Industrial fire simulation and uncertainty associated with the Emission Dispersion Model

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Uncertainty in the Dynamic LCA- Fire methodology to assess the environmental fire effects
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S. Chettouh, R. Hamzi, F. Innal, D. Haddad

Abstract— **Life Cycle Impact Assessment, LCIA, is the third phase of Life Cycle Assessment (LCA) described in ISO 14042. The purpose of LCIA is to assess a product system's life cycle inventory analysis (LCI) in order to better understand its environmental significance. However, LCIA typically excludes spatial, temporal, threshold and dose-response information, and combines emissions or activities over space and/or time. This may diminish the environmental relevance of the indicator result. The methodology, Dynamic LCA -Fire proposed in this paper to complete the International Standard ISO 14042 in the fire field, combines the LCA - Fire method with the Dispersion Numerical Model. It is based on the use of the plume model used to assess pollutant concentrations and thermal effects from fire accident scenarios and to cope with the presence of uncertainties in the input data we propose an 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, The Dynamic LCA - Fire methodology is applied to a case study for petroleum production process management and we are interested in the uncertainty propagation related to NO2 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.**

I. INTRODUCTION

Life-Cycle Assessment (LCA) is a versatile tool to investigate the environmental aspects of a product, a process or an activity by identifying and quantifying energy and material flows for the system, it is the most common method to assess the environmental impact of a product or activity is through the use of life-cycle assessment methodology [1]. The standard LCA method aim to assess the overall environmental impact throughout the life of a product or service [2], however, excludes the impact of accidents, such as fires or accidental pollution incidents.

Recently a Fire-LCA model was developed that also includes fires and their impact on the environment [3]. Fire-LCA is an LCA method that incorporates fires as one possible end of life scenario [4] and takes account in the Life Cycle Assessment the impact of accidental fires was originally developed by SP and IVL in order to be able to assess lifecycle aspects of the fire performance of products [3]. The LCA-Fire model will therefore include modules to describe the fire behavior for the different types of fires. Fire statistics are used to quantify the amount of material involved in the different types of fires. In addition, the model should include modules for handling the production of replacement materials that are needed due to the shortening of lifetime that the fires have caused. If possible the model should also include modules for the handling of the fire extinguishing process and the decontamination process [5].

The "dynamic LCA -Fire" is a proposed approach that combines two tools: LCA-Fire and Dispersion Numerical Model (DNM) within the inclusion of spatial and temporal aspects in LCIA in order to give information post-process such as the residence time or the concentration of the pollutant resultant from the Fire; One important purpose of such tools is to provide relevant and structured information in decision-making processes. 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. The first problem that has been partly overlooked is accuracy of results from mathematical models is often complicated by the presence of uncertainties in their inputs data. Uncertainty analysis investigates the effects of lack of knowledge and other potential sources of error in the model [6]. 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. That is what; we study the uncertainty propagation of input parameters of NO_2 atmospheric dispersion model on the variation of its output (NO_2 concentration).

S. Chettouh is with the Laboratory of Research in Industrial Prevention, Institute of health and industrial safety, University of Batna, Algeria (corresponding author to provide phone: +213662475170; fax: +21333865728; e-mail: samia.chettouh@ yahoo.com).

R.Hamzi is with the Laboratory of Research in Industrial Prevention, Institute of health and industrial safety, University of Batna, Algeria (e-mail: hamzi_hr@yahoo.fr).

F. Innal is with the Laboratory of Research in Industrial Prevention, Institute of health and industrial safety, University of Batna, Algeria. (e-mail: innal.fares@hotmail.fr).

D.Haddad is with the Laboratory of Research in Industrial Prevention, Institute of health and industrial safety, University of Batna, Algeria. (e-mail: djamel_hd2@yahoo.fr).

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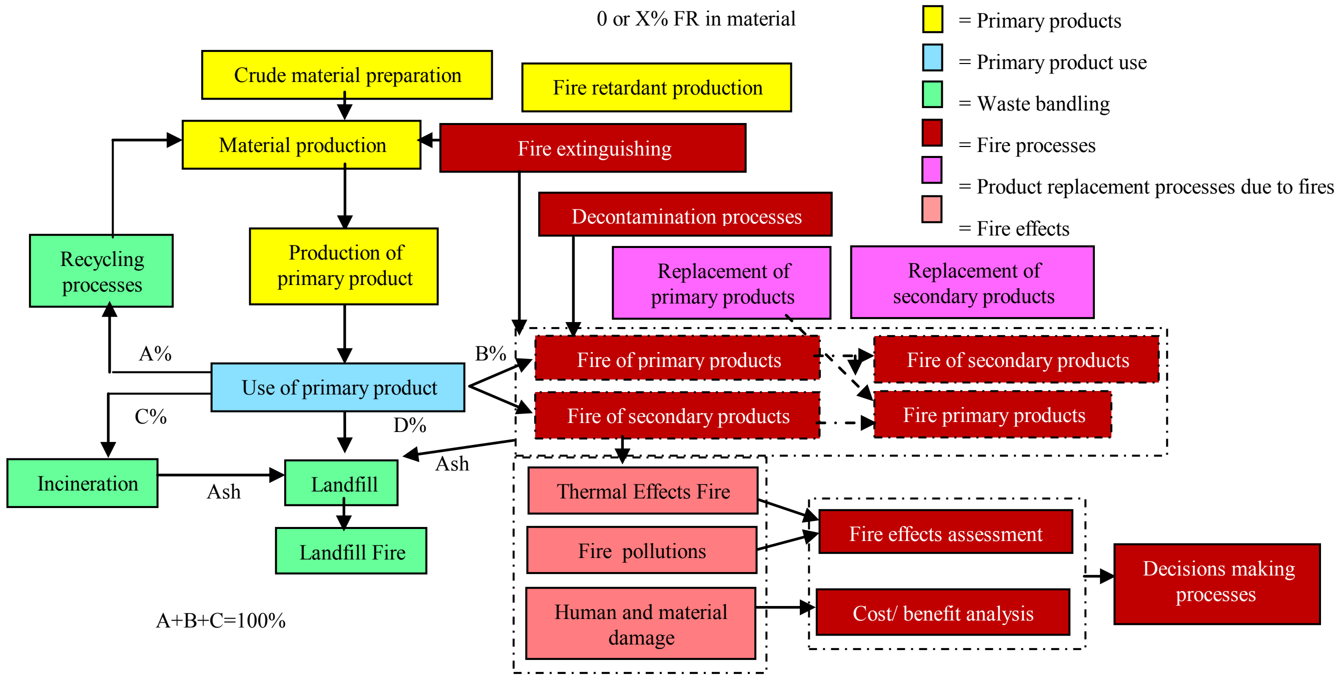

Figure 1. The three modules of Dynamic Fire –LCA model

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.

II. DYNAMIC LCA – FIRE METHODOLOGY

The Dynamic LCA - Fire model is essentially equivalent to a traditional LCA approach with the inclusion of emissions from fires and the dispersion of the emitted pollutants in the atmosphere. During the lifetime of the products to be analyzed, some products will be involved in different types of fires. The Dynamic Fire-LCA model is composed of the following modules: LCA method with fire considerations, Statistical fire model and Dispersion numerical model, see Fig 1. LCA model will therefore include modules to describe the fire behavior for the different types of fires. Fire statistics are used to quantify the amount of material involved in the different types of fires [7]. In addition, the model also includes modules for evaluating the pollution produced from the fire that are needed due to the shortening of lifetime that the fires have caused.

A. LCA method with fire considerations

The Life Cycle Assessment methodology also needs continuous improvements to incorporate new aspects and processes. An LCA typically describes a process during normal operation and abnormal conditions such as accidents are left out of the analysis, usually due to lack of a consistent methodology or relevant data [3]. For example, LCA data for power production usually assume normal conditions without any accidents.

Provisions for certain accidents in the analysis of the life-cycle could be included provided these could be specified in sufficient detail and occurred with sufficient regularity to make their inclusion relevant. The Fire-LCA model is essentially equivalent to a traditional LCA approach with the inclusion of emissions from fires being the only real modification.

B. Statistical fire model

The fire statistics that are used to develop the fire model must be detailed. One must be able to determine the number of primary and secondary fires each year. In addition one must be able to estimate the size of these fires, i.e., the number of fires that grow to involve the rest of the room and/or the rest of the building. Fire statistics tend only to include fires that are large enough for the fire brigade to be summoned. In many cases small fires are extinguished by people nearby and the fire brigade is not called. These fires are, however, often reported to insurance companies as part of an insurance claim. Therefore statistics from insurance companies should also be included in construction of the fire model.

Also, The quantitative output of the statistical analysis of a scenario constitute parameters for the adjustment model, resulting in an equation that can be used to make conservative adjustments of model predictions, by the modeling of the uncertain parameters of the model by means of random variables and then construct explicitly the probabilistic model of these random variables using the available information [8]. This approach is the most appropriate and most effective way to take into account the uncertainties in the model parameters when the probability theory can be used.

TABLE I. NUMERICAL DISPERSION MODEL EQUATIONS

<table>
<tr><td>Transport equation</td><td colspan="5">$\frac{\partial\Phi}{\partial t}+\frac{\partial U\Phi}{\partial x}+\frac{\partial V\Phi}{\partial y}=\Gamma\left(\frac{\partial^2\Phi}{\partial x^2}+\frac{\partial^2\Phi}{\partial y^2}\right)+S \qquad (1)$</td></tr>
<tr><td rowspan="4">Numerical Dispersion Model (NDM)</td><td colspan="5"><i>Continuity equation:</i>
$\frac{\partial U}{\partial x}+\frac{\partial V}{\partial y}=0$</td></tr>
<tr><td colspan="5"><i>Movement equation:</i>
$\frac{\partial U}{\partial t}+\frac{\partial U.U}{\partial x}+\frac{\partial V.U}{\partial y}=\frac{1}{Re}\left(\frac{\partial^2 U}{\partial x^2}+\frac{\partial^2 U}{\partial y^2}\right)-\frac{\partial P}{\partial x}$;
$\frac{\partial V}{\partial t}+\frac{\partial U.V}{\partial x}+\frac{\partial V.V}{\partial y}=\frac{1}{Re}\left(\frac{\partial^2 V}{\partial x^2}+\frac{\partial^2 V}{\partial y^2}\right)-\frac{\partial P}{\partial y}+(Gr_m.C+Gr_T.T)/Re^2$</td></tr>
<tr><td colspan="5"><i>Equation of energy:</i>
$\frac{\partial T}{\partial t}+\frac{\partial U.T}{\partial x}+\frac{\partial V.T}{\partial y}=\frac{1}{Re.Pr}\left(\frac{\partial^2 T}{\partial x^2}+\frac{\partial^2 T}{\partial y^2}\right)$</td></tr>
<tr><td colspan="5"><i>Equation of conservation of mass:</i>
$\frac{\partial C}{\partial t}+\frac{\partial U.C}{\partial x}+\frac{\partial V.C}{\partial y}=\frac{1}{Re.Sc}\left(\frac{\partial^2 C}{\partial x^2}+\frac{\partial^2 C}{\partial y^2}\right)$</td></tr>
<tr><td>Adimensionnal Numbers</td><td><i>Reylonds Number:</i>
$Re=\frac{U_{jet}.L}{\nu}$</td><td><i>Grashof thermique Number:</i>
$Gr_T=\frac{\beta_T.g.\Delta T_{max}.L^3}{\nu^2}$</td><td><i>Grashof massique Number:</i>
$Gr_m=\frac{\beta_m.g.\Delta C_{max}.L^3}{\nu^2}$</td><td><i>Schmidt Number:</i>
$Sc=\frac{\nu}{D_m}$</td><td><i>Prandtl Number:</i>
$Pr=\frac{\nu}{D_T}$</td></tr>
</table>

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;

ΔT_{max} : Maximum thermal gradient;

D_m : Coefficient of mass diffusion;

ΔC_{max} : Maximum concentration gradient.

C. Dispersion Numerical Model (DNM)

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 [9]. 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.

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 above.

III. MODEL APPLICATION

A. Fire - LCA results

Fire - LCA process:

The aim of this section is to obtain a measure of the environmental impact of the choice of a given level of fire safety. Implicit in this model is the fact that to obtain a high level of fire safety some fire performance improvement measures need to be taken, these could be for example the addition of flame retardants (FR) or a fire extinguishing system or to change the design of the product. The case chosen for this application represent an industrial fire illustrated by the refinery products (essence and gasoil) [10].

Fire – LCI (Life Cycle Inventory):

The fire - LCI phase concern the determination of the pollutant quantity emitted from the fire and also we could take into account the heat flux generated from the fire and represented by the elevation of temperature. The data of this part could be acquired from the database of fires occurred in the refineries. For this, we could reference to a fire which took place in the refinery of Skikda (city in Algeria). The fire started on the first crude oil tank (S106) and it was extended to adjacent tank (S105). The source (S106) was in filling at 70%, the specification of maximum RVP (Reid vapor pressure) is of 0.75 kg/cm^2 for a floating roof tank. The estimate of the contents in LPG (Liquefied petroleum gas): 3% (mole) with 0.75 kg/cm^2 and 5% mole with 0.95 kg/cm^2 [11]. This investigated is carried out by a team of experts [12], showed also that smoke contains gaseous pollutants in particular NO_x (Oxides of Nitrogen) and VOCs (Volatile Organic Compounds). These two pollutants could be simulated by the dispersion model, for NO_x chosen to be

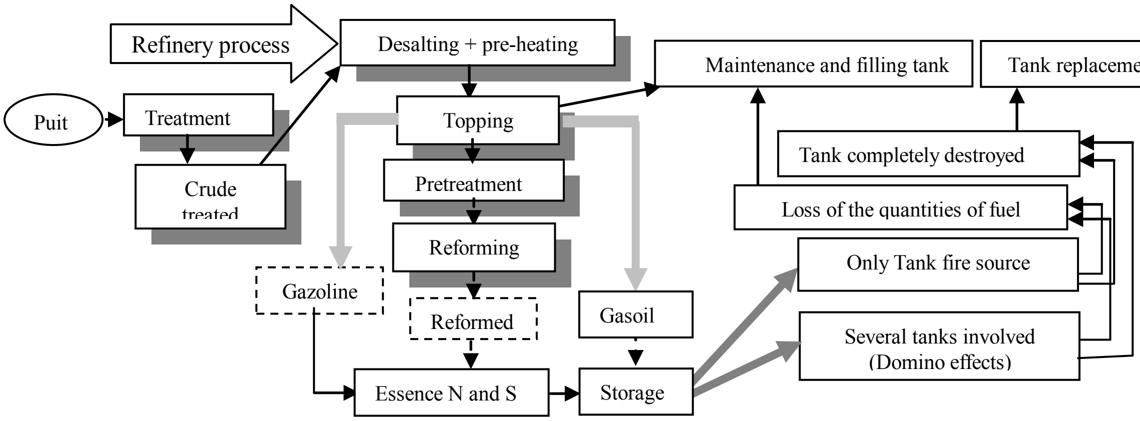

Figure 2. LCA model for each product: Essence and Gasoil.

modelled in the following section, and VOCs can be simulated by the software SLAB View in future work.

B. Fire statistics

Using the complete database of the 448 fire incidents from 1960 to 2005 where it is possible to obtain full or almost full information about the fire size, the number of fires that are confined to the original tank fire (only tank fire) and those that fire spread beyond the original tank to other tanks in area (involved several tanks: domino effects). The statistics concerning distribution of the size of the fire, describe the number of tanks which are destroyed only and those involved in the original tank fire [13].

The fire occurred in the refinery of Skikda (2005), represent serious accident that involved two tanks and have a considerable human and material damage (27 dead and completely destroyed two tanks).

	Fire	% of 448 fires
Only tank fire	143	30
Involved several tank	139	29

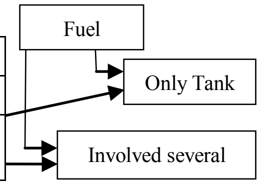

Figure 3. The incorporation of fire statistics in the LCA model of Essence and Gasoil.

These values are used as input in the model, see Fig. 3. It is assumed that the same percentage (30%) of 448 tank fires is in the "only tank fire" and "domino effects".

IV. ANALYSIS RESULTS AND DISCUSSION

The solution of the partial differential equation described by the general formula (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 Fig. 2, Fig. 3 and Fig. 4. These figures present, the NO_2 atmospheric dispersion (plume) at time t = 100 s and 1200s from the beginning of the tank fire, NO_2 concentration profile for cloud height y=50 and 500 m against the Downwind distance (x) and NO_2 concentration profile for a fixed Downwind distances x= 500m and 1.5Km 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:

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

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

For 90% confidence interval, E equals to 1.64. This being the case, the NO_2 cloud dispersion related to Fig. 4.(a) and Fig. 4.(c) (resp. Fig. 5.(a) and Fig. 5.(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 two 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, Fig. 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 II. [14].

TABLE II. 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

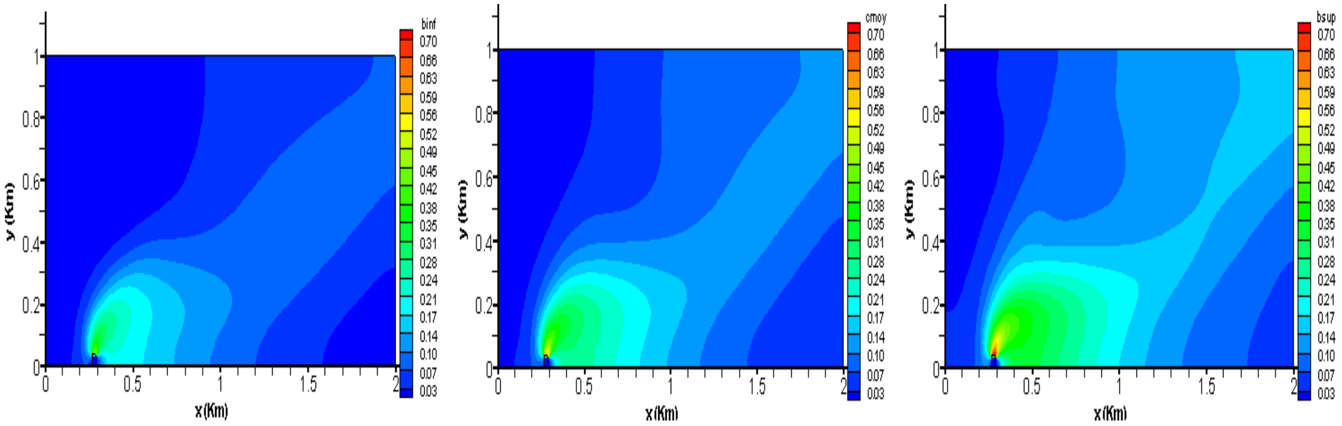

Figure 4. NO_2 plume dispersion for t= 1200 s: (a) Lower bound (5th percentile); (b) Mean bound; (c) Upper bound (95th percentile).

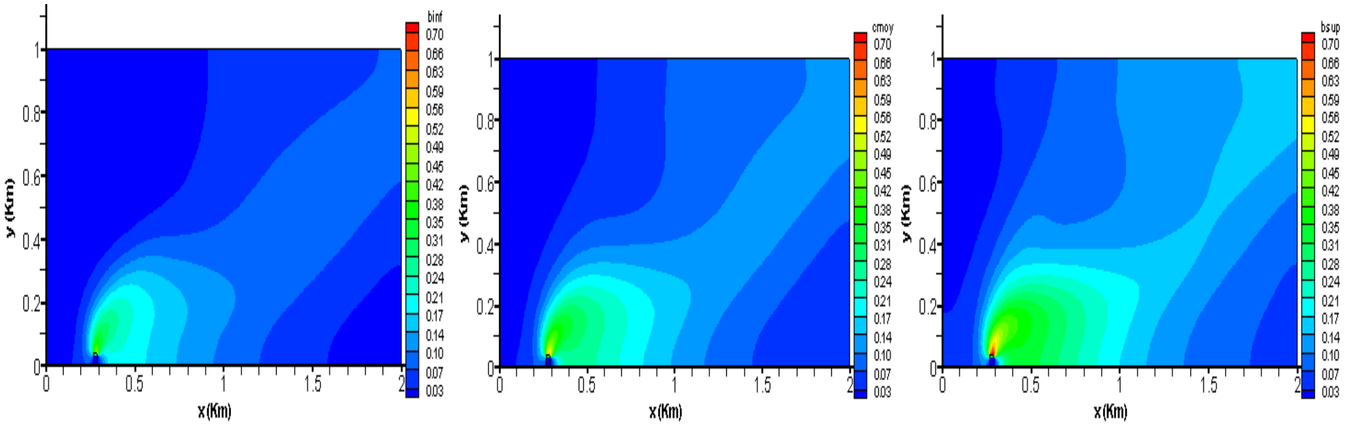

Figure 5. NO_2 plume dispersion for t= 100 s: (a) Lower bound (5th percentile); (b) Mean bound; (c) Upper bound (95th percentile)

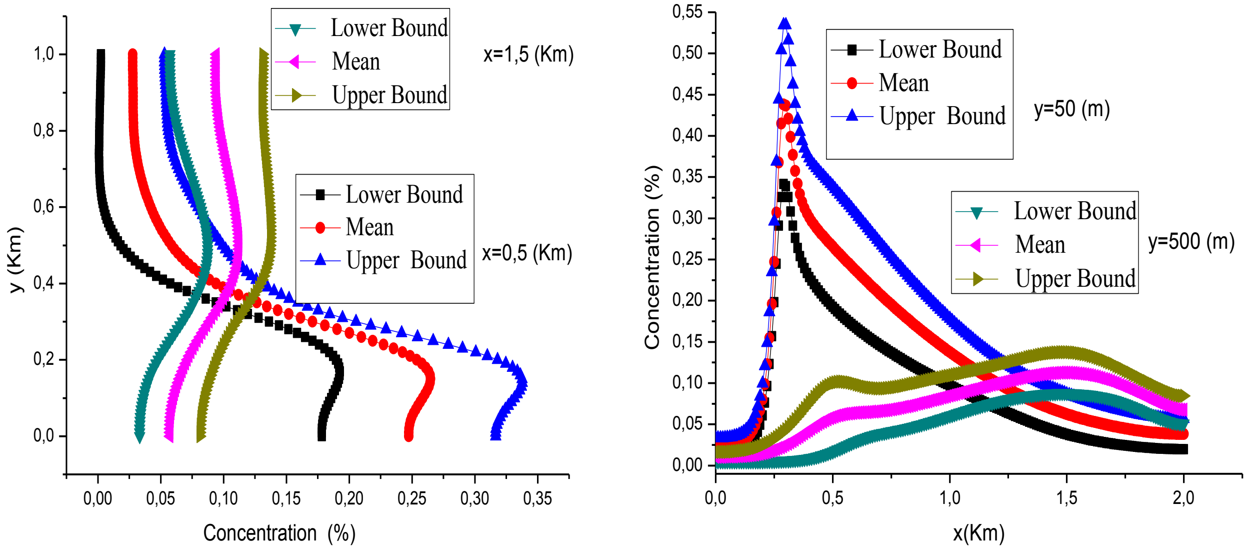

Figure 6. NO_2 plume dispersion at t= 1200 s for (a) fixed x; (b) for fixed y.

Fig 5. and Fig 6 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.

V. CONCLUSION

There is no easy way to collect detailed information about tank fires, in the Fire – LCA analysis, especially to `complete LCI, very little fire emission data is reported in the literature and also data at industrial sites is confidential. One of the objectives of this work is to propose a methodology approach easy to collect all information of the site sinister before and after accident, this help to elaborate a database of statistics and the different fire effects. There are two alternatives for combating a tank fire, either to let it burn out and thereby self-extinguish or, alternatively to actively extinguish the fire, using fire fighting foams.

As the burn out procedure will result in a fire that is likely to last several days, complete loss of stored product, environmental problem, large cooling operation to protect fire spread to adjacent tanks. In another case, when the amount of fuel in fire is important, the heat generated can destroy the tank and we have then to replace it.

While the Fire-LCA tool provides a good starting point for a holistic interpretation of a realistic life – cycle of a product including information concerning the probability that the product may be involved in a fire it does not provide information concerning, for example, the effect of the toxicity of chemicals used in the product or the fate of pollutants emitted during the fire in the atmosphere. The dispersion numerical model responds to this limit by determining the residence time of the pollutant in atmosphere and other parameters like temperature. The dynamic fire- LCA is an organized approach to be used as an aid decision-making tool and experience feedback.

In this study, we also 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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