirical models;

(2) Semi-empirical models;

(3) Deterministic models.

Due to the difficulties inherent with experiments, particularly for large-scale fires, deterministic fire modeling is become widely used to study ignition, fire behavior and fire spread (Ahmadi *et al.*, 2019; Koo *et al.*, 2020). Three main classes of deterministic models are available: Gaussian models, zone models and computational fluid dynamics models (Ralph and Carvel, 2018).

2.1 Emission dispersion model

The atmospheric dispersion model used in this work is the EDM, which is a computer program that uses an elaborate mathematical algorithm to describe the complex interactions between the thermal effects of a fire and the released pollutants by calculating the resulting particle dispersion concentration resulting from a fire. The EDM is a general model that takes into account all phenomena to which, a pollutant generated during a fire in the atmosphere is subjected, including diffusion, transport and chemical kinetics accompanying the effects representing the fire (Chettouh *et al.*, 2014).

Since the EDM was based on the fire–environment interaction, i.e. the coupling between heat and mass transfer modes, the fire plume is considered to have been described in terms of a two-dimensional, compressible, turbulent, stationary flow regime with a uniform wind speed. Further details about the model can be found in (Chettouh *et al.*, 2014).

With:

U_{jet}: Rate of pollutant; β_{T}: Coefficient of thermal expansion;

ν: Viscosity; β_m: Coefficient of mass expansion;

D_T: Coefficient of thermal diffusion; $\Delta T_{\max}$: Maximum thermal gradient;

D_m: Coefficient of mass diffusion; $\Delta C_{\max}$: Maximum concentration gradient.

The results that can be obtained from this model are:

(1) Pollutant concentration fields that show the significant impact of fires on local air quality;

(2) Thermal fields, which are due to the dispersion of pollutants.

Thus, EDM allows us to track the plume by determining the quantities of pollutants at each position and at any time during the life cycle of the plume, which will allow the determination of the residence time of the pollutant.

This shows the importance of numerical modeling as a decision-making tool and in particular for feedback (Koo *et al.*, 2020). The theory of the EDM is based on the fire–environment dynamic, the interaction between the heat transfer modes and mass. The development of the EDM (See Table 1) is presented in (Hamzi, 2008).

However, even with the development of numerical modeling, models are not yet able to predict accurately fire phenomena. This gap between the reality and simulations is probably due to the presence of uncertainties in their input data. Therefore, to be used in an effective decision-making process, the uncertainties in our model must be quantified and its sensitivity to the input parameters must be analyzed. When carried out, sensibility analysis allows the EDM users to be better informed about the confidence that can be placed in the model's results and thus becomes a quality assurance factor (Chettouh *et al.*, 2014).

Transport equation	$\frac{\partial \Phi}{\partial t}+\frac{\partial U\Phi}{\partial x}+\frac{\partial V\Phi}{\partial y}=\Gamma\left(\frac{\partial^2\Phi}{\partial x^2}+\frac{\partial^2\Phi}{\partial y^2}\right)+S$				
Emission dispersion model (EDM)	Continuity equation: $\frac{\partial U}{\partial x}+\frac{\partial V}{\partial y}=0$ Movement equation: $\frac{\partial U}{\partial t}+\frac{\partial U.U}{\partial x}+\frac{\partial V.U}{\partial y}=\frac{1}{\mathrm{Re}}\left(\frac{\partial^2 U}{\partial x^2}+\frac{\partial^2 U}{\partial y^2}\right)-\frac{\partial P}{\partial x}$ $\frac{\partial V}{\partial t}+\frac{\partial U.V}{\partial x}+\frac{\partial V.V}{\partial y}=\frac{1}{\mathrm{Re}}\left(\frac{\partial^2 V}{\partial x^2}+\frac{\partial^2 V}{\partial y^2}\right)-\frac{\partial P}{\partial y}+(\mathrm{Gr}_m.C+\mathrm{Gr}_T.T)/\mathrm{Re}^2$ Equation of energy: $\frac{\partial T}{\partial t}+\frac{\partial U.T}{\partial x}+\frac{\partial V.T}{\partial y}=\frac{1}{\mathrm{Re.Pr}}\left(\frac{\partial^2 T}{\partial x^2}+\frac{\partial^2 T}{\partial y^2}\right)$ Equation of conservation of mass: $\frac{\partial C}{\partial t}+\frac{\partial U.C}{\partial x}+\frac{\partial V.C}{\partial y}=\frac{1}{\mathrm{Re.Sc}}\left(\frac{\partial^2 C}{\partial x^2}+\frac{\partial^2 C}{\partial y^2}\right)$				
Adimensional number	Reynolds Number $\mathrm{Re}=\frac{U_{jet}.L}{v}$	Grashof thermique Number $\mathrm{Gr}_T=\frac{\beta_r.g.\Delta T_{\max}.L^3}{v^2}$	Grashof massique Number $\mathrm{Gr}_m=\frac{\beta_m.g.\Delta C_{\max}.L^3}{v^2}$	Schmidt Number $\mathrm{Sc}=\frac{v}{D_m}$	Prandtl Number $\mathrm{Pr}=\frac{v}{D_T}$

Table 1.
Emission dispersion model equation (Chettouh *et al.*, 2014)

3. Sensitivity analysis

The deterministic modeling techniques have a series of limitations from which the lack of accuracy and/or proper validation and thus, they do not provide complete information about the modeling accident scenarios and considerably complex and require large number of input parameters (operating temperature and pressure, wind speed, etc.) (Bley *et al.*, 2003; Li *et al.*, 2018; Pandya *et al.*, 2012; Salvador *et al.*, 2001). When model results are used in risk assessment and decision-making, good practice suggests providing best quantitative estimates of the level of uncertainty and sensitivity (such as confidence intervals) (Briggs *et al.*, 2012; De Rocquigny *et al.*, 2008).

The purpose of SA is to determine which factors contribute the most to the amount of uncertainty in model output (Debnath *et al.*, 2015, Gant *et al.*, 2013; Massada and Carmel, 2008; Zhan and Zhang, 2013). Such analysis lead to a better understanding of how to structure the model with respect to reality (Dimitrakopoulos and Omi, 2003; Hall *et al.*, 2009).

3.1 Sensitivity analysis methodology

Because SA is associated with uncertainty analysis, Monte Carlo method (Derwent *et al.*, 2018; Lemieux, 2009; Mycek and De Lozzo, 2019; Nezaratian *et al.*, 2018) is usually used to conduct both of them. It comprises the following steps:

(1) Assign a probability density function (PDF) to each input parameter;

(2) Generate a set of input parameters using random numbers (uniformly distributed between 0 and 1) according to the PDF assigned to these parameters;

(3) Quantification of the output function using a set of random values according to the model in question. The value obtained is a realization of a random variable (X) ;

(4) Repeat steps 2–3, N times (until a sufficient number, e.g. 1,000) producing N independent output values. These N output values represent a random sample from the probability distribution (empirical distribution) of the output function. The accuracy in the statistics produced is improved by increasing the number of iterations. It is therefore important to perform enough iterations so that the statistics are stable;

(5) Generate statistics from the obtained sample for the output result: mean, SD, confidence interval (percentiles), etc. (Chettouh *et al.*, 2014; Innal *et al.*, 2013).

By investigating the sensitivity of model parameters, a user can become knowledgeable of the importance of those parameters in the model (Nezaratian *et al.*, 2018; Price, 2011). There are a large number of approaches to perform a SA depending on the features of the model at hand (computational expense, correlated inputs, model interactions, nonlinearity, etc.) (Li and DeLiberty, 2020).

3.2 Existing methods for sensitivity analysis

The literature contains details on the types of SA tools used for various modeling situations. According to (Saltelli *et al.*, 2004) SA methods may be classified into three types:

(1) *Screening methods:* Allow the analysis the importance of parameters and determine the most influential among a large number that affect the results of the models. The analysis is done qualitatively with a small number of simulations (Saltelli *et al.*, 2004). These methods are useful for models that are expensive to compute and have a large number of input parameters because they are generally less computationally demanding than other methods and are therefore useful for more complex problems (Pandya *et al.*, 2012).

(2) *Local sensitivity methods:* Methods based on the calculation of a partial derivative at a point (Saltelli *et al.*, 2004), this derivative presents the sensitivity index, which represents the variations of an output of the model following a small variation of an input parameter (Li and DeLiberty, 2020). In this method only one parameter varies at a time, the others remain at their nominal value; this avoids problems of cancellation effects (when the effects of two factors influencing the output cancel each other out). This method is simple to implement because it does not require a complex mathematical procedure (Spitz, 2012), but may appear insufficient to characterize the sensitivity of complex models because it does not take into account the interactions between the parameters (Spitz, 2012).

(3) *Global sensitivity methods:* This analysis consists of evaluating the effect of one parameter while all other parameters are varied simultaneously (Li and DeLiberty, 2020; Sun *et al.*, 2020). Global SA focuses on the variability of the model output within its range of variation. These methods take into account the interactions between parameters without depending on the stipulation of a nominal point (they explore the full range of each parameter). They focus on the overall effect of input variables on the model output by varying the input parameters and vary each over the range of the input parameter to calculate their influence on the output (Rodriguez-Fernandez *et al.*, 2012). The statistical distributions for each input variable are defined in the analysis, which explains the degrees of knowledge of the input parameters. The most popular methods of global analysis are the Sobol method, the FAST (Fourier Amplitude Sensitivity Test) method, the DGSM (derivative-based global sensitivity measures) method (Kucherenko *et al.*, 2009; Sobol, 2001), the linear regression method, etc.

4. Performing a sensitivity analysis for EDM

In order to determine the most influential parameters on the numerical dispersion model, several methods of SA were used.

4.1 Local sensitivity analysis

There are several ways to define the sensitivity of a model in relation to its input parameters. In this section, the sensitivity to a single input factor is first considered. In order to further, investigate the impact of variation of the input parameters with respect to NO_2 concentration

This method is simple to implement and the results are easy to communicate, this is why this kind of techniques have been the most used among the scientific community for years (Li and DeLiberty, 2020). Many works on SA in fire research and atmospheric dispersion have adopted the OAT method such as the studies achieved by (Bessie and Johnson, 1995; Bevins and Martin, 1978).

To carry out a local SA for EDM, the index (S_i), which is proposed by Hoffman and Miller, 1983, and Bauer and Hamby, 1991, is calculated from the percentage difference in the output when an input parameter varies from its minimum to its maximum value. Both studies advocated the use of the full range of possible values for each parameter to assess the sensitivity to the input parameters.

$$S_i = \frac{C_{\text{Upper}} - C_{\text{Lower}}}{C_{\text{Upper}}} \tag{1}$$

The output of each of 1,000 iterations is stored in a matrix, which gives the NO_2 concentration for all coordinates (x, y): c_{xy}. Based on the resultant matrix, 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 (Chettouh, 2016):

$$c_{xy}^{\text{Mean}} = \frac{\sum_N c_{xy}}{N} \tag{2}$$

$$c_{xy}^{\text{Lower}} = c_{xy}^{\text{Mean}} - E \cdot \frac{\sqrt{\sum_N \left(c_{xy}^{\text{Mean}} - c_{xy}\right)^2 / N}}{\sqrt{N}} \tag{3}$$

$$c_{xy}^{\text{Upper}} = c_{xy}^{\text{Mean}} + E \cdot \frac{\sqrt{\sum_N \left(c_{xy}^{\text{Mean}} - c_{xy}\right)^2 / N}}{\sqrt{N}} \tag{4}$$

4.2 Global sensitivity analysis

Various technical and overall sensitivity estimators are available and can be used to quantitatively analyze the influence of input factors on the model output (Koo *et al.*, 2020; Sun *et al.*, 2020). Among these techniques, we select the method of linear regression. Several sensitivity indices are defined by this method, which studies the linear relationship between the model output and input variables (García-Díaz and Gozálvez-Zafrilla, 2012). In our study, we will use the Pearson coefficient, which represents a sensitivity index named SRC (sensitivity regression correlation) (Pagnon, 2012; Volkova *et al.*, 2008). This index, through correlation and regression analysis, allows us to perform SA's based on the objective of measuring the importance of each input parameter. This method is applicable to the cases that have a linear relationship between input parameters and model output (LIU *et al.*, 2007; Suard *et al.*, 2013). In our case, it is the NO_2 concentration.

Assuming that EDM is linear, we can then write it in the subsequent form:

$$Y = \beta_0 + \sum_{i=1}^{p} \beta_i X_i \tag{5}$$

where: $\beta_i (i = 1, \ldots, p)$ is the regression coefficient.

Additionally, because the variables X_i are independent, the variance of Y can be written as follows [11, 59]:

$$V(Y) = \sum_{i=1}^{p} \beta_i^2 V(X_i) \tag{6}$$

Knowing that $\beta_i^2 V(X_i)$ is the variance part due to the X_i variance. We define the SRC index representing the variance part of Y response due to the variance of the variable X_i.

$$\text{SRC} = \frac{\beta_i^2 V(X_i)}{V(Y)} = \beta_i^2 \frac{\sigma_{x_i}^2}{\sigma_Y^2} = \left(\beta_i \frac{\sigma_{x_i}}{\sigma_Y}\right)^2 \tag{7}$$

where $\sigma_{X_i}^2$, σ_Y^2 represent the variances of X_i and Y_i respectively.

Knowing that the Pearson coefficient is $\rho_{X_i,Y} = \frac{\text{Cov}(Y; X_i)}{\sigma_{X_i}\sigma_Y}$ and $\text{Cov}(Y; X_i) = \beta\sigma_{X_i}^2$

So:

$$\rho_{X_i,Y} = \frac{\sigma_{X_i}}{\sigma_Y}\beta \tag{8}$$

and finally:

$$\mathrm{SRC} = \rho^2_{X_i,Y} \tag{9}$$

The Pearson coefficient noted ρ for X_j and Y_i is defined by the following relationship (Monod *et al.*, 2006):

$$\rho_{X_jY_i} = \frac{\sum_{k=1}^{N}\left([X_j]^k - \overline{[X_j]}\right)\left([Y_i]^k - \overline{[Y_i]}\right)}{\sqrt{\sum_{k=1}^{N}\left([X_j]^k - \overline{[X_j]}\right)^2\left([Y_i]^k - \overline{[Y_i]}\right)^2}} \tag{10}$$

where:

$\overline{[X_j]}$ and $\overline{[Y_i]}$ are the mean values of ($[X_j]_1,\ldots,[X_j]_N$) and ($[Y_i]_1,\ldots,[Y_i]_N$).

The Pearson coefficient ranges from -1 to 1 and allows the ranking of parameters according to their absolute values. If the Pearson coefficient is close to -1 or 1, it means that the relationship between X and Y is linear (Liu *et al.*, 2007). To measure the degree of linearity between the input parameters X_i ($i = 1,\ldots,p$) and the output Y, we shall calculate R^2:

$$R^2 = 1 - \frac{\sum_{i=1}^{N}\left(Y_i - \tilde{Y}_i\right)^2}{\sum_{i=1}^{N}\left(\overline{Y}_i - Y_i\right)^2}$$

where:

$\overline{Y}_i$ is the mean of Y_i;

$\tilde{Y}$ is the value of the linear model found by linear regression.

The relationship between the input parameters and the output of the model is linear when R^2 is close to 1. Based on this result, we can classify the input parameters by their degree of influence on the model output.

4.3 Industrial case study

The analyzed case study in this paper is based on a real accident occurred in an Algerian refining site "Skikda refinery" which is the largest refinery in Africa, wherein a tank fire took place in the 5th October, 2005. The fire started on a first crude oil tank (S106) and extended to an adjacent tank (S105). The tank (S106) was being filled at the time (70% full); the specification of maximum RVP (Reid Vapour Pressure) was 0.75 kg/cm^2 for a floating roof tank (Chettouh *et al.*, 2018). The estimate of the contents in LPG (Liquefied petroleum gas) was 3% mole with 0.75 kg/cm^2 and 5% mole with 0.95 kg/cm^2 (Chettouh *et al.*, 2018).

The deterministic results are obtained by solving the EDM using the finite volumes method within FORTRAN environment (FORTRAN 6.6). The correlation analysis results are obtained using STATISTICA 12 Software.

4.4 Estimation of SA indices

In this part, we present the conducted SA. Among the range of conditions modeled using in EDM, four input parameters are chosen for the SA. Table 2 describes the input parameters studied in this work: the wind speed (U), the initial concentration of NO_2 (C_0) the diffusion coefficient (Sch) and the viscosity coefficient (Re). The generally used reference values are also indicated. The Minimum and Maximum values are based on the estimated uncertainty band, coming from the measurement of uncertainty, lack of knowledge or the variation of the concerned factor depending on the fire scenarios.

Uniform probability distributions have been used for each variable except the wind speed, for which we have attributed the triangular distribution.

These positions represent the location of two different agglomerations in relation to the accident (fire) (See Figure 1).

These positions represent the location of two different agglomerations in relation to the emission source point (Location of burnt tank).

(1) Position A: $y = 100$ m (cloud height) and $x = 0.5$ km (down distance) presents the industrial site area;

(2) Position B: $y = 200$ m and $x = 1.5$ km presents the area neighboring the industrial site.

Table 2.
Input parameters for sensitivity analysis with reference values, distribution type and intervals of distribution parameters variation

Inputs parameters	Ref. Values	Distribution	Intervals of distribution parameters Min	Max	Unit
Wind speed (U)	5	Triangular	2	7	$m.s^{-1}$
NO_2 initial concentration (C_0)	0.45	Continuous uniform	0.1	0.8	%
NO_2 diffusivity coefficient characterized via the Schmidt number (Sch)	0.85	Continuous uniform	0.7	1	–
NO_2 viscosity characterized via the Reynolds number (Re)	1,650	Continuous uniform	1,000	2,300	–

Note(s): In the current study, the outputs are the concentrations of NO_x in two different positions (A, B). (Chettouh *et al.*, 2018)

Figure 1.
Presentation of the industrial site with two positions (A, B)

5. Results and discussions

To perform the SA, the Monte Carlo method presented in Section 3.1 was used. This step was preceded by running the EDM to predict the NO_2 concentration under the conditions that we have described in Table 1, the result is presented in Figure 2.

Figure 2 depicts the spatial distribution of the NO_2 concentration plume at the point time t = 1,200 s from the beginning of the tank fire, where all the uncertain parameters are considered.

5.1 Local sensitivity analysis results

The local sensitivity index (Si) (see Eqn (1)) is calculated using the minimum and maximum value of the output. Obviously, Figure 3 shows that the variation of the initial concentration of NO_2 has the highest impact in the first position A (y = 100 m and x = 0.5 km) while the wind speed is the most important parameter for the second position B (y = 200 m and x = 1.5 km). The other parameters such as Reynolds (Re) and Schmidt (Sch) have almost no effect on the first position, while for the second position; we can notice that they can influence the output by 10 and 20%, respectively.

To complete the analysis and basing on Eqn (1), S_i^{Inf}, S_i^{Moy}, S_i^{Sup} are proposed:

$$S_i^{\mathrm{Inf}} = \frac{C_i^{\mathrm{Inf}} - C^{\mathrm{Inf}}}{C^{\mathrm{Inf}}}; \; \ldots S_i^{\mathrm{Moy}} = \frac{C_i^{\mathrm{Moy}} - C^{\mathrm{Moy}}}{C^{\mathrm{Moy}}}; \; \ldots S_i^{\mathrm{Sup}} = \frac{C_i^{\mathrm{Sup}} - C^{\mathrm{Sup}}}{C^{\mathrm{Sup}}}$$

These sensitivity indices are defined to illustrate the sensitivity of each input parameter on the variation of the lower, mean and upper limit of the NO_2 concentration.

Figures 4 and 5 indicate the importance of the relative difference between the values obtained when a single input parameter is varied (i parameter) and those observed when all parameters uncertainties are taken into account. Indeed, this importance presents the direction of variation of the NO_2 concentration following the effects of the uncertainties in the input data (increase or decrease).

Regarding safety, only the impact of the input parameters of the concentration variation related to the mean and upper limit will be discussed. For the first position (A), it can be seen from Figure 4 that the coefficient of viscosity, the coefficient of diffusivity and the wind speed are the input parameters that have the significant impact on the mean and upper

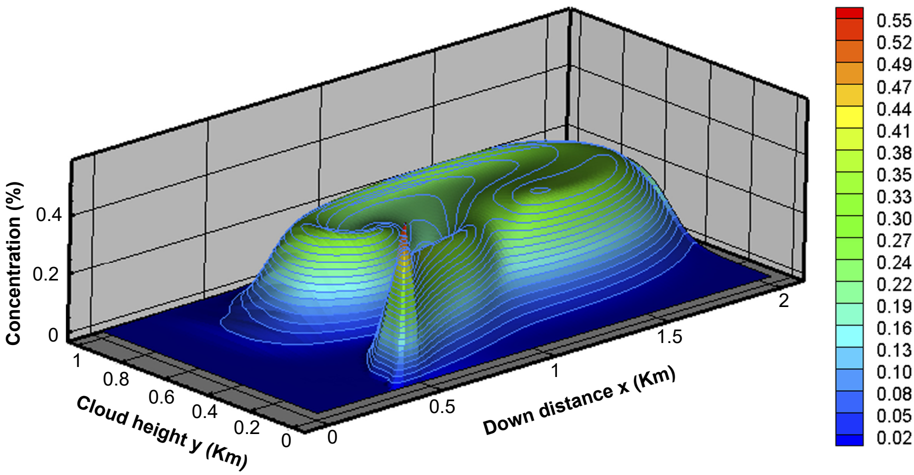


Figure 2.
Spatial distribution of the NO_2 concentration plume

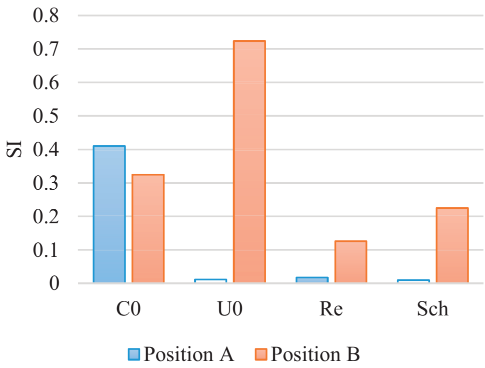


Figure 3.
Local sensitivity index S_i for the positions A and B

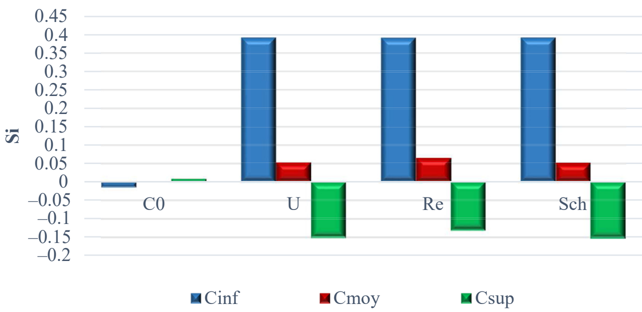


Figure 4.
Impact of the variation of the input parameters on the NO_2 concentration for the first position(A)

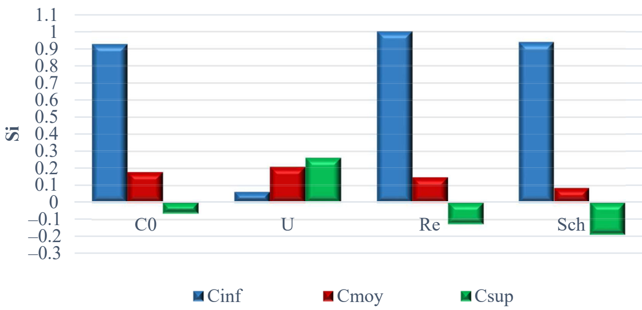


Figure 5.
Impact of the variation of the input parameters on the NO_2 concentration for the second position(B)

concentrations, respectively. For the second position (see Figure 5), wind speed is claimed to be the most important parameter for the mean and upper concentration limits, followed by the initial NO_2 concentration.

5.2 Global sensitivity analysis results

The results of the correlation analysis technique are presented in a scatter plot for each input parameter relative to the two positions (A, B). The statistical methods related to the regression are then used to represent and measure the sensitivity of the output variables with respect to input parameters through the SRC index. The correlation coefficient R are used to determine the direction of influence of the parameter on the model output and the relationship between the input and EDM output. $N = 1{,}000$ scenarios were generated in STATISTICA for uniform and triangular distributions. Figures 6–9 show the correlation of EDM simulations, linear regressions between the input parameters (wind speed, initial concentration, viscosity coefficient and diffusion coefficient) and the EDM output (NO_2 concentration).

As known in previous studies, (e.g. Bubbico and Mazzarotta, 2008; García-Díaz and Gozálvez-Zafrilla, 2012), Figure 6 presents a positive correlation in the two positions (A, B) with a low influence in the first position with an $R = 0.1954$ and a moderate influence in the second position including $R = 0.5308$. This means that the EDM has a remarkable sensitivity to wind speed in position B (agglomeration zone) and this influence increases the estimate of the NO_2 concentration.

Figure 7 gives us the value of $R = 0.9946$. This value shows the existence of a significant positive correlation between the initial concentration of NO_2 the NO_2 concentration in the first position (Refinery area), this result is consistent with a previous study of (García-Díaz and Gozálvez-Zafrilla, 2012). While this correlation decreases considerably in the second position to reach $R = 0.6258$.

Figure 8 presents the correlation between the viscosity coefficient and the NO_2 concentration which is very low and positive in position A, with an $R = 0.0334$. On the other hand, a small increase in this correlation in the position B with $R = 0.1001$.

Figure 9 shows a very low negative correlation in the two positions A and B with a regression coefficient $R = -0.1174$ and $R = -0.1170$, respectively. This means that the NO_2 concentration decreases with the variation of the diffusion coefficient

PEARSON and SRC coefficients for EDM inputs are given in Table 3. They are calculated using the linear model function in the statistical package of STATISTICA from the 1,000 simulations. The results are shown in Figure 10.

Figures 6 and 7 show that the most important parameter uncertainty is the NO_2 initial concentration and a negative relationship between NO_2 concentration and the diffusivity coefficient, where NO_2 concentration decreases as the diffusivity coefficient increases as previously indicated in the study of (García-Díaz and Gozálvez-Zafrilla, 2012).

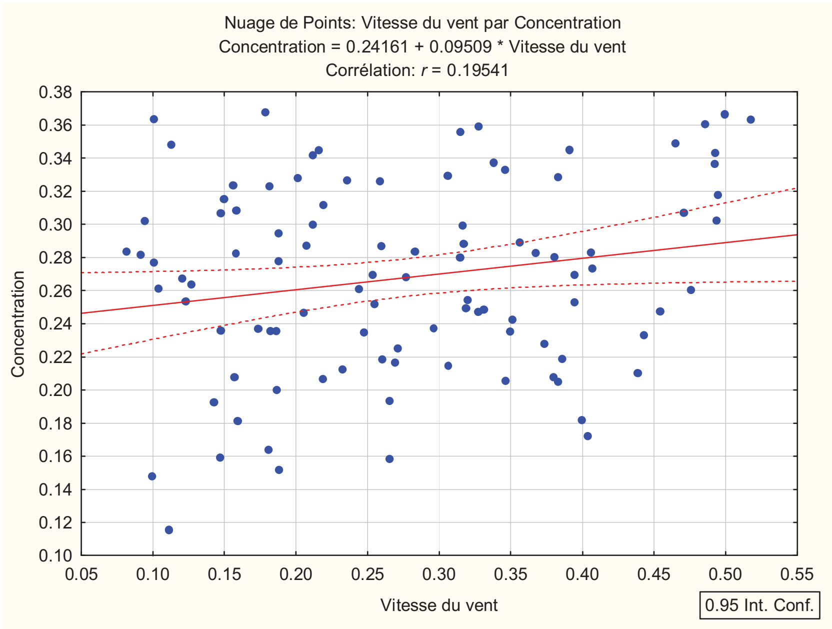
The SRC is used as a sensitivity measure. Figure 10 presents the obtained SRC coefficients. The most important parameter is the NO_2 initial concentration for both positions. NO_2 concentration is also sensitive to wind speed in the position B.

Figure 10 shows the SRC sensitivity index between the output variable (NO_2 concentration) and the input parameters (wind speed, initial concentration, viscosity coefficient and diffusion coefficient).

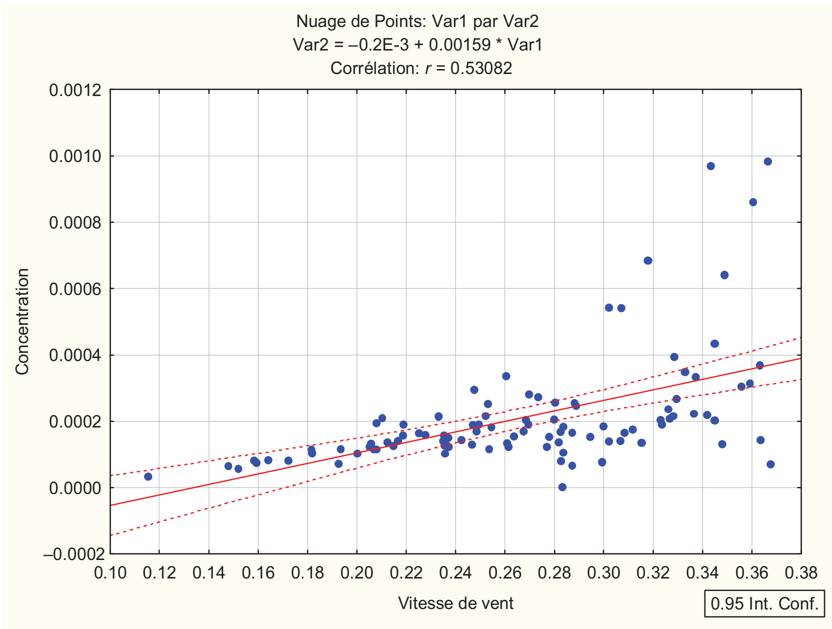
The results of the local and global SA (see Figures 3–8) are coherent in many respects, but also oppose each other in some cases. These results showed that for both analyses, the initial concentration of NO_2 is the most important input parameter in position A, while in the second position (B), the local SA shows that wind speed is the most influential parameter, while this parameter plays a secondary role in the global SA (see Figures 3–10).

For the viscosity and diffusion coefficients, the local sensitivity showed that they have a minor effect on the output in B position (see Figures 8 and 9). However, the global SA affirmed that these two parameters had almost no effect on position B. Finally, both analyses showed that the viscosity and diffusion coefficients had no effect in position A.

Figure 10 shows that the model output (NO_2 concentration) is much more influenced by the initial NO_2 concentration in the first position than in the second position as shown in Figure 8. This comes back to the high NO_2 concentration released by the fire at the industrial site (Position A), whereas as one moves away from the fire, this concentration will progressively decrease as well as its effect on the model output, but it is still the most important parameter in both positions A and B.

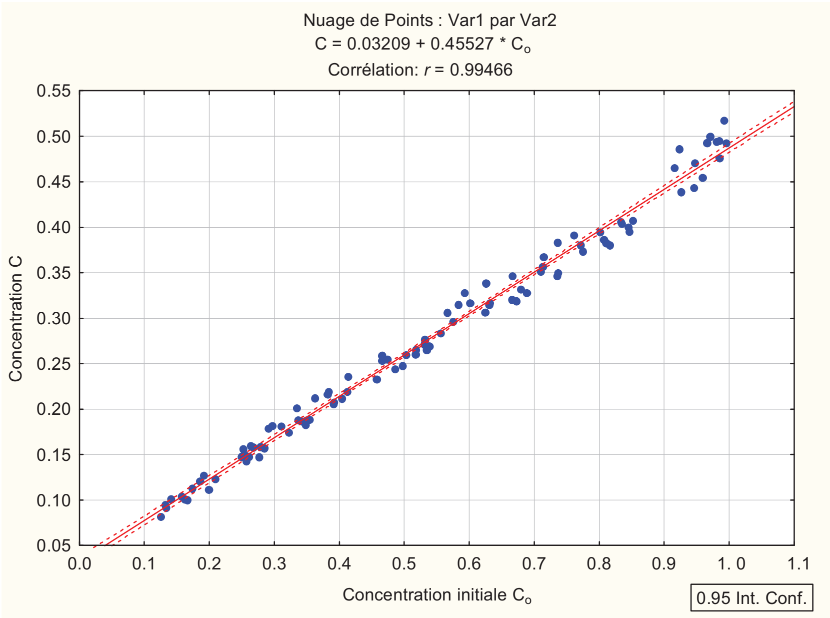


(a)

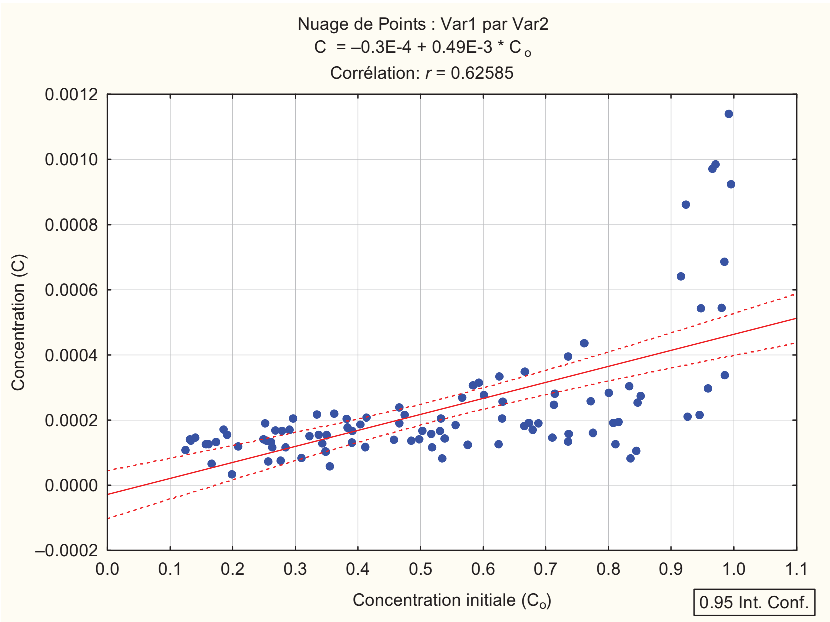


(b)

Figure 6.
Correlation between wind speed and NO_2 concentration over its range of uncertainty for positions A and B

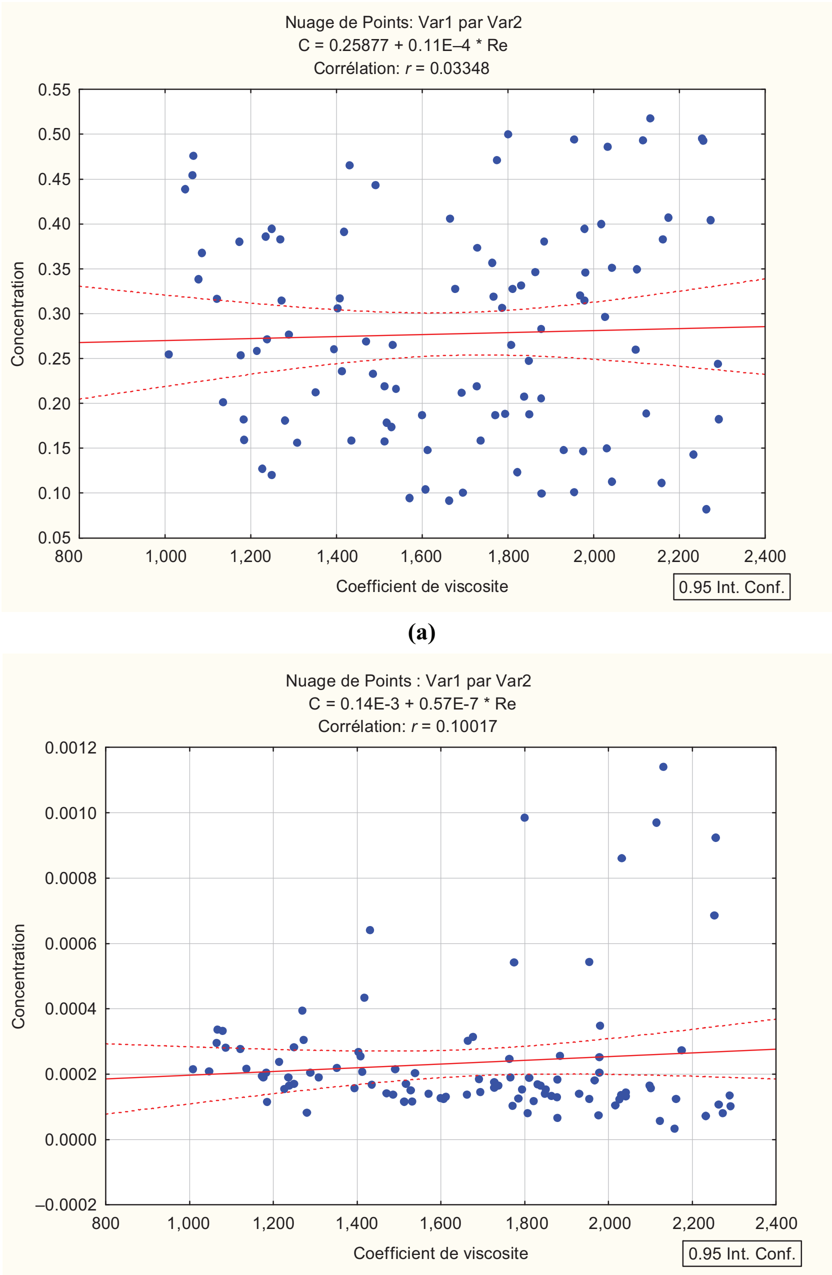


(a)



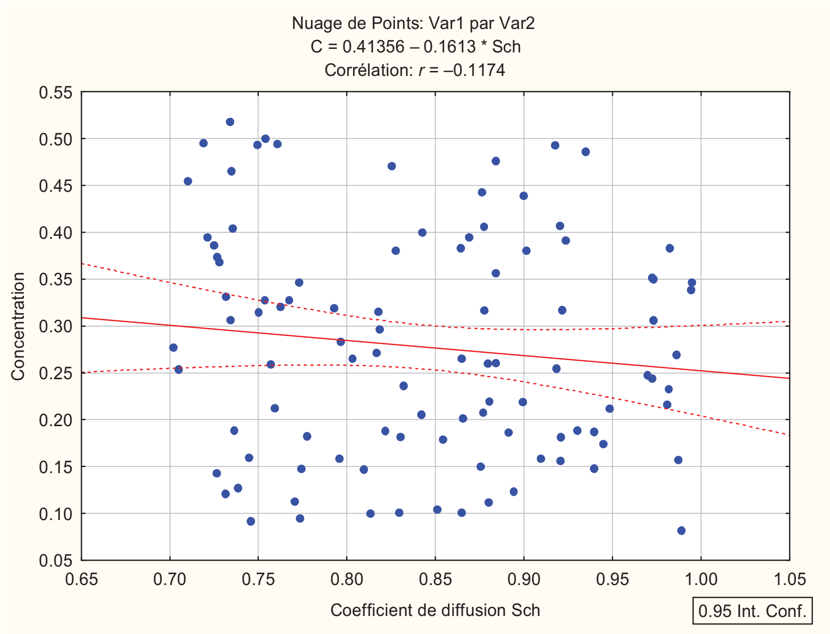
(b)

Figure 7.
Correlation between initial NO_2 concentration and NO_2 concentration over its range of uncertainty for positions A and B

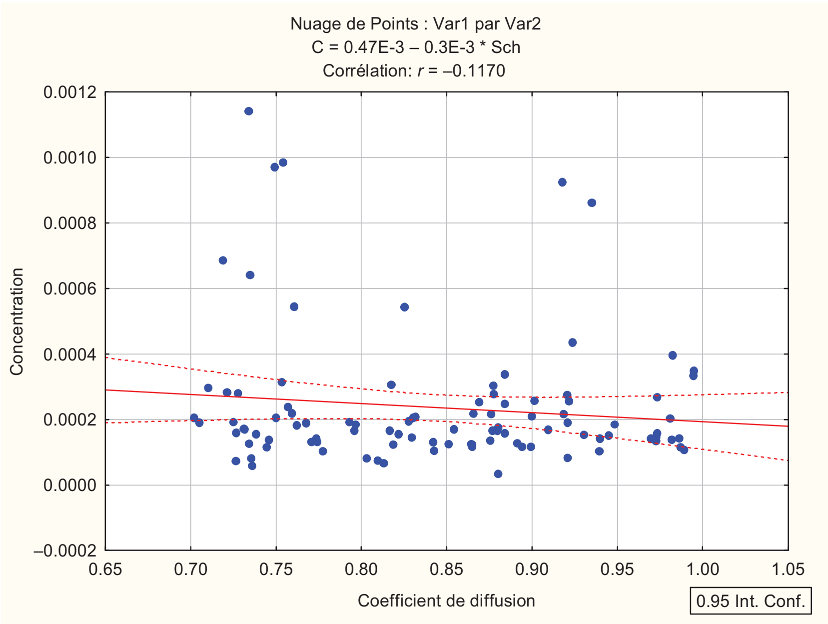


(b)

Figure 8.
Correlation between viscosity coefficient and NO_2 concentration over its range of uncertainty for positions A and B



(a)



(b)

Figure 9.
Correlation between diffusion coefficient and NO_2 concentration over its range of uncertainty for positions A and B

The NO_2 concentration appears to be quite sensitive to wind speed at position B and very insensitive at position A. This can be explained by the fact that at position A, the plume released by the fire is very dense and driven at a high speed (jet speed) which will control its transport and orientation and thus the variation in wind speed cannot have a great effect. However, in the second position, the density of the plume decreases and subsequently the dispersion of the plume will be dominated by the effect of the wind speed and especially when it increases in altitude and thus the variation of the wind speed will have a considerable effect on the output of the EDM.

The variation in the viscosity coefficient and diffusion coefficient does not seem to have too much influence on the NO_2 concentration. Indeed a variation of the viscosity coefficient induces a change of 0.11% at the outlet in position A and 1% in position B. At this level, it should be pointed out that this parameter varies in the opposite direction to the NO_2 concentration in position A and this means that its variation leads to a decrease in the estimate of the level of NO_2 concentration and this is very dangerous from the point of view of industrial safety, since it can lead to underestimates of NO_2 levels and this can be detrimental to the health of the population.

While for the diffusion, coefficient its variation leads to a change in the NO_2 concentration of 1.37% at position A and 1.4% at position B.

Therefore, some input parameters may have gained more importance in the global SA and others have lost it, and the same applies to the local SA. This discrepancy in some of the results of the local and global SA may be due to the nature of each analysis, in that one focuses on the value of the response (local sensitivity), while the other focuses on its variability (global sensitivity) and considers the effects of other input parameters on the input parameter in question. In addition, the signs of the coefficients are identical between the local and global analyses.

It may be noted that the same input parameters may have more importance in the global SA and less importance in the local SA. This is due to the nature of each analysis; the local SA is concerned with the value of the response, while the global SA is interested in its variability and takes into account the effects of the other input parameters on the concerned input parameter.

Table 3.
Pearson coefficient and SCR for the EDM estimated from 1,000 Monte Carlo samples

	Position A		Position B	
	Pearson ρ	SRC = ρ^2	Pearson ρ	SRC = ρ^2
U_0	0.1954	0.03818	0.5308	0.28174
C_0	0.9946	0.98922	0.6260	0.39187
Re	0.0334	0.00111	0.1000	0.01000
Sch	0.1173	0.01375	−0.1169	0.01430

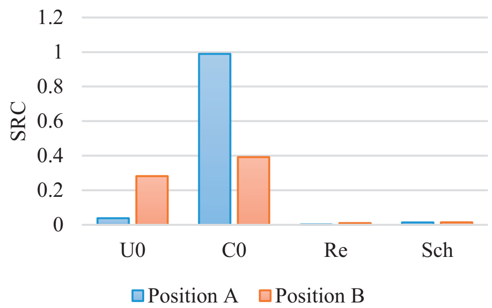


Figure 10.
Sensitivity regression correlation (SRC)

The results of this study can be of some help for risk analysts in optimizing the resources allocation when carrying out industrial risks analysis studies.

6. Conclusion

Fire deterministic modeling does not consider uncertainty and provide complete information about the modeling scenario because of the lack of information in the input parameters. Additionally, SA represents an essential tool for the decision-making processes.

The novelty of this study is the SA of EDM, to determine the effect of four parameters on the estimation of NO_2 concentration generated by an industrial fire. This can determine the performance of the EDM considering uncertainty in input parameters.

First, the model was run to predict deterministic dispersion of NO_2 from an industrial fire under conditions that were described in Section 4, and the spatial distribution of the concentration plume was determined. Next, we have performed a local and global SA to determine the influence of four input parameters uncertainties on the NO_2 concentration. The local SA was carried out. We opted to carry out this study using new sensitivity indicators that allow the identification of which parameters have the most influence on the EDM output at two different agglomerations (Position A and B). The Global SA was carried out using the correlation analysis and results have been obtained using STATISTICA Software. The results showed that the output of the EDM is highly sensitive to the initial NO_2 concentration, whereas it is significantly affected by wind speed. While the effect of the two coefficients of viscosity and diffusion is insignificant. The SA performed using the linear regression method and the SRC sensitivity index confirmed the results obtained by the local SA and added information on the direction of influence of each input parameter on the NO_2 concentration.

It has been shown that, for the far field, the initial concentration and the wind speed have the most impact on the NO_2 concentration estimation. The study also has shown that an effective decision-making process should not be based only on the mean values of the plume concentration, but it should, in particular, consider the upper bound plume concentration. Finally, this study indicate that, after performing an uncertainty and SA, the EDM becomes very useful for estimating NO_2 concentration at different distances in the field of hydrocarbon industries.

Due to the lack of information, our study was limited to four input parameters and only one interest value. In order to make the EDM results more realistic, it is recommended to carry out further studies by analyzing more input parameters for several interest values (thermal effect T) using other more complex SA techniques such as the Sobol method, the FAST (Fourier Amplitude Sensitivity Test) method and the DGSM.

References

Ahmadi, O., Mortazavi, S.B., Pasdarshahri, H. and Mohabadi, H.A. (2019), "Consequence analysis of large-scale pool fire in oil storage terminal based on computational fluid dynamic (CFD)", *Process Safety and Environmental Protection*, Vol. 123, pp. 379-389.

Ali, I. and Bruen, M. (2016), "Methodology and application of the combined SWAT-HSPF model", *Environmental Processes*, Vol. 3 No. 3, pp. 645-61.

Alzbutas, R., Iešmantas, T., Povilaitis, M. and Vitkutė, J. (2014), "Risk and uncertainty analysis of gas pipeline failure and gas combustion consequence", *Stochastic Environmental Research and Risk Assessment*, Vol. 28 No. 6, pp. 1431-46.

Bauer, L. and Hamby, D. (1991), "Relative sensitivities of existing and novel model parameters in atmospheric tritium dose estimates", *Radiation Protection Dosimetry*, Vol. 37 No. 4, pp. 253-60.

Bessie, W. and Johnson, E. (1995), "The relative importance of fuels and weather on fire behavior in subalpine forests", *Ecology*, Vol. 76 No. 3, pp. 747-62.

Bevins, C.D. and Martin, R.E. (1978), *An Evaluation of the Slash (I) Fuel Model of the 1972 National Fire Danger Rating System*, Vol. 247, Department of Agriculture, Forest Service, Pacific Northwest Forest and Range Experiment Station.

Bley, D.C., Droppo, J.G., Eremenko, V.A. and Lundgren, R. (2003), "Quantitative risk assessment methods of accounting for probabilistic and deterministic data applied to complex systems", *Risk Methodologies for Technological Legacies*, Springer, pp. 183-99.

Briggs, A.H., Weinstein, M.C., Fenwick, E.A., Karnon, J., Sculpher, M.J., Paltiel, A.D. and Force, I.S.M.G.R.P.T. (2012), "Model parameter estimation and uncertainty: a report of the ISPOR-SMDM modeling good research practices task force-6", *Value in Health*, Vol. 15 No. 6, pp. 835-42.

Bubbico, R. and Mazzarotta, B. (2008), "Accidental release of toxic chemicals: influence of the main input parameters on consequence calculation", *Journal of Hazardous Materials*, Vol. 151 Nos 2-3, pp. 394-406.

Cao, B., Cui, W., Chen, C. and Chen, Y. (2020), "Development and uncertainty analysis of radionuclide atmospheric dispersion modeling codes based on Gaussian plume model", *Energy*, Vol. 194, p. 116925.

Chettouh, S. (2016), "Modèles statistiques pour l'évaluation des incertitudes associées aux effets du risque incendie", Doctoral dissertation, University of Batna 2, Batna.

Chettouh, S., Hamzi, R. and Chebila, M. (2018), "Contribution of the lessons learned from oil refining accidents to the industrial risks assessment", *Management of Environmental Quality an International Journal*, Vol. 29, pp. 643-665.

Chettouh, S., Hamzi, R., Innal, F. and Haddad, D. (2014), "Industrial fire simulation and uncertainty associated with the emission dispersion model", *Clean Technologies and Environmental Policy*, Vol. 16 No. 7, pp. 1265-73.

Clark, R., Hope, A., Tarantola, S., Gatelli, D., Dennison, P.E. and Moritz, M.A. (2008), "Sensitivity analysis of a fire spread model in a chaparral landscape", *Fire Ecology*, Vol. 4 No. 1, pp. 1-13.

Dadashzadeh, M., Khan, F., Abbassi, R. and Hawboldt, K. (2014), "Combustion products toxicity risk assessment in an offshore installation", *Process Safety and Environmental Protection*, Vol. 92 No. 6, pp. 616-24.

De Rocquigny, E., Devictor, N. and Tarantola, S. (Eds) (2008), *Uncertainty in Industrial Practice: A Guide to Quantitative Uncertainty Management*, John Wiley & Sons.

Debnath, S., Adamala, S. and Raghuwanshi, N. (2015), "Sensitivity analysis of FAO-56 Penman-Monteith method for different agro-ecological regions of India", *Environmental Processes*, Vol. 2 No. 4, pp. 689-704.

Derwent, R.G., Parrish, D.D., Galbally, I.E., Stevenson, D.S., Doherty, R.M., Naik, V. and Young, P.J. (2018), "Uncertainties in models of tropospheric ozone based on Monte Carlo analysis: tropospheric ozone burdens, atmospheric lifetimes and surface distributions", *Atmospheric Environment*, Vol. 180, pp. 93-102.

Dhyani, R. and Sharma, N. (2018), "Meteorological factors influencing dispersion of vehicular pollution in a typical highway condition", *Environmental Pollution*, Springer, pp. 65-75.

Dimitrakopoulos, A. and Omi, P. (2003), "Evaluation of the fire simulation processes of the national fire management system's initial attack analysis processor", *Environmental Management*, Vol. 31 No. 1, pp. 0147-56.

Gant, S., Kelsey, A., McNally, K., Witlox, H. and Bilio, M. (2013), "Methodology for global sensitivity analysis of consequence models", *Journal of Loss Prevention in the Process Industries*, Vol. 26 No. 4, pp. 792-802.

García-Díaz, J.C. and Gozálvez-Zafrilla, J.M. (2012), "Uncertainty and sensitive analysis of environmental model for risk assessments: an industrial case study", *Reliability Engineering and System Safety*, Vol. 107, pp. 16-22.

Gernay, T., Khorasani, N.E. and Garlock, M. (2019), "Fire fragility functions for steel frame buildings: sensitivity analysis and reliability framework", *Fire Technology*, Vol. 55 No. 4, pp. 1175-210.

Girard, S., Korsakissok, I. and Mallet, V. (2014), "Screening sensitivity analysis of a radionuclides atmospheric dispersion model applied to the Fukushima disaster", *Atmospheric Environment*, Vol. 95, pp. 490-500.

Hall, J.W., Boyce, S.A., Wang, Y., Dawson, R.J., Tarantola, S. and Saltelli, A. (2009), "Sensitivity analysis for hydraulic models", *Journal of Hydraulic Engineering*, Vol. 135 No. 11, pp. 959-69.

Hamzi, R. (2008), "Modélisation et impacts à court terme d'un incendie en milieu ouvert sur l'environnement", Doctoral dissertation, University of Batna.

Hasofer, A.M. (2009), "Modern sensitivity analysis of the CESARE-Risk computer fire model", *Fire Safety Journal*, Vol. 44 No. 3, pp. 330-8.

Hoffman, F.O. and Miller, C.W. (1983), "Uncertainties in environmental radiological assessment models and their implications", *Oak Ridge National Lab*.

Hopkin, C., Spearpoint, M. and Bittern, A. (2018), "Using experimental sprinkler actuation times to assess the performance of Fire Dynamics Simulator", *Journal of Fire Sciences*, Vol. 36 No. 4, pp. 342-61.

Innal, F., Dutuit, Y. and Chebila, M. (2013), "Monte Carlo analysis and fuzzy sets for uncertainty propagation in SIS performance assessment", *International Journal of Mathematical, Computational, Physical and Quantum Engineering*, Vol. 7 No. 11, pp. 1063-71.

Koo, H., Chen, M., Jakeman, A.J. and Zhang, F. (2020), "A global sensitivity analysis approach for identifying critical sources of uncertainty in non-identifiable spatially distributed environmental models: a holistic analysis applied to SWAT for input datasets and model parameters", *Environmental Modelling and Software*, p. 104676.

Kucherenko, S., Rodriguez-Fernandez, M., Pantelides, C. and Shah, N. (2009), "Monte Carlo evaluation of derivative-based global sensitivity measures", *Reliability Engineering and System Safety*, Vol. 94 No. 7, pp. 1135-48.

Lemieux, C. (2009), *Monte Carlo and Quasi-Monte Carlo Sampling*, Springer Science & Business Media.

Li, Y. and DeLiberty, T. (2020), "Assessment of urban streamflow in historical wet and dry years using SWAT across Northwestern Delaware", *Environmental Processes*, Vol. 7 No. 2, pp. 597-614.

Li, X., Hadjisophocleous, G. and Sun, X.-q. (2018), "Sensitivity and uncertainty analysis of a fire spread model with correlated inputs", *Procedia Engineering*, Vol. 211, pp. 403-14.

Liu, Z.Q., Zhang, Y.H., Li, G.H. and Zhang, X. (2007), "Sensitivity of key factors and uncertainties in health risk assessment of benzene pollutant", *Journal of Environmental Sciences*, Vol. 19 No. 10, pp. 1272-80.

Massada, A.B. and Carmel, Y. (2008), "Incorporating output variance in local sensitivity analysis for stochastic models", *Ecological Modelling*, Vol. 213 Nos 3-4, pp. 463-7.

Monod, H., Naud, C. and Makowski, D. (2006), "Uncertainty and sensitivity analysis for crop models", *Working with Dynamic Crop Models: Evaluation, Analysis, Parameterization, and Applications*, Vol. 4, pp. 55-100.

Mycek, P. and De Lozzo, M. (2019), "Multilevel Monte Carlo covariance estimation for the computation of Sobol'indices", *SIAM/ASA Journal on Uncertainty Quantification*, Vol. 7 No. 4, pp. 1323-48.

Nezaratian, H., Zahiri, J. and Kashefipour, S.M. (2018), "Sensitivity analysis of empirical and data-driven models on longitudinal dispersion coefficient in streams", *Environmental Processes*, Vol. 5 No. 4, pp. 833-58.

Pagnon, S. (2012), "Stratégies de modélisation des conséquences d'une dispersion atmosphérique de gaz toxique ou inflammable en situation d'urgence au regard de l'incertitude sur les données d'entrée", Doctoral dissertation, Ecole Nationale Supérieure des Mines de Saint-Etienne.

Pandya, N., Gabas, N. and Marsden, E. (2012), "Sensitivity analysis of Phast's atmospheric dispersion model for three toxic materials (nitric oxide, ammonia, chlorine)", *Journal of Loss Prevention in the Process Industries*, Vol. 25 No. 1, pp. 20-32.

Perry, G. (1998), "Current approaches to modelling the spread of wildland fire: a review", *Progress in Physical Geography*, Vol. 22 No. 2, pp. 222-45.

Poudyal, N.C., Johnson-Gaither, C., Goodrick, S., Bowker, J. and Gan, J. (2012), "Locating spatial variation in the association between wildland fire risk and social vulnerability across six southern states", *Environmental Management*, Vol. 49 No. 3, pp. 623-35.

Price, R.K. (2011), *Urban Hydroinformatics: Data, Models, and Decision Support for Integrated Urban Water Management*, IWA Publishing, London.

Ralph, B. and Carvel, R. (2018), "Coupled hybrid modelling in fire safety engineering; a literature review", *Fire Safety Journal*, Vol. 100, pp. 157-70.

Ramroth, W., Krysl, P. and Asaro, R. (2006), "Sensitivity and uncertainty analyses for FE thermal model of FRP panel exposed to fire", *Composites Part A: Applied Science and Manufacturing*, Vol. 37 No. 7, pp. 1082-91.

Rodriguez-Fernandez, M., Banga, J.R. and Doyle, F.J. III (2012), "Novel global sensitivity analysis methodology accounting for the crucial role of the distribution of input parameters: application to systems biology models", *International Journal of Robust and Nonlinear Control*, Vol. 22 No. 10, pp. 1082-102.

Saltelli, A., Tarantola, S., Campolongo, F. and Ratto, M. (2004), *Sensitivity Analysis in Practice: A Guide to Assessing Scientific Models*, Vol. 1, Wiley, New York.

Salvador, R., Pinol, J., Tarantola, S. and Pla, E. (2001), "Global sensitivity analysis and scale effects of a fire propagation model used over Mediterranean shrublands", *Ecological Modelling*, Vol. 136 Nos 2-3, pp. 175-89.

Sobol, I.M. (2001), "Global sensitivity indices for nonlinear mathematical models and their Monte Carlo estimates", *Mathematics and Computers in Simulation*, Vol. 55 Nos 1-3, pp. 271-80.

Spitz, C. (2012), *Analyse de la fiabilité des outils de simulation et des incertitudes de métrologie appliquée à l'efficacité énergétique des bâtiments*, Doctoral dissertation, Université de Grenoble.

Srinivas, C., Prasad, K.H., Naidu, C., Baskaran, R. and Venkatraman, B. (2016), "Sensitivity analysis of atmospheric dispersion simulations by flexpart to the WRF-simulated meteorological predictions in a coastal environment", *Pure and Applied Geophysics*, Vol. 173 No. 2, pp. 675-700.

Suard, S., Hostikka, S. and Baccou, J. (2013), "Sensitivity analysis of fire models using a fractional factorial design", *Fire Safety Journal*, Vol. 62, pp. 115-24.

Sun, X., Choi, Y.Y. and Choi, J.I. (2020), "Global sensitivity analysis for multivariate outputs using polynomial chaos-based surrogate models", *Applied Mathematical Modelling*, Vol. 82, pp. 867-87.

Tondini, N., Thauvoye, C., Hanus, F. and Vassart, O. (2019), "Development of an analytical model to predict the radiative heat flux to a vertical element due to a localised fire", *Fire Safety Journal*, Vol. 105, pp. 227-43.

Volkova, E., Iooss, B. and Van Dorpe, F. (2008), "Global sensitivity analysis for a numerical model of radionuclide migration from the RRC 'Kurchatov Institute' radwaste disposal site", *Stochastic Environmental Research and Risk Assessment*, Vol. 22 No. 1, pp. 17-31.

Zhan, Y. and Zhang, M. (2013), "Application of a combined sensitivity analysis approach on a pesticide environmental risk indicator", *Environmental Modelling and Software*, Vol. 49, pp. 129-40.

Corresponding author
Samia Chettouh is the corresponding author and can be contacted at: samia.chettouh@yahoo.com