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Study of the air pollutants dispersion from several point sources using an improved Gaussian model

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Abstract
This work presents a study of the atmospheric dispersion of emissions, particularly those of NOx (NO + NO_2), generated by one or more stacks (five in our case). A numerical simulation of the dispersion of pollutants emitted by sources was performed on an area up to 3 Km^2 using an improved Gaussian model. A validation of this model was performed using a close comparison with measurements (previous works) .Finally, a study of various scenarios aimed to reducing the impact of these pollutants on the area was carried out by studying the influence of different parameters (the number of emission points, stack height, atmospheric stability, speed and wind direction,...) on the dispersion of pollutants. The obtained results are of great interest for the improvement of evacuation devices to significantly reduce emissions and improve the air quality in the surrounding industrial sites.

Keywords: Air pollution, simulation, smokestack, emissions, NO_x, dispersion.

1 Introduction
Epidemiological studies have consistently shown an association between air pollution, mainly by particles and gases, not only with disease exacerbations in people with respiratory problems, but also increases in the number of deaths from disease cardiovascular and respiratory function of older people [1]. However, despite technological advances in filtration of particles in evacuation systems, the problem is still persistent in fine particles (gas), which cannot be hindered from discharging into the atmosphere.This is why a study of the transport and diffusion of air emissions to the output smokestacks depending on weather conditions, geometric parameters and evacuation conditions gives a better understanding of the physicochemical mechanisms that influence these phenomena. It also allows to anticipate problems and to propose solutions to take over the risk of these emissions on the neigh boyhood.
The numerical models used to determine the fields of continuous or instantaneous concentrations of pollutants emitted by smokestacks, are tools for decision support, their results are used to determine areas of potential risk, and then to propose scenarios aiming the reduction of these impacts.
Previous works in this field have focused on identifying, on one side, the influence of the height of the chimney and the presence of obstacles on the dispersion process by using experimental models, and comparing calculation approaches on the other side. The works of Huber Adhikari [2], [3] and Erbrink [4] have contributed to the improvement of air dispersion factors used in previous works in particular those of Roy M. Harrison, [5] by specifying the impact of the existence of obstacles. These studies are based on an experimental approach (controlled atmosphere), within the same frame work Hyojoon Jeong [6] and Dietmar Oettl [7] showed clearly the impact of profiles at low speeds on the atmospheric dispersion factors.
The work reported by Smith, [8] demonstrated that the stack height affects the dispersion in the case of thermal inversion, when one or more pollutants are emitted by a low stack, discharging under the inversion thermal layer, an accumulation of these pollutants below this layer is observed, however if the chimney opens above this layer, the pollutants normally diffuse. These works were complemented by two numerical studies, that of Benkoussas Bouzid, [9] and Carlos S. Borrego, [10]. The first is based on CFD-fluent, which demonstrated the influence of

the ratio of the exhaust velocity and the wind speed, the stack height and roughness on the dispersion of particles ejected and the second based a simple Gaussian model that took into account the roughness of the area.

The present work is achieved, on two steps, using a dispersion improved Gaussian model. We started this work with a validation study of the model by comparing our results with measurements carried out as part of the work of Roy M. Harrison, [5] at the Earth's surface and aloft. In a second time, we discuss the improvement, of the same work, articulated around a different view of the impact of a number of parameters on the pollutants dispersion throughout the study area.

2 Equations

The Gaussian model is based on the general advection-diffusion equation **(2.1)**of particles or gases. We assume that the dispersion is stationary and the Gaussian distribution that is typical with a stochastic process.

$$\frac{\partial c}{\partial t} = -v\frac{\partial c}{\partial x} + \frac{\partial c}{\partial y}\left(k_y \frac{\partial c}{\partial y}\right) + \frac{\partial c}{\partial z}\left(k_z \frac{\partial c}{\partial z}\right) + S \qquad \textbf{(2.1)}$$

Where $S = Q\delta(x)\delta(\mathrm{y})\delta(\mathrm{z})$

The integral of the concentration in a transverse plane of the plume multiplied by the wind speed must be equal to the source rate (mass conservation), the equation **(2.1)** has an exact solution given by equation **(2.2)**:

$$c(x,y,z,t) = \frac{Q}{2\pi\sigma_y\sigma_z v}\exp\left[-\frac{y^2}{2\sigma_y{}^2}\right]\left\{\exp\left[-\frac{(z-H)^2}{2\sigma_z{}^2}\right] + \exp\left[-\frac{(z+H)^2}{2\sigma_z{}^2}\right]\right\} \qquad \textbf{(2.2)}$$

The convective strength flow and buoyancy due to heat plume compared to the environment are the two phenomena that contribute to the elevation of a plume emitted from a point source. The elevation is given by the equation of Holland (2.3) Peavy, 1987 [11]

$$H = \left(\frac{V_s d}{v}\right)\left(1.5 + 2.68.10^3 Pd\,\frac{T_s - T_a}{T_s}\right) \qquad \textbf{(2.3)}$$

As first point of improvement, and after an impact study that we performed, the influence of buoyancy due to heat, on the form of the plume and concentrations at different altitudes, is negligible in the case where the evacuation temperatures (T_s) is close to the ambient temperature (T_a) and in the case of relatively open ground surface and flat (low roughness). Therefore, only the strength of convective flow contributes to the elevation (2.4).

$$H = 1.5\left(\frac{V_s d}{v}\right) \qquad \textbf{(2.4)}$$

Where:

$c(x,\mathrm{y},\mathrm{z},\mathrm{t})$ = concentration of pollutant (µg m^{-3})

Q = Emission Rates (g s^{-1})

H = Effective height (elevation) (m)

$(k_y)\, and\, (k_z)$ Horizontal (y) and vertical (z) diffusion coefficients

σ_y, σ_z = Horizontal (y) and vertical (z) values of the dispersion factors (m); the standard deviation of profiles that have a Gaussian distribution**.**

V_s and v are respectively the gas velocity and the horizontal windvelocity (m s^{-1})

d = stack diameter

S describes source or sink of c

3 Sampling sites and emission sources

The source of the pollution chosen for the study was a fertilizers production unit based on ammonium nitrate located on the area of Heysham near Lancaster. The site is considered as a source of nitric oxide and nitrogen dioxide emitted during the production of nitric acid. A description of the production process and the rate of evacuation were described by Harrison and McCartney, [5].

Figure1. Maps showing measurement sites, sources (S), and land-sealimits. On the right, MLC the mobile measuring station; big black circle represents the balloon measurement site (altitude), the left map shows a large-scale land-sea boundaries

The pollutants emitted from five sources are grouped into a distance that does not exceed 280m **(Fig. 1)**. For this study we considered the individual effect of each source, instead it acts as a virtual point source.
The ground level concentrations of both NO and NO_2 were measured using a mobile station (MLC) located at 1.2 km to the north of the plant **(Fig.1)**. The measurements of vertical concentration profiles were made at sites close to the source. Access to the plant was limited only allowing sites to the east of the sources to be used for measurements **(Fig.1)**. The area surrounding the fertilizer plant was flat with a low altitude above sea level (elevation sites within 2 km of works ranges from less than 20m elevation to that of the work). A map of the area is given by an overview from free version of google-earth **(Fig. 1)**.

The area, to the north, east and south of the study location, is open with some hedges and small trees pasture [5]. The area to the west is an industrial site with a few buildings. The coastline to the west is between 1.7 and 2.5km, and around 4km to the southwest. The pollutants were emitted by five sources of the same height (46 + 1 m) and there were no buildings of significant height (roughness is zero).

4 Data preparation and measurement methodology

4.1 Approach and Methodology

Unlike the work of Roy M. Harrison [5], the deposit of pollutants on the ground levelis taken into account. NO_2 and NO, however, are deposited on vegetated surfaces Hill, 1971 [12]; the elevation of the plume was calculated by the equation of Holland **(1.3)** for the five sources, and finally we took into account all emissions sources as real point sources, and cannot act as a single point one, with same strength source located at a larger downwind distance, to not reduce as well, the concentrations at ground level and low altitudes, compared to measurement.
The rate of emission sources is estimated from the daily production rate of one hundred percent of HNO_3, (NO and NO_2 are released during HNO_3: production process) [18-20]. This is achieved by adjusting operating conditions in the absorption unit of the acid to control emissions of NOx, instead of subsequent gas treatment. A typical emission factor is between 25 and 27.5kg NO emitted per ton of HNO_3 product Sitting, [13-22]; and the intensity of the daily average sources could be estimated.
The concentrations of pollutants at various heights were measured by collecting samples of air bags in Teflon FEP (Fluor Ethylene Propylene) suspended within a captive balloon; Samples were collected and analyzed using the analyzer of the mobile station MLC [5].The simulations were performed by an approach based on the Gaussian model that we developed. The calculations were performed considering the data of the day when the measurements were recorded [5, 16-21].

4.2 Site and meteorological data

Speed and wind direction were recorded at 5m, every two minutes during the measurement campaign conducted in the work of Roy M. Harrison, [5]. The ambient temperature and the state of the atmosphere (1 low radiation, 2 moderate radiation, 3strong radiation, 4 uncovered Night, 5 very covered Night) are also recorded every two hours. The schedule evolution of all parameters is detailed in the table **(Tab.1)**. the Pasquill atmospheric stability classes Pasquill, [14] (A very stable to very unstable F) are defined, based on wind speed and atmospheric states (Tab.2), in order to calculate horizontal (y) and vertical (z) values of dispersion factors.

Table 1. Changing weather parameters during the simulation day

Year	**Month**	**Day**	**Hour**	**Wind speed* [ms^{-1}]**	**Wind direction [°]**	**Atmospheric State² (from 1 to 5)**	**Atmospheric temperature [°C]**
1978	07	13	2	6.	40.	5	12.0
1978	07	13	4	6.	40.	5	15.0
1978	07	13	6	6.5	40.	3	15.5
1978	07	13	8	6.5	40.	3	17.5
1978	07	13	10	6.5	40.	2	18.0
1978	07	13	12	7.	40.	1	20.0
1978	07	13	14	7.	90.	1	21.5
1978	07	13	16	7.	0.	1	22
1978	07	13	18	6.5	0.	2	20.5
1978	07	13	20	6.5	0.	3	19.0
1978	07	13	22	6.5	0.	4	15.0
1978	07	13	24	6.	0.	4	13.5

*The wind speed at the elevation of the stack is calculated by relationship Smith, [15]:

²The state of the atmosphere and wind speed are essential for determining the classes of atmospheric stability **(tab.2)**

Table 2. Pasquill stability classes

Wind speed (ms^{-1})	**Day Insolation**			**Night Cloud cover**	
	Strong (1)	Moderate (2)	Slight (3)	<3/8 (4)	>1/2 (5)
< 2	A	A-B	B	F	F
2-5	A-B	B	C	E	F
5-7	B	B-C	C	D	E
7-9	C	C-D	D	D	D
> 9	C	D	D	D	D

5 Results and Discussion

5.1 Model validation

In this section, we performed, at different altitudes **(Fig. 2**), a comparison between the concentrations of NO_x ($NO + NO_2$) predicted by the improved Gaussian model and those measured in the works of Harrison & McCartney [5]. The simulations performed by our model, including meteorological data and data from the site (on the same day where the measurement campaign took place) gave great satisfaction at all levels and particularly at the levels surrounding the stacks height (Z = 40 ~ 50 m).

The model predicts the dispersion of emissions from the five chimneys, and simulates the concentrations throughout the surrounding area and at different altitudes without taking into account the already existing elements in the atmosphere or deposited on the ground, or even emissions from natural sources or other areas. This point is deterministic to explain some inconsistencies between measurements and simulations at altitudes much lower or higher than the height of the chimneys.

On many occasions, visual observation indicated that the plume elevation was generally low and was estimated to an average value between 5 and 10 m giving an effective height, H, 51 m to 60 m for each chimney. The simulations carried out using our model confirm these observations **(Fig. 3)**.

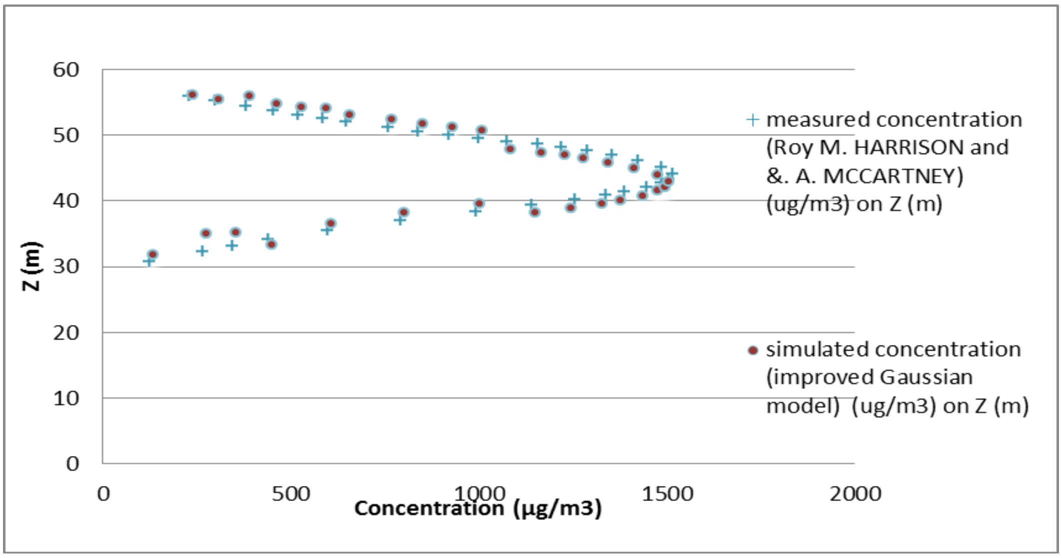

Figure2. Comparison between concentrations measured by balloon (Harrison & McCartney) and concentrations simulated using the improved Gaussian model.

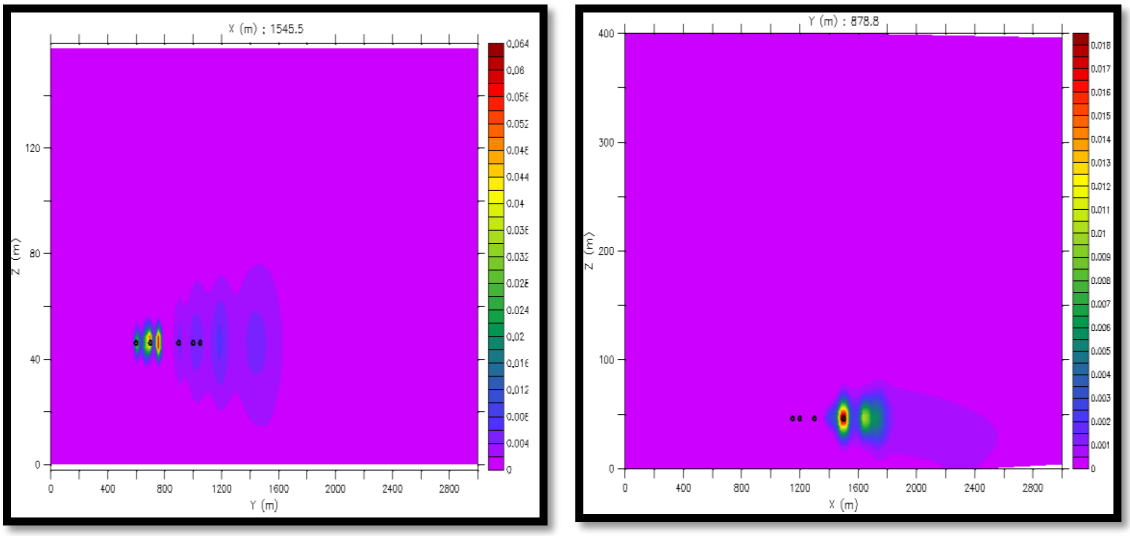

Figure 3. The XZ and YZ planes of the plume generated by the five stacks simulated using the improved Gaussian model.

5.2 Simulation of emission dispersion on horizontal surfaces

The NO_x emissions generated by the chimneys are transported away and diffused throughout the surrounding area up to $2km^2$ and a part of these emissions is deposited on the ground. The averaged concentrations of NO_x at ground level **(Fig.4 a)**, above ground **(Fig.4, b)**, at the height of the chimneys **(Fig.4, c)** and above, of the stacks height **(Fig.4, d)** are chosen for the simulations to give an overview on the dispersion process through the most representative levels.

The NO_x concentrations were calculated for periods when the plume passed over the site, by the interpolation of the discontinuous record. The simulation shows that the quantity of NO_x emitted by the five sources from the industrial unit is subsequently dispersed in the neighboring area. The dispersion is much higher on the earth's surface compared to the other levels, but the NO_x concentrations are relatively low (0 to 1.610^{-3} mg/m^3). At the stacks height, the pollutants are not dispersed enough, but the concentrations (up to 0.15 mg/m^3) are largely high compared to higher or lower levels. A large part of these emissions is transported and distributed to the north from the industrial unit. This is essentially due to the intersection of two parameters: the direction of a relatively strong winds and peak hours at the unit (during the moderate insolation day), which generated more than averaged atmospheric instability class.

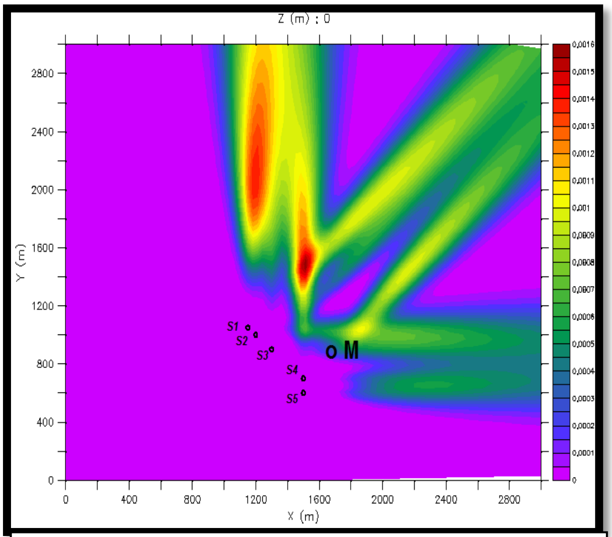

Figure 4,a : NOx concentrations (mg/m3) at ground level (Z m = 0). O the site where the balloon measurements are made

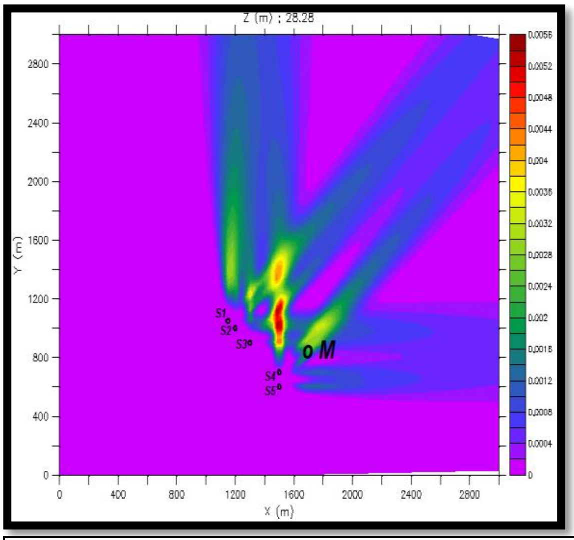

Figure 4,b : NO_x concentrations (mg/m^3) above the ground (Z = 28.28 m). **O** measurement site

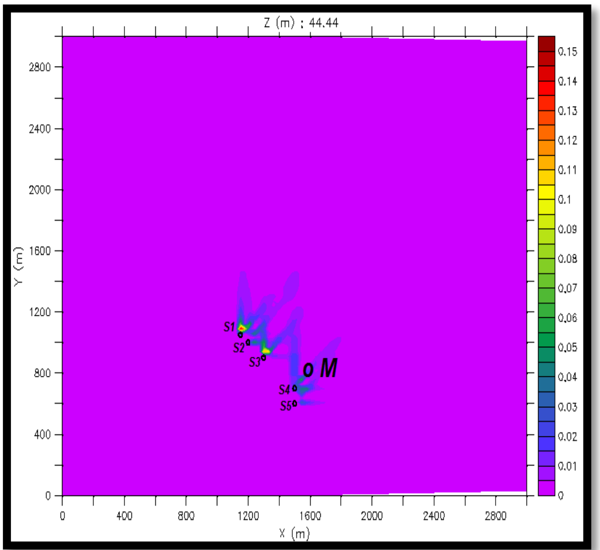

Figure 4,c : NOx concentrations (mg/m3) just below the chimneys (Z = 44.44 m). **O** measurement site

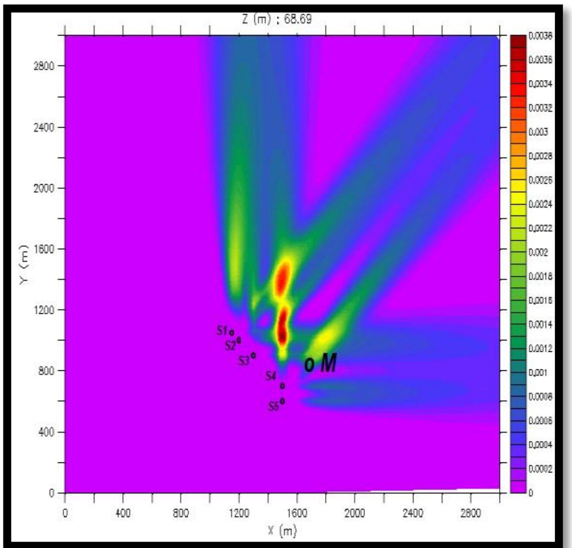

Figure 4,d : NO_x concentrations (mg/m^3) above the chimneys (Z = 68.69 m). **O** measurement site

6 Reductions cenarios

6.1 Stack height

The stack height is a decisive parameter for the dispersion of pollutants in the atmosphere, especially in the lower layers which contain mainly air breathed by living beings.

In this first scenario we increase the height of all the chimneys of the site, to 34m giving a real height of 80m. The NO_x emissions generated from stacks dispersed throughout the surrounding area, except this time, the averaged concentrations of NO_x at ground level and just above **(Fig.5, a and b)** are remarkably low (0 to 0.5210^{-3} mg/m^3) compared to the recorded concentrations at the current stacks heights (0 to 1.610^{-3} mg/m^3). But concentrations at levels of stacks heights and above **(Fig.5, c and d)** are remarkably high (until 0.8 mg/m^3) compared to similar cases recorded for the current stack heights concentrations (0.15 mg/m^3).

The potential explanation for these results is up to phenomena of atmospheric thermal inversion layers at the height of the chimney which prevents the gases to diffuse quickly to the lower layers (at least close to the site) and therefore, keeps these pollutants with high concentrations on higher level.

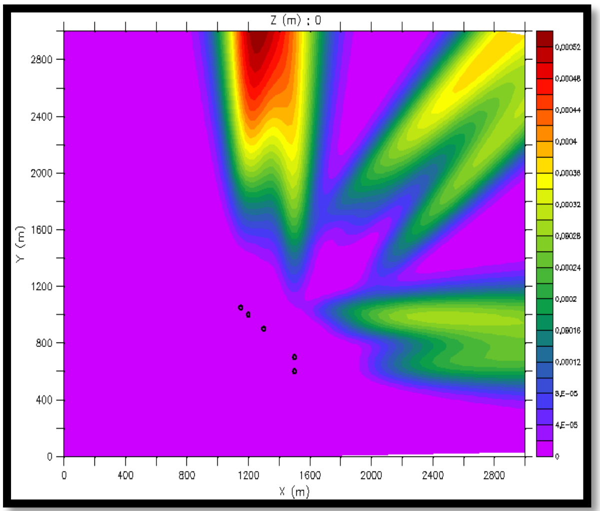

Figure 5.a . NO_x concentrations (mg/m^3) at ground level (Z = 0 m).

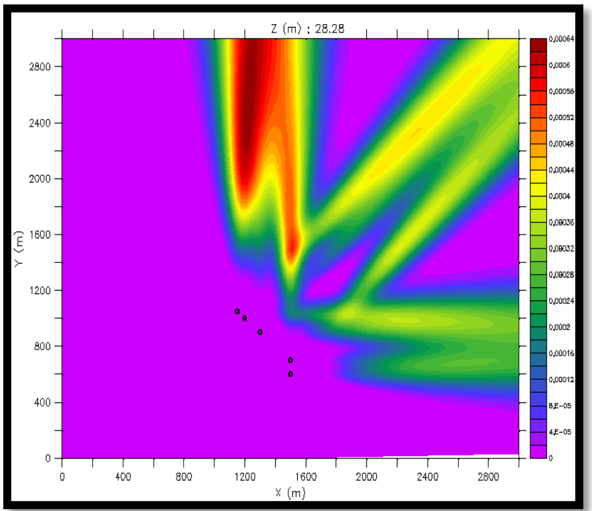

Figure 5. b . NO_x concentrations (mg/m^3) above the ground level(Z = 28.28 m).

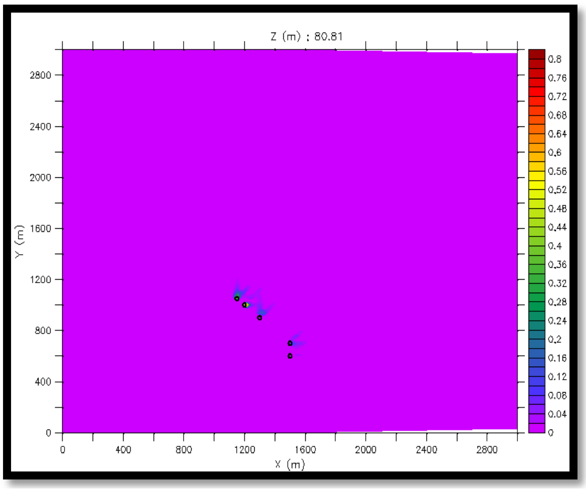

Figure 5.c . NO_x Concentrations (mg/m3) just below the chimneys (Z = 80.81 m).

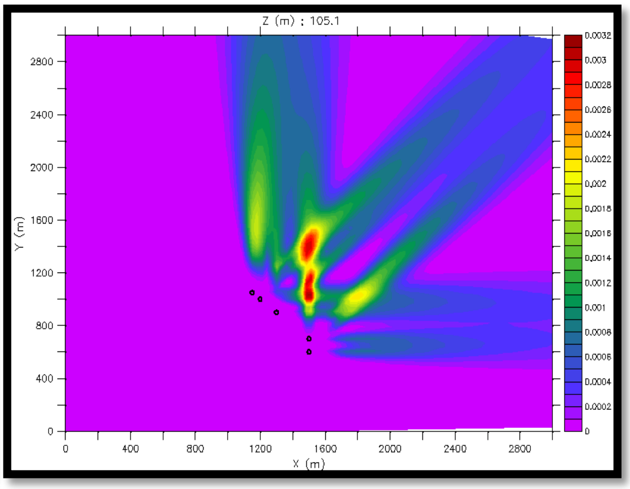

Figure 5. d . NO_x Concentrations (mg/m^3) above the chimneys(Z = 105.1 m).

6.2 Reduction of emission points

Another solution that seems much more relevant, is based on the idea of bringing the five current evacuation outputs into one output (chimney) with an intensity equivalent to the sum of intensities of the five chimneys with an effective height of 80m as we have already indicated in the previous section **(Fig. 6, a and b).**

Emissions still continue to disperse but this time just on specific areas and not on the entire region. Increasingly, the concentrations are largely low compared to the recorded concentrations in the first scenario studied in the previous section whatsoever, at ground level or at the stack height level (80 m). The superposition of the emissions generated by the five chimneys coupled with the roughness that presents one smokestack to others; contribute in the diffusion process of pollutants to the lower layers, which consequently increases the concentrations at ground level.

Conclusion

The results of comparisons between the concentrations simulated by our model, and concentrations measured by Roy M. Harrison [5] indicate that our model, which takes into account a number of parameters that usually neglected by classical models, can predict not only the concentrations on the ground level and at different altitudes, but also the geometry (elevation, length and width) of the plume, with acceptable accuracy.

Increasing the height of the chimney reduces significantly the concentrations of pollutants emitted by the chimney on the ground level of the region in the proximity and below the stack height levels. But the concentrations remains important on higher levels and which may be deposited thereafter on a remote areas.

However, reducing the number of emission points with a correct height contributes to a significant reduction of concentrations on all levels including the ground level, and a large part of this area will not be affected by pollution.
The model provides certainly encouraging results. However, some improvements remain to be developed in order to make it applicable to surfaces exhibiting particular complexities such as the existence of buildings and obstacles and thus generating wind convergences

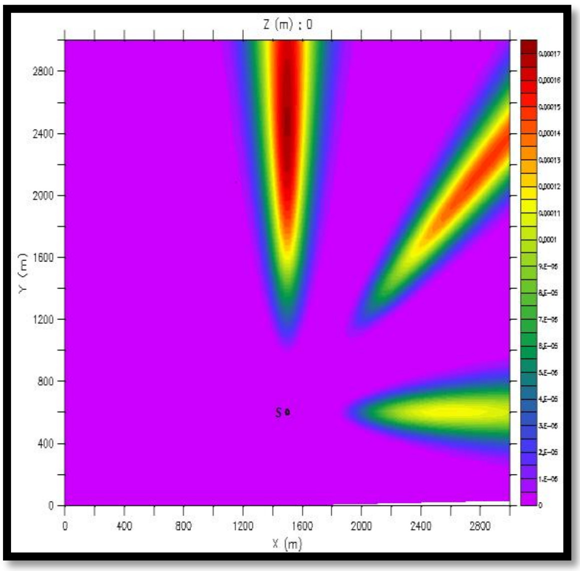

Figure 6.a. NOx concentrations (mg/m^3) at ground level (Z = 0 m).

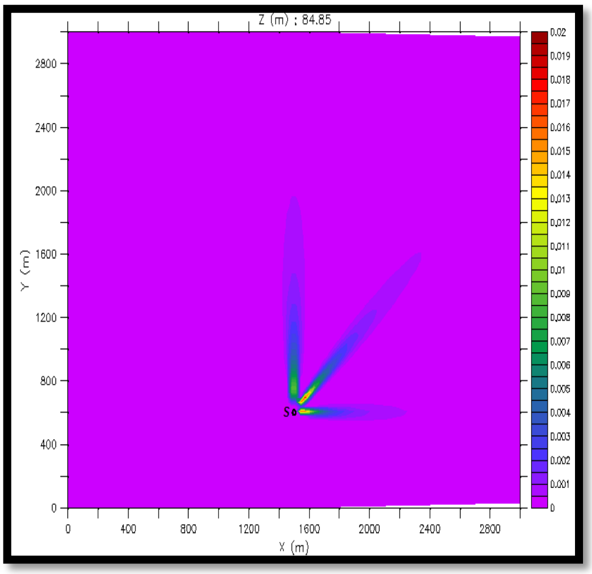

Figure 6.b. NOx concentrations (mg/m3) just above the level of the chimney Z = 84.85 m).

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