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STUDY REGARDING THE DISPERSION OF FLUE GASES IN THE ATMOSPHERE

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ABSTRACT

This paper deals with the comparative study of the dispersion of some components of flue gases in the atmosphere. Mathematical modelling of the dispersion of pollutants discharged from technological furnaces in refineries is carried out using high-performance software. Thus, taking into account the meteorological conditions and the pollutant concentrations, the level of atmospheric pollution can be determined.

The aim of the paper is to compare the values of NO_2 and CO concentrations obtained with the classical Gaussian dispersion model algorithm with the values of pollutant concentrations estimated using the SCREEN View simulation software.

The determinations were made taking into account receivers located at distances of 100 m, 500 m, 2500 m and 5000 m from the emission source, thus it was established at which distance from the source the maximum pollutant concentrations resulted. For atmospheric stability class, A and F (very unstable and stable). For A stability class, the maximum concentrations pollutant resulted at a distance of 500m from the emission source, and for F stability class, the maximum pollutant concentrations resulted at a distance of 2500 m from the emission source.

Both with the classic work methodology and with the SCREEN View software, the concentration values are comparable, this underlines the precision of the software.

Also, with the classic Gaussian modelling algorithm, the maximum height of the smoke plume was calculated. This is higher for stability class A, compared to F.

Keywords: dispersion, flue gases, chimney, refineries, pollutant

INTRODUCTION

Internationally, the oil industry is facing increasing pressure from governments and civil society to continuously improve its environmental performance.

The increasingly poor quality of crude oil can obviously lead to high sulphur content in petroleum products, which favours equipment corrosion, catalyst poisoning, environmental pollution and other negative consequences. Treatment of high-sulphur crude oil is becoming the focus of research in the oil refining industry. To meet the needs of producing green fuels, lowering the sulphur content of crude oil becomes an urgent task [1].

Romania, as a member of the European Union, has assumed the responsibility of complying with the strict conditions for reducing greenhouse gas emissions generated by the use of gasoline and diesel during the life cycle, implicitly to reduce the sulphur content of these fuels. Thus, by Decision no 928/2012 on establishing the conditions for placing gasoline and diesel on the market, the technical specifications are established, based on health and environmental considerations [2].

Thus, at the level of refineries, hydrogen treatment processes such as hydrofining arose out of necessity to desulfurize atmospheric distillates, in order to comply with the norms imposed on the final products or, in the case of gasoline, to make them suitable for fueling catalytic reforming that used catalysts containing platinum. Later, attention was also paid to the elimination of nitrogen, which decreased the oxidation stability of the products.

Human activities have led to negative effects on air, one of the environmental factors, reacting most quickly to harmful substances.

Any change in the air quality is felt by the organism, which can lead to a change in the health of the population.

One of the biggest equipment in the refinery is the technological furnace. The combustion process takes place there, resulting in flue gases [3].

Combustion calculation involves establishing the composition and characteristics of the flue gases resulting from the reactions between fuel and oxygen in the air. During the operation of the furnace, a series of changes in the working parameters occur that lead to variations in the flow rate and the composition of the flue gases.

According to the legislation in force, atmospheric pollutant is any substance present in the surrounding air that can have harmful effects on human health and/or the environment as a whole. Polluting substances are released into the atmosphere especially in urban areas and heavily industrialized regions [4].

The movement, in time and space, of a group of particles (aerosols, gases, powders) released into the atmosphere, represents atmospheric dispersion [5].

The dispersion phenomenon is influenced by atmospheric conditions, soil parameters and the level of emission concentrations [5].

The mathematical simulation of the spread of pollutants in the atmosphere represents the atmospheric dispersion model [6].

The aim of the paper is to compare the values of NO_2 and CO concentrations obtained with the classical Gaussian dispersion model algorithm with the values of pollutant concentrations estimated using the SCREEN View simulation software. The maximum height of the smoke plume will also be calculated, using the dispersion model algorithm.

ATMOSPHERIC DISPERSION MODELS APPLIED FOR FLUE GASES

The mathematical simulation of pollutants spreading in atmosphere is used to estimate the concentration of pollutants emitted from the industrial activity or automobile traffic, depending on the wind direction [4, 7].

The Pasquill stability scheme is only one of a number of methods used to determine pollutant concentrations, and several studies have compared the effectiveness of the Pasquill scheme against these other methods. Method of choosing each Pasquill stability class based on surface wind speed and sky conditions. Pasquill determined six stability classes, A-F, for use in dispersion model calculations [7, 8].

Table 1. *Pasquill-Gifford Turner Stability Classifications* [9, 10].

Surface wind speed[a] (m/s)	Day solar insolation			Night cloudiness*	
	Strong[b]	Moderate[c]	Slight[d]	Cloudy (≥4/8)	Clear (≤ 3/8)
< 2	A	A-B[f]	B	E	F
2-3	A-B	B	C	E	F
3-5	B	B-C	C	D	E
5-6	C	C-D	D	D	D
> 6	C	D	D	D	D

[a]Surface wind speed is measured at 10m above the ground.

[b]Corresponds to clear summer day with sun higher than 60° above the horizon.

[c]Corresponds to a summer day with a few broken clouds, of a clear day with sun 35-60° above the horizon.

[d]Corresponds to a fall afternoon, or a cloudy summer day, or clear summer day with the sun 15-35° above the horizon.

[e]Cloudiness is defined as the fraction of sky covered my clouds.

[f]For A-B, B-C, or C-D conditions, average the values obtained for each.

Note: A, very unstable; B, moderately unstable; C, slightly unstable; D, neutral; E, slightly unstable; F, stable. Regardless of wind speed, class D should be assumed for over cast conditions, day or night.

In this paper, the concentrations of two toxic pollutants from the flue gases, from the furnace of the diesel hydrofining plant in a refinery, were calculated, for two stability classes: A- very unstable and F - stable.

The domain for the evaluation of immissions, caused by the hydrofining plant, is the surface that is completely inside the circle around the chimney, which is 50 times higher than the actual height of the chimney (according to the TA Luft guide) [11].

The calculation of the maximum concentrations at ground, for two possible pollutant components present in the flue gases from a technological furnace into a hydrofining plant was performed [3]:

- NOx (assimilated with NO_2) - nitrogen oxides and
- CO - carbon monoxide.

The concentrations of NO_2 and CO pollutants were determined with the Gaussian dispersion model [6].

Required data to calculate the pollutant concentrations were known and are specified in table 2. These data were taken from the technological furnace at the diesel hydrofining plant in a refinery.

Table 2. Input data necessary the pollutant concentrations.

Source	Pollutant	Flow rate q,[g/s]	Height chimney [m]	Inner Diameter at the top of the chimney [m]	Outlet temperature [K]	Outlet velocity flue gases [m/s]
Chimney stack	NO_2	8,63	100	3,8	373	4
	CO	3,5	100	3,8	373	4

Gaussian model of dispersion – classical algorithm

Figure 1 shows the variation profile of the pollutant cloud concentration, from the exit through the furnace chimney, in the direction of the wind and at the height from the ground.

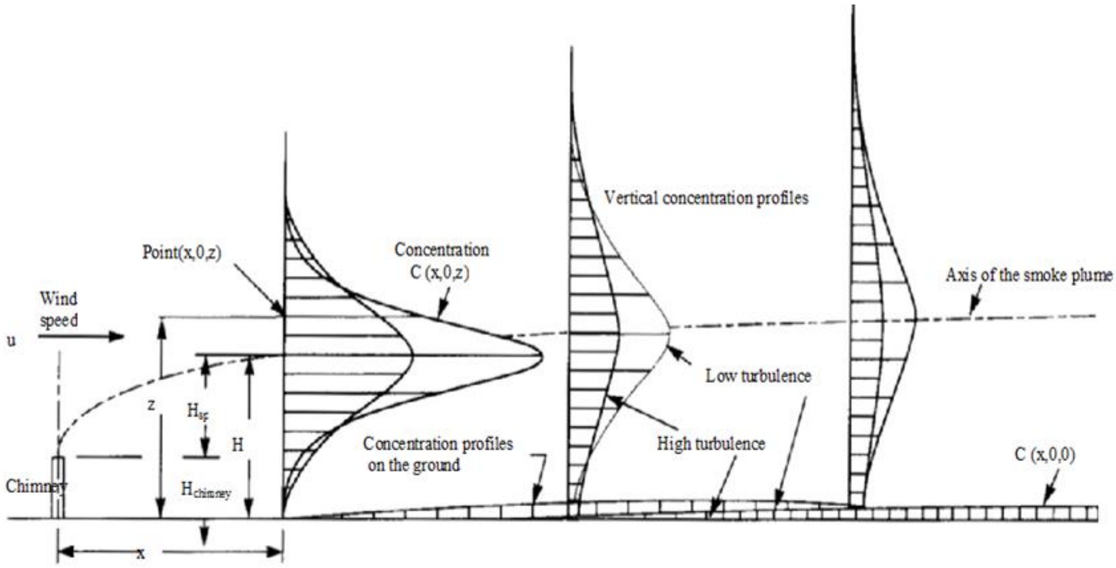

***Figure 1**. The Gaussian Plume Model* [6, 12].

The Gaussian model is the most widely used model for analyzing the dispersion of atmospheric pollutants. The hypothesis underlying the model is that in any direction of the wind, the smoke cloud has a Gaussian distribution, independent horizontally, but also vertically.

For a continuous point source of pollutants, considering the flow of combustion gases from the chimney of the technological furnace, the general dispersion relation of Gauss is applied:

$$c_{(x,y,z)}=\frac{q}{2\cdot\pi\cdot u\cdot\sigma_y\cdot\sigma_z}\cdot e^{-0,5\cdot\left(\frac{y}{\sigma_y}\right)^2}\cdot\left(e^{-0,5\cdot\left(\frac{z-H}{\sigma_z}\right)^2}+e^{-0,5\cdot\left(\frac{z+H}{\sigma_z}\right)^2}\right) \qquad (1)$$

Where:

c - the emission concentration [g/m^3],

q – emission source rate [g/s],

u – horizontal wind speed, [m/s],

y – lateral distance from the plume center,

H– the effective plume height above the ground [m],

σ_z – dispersion coefficient of the vertical distribution emission [m],

σ_y – dispersion coefficient of the horizontal distribution emission [m].

The highest concentration that occurs at ground level is located in the center of the smoke plume, for y = 0 and z = 0

$$c_{(x,0,0)}=\frac{q}{\pi\cdot u\cdot\sigma_y\cdot\sigma_z}\cdot e^{-0,5\cdot\left(\frac{H}{\sigma_z}\right)^2}\left[\frac{g}{Nm^3}\right] \quad (2)$$

The dispersion coefficients can be found in the relationships for determining the concentrations. The values of these coefficients, which represent, in fact, standard deviations, are the basis of the results of experimental data, following the studies on the evolution of gases [13].

The dispersion coefficients used are:

- Pasquill-Gifford coefficients – called rural Pasquill coefficients;
- McElroy-Pooler coefficients – called urban Briggs coefficients.

For the case of pollution sources located in urban areas, the dispersion coefficients in z and y directions are determined with the relationships listed in table 3, respectively in table 4. The values written in bold are those used in the following steps.

Table 3. *Calculation of the dispersion coefficient along the y direction [14].*

Stability class	**Relationship σ_y**	**x=100m**	**x=500m**	**x=2500m**
A				
B	$0,32\cdot x\cdot(1,0+0,0004\cdot x)^{-1/2}$	31.38	146.06	565.69
C	$0,22\cdot x\cdot(1,0+0,0004\cdot x)^{-1/2}$	21.57	100.42	388.91
D	$0,16\cdot x\cdot(1,0+0,0004\cdot x)^{-1/2}$	15.69	73.03	282.84
E				
F	$0,11\cdot x\cdot(1,0+0,0004\cdot x)^{-1/2}$	10.79	50.21	194.45

Table 4. *Calculation of the dispersion coefficient along the z direction [14].*

Stability class	**Relationship σ_z**	**x=100m**	**x=500m**	**x=2500m**
A				
B	$0,24\cdot x\cdot(1,0+0,001\cdot x)^{1/2}$	25.17	146.97	1122.5
C	$0,20\cdot x$	20	100	500
D	$0,14\cdot x\cdot(1,0+0,0003\cdot x)^{-1/2}$	13.79	65.28	264.58
E				
F	$0,08\cdot x\cdot(1,0+0,0015\cdot x)^{-1/2}$	7.46	30.24	91.77

In order to calculate the concentration of the pollutant, the effective height from which the dispersion takes place must be known, this involves the calculation of the height of the plume, H_p. The Briggs method is used in the calculations, which considers the height of the plume as a function of the distance x, along the wind direction, the lift of the plume and the wind speed [15].

Calculations were made for stability class A and F as follows [7, 12]:

- Ascending F (or buoyancy factor) calculation:

$$F=\frac{g}{4}\cdot D_{i,chimney}^{2}\cdot w_{o,chimney}\cdot\frac{T_{o,chimney}-T_{air}}{T_{o,\ chimney}}\left[\frac{m^4}{s^3}\right] \qquad (3)$$

Where F is buoyancy factor – the ascending flow;

$D_{i,chimney}$ – the inner diameter of chimney – 3,8 m;

$w_{o,\ chimney}$ – the flue gases velocity from chimney – 4 m/s;

$T_{o,chimney}$ – the absolute outlet temperature of the flue gases from chimney - 373 K;

T_{air} – the absolute air temperature – 293 K;

g = 9.80665 [m/s^2] – the gravitational acceleration;

- Calculating the distance x_f from the emissions source where the plume height is maximum:

For unstable and neutral conditions (stability class A, B, C, D):

$$x_f=49\cdot F^{\frac{5}{8}}\ [m]\ \text{for}\ F<55 \qquad (4)$$

$$x_f=119\cdot F^{\frac{2}{5}}\ [m]\ \text{for}\ F\geq 55 \qquad (5)$$

$$x_f=3{,}14\cdot\frac{u}{S^{0,5}}\ [m]\ \text{for stable conditions (E, F)} \qquad (6)$$

Where: u – wind velocity to chimney height [m/s];

s – the atmospheric stability parameter [s^{-2}]

For E stability class s = 0,02·g/T_a (7)

For F stability class s = 0,035·g/T_a (8)

- Calculating the lifting height of plume, H_p:

For unstable and neutral conditions (stability class A, B, C, D)

$$H_p=1{,}6\cdot F^{\frac{1}{3}}\cdot\frac{x^{\frac{2}{3}}}{u}\ [m]\ \text{pentru}\ x < x_f \qquad (9)$$

$$H_p=1{,}6\cdot F^{\frac{1}{3}}\cdot\frac{x_f^{\frac{2}{3}}}{u}\ [m]\ \text{pentru}\ x \geq x_f \qquad (10)$$

For stable conditions (stability class E, F)

$$H_p=\min(H_{p1},H_{p2},H_{p3})[m], \qquad (11)$$

$$H_{p1}=2{,}4\cdot\frac{F^{\frac{1}{3}}}{u\cdot S}\ [m], \qquad (12)$$

$$H_{p2}=5\cdot\frac{F^{\frac{1}{4}}}{S^{\frac{3}{8}}}\ [m], \qquad (13)$$

$$H_{p3}=1,6\cdot\frac{F^{\frac{1}{3}}\cdot x_f^{\frac{2}{3}}}{2}\ [m] \quad (14)$$

- Height of the smoke plume, H: $H = H_c + H_p$ (15)

For stability class A, resulted H = 266.2 m

For stability class F, resulted H= 187.4 m

Taking into account receivers located at 100 m, 500 m, 2500 m and 5000 m within a radius of 5 km from the source, the calculations of CO and NO_2 pollutant concentrations showed that for stability class A, the maximum concentrations are reached at 500 m from the source, and for stability class F, maximum concentrations are reached at 2500 m.

The values of NO_2 and CO concentrations can be seen in the table 6.

Gaussian model of dispersion - SCREEN View simulation

A simulation program was used to estimate concentrations of gaseous pollutants at ground level [16].

This program was developed by the American company Lakes Environmental, well known for the varied range of software it has developed for modelling air dispersion. These software are used by various companies, in industry, by governmental environmental agencies, as well as by the academic environment [16].

Taking into account the type of source, the height of the chimney, the meteorological conditions, the pollutant flows, with the help of the program their concentrations are determined depending on the distance from the source.

SCREEN View can be applied to simple or complex terrains, with or without buildings, and provides results for appreciable distances.

Applying the SCREEN View program can save time and resources, not requiring more complicated modelling.

SCREEN View is based on the more complex program ISC3 (Industrial Source Complex) used to determine pollutant emissions at different types of sources [16].

Figures 2, 3, 4 and 5 are print screens of the windows in the SCREEN View program, where the required data for the simulation were entered, as well as those used in the classical calculation variant.

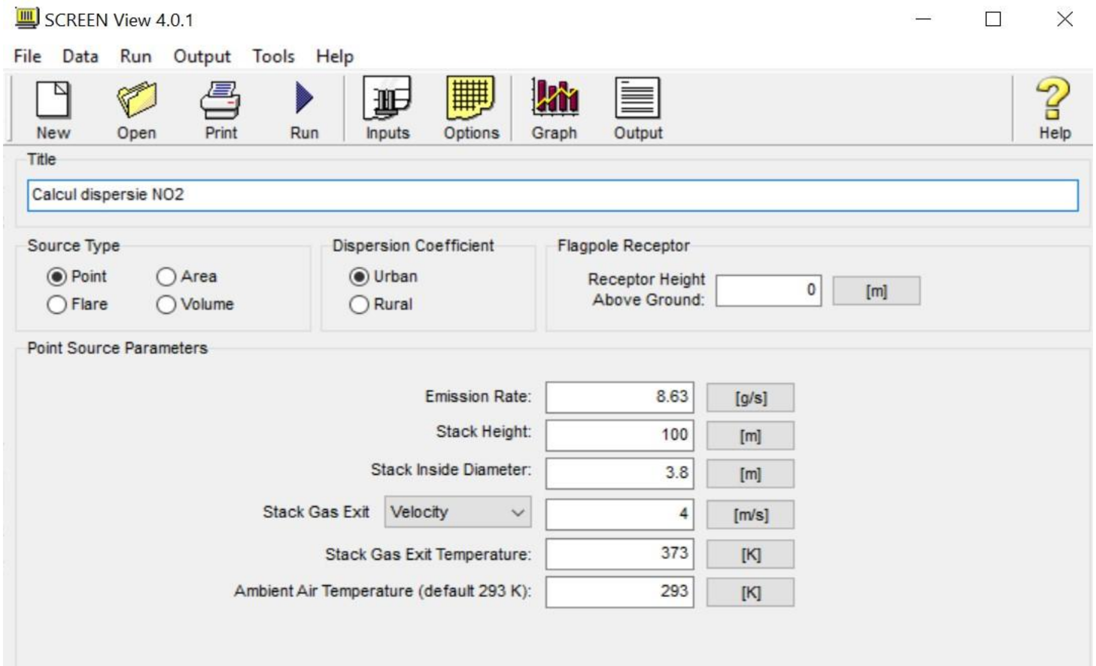

Figure 2. *Screen View input data window for NO_2 pollutant.*

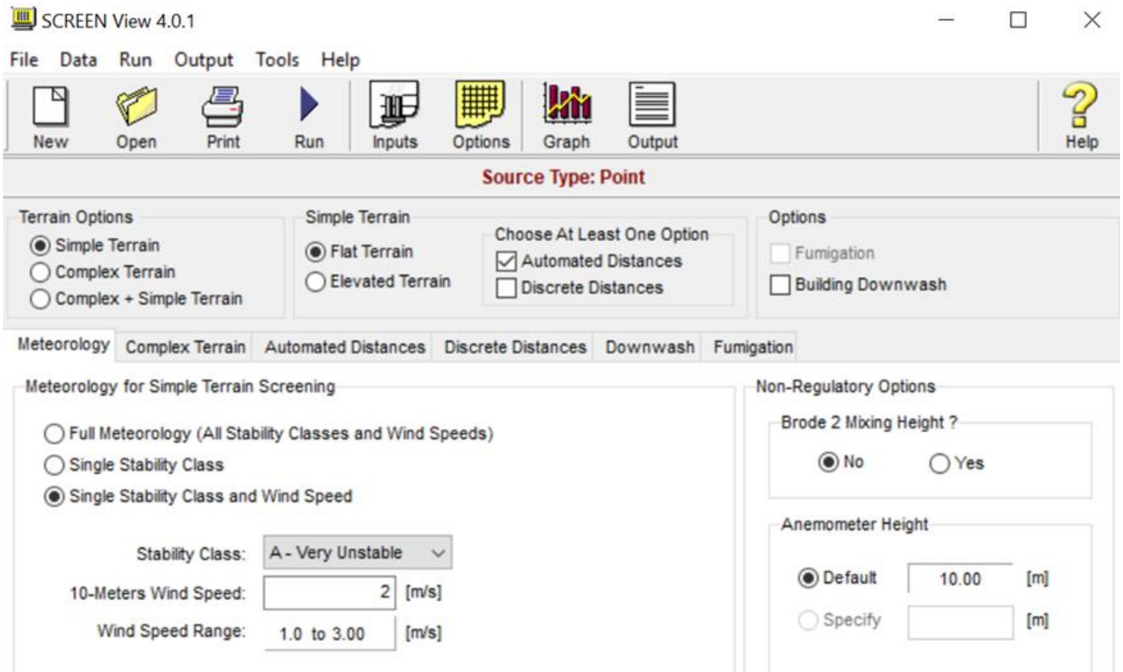

Figure 3. *Weather input data window – A stability class.*

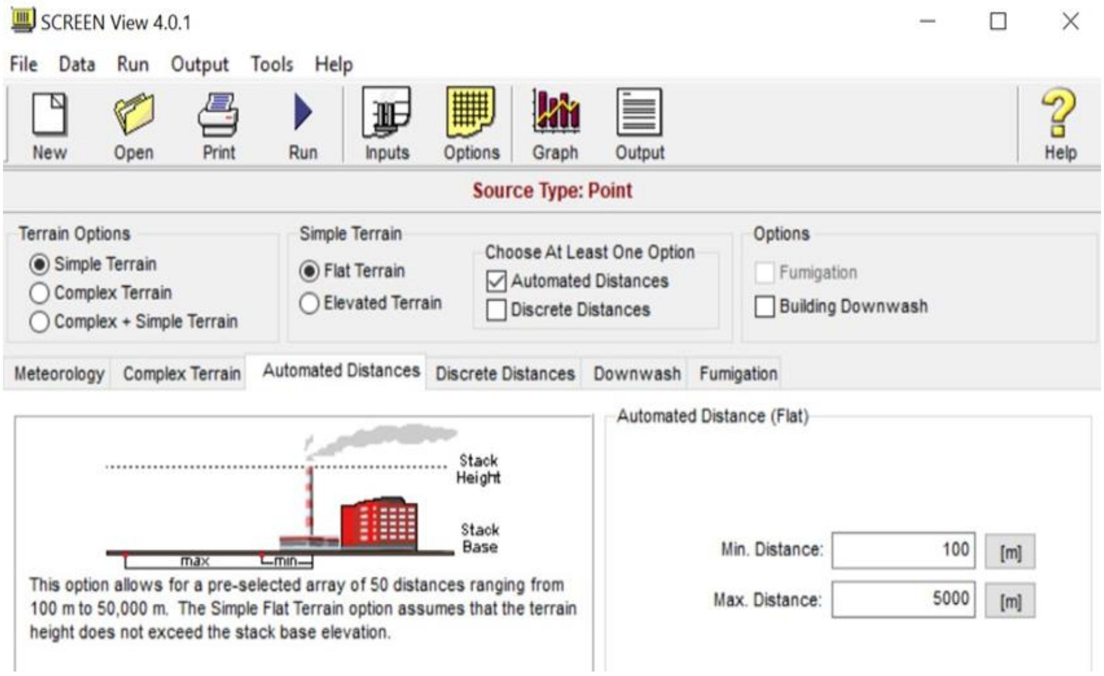

Figure 4. *Input data window of the field of study of immissions.*

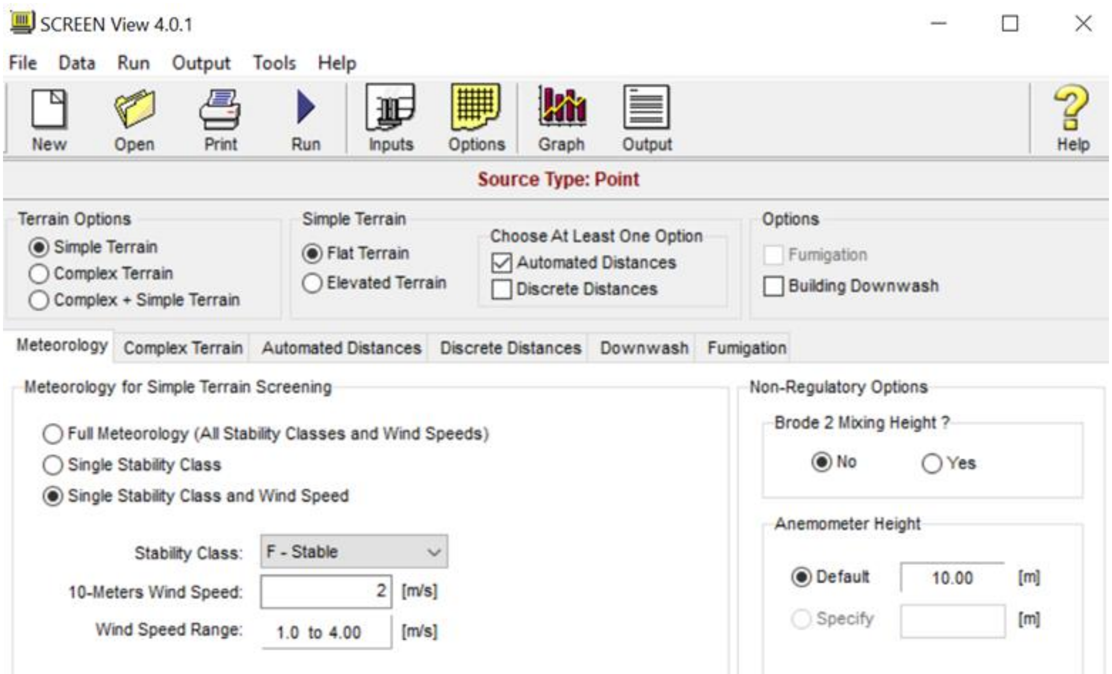

Figure 5. *Weather input data window – F stability class.*

RESULTS

The results obtained after the simulation are expressed in tables or graphs.

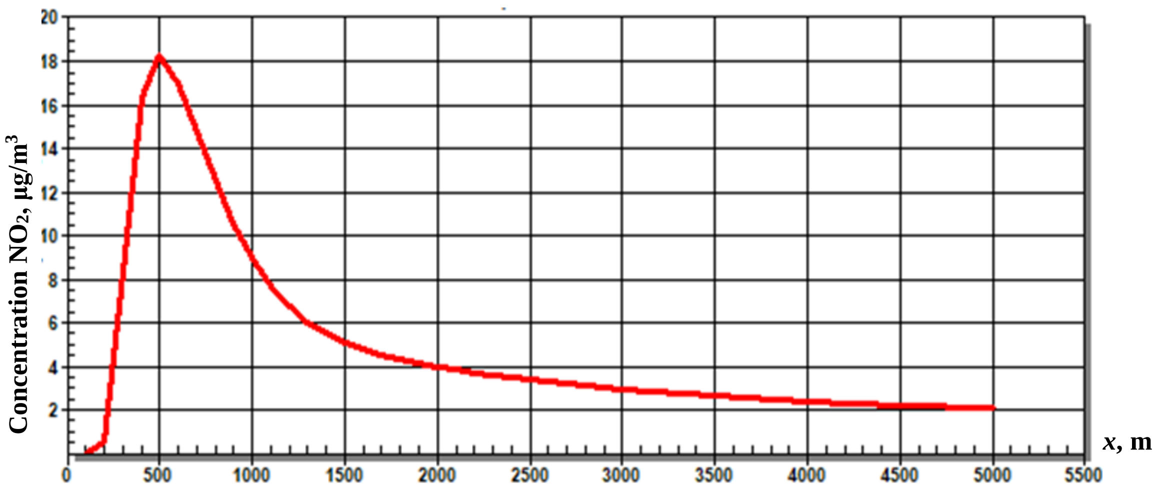

Figure 6. *Variation of NO_2 concentration depending on distance x, for A – stability class.*

At 100 m distance from the source, the pollutant begins to settle in low concentrations at ground level, reaching a maximum concentration of 18.29 µg/m3 at a distance of 494 m.

Restarting the simulation and using the same input data, but reducing the chimney height to 50 m, the result showed a doubling of the pollutant concentration and a reduction in the distance for the maximum concentration point as can be seen in the figure 6. More precisely, a concentration of 30 µg/m^3 is reached at a distance of 400 m from the source.

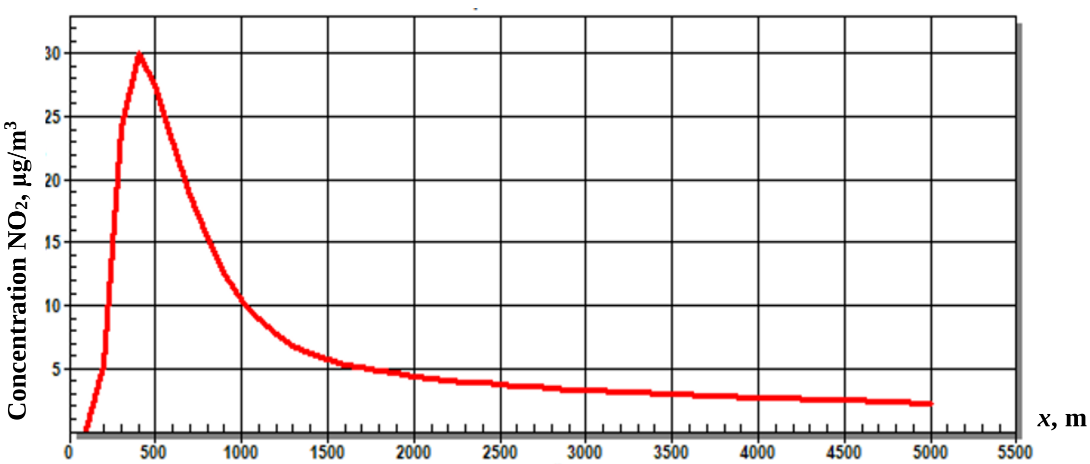

Figure 7. *Variation of NO_2 concentration pollutant with distance x,*
for a 50 m chimney height, A stability class.

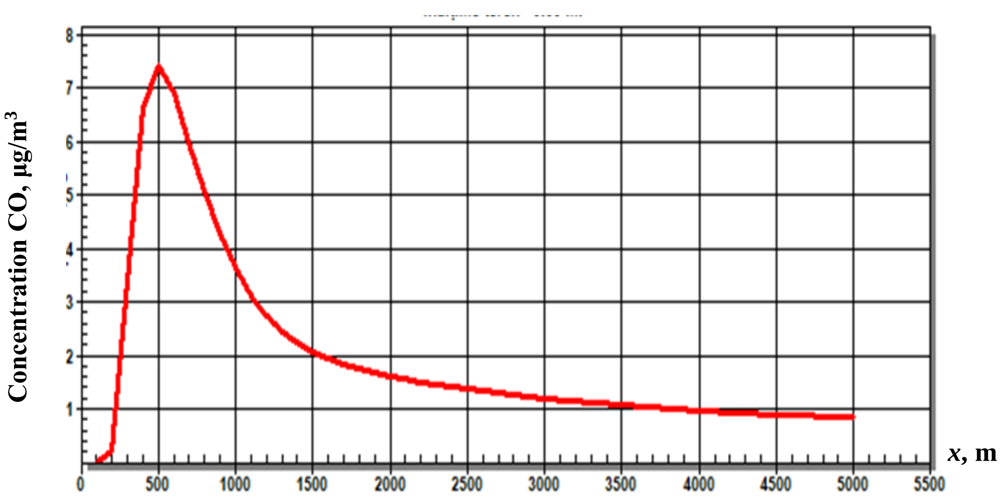

Figure 8. *Variation of CO concentration pollutant with distance x, A stability class.*

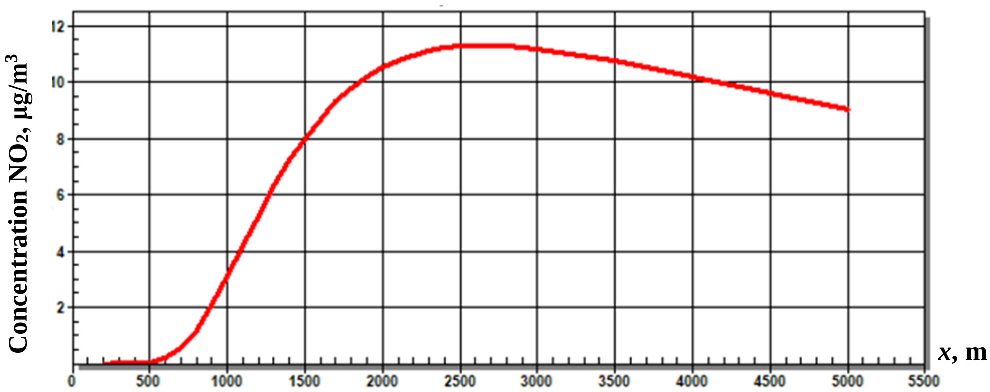

Figure 9. *Variation of NO_2 concentration pollutant with distance x, F stability class.*

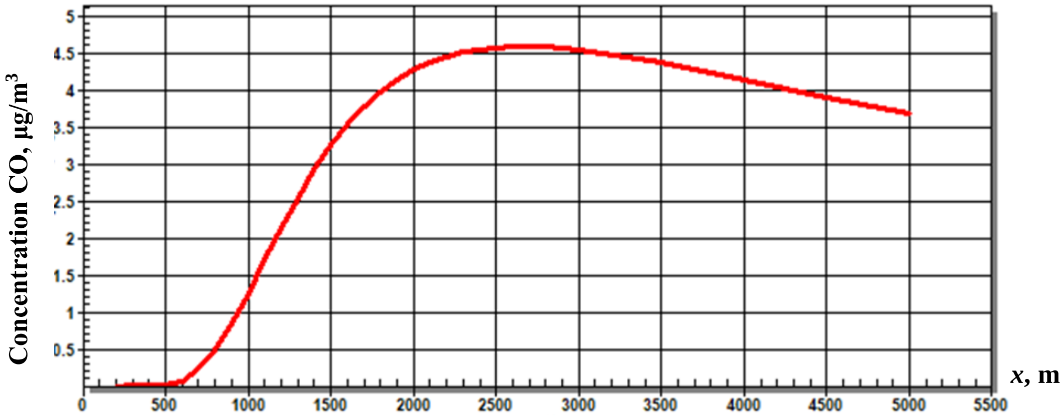

Figure 10. *Variation of CO concentration pollutant with distance x, F stability class.*

The results obtained with the SCREEN View software are presented in table 3.

It is observed that the maximum values of the pollutant concentrations are at a distance of 500 m from the source of emissions, for stability class A and at 2500 m from the source of emissions, for stability class F.

Table 5. *The NO_2 and CO pollutant concentrations with SCREEN View.*

Stability Class	Pollutant	Highest Concentration of pollutant [μg/m³]				
		Distance from the source [m]				
		200	**500**	**1000**	**2500**	**5000**
A	NO_x	0.472	18.29	8.94	3.27	2.06
	CO	0.192	7.42	3.63	1.36	0.836
F	NO_x	0.111E-09	0.308E-01	3.11	11.28	9.05
	CO	0.451E-10	0.125E-01	1.26	4.55	3.7

The table 6 shows only the maximum values of the NO_2 and CO pollutant concentrations, correlated with the distances from the emission source, determined by the classical algorithm of the dispersion model.

Table 6. *The NO_2 and CO pollutant concentrations with Gaussian model dispersion.*

Stability Class	Pollutant	Highest Concentration of pollutant [μg/m³]	
		Distance from the source [m]	
		500	**2500**
A	NO_x	17.1	-
	CO	6.95	-
F	NO_x	-	11.1
	CO	-	4.5

Also, with the classical calculation algorithm of the dispersion model, the maximum height of the smoke plume was also determined, thus the following results were obtained:

For stability class A, resulted H = 266.2 m

For stability class F, resulted H = 187.4 m

This fact demonstrates the fact that the meteorological condition, the stability class, favours a rise in the smoke plume as the degree of instability increases.

CONCLUSIONS

The present work achieved two objectives:

1. Determining the maximum concentrations of NO_2 and CO pollutants and the maximum height of the smoke plume, by calculation with the classical algorithm of the Gaussian dispersion model, at a distance from an emission source, for two classes of atmospheric stability;

2. Determining the maximum concentrations of NO_2 and CO pollutants with the SCREEN View simulation program.

The values of the maximum concentrations of NO_2 and CO obtained by the two variants are comparable. This fact shows the accuracy of the simulation program and also the importance of its use, simplifying the use of resources and reducing work time.

In the simulation program, the 100 m height of the furnace chimney was used, but a simulation with a height of 50 m was also carried out, for stability class A.

In figure 6, an increase in the pollutant concentration can be observed, when the chimney height of the furnace is reduced, and this has an environmental impact at a smaller distance from the emission source, compared to the variation of the pollutant concentration in figure 7, when the furnace chimney has a height of 100 m.

The impact of the maximum concentrations of NO_2 and CO pollutants occurs at receptors located on 500 m distance, for A class atmospheric stability, and at receptors located on 2500 m distance, for F class atmospheric stability.

It is also worth noting that, after reaching the maximum level of concentration, for stability class F, the decrease in pollutant concentrations is slower than in stability class A. This means that the persistence of the components in the atmosphere is greater.

The height of the smoke plume increases with the increase of atmospheric instability.

The mixing consistency between the states is determined by the static stability. In general, an unstable atmospheric layer produces high mixing and dispersion if there is cold air above it. This means that temperature plays a very important role in the dispersion process.

An atmospheric layer is considered stable, if the warmer air is above it, thus the mixing and uptake of the smoke are difficult.

REFERENCES

[1] Lin, L., Hong, L., Jianhua, Q., Jinjuan, X., Progress in the technology for desulfurization of crude oil, in China petroleum processing and petrochemical technology, vol. 12, no. 4, pp1-6, 2010.

[2] https://legislatie.just.ro/Public/DetaliiDocumentAfis/170859

[3] Dobrinescu, D., Procese de transfer termic și echipamente specifice, Editura Didactică și Pedagogică, București, 1983.

[4] http://mmediu.ro/app/webroot/uploads/files/2015_06_17_Ghid_monitorizare_lcp.pdf

[5] www.scientificbulletin.upb.ro/rev_docs_arhiva/full677_521179.pdf

[6] https://faculty.washington.edu/markbenj/CEE357/CEE%20357%20air%20dispersion%20models.pdf

[7] Mărunțelu, O., Lăzăroiu, G., Bondrea, D.A., Mathematical model for air pollutants dispersion emitted by fuel combustion, U.P.B. Sci. Bull., Series D, Vol. 77, Iss. 4, ISSN 1454-2358, 2015.

[8] https://dc.uwm.edu/cgi/viewcontent.cgi?article=2458&context=etd

[9] http://www.webmet.com/met_monitoring/64.html

[10] Ashrafi, Kh., Hoshyaripour, Gh.A., A Model to Determine Atmospheric Stability and its Correlation with CO Concentration, World Academy of Science, Engineering and Technology International Journal of Environmental and Ecological Engineering, Vol. 2, No, 8, pp 96-101, 2008.

[11] https://www.bmuv.de/fileadmin/Daten_BMU/Download_PDF/Luft/taluft_engl.pdf

[12] Tița, M.C., Modelarea dispersiei atmosferice a poluanților, Universitatea din Craiova, Buletin AGIR, Supliment 2/2012, pp 70-75;

[13] Essa, K.S.M., El Saied, S.I.M., Maximum ground level concentration for Gaussian plume formula using standard and Briggs methods. Environmental Quality Management, 32 (4), 73–81, 2023

[14] Cîndea, L.A., Modelarea dispersiei poluanților gazoși cu SCREEN View, Simpozion științific studențesc HD-47-STUD, Hunedoara, 26-27 mai 2017.

[15] https://www.chemeurope.com/en/encyclopedia/Atmospheric_dispersion_modeling.html

[16] Lakes Environmental Software, SCREEN View, Screening air dispersion model (SCREEN3), User's Guide ©1995-2016.

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