

Simulation Effect of Stability Classes on SO₂ Concentration in Daura Refinery and Neighboring Regions

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Abstract

Sulfur dioxide (SO₂) is one of the most dangerous pollutants in the air. Most of the gas is emitted from industrial sources, mainly steam power plants, which account for more than 50% of it. Its consider toxic gas that cause irritating respiratory effects in this study the effect of air pollution around Durra refinery and its neighborhood. Where adopted in the study. the data of gaseous pollutants in the air (sulfur dioxide) were analyzed in the area south of Baghdad at January month that is have high frequent of stability condition . The data provided by the Ministry of Oil / Baghdad for 2017. In addition, the effect of air stability classes on the quantities of this pollutant. The results of the study showed that the in atmospheric stability class (F) concentrations of sulfur oxides is (54442mg/m³) at distance 100m and (5127 mg/m³) at distance 10000m were the highest in the region. Overall results show that the concentration rates reached relatively high values during the stable and very stable atmospheric stability and that the values for the month of January for sulfur dioxide were found to be high and are inversely proportional to the speed of the wind.

Keywords: Effect of stability, SO₂ concentration, Gaussian Plume Model.

الخلاصة

ثاني أكسيد الكبريت (SO₂) ، هو واحد من أخطر الملوثات في الهواء. ينبعث معظم الغاز من مصادر صناعية ، خاصة محطات توليد الطاقة البخارية ، التي تمثل أكثر من ٥٠٪ منها. اعتبر الغاز سام الذي يسبب تأثيرات تنفسية مزعجة. في هذه الدراسة تأثير تلوث الهواء حول مصفاة الدورة وجوارها. تم تحليل بيانات الملوث الغازية في الهواء (ثاني أكسيد الكبريت) في المنطقة الواقعة جنوب بغداد في شهر كانون الثاني / يناير. البيانات المقدمة من وزارة النفط / بغداد لعام ٢٠١٧. بالإضافة إلى تأثير فئات استقرار الهواء على كميات هذا الملوث. وأظهرت نتائج الدراسة أن تركيزات أكاسيد الكبريت في درجة حرارة الغلاف الجوي وصنف الاستقراريه مستقر بشكل كبير هي (54442mg/m³) على مسافة ١٠٠ متر و (5127 mg/m³) على مسافة ١٠٠٠٠ متر كانت الأعلى في المنطقة. تظهر النتائج الإجمالية أن معدلات التركيز وصلت إلى قيم عالية نسبياً خلال الاستقرار الجوي المستقر والثابت جداً وأن قيم شهر كانون الثاني (ثاني أكسيد الكبريت) كانت عالية وتناسب عكسياً مع سرعة الرياح.

Introduction

Air pollution is the exposure of the atmosphere to chemicals, physical particles or biological compounds, or is a chemical alteration of the natural composition of the atmosphere [1], which causes damage and harm to humans and other living organisms. Stability effect on the spread of pollutants it determines by the difference in temperature between a sample of air and its surroundings. This difference is caused by the vertical movement of the air sample (up or down). This movement has four basic conditions that describe the state of

stability in general. When the vertical motion is disabled, it is classified as a stable condition. Unstable Condition founded When the sample does not rise or fall, the adiabatic rate is cooled or heated and is under Neutral Condition. In Very stable conditions air near the surface is cold and warmer layer above and occur in the case of heat coupling the four cases have a direct effect on the concentration of contaminants in the ambient air [2]. The air moves in three directions (x, y, z), In the case of thermal coupling, the vertical motion is active so that the pollutants are transported by

vertical motion [3]. This consider the best conditions for the spread of contaminants [4]. It is known that SO₂ is a substance that is used to treat all mucous membranes in the human body that are exposed to contact, especially for people with respiratory problems and accelerate the development of chronic respiratory diseases [5]. In this study, we will discuss the effect of stable classes on the spread of sulfur dioxide, which is considered to be one of the main pollutant gases produced by fuel combustion in oil refineries and power generation units.

Location and Data

Durra Refinery is the main refinery of Midland Refineries Company in Iraq. It is located on the western side of the Tigris River and south of Baghdad, kilometers from the city center, which is flat ground. Dimensions of length 1620 m and width of 860m the urban area with a few palm trees is located around the refinery. A small liquid gas filling plant, and the Imam Hassan neighborhood is located on the east side, the university district in the west and south-west, the residence of employers near the borders of the refinery in the west. The highway and the highway are located on the east, south-east and south sides. Finally, on the northern side, a small flat area extends across the Tigris River, Figure 1. The Dura refinery operates 24 hours,

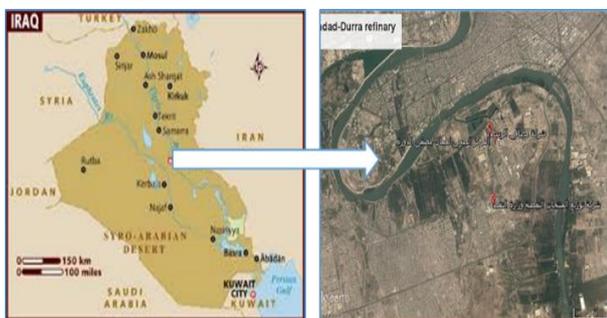


Figure 1: location of Durra refinery in Iraq.

a day and very large quantities of crude oil are refined to produce oil products [6]. However, it represents one of the biggest air pollution problems in Baghdad. The Dura refinery includes 30 plants represented in twelve units [7]. as shown in Table 1.

Table 1: The production units in Daura refinery which are used in present study; Symbols, Number of stacks.

Item	Name of operation unit	Symbols	Stack's
1	Crude Distillation	CDU_1	1
	unit_70000 barrel_1		
2	Crude Distillation	CDU_2	1
	unit_70000 barrel_2		
3	Catalytic Reformer_1	CR_1	4
4	Kerosene	KH	2
	Hydrogenation		
5	Catalytic Reformer_2	CR_2	5
6	Distillation of Crude oil	DCU_1_3	3
	units_1, and 3.		
7	Power unit_1	PU_1	4
	(Boiler_1,2,3,4,5,6,7,8)		
8	Power unit_3	PU_3	1
	(Boiler_11& 12)		
9	Lube oil_1	LO_1	3
10	Lube oil_2	LO_2	5
11	Lube oil_3	LO_3	5
12	Power unit_2	PU_2	1
	(Boiler_9& 10)		

In the current work, these units are considered as sources of 12 points since the distance between them is close to each other, and some units share the same group The fuel used in the refinery is the monthly fuel oil and fuel gas, Table 2 show the summed consumption fuel at year 2017.

Methodology

1. Atmospheric Stability Classes

There are several classes that refer to specified atmospheric stability condition such as [8]:

1- *Class A*: a state of instability with light winds, high vortex, adiabatic or adiabatic thermal decline, accompanied by looping shape of looping. Pollution concentration values are high in the vicinity of the chimney. This condition occurs during the day when the sky is clear and solar radiation Strong and even in the case of a few clouds.

2- *Class B*: a state of instability is relatively long if accompanied by light winds and air disturbance with a thermal gradient under the top of the chimney, the form of the cloud of smoke trapezoidal movement trapping and get this situation in the early morning with the possibility of touching the smoky clouds Earth.

Table 2: The Fuel Oil and Fuel gas used in production units in Daura refinery.

month	Type of fuel	month/m ³	hour in month	m ³ /hour	kg/hour
Jan.	Fuel Oil	46606.1	744	62.6426	60011.6
	Fuel gas	6417115	744	8625.15	9918.93
Feb.	Fuel Oil	23336	672	34.7262	33267.7
	Fuel gas	6874422	672	10229.8	11764.3
March	Fuel Oil	28198.7	744	37.9015	36309.6
	Fuel gas	9461812	744	12717.5	14625.1
April	Fuel Oil	27725.3	720	38.5074	36890.1
	Fuel gas	6989075	720	9707.05	11163.1
May	Fuel Oil	25728.7	744	34.5816	33129.2
	Fuel gas	1021576.5	744	1373.09	1579.05
June	Fuel Oil	29945.389	720	41.5908	39844
	Fuel gas	88777791	720	123302	141798
July	Fuel Oil	31436.1	744	42.2528	40478.2
	Fuel gas	9290553.9	744	12487.3	14360.4
Aug.	Fuel Oil	224199.7	744	301.344	288687
	Fuel gas	87240721	744	117259	134848
Sep.	Fuel Oil	28277.5	720	39.2743	37624.8
	Fuel gas	8511023	720	11820.9	13594
Oct.	Fuel Oil	26906.8	744	36.1651	34646.1
	Fuel gas	10417273	744	14001.7	16102
Nov.	Fuel Oil	29150.1	720	40.4863	38785.8
	Fuel gas	10644529	720	14784.1	17001.7
Dec.	Fuel Oil	28706.1	744	38.5835	36963
	Fuel gas	9898296	744	13304.2	15299.8

3- *Class C:* the case of the stability of a neutral air or lack of stability, mechanical disturbance and an arbitrary thermal decline, the cloud of smoke in the form of Cone movement is likely to touch the cloud of smoke Earth, and get this situation at night and day and in extreme wind conditions with concentration values Relatively few and relatively stable.

4- *Class D:* high stability situation and minor disturbance accompanied by a thermal coup with light winds and clear sky, the form of smoke cloud Fanning helicopter movement and get this situation in the early hours of the night and early morning, concentration values are high and far from the chimney, Smoke touches the earth.

5- *Class E:* This condition occurs when the chimney nozzle is located under the base of the thermal coup when changing from the state of the coup to the state of the adipatic or adipatic thermal regression, and moderate winds and the form of smoke cloud Fumigation and get this situation in the early morning.

6- *Class F:* shows with the transition from instability to the state of stability, which is the opposite of the smoking situation, and the thermal gradient adiabatic at the top of the chimney and the case of a coup under it, and the wind is light when the shape of the smoke fume Moved to the top Lofting and get this situation before sunset, If the chimney height is short, there may be concentration at the ground level. Figure 2 shows the class of stability.

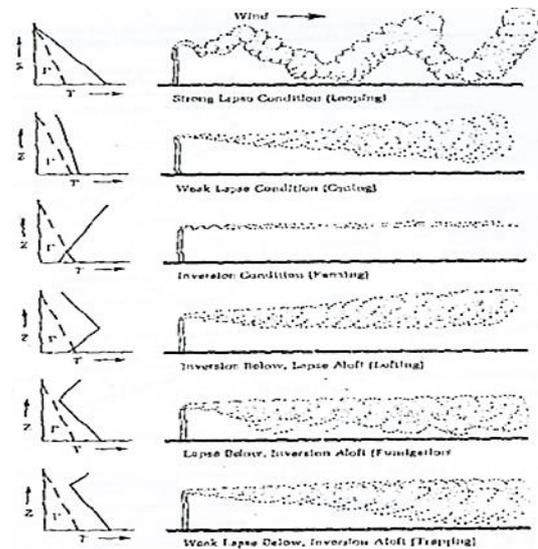


Figure 2: shown the plume in class's stability.

2. Gaussian Plume Model

The Gaussian model is one of the earliest models used to solve air pollution problems because the contaminants are similar in their propagation to the normal distribution near the Gaussian model. Figure 3 shows the Gaussian curve used to describe probability propagation. The curve width is defined by standard deviation, so the causal distribution of contaminants in the horizontal and y directions is given by the following relations [8]. The Gaussian model is one of the earliest models used to solve air pollution problems. Thus, the causal distribution of contaminants in the horizontal y and vertical directions is given by the following two relations [8].

$$G_y = \frac{1}{(2\pi)^{1/2}\sigma_y} \exp\left[-\frac{1}{2}\left(\frac{y}{\sigma_y}\right)^2\right] \quad (1)$$

$$G_z = \frac{1}{(2\pi)^{1/2}\sigma_z} \exp\left[-\frac{1}{2}\left(\frac{z}{\sigma_z}\right)^2\right] \quad (2)$$

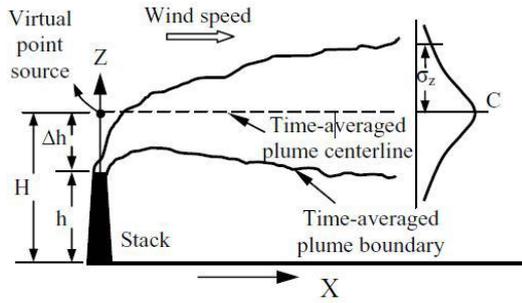


Figure 3: sketch of the plume dispersion.

G_y, G_z : is the calibrated Gaussian curve at the level (y-z).

σ_y = horizontal dispersion coefficient (standard deviation), m σ_z = vertical dispersion coefficient (standard deviation), m In this equation, the ground is usually assumed to be a perfect:

$$\sigma_y = a \times 0.894 \quad , \quad \sigma_z = c \times d + f$$

Constant a, b, c, f, d can obtain from Table 3 [9].

Table 3: Effect of stability classes on SO₂ dispersion.

stability	X ≤ 1 km					X ≥ 1 km		
	a	b	c	f	d	c	d	f
A	213	440.8	81.941	9.27	459.7	2.094	-9.6	
B	156	106.6	61.149	3.3	108.2	1.098	2	
C	104	61	0.911	0	61	0.911	0	
D	68	33.2	0.725	-1.7	44.5	0.516	-13	
E	50.5	22.8	0.678	-1.3	55.4	0.305	-34	
F	34	14.35	0.74	-0.35	62.6	0.18	-48.6	

The concentration of contaminants for smoke fumes can be calculated in the directions (x, y, z) of the following propagation equation [10].

$$C(x, y, z) = \frac{Q}{2\pi\sigma_y\sigma_zU} \exp\left[-\frac{1}{2}\left(\frac{y}{\sigma_y}\right)^2\right] \exp\left[-\frac{1}{2}\left(\frac{z}{\sigma_z}\right)^2\right] \quad (3)$$

and at the top of the chimney x = 0, at the central line of the smoke fume y = 0, and at the ground level z = 0 if the effective rise of chimney H, Since z is calculated from the ground level to the top so the propagation equation is as follows [11].

$$C(x, y, z) = \frac{Q}{2\pi\sigma_y\sigma_zU} \exp\left[-\frac{1}{2}\left(\frac{y}{\sigma_y}\right)^2\right] \exp\left[-\frac{1}{2}\left(\frac{z-H}{\sigma_z}\right)^2\right] \quad (4)$$

On the assumption that the mass is reserved, all the smoke clouds that are in contact with the earth are fully reflected in the atmosphere. Therefore, the second limit must be added to calculate the reflective smoke cloud [13], Shown in Figure 2.

$$C(x, y, z) = \frac{Q}{\pi\sigma_y\sigma_zU} \exp\left[-\frac{1}{2}\left(\frac{y}{\sigma_y}\right)^2\right] \left\{ \exp\left[-\frac{1}{2}\left(\frac{z-H}{\sigma_z}\right)^2\right] + \exp\left[-\frac{1}{2}\left(\frac{z+H}{\sigma_z}\right)^2\right] \right\} \quad (5)$$

Evolution of reflections of the ground level of smoke fumes [11]. For earth-level emissions, such as fires, explosions, and chimneys in industrial areas, equation becomes as follows [14]:

$$C(x, y, z) = \frac{Q}{\pi\sigma_y\sigma_zU} \exp\left[-\frac{1}{2}\left(\frac{y}{\sigma_y}\right)^2\right] \exp\left[-\frac{1}{2}\left(\frac{z}{\sigma_z}\right)^2\right] \quad (6)$$

Where C(x,y,z)= concentration at ground level at the point (x,y), μg/m³.

X= distance directly downwind, m

Y= horizontal distance from the plum center line, m

Z= vertical direction, m

Q= emission rate of pollutants, μg/s

H= effective stack height, m, (= h + Δh),

where h = actual stack height, and Δh=plume rise) = average wind speed at the effective height of the stack, m/s

3. Emission rate of SO₂

Emission rate of SO₂: The amount of fuel oil burned within one hour = 60011 kg.

The percentage of sulfur (S) in fuel oil = 3.8%.

The amount of sulfur in fuel oil = $\frac{60011 \text{ kg fuel oil} \times \text{SO}_2 \text{ kg}}{\text{fuel oil kg}} = 2280 \frac{\text{kg sulfur}}{\text{hour}}$

The number of Sulfurized Soles is equal to the number of S + O₂ → SO₂

The atomic weight of sulfur is 32 and the molecular weight of SO₂ is 64. Therefore,

Number of sulfur moles (S) = (2280.4 kg) / (32 kg / kg mol) = 71.26 kg of SO₂ produced Kg SO₂ = (64 kg SO₂ / kg m) × kg mol SO₂= 64 × (2280.4 / 32) = 4560.64kg / hr = (12668g / sec) SO₂ emission rate.

Results and Discussion

Calculate emission Rate

Through the equations that used, the emission ratios for the SO₂ gas emitted from the chimneys of the cycle refinery were calculated during a period of one year and the liquidator was considered one distribution point. The data

were transferred from the quantity of fuel per cubic meter / month to the quantity of fuel per ton / month and then divided by the number of hours per month to obtain quantity The fuel consumed in the refinery within one hour and then the quantity of fuel consumed within an hour was converted to emissions and as detailed in Table 4. From the table, the highest value of the SO₂ gas emission is in November and the lowest value of the gas emission is in April. It is noted that the high values of polluted emissions are in the winter and autumn and the low values in the spring and summer.

Dispersion coefficients

The horizontal and the vertical of the dispersion coefficient is estimated according to stability class. In Table 4, for the distance if it's greater than 1 kilo mater or less than one kilo mater .shown in Figure 3. A, Very unstable; B, moderately unstable; C, slightly unstable; D, neutral; E, slightly stable; F, stable. Regardless of wind speed, class D should be assumed for overcast conditions, day or night [15]. In order to use Eq. (5) in practical applications, it is required to know the dispersion coefficients σ_y and σ_z . These will be functions of downwind distance x and will also be unequal, since the characteristic turbulence velocities are

expected to be different in the horizontal and vertical directions.

Finally, they are expected to be depends on atmospheric conditions: for stable conditions, the r.m.s. velocities are very low and hence the dispersion coefficients small; for unstable conditions, the turbulence is vigorous and we expect much larger dispersion coefficients. The σ 's can be estimated at a given downwind distance from the following equations and hence Eq. (1) can be applied to give the mean pollutant:

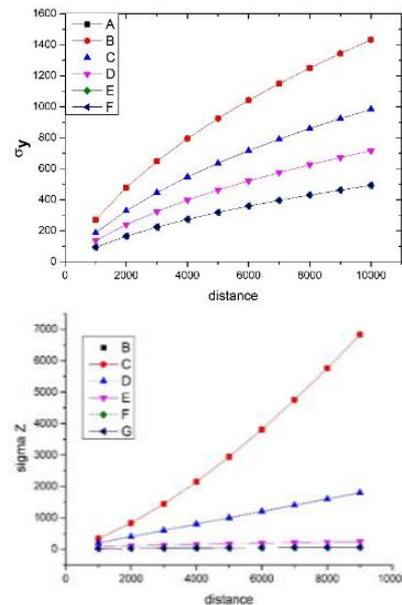


Figure 3: show the σ_y and σ_z .

Table 4: Details of the amount of sulfur dioxide emissions from the amount of fuel used in the refinery at all months 2017.

Item	month	fuel oil	h- month	fuel oil m ³ /h	fuel oil kg/h	fuel oil t/h	total mass out	mass s on fuel oil	SO ₂ kg/h	SO ₂ g/s
1	Jan.	46606.1	744	62.642608	60011.618	60.011618	1197231.8	2280.4	4560.883	1266.91
2	Feb.	233336	672	347.22619	332642.69	332.64269	6636221.7	12640	25280.844	7022.46
3	March	28198.7	744	37.901478	36309.616	36.309616	724376.85	1379.8	2759.5308	766.536
4	April	27725.3	720	38.507361	36890.052	36.890052	735956.54	1401.8	2803.6439	778.79
5	May	25728.7	744	34.581586	33129.159	33.129159	660926.73	1258.9	2517.8161	699.393
6	Jun	29945.4	720	41.590819	39844.005	39.844005	794887.9	1514.1	3028.1444	841.151
7	Jul	31436.1	744	42.252823	40478.204	40.478204	807540.17	1538.2	3076.3435	854.54
8	Aug.	224200	744	301.34368	288687.25	288.68725	5759310.6	10970	21940.231	6094.51
9	Sep.	28277.5	720	39.274306	37624.785	37.624785	750614.46	1429.7	2859.4836	794.301
10	Oct.	266907	744	358.7457	343678.38	343.67838	6856383.7	13060	26119.557	7255.43
11	Nov.	299150	720	415.48625	398035.83	398.03583	7940814.8	15125	30250.723	8402.98
12	Dec.	287706	744	386.70175	370460.27	370.46027	7390682.5	14077	28154.981	7820.83



Relationship between stability classes and SO₂ concentration

After emission rate and dispersion coefficient is calculated in the previous state, Gaussian model can be applied, where there is program software built in to estimated concentration of SO₂ the input of this program is taken in Table 5, stability classes is compared with concentration in each case, where every class is studied separately as:

Table 5: Constant parameters for model validation.

PARAMETER	Symbol	Value
Emission rate g/s	Q	1266.91 g/s
Height of the stack (m)	H	30
Exit velocity of the gas (m/s)		5
Diameter of the stack meters	D	2
Temperature of the exiting gas (C°)		200
Ambient temperature of the air (C°)		20
Atmospheric condition	stability	A;B;C;D;E;F
Wind velocities (m/s have 11 points)		1,3...21
Distances downwind (m)	x-distance	100, 1000, 2000, ..10000

Class A: This type of stability is highly unstable (A) Note that the concentrations of pollutants in the A class are very low (1-30 mg/m³) and are spread at a distance of 100-1000m towards the prevailing wind and at a speed of m / s and at a speed of 5 m / s with a concentration of 6 mg/m³. In the direction of the prevailing winds. Concentrations continue to decrease in the A class with increasing wind speed. This means that the concentration of pollutants is inversely proportional to the wind speed in the A class and is centered around the smoker's surroundings within 100 m.

Class B: In the stability category, Note that the concentrations of pollutants in the stability class B are very low (1 - 70 mg/m³) and are spread at a distance of 100-2000 m in the direction of prevailing winds and at the speed of m/s winds and at a speed of 5 m/s, the concentrations decrease significantly (14 mg/m³), in the direction of the prevailing winds. Concentrations continue to decrease in the stability class B with increasing wind speed. This means that the concentrations of

pollutants are inversely proportional to the wind speed in the B class and are centered around the smoker within 100 m towards the prevailing wind.

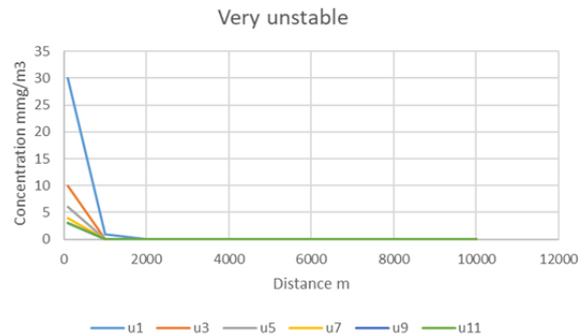


Figure 4: show the effect of stability class (A) prevailing wind.

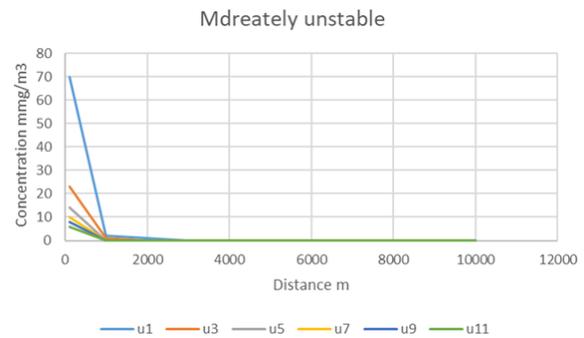


Figure 5: show the effect of stability class (B).

Class C: In the stability category, Note that the concentration of pollutants in the class C is (6-663 mg/m³) and is spread at a distance of 100-10000m towards the wind prevailing, at the speed of the wind 1 m / s, and at a speed of 5 m/s, the concentrations decrease 1-139 mg/m³), in the direction of prevailing winds. Concentrations continue to decrease in the C class with increasing wind speed. This means that concentrations of pollutants are inversely proportional to the wind speed in the C class and are diffused within 100-10000m towards the prevailing wind.

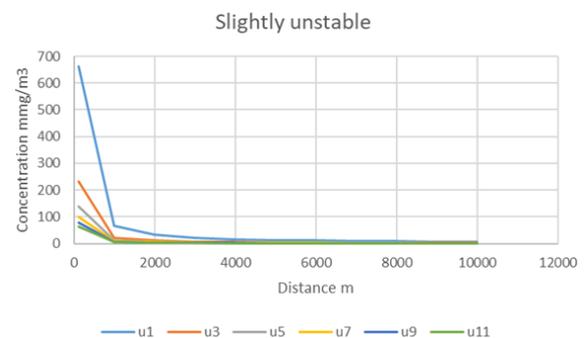


Figure 6: show the effect of stability class (C).

Class D: In the stability category In this form we observe a clear effect of the class D on concentrations of contaminants (1839-32 mg/m³) and spread at a distance of 100-10000 m towards the wind prevailing at the speed of wind m/s and at a speed of 5 m/s, the concentrations decrease 660-7 mg/m³) (308-3 mg/m³). This means that concentrations of pollutants are inversely proportional to the speed of the wind in the class of stability D and are spread within 100-10000 m towards the prevailing wind

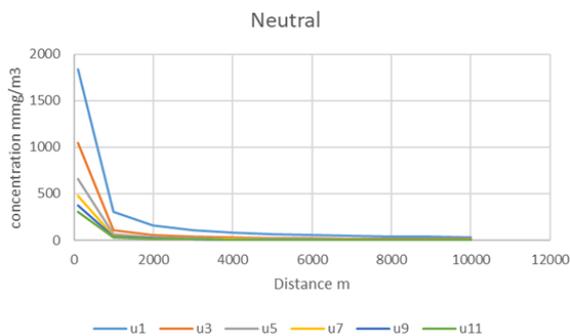


Figure 7: show the effect of stability class (D).

Class E: In this form, we observe a clear effect of the class E on concentrations of pollutants (21907-2033 mg/m³) and are spread at a distance of 100-10000 m towards the wind prevailing at the speed of the wind m/s and at a speed of 5 m/s, the concentrations decrease (4381-407 mg/m³) Within the range of -10000100 m in the direction of the prevailing winds and the concentration continues to decrease in the category of stability E with increasing the speed of the wind and become at a speed of 11 m/s (1992-182 mg/m³) This means that concentrations of pollutants inversely proportional to the speed of the wind in the category of stability E and diffuse I within 100-10000 m towards the prevailing wind.

Class F: In this figure we observe a clear effect of the concentration class F on concentrations of contaminants (54442-5127 mg/m³) and spread at a distance of 100-10000 m towards the wind prevailing at the speed of the wind m/s and at a speed of 5 m/s, the concentrations decrease 10888-1025 mg/m³) Within the range of -10000100 m in the direction of the

prevailing winds and the concentration continues to decrease in the class of stability F with increasing wind speed and become at a speed of 11 m/s (494-466 mg/m³) and this means that concentrations of pollutants inversely proportional to the speed of wind in the class F stability and diffuse Within 100-10000 m towards the prevailing wind.

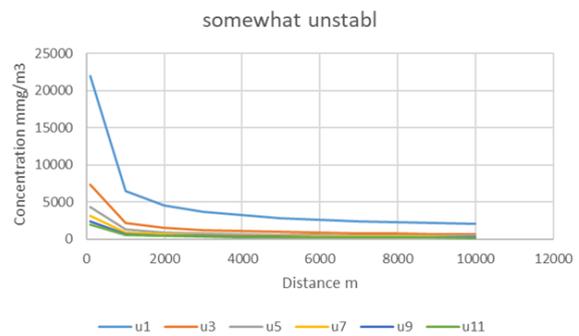


Figure 8: show the effect of stability class (E).

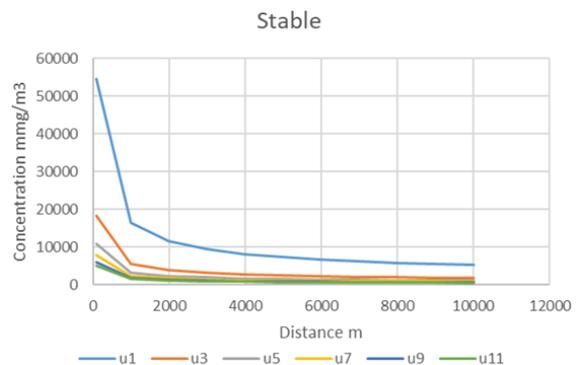


Figure 9: show the effect of stability class (F).

Conclusion

1. Increasing temperature reduces pollution. The high temperature of the surface of the earth during daylight hours and the proximity of air to near-ground air, leads to active upward air movements that work to spread the pollutants as horizontally as possible. In the night, due to the coldness of the surface of the earth and the near air. If the ascending vertical air currents lead to the control of the downward movement of the air and the air recession resulting from the concentration of air pollutants near the surface of the earth and the vertical spread in this case specific, which increases the density of pollutants near the surface of the earth This means that total control of the stable species

(D, E, F) will spread the pollutants over a wide range with prevailing wind direction.

2. Increase wind speed reduces pollution, wind speed plays a major role in influencing the spread of pollutants in the direction of wind blows from one place to another and the speed of the wind to reduce the concentration of pollutants directly as soon as starting from the source that the increase in wind speed leads to increasing distances between The concentration of the particles is therefore proportional to the speed, because the rapid movement acts on dispersing the contaminants. Thus, the diffusion inside the air mass will reduce the concentration of the pollutants and the wind speed has the added effect of controlling the turbulent mixing.

3. There is no clear effect of the direction of wind on pollution concentrations.

4. We observe very high concentrations of pollutant SO₂, which requires the authorities concerned to control sulfur emissions .We observed that atmospheric stability classes had a major effect on the spread of pollutants towards prevailing winds and were as follows:

5. In Class A stability where it is noted that the spread of pollutants is a little and concentrated in the first 100-1000m and the reason is that the speed of the little wind helps the rise of pollutants higher than the layer of the thermal coup Mambwe to rise to the highest layers of the atmosphere so Langhe at the ground level. In the class B, the same is the case in the A class with a slight difference due to the increase in the speed of the wind where the spread of pollutants extends to a distance of 2000 meters with the direction of the wind.

In the category of stability C noted the spread of pollutants in small amounts to a distance of 10000 m with the direction of the wind and the reason for this is the occurrence of smoke chimney near the layer of thermal coup.

7. In the classes of stability D, E, F spread pollutants along the direction of the wind and in large quantities, reaching the highest concentrations in the class stability F because of the high stability of the atmosphere and the occurrence of the top of the smoker under the mixing layer, reaching the ground level with high concentrations to a distance of 10000 m.

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