INTEGRATED SYSTEM FOR AIR POLLUTION AROUND REFINERIES

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ABSTRACT

A mathematical model for integrated air pollution modelling around refineries is built and named as Computerized System for Integrated Air Pollution Modelling Around Oil Refineries (CSIAPMAOR).The model based on Gaussian equation to estimate concentration of pollutants (SO_2, NO_2, CO, Particulates) that are emitted from a continuous air pollution elevated source. The model is designed by using Visual Basic as a main core of the system and linked with auxiliary models such as ArcMap (GIS), Surfer software, Ms-Excel and Ms-Access. The model has flexibility to select either rural, urban or stability (Smith equation) wind speed profile. It also has the option of using three types of dispersion coefficients equations for rural condition (PGT-Briggs-Martin equation) and one equation for urban condition (Briggs equation).The model has many options to display results as concentrations versus center line-downwind distance or as Three-Dimensional (3D) map. The model can compute maximum concentration with the contribution of each stack to the overall maximum concentration. Moreover the model has the ability to perform a sensitivity analysis for the effect of the most important parameters according to the Gaussian equation. AL-Doura Oil Refinery was taken as a case study using the available observed data of two sites1 and 2 for periods 15^{th} -21^{st} and 23^{rd} -29^{th} August 1997 in order to check the performance potential of the model. Results showed that Briggs equation for dispersion coefficients with rural wind speed profile has the best degree of agreement with the observed values of 0.86, 0.90 for SO_2; 0.69, 0.80 for NO_2; 0.73, 0.79 for CO; 0.63, 0.60 for particulates at site 1 and 2 respectively. It is found, that for AL-Doura Oil Refinery stacks number 6, 2, 7, and 3 have a large contribution on the overall maximum concentration. The model demonstrates the influence of atmospheric stability, wind speed, emission rate, exit velocity, physical height, exit temperature and rural-urban area in reducing the concentrations of pollutants. Sensitivity analysis shows that the concentrations are sensitive to stability class in comparison with other input parameters.

الخلاصة:

في هذا البحث تم بناء نظام مبرمج في الحاسوب لنمذجة متكاملة لتلوث الهواء حول المصافي وسمي ب CSIAPMAOR. النموذج مبني اساسا" على معادله گاوس لتخمين ملوثات الهواء مثل ثنائي اوكسيد الكبريت وثنائي اوكسيد النتروجين واول اوكسيد الكاربون والدقائق العالقه المنبعثة من مصادر تلوث الهواء المستمر . النموذج تم تطويرة باستخدام برنامج Visual Basic كلغة برمجيه اساسيه للنظام مع ربط النظام ببرامج مساعدة وهي: اولا" برنامج ArcMap(GIS) تم استخدامه لاعطاء احداثيات حقيقية للخارطة الاساسية مع رسم طبقات كنتورية ذات ثلاثة ابعاد TINs. ثانيا" برنامج Surfer وذلك لرسم خرائط كنتورية لتحليل الحساسية . ثالثا" برنامج Ms Excel وبرنامج Ms Access وذلك لخزن كل مدخلات و نتائج البرنامج. . النموذج ذو قابلية لاختياروا حدة من ثلاث حالات لحساب تغاير سرعة الرياح في المناطق الحضرية او الريفية او بالاعتماد على الاستقرارية (معادله سمث). النموذج ايضا" له القابلية لاختيار واحدة من ثلاث معادلات للمناطق الريفية. والمعادلات هي (PGT – Briggs –

Martin equation) و معادله واحدة للمناطق الحضرية (Briggs) لحساب معاملات التشتت . بالاضافة الى امكانية النموذج لعرض نتائج تغير التراكيز مع خط منتصف الدخان المنبعث أو بشكل خارطة ثلاثية الابعاد. بالاضافة الى امكانية النموذج في حساب التركيز الاقصى للملوثات مع تحديد مساهمة كل مصدر من مصادر التلوث في قيمة هذا التركيز كما أن له امكانيه استخدام تحليل الحساسيه لتبيان تأثير تغير المعاملات المهمة على معادلة گاوس. البرنامج يتناول مصفى الدورة كموضوع دراسة باستخدام البيانات المتوفرة التي تمت ملاحظتها لموقعين عند جنوب شرق المصفى للفترتين (15-21) و(23- 29) من اب للعام 1997 . أستخدمت هذة البيانات للتحقق من كفاءة اداء البرنامج .النتائج المستحصلة من استخدام معادلة Briggs لمعاملات التشتت مع مؤشرات سرعة الرياح في المناطق الريفية أعطت توافقية عالية مع القيم المقاسة. وقيم معامل التوافق البالغة 0.86 و 0.90 لثنائي اوكسيد الكبريت و 0.69 ، 0.80 لثنائي اوكسيد النترجين و0.73 ، 0.79 لأول اوكسيد الكربون و 0.63 ، 0.60 للدقائق العالقة في الموقعين 1 و 2 على التوالي . وايضا" وجد من خلال تحليل المساهمة بأن ثنائي اوكسيد الكبريت له التركيز الاقصى في الساعة للفترات آنفة الذكر و بذلك يفوق المعايير المسموح بها في العراق لكلا الموقعين. مداخن مصفى الدورة رقم 6 و2 و7 و3 كانت لها مساهمة كبيرة في تكوين التراكيز القصوى. و تم استعرض تأثير كل من استقرارية الجو و سرعة الرياح و معدل و سرعة الانبعاث و ارتفاع المداخن و حرارة الانبعاث و تأثير المناطق الحضرية و الريفية في تخفيض تراكيز الملوثات المنبعثه.

KEYWORDS
Air Pollution, Gaussian Model, GIS and Environmental Modeling, Designed Model

INTRODUCTION

Urban air pollution due to activities of the process petroleum refinery industries is one of the main problems faced by the industrial area worldwide. Many experimental analyses were carried out to determine the extent of air pollution due to the petroleum refinery industry, focusing on the concentrations of NO_2, CO, SO_2 [Abdulkareem, 2005].

The development of an air pollution model for multi-sources is no doubt useful. Integrated models using available nowadays softwares will be useful in many ways. These models can be used to predict different pollutants levels spread over the nearby area, due to different properties of multipoint sources. The integrated model can allow the variation of sources properties, such as emission rate, exit velocity, etc. Integrated models are those models that use different softwares linked in a proper way to transfer data between these softwares to achieve certain tasks. Integrated models are rather rare or expensive, while each of the softwares contributing in the developed model is available and free. For example, Visual Basic, Ms Excel, Ms Access, ArcMap (GIS), are available softwares nowadays, whereas a specialized integrated model for air pollution modelling is not freely available. Hence the development of such model is essential. The main challenge in building an integrated model for a special purpose is the proper linkage between the available softwares, i.e. the way to transfer data between these softwares.

GAUSSIAN MODEL

The Gaussian model is perhaps the oldest (Circa 1936) [Bosanquet, 1936 as cited in Wikipedia, 2008] and is the most commonly used dispersion model to estimate the concentration of a pollutant because of its simplicity [Awasthi et al., 2006]. It assumes that the air pollutant dispersion has a Gaussian distribution, meaning that the pollutant distribution has a normal probability distribution. The primary algorithm used in Gaussian model is the Generalized Dispersion Equation for a Continuous Point-Source Plume [Beychok, Milton, 2005 as cited in Wikipedia, 2008].

GIS AND ENVIRONMENTAL MODELING

Geographical Information System (GIS) is a computer based information system that enables capturing, modelling, manipulation, retrieval, analysis, and presentation of geographically referenced data [Aronoff, 1991 as cited by Rahmatizadeha et al., 2002]. The basic advantage of this science and technology is its ability to manage and integrate with the present database and for spatial analysis such as (overlay, buffering and zoning) which provides an environmental alarming system [Rahmatizadeha et al., 2002]. By doing air quality modelling in a GIS environment, the output of the pollutant records can be obtained as spatial records in the form of map layers, which can visualize real objects by vector and raster data formats together with graphs and multimedia presentations [Matejicek et al., 2002].

THE COMPUTERIZED SYSTEM FOR INTEGRATED AIR POLLUTION MODELLING AROUND OIL REFINERIES (CSIAPMAOR):

The designed model provides options to model point source emissions from stacks present at industrial areas. The basic equation governing the phenomena is the straight-line, steady-state Gaussian plume equation for a continuous air pollution elevated source [Kiely, 1997]:

$$C(x,y,z,H_e)=\frac{Q}{2\pi\sigma_y\sigma_z U}\exp\left[-\frac{1}{2}\left(\frac{y}{\sigma_y}\right)^2\right]\left\{\begin{array}{l}\exp\left[-\frac{1}{2}\left(\frac{z-H_e}{\sigma_Z}\right)^2\right]\\+\exp\left[-\frac{1}{2}\left(\frac{z+H_e}{\sigma_Z}\right)^2\right]\end{array}\right\} \qquad (1)$$

Where: C (x, y, z) is the concentration of pollutant (g/m^3) at a receptor located at (x, y, z), x is downwind distance from the source point (m), y is crosswind distance from the plume centreline (m), z is height above ground level (m), Q is pollutant emission rate (g/s), U is mean wind speed at release height (m/s), H_e is the effective height of release of the point source (m), σy and σz are horizontal and vertical standard deviations of the emission distribution (m).

Softwares Used in the CSIAPMAOR Model

The **CSIAPMAOR** program was designed using Visual Basic (version 6.0) as the basic programming language and as a control tool for integrating the system with auxiliary models. These auxiliary softwares are Ms Access, Ms Excel for storing output results, ArcMap (GIS) (version 8.1) for Georeference of the base map, in addition for drawing TINs layers to show the spatial variation in the contaminant levels over the area under study, Surfer (version 7.0) for drawing contour maps of the sensitivity analysis.

Features and Capabilities of the Designed Model

- The model can be used to predict short-term concentrations (for periods of 24 hours or less) for pollutants SO_2, NO_2, CO and Particulates resulted from a point source or from multisources, instantaneously.
- The model offers three options for computing wind speed profile: rural, urban, and stability (Smith equation) wind speed profile.
- The model offers flexibility to select either rural or urban dispersion parameters, depending on the characteristics of the source location. Three options for rural dispersion coefficients: PGT, Briggs, and Martin equation, and just one option for urban condition (Briggs equation), are available.
- The model can estimate maximum hourly concentration, in addition to the location of the receptor and the hour at which it happens.
- The model can perform contribution analysis for each point source to the overall maximum concentration.
- The model has an option of drawing hourly concentration for continuous emitting from multisources as 3D TINs layer or as a contour map to show the influence of the different concentration levels extended over a base map of the area around these sources.

- The model has option for displaying hourly concentration emitting from each stack with center-line downwind distance by a bar chart.
- The model can determine the required calibration factor between the model results and a set of measured values.
- The model provides tabular printed outputs with many options
- The model has option to test sensitivity of the Gaussian model to the variation in its parameters by four options for stability class, wind speed, stack properties (exit velocity, exit temperature, physical height, emission rate) and rural versus urban area.

The model built here, has the following limitations:

- Estimate pollutants emitted from elevated point source.
- Valued for non-reactive pollutant only.
- The effect of momentum force in plume rise is neglected and only buoyancy force is considered.
- Particulates are limited for spherical shape only.
- All pollutants are totally reflected.

APPLICATION OF THE DESIGNED MODEL: CASE STUDY AL-DOURA OIL REFINERY

The model has been used first for a Cartesian receptor grid with 25 meters for a small area of (1700m × 1700m) with origin point (0 E, 0 N) in the lower left corner of the area. The (UTM) coordinates of this point are (446100.73 E, 3680688.62 N) as shown in Figure (1). This area covers all stacks of AL-Doura Oil Refinery in addition to the two sites (receptors) where measured data are available for the designed model validation; dense grid is used because these receptors are very close to AL-Doura Oil Refinery. The model is then used for a Cartesian receptor grid with 100 meters for a large area of (14000m × 11000m) as shown in Figure (1) to cover all the area surrounding the refinery in the eastern south direction. The origin point (0 E, 0 N) of this area with corresponding UTM coordinates are (443382.21 E, 3672874.80 N). The second application of the model to such an area is used to show the impact of the refinery on the large adjacent areas using contour maps which clarify the maximum concentrations and the contribution of each stack on this maximum concentration.

The model is applied using two cases, the first case with stability wind speed profile (Smith equation) using three equations for calculating the dispersion coefficients of the rural area (PGT equation, Briggs equation and Martin equation), the second case with rural wind speed profile using the same equations for the dispersion coefficients to select which case will be suitable to represent the case study.

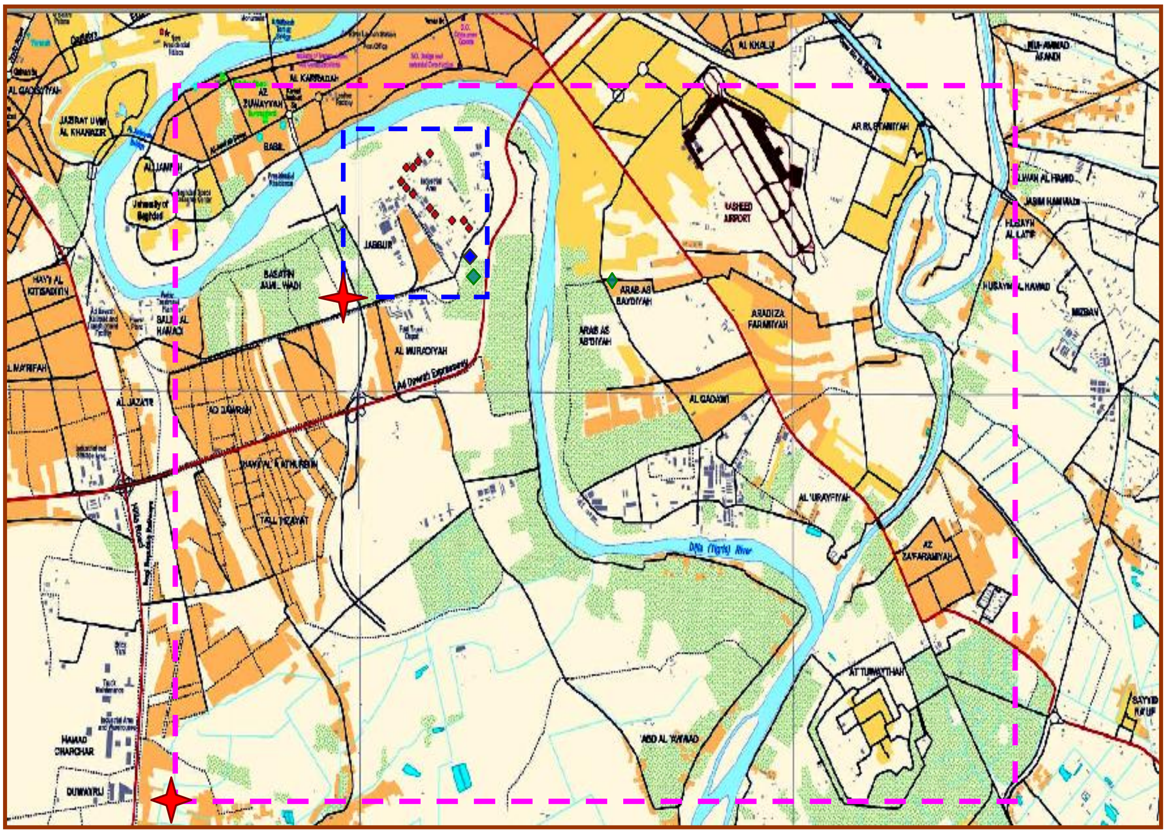
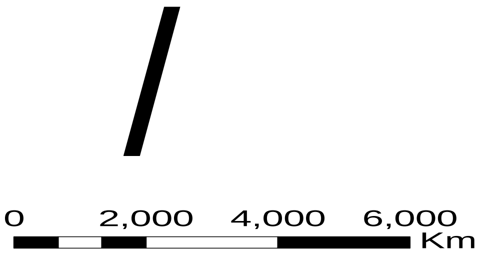
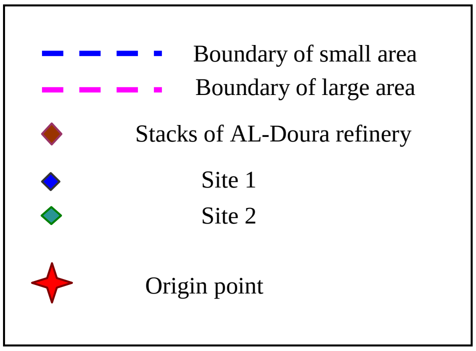


Fig (1) Boundaries of the Small and Large Area for Which the Model was Applied





Comparison of the Model Results with the Measured Concentrations

The results obtained from the model application have been compared to the observations of the hourly concentrations measured at sites 1, and 2 for periods from (15^{th} to 21^{st} August 1997 at site 1) and (23^{rd} to 29^{th} August 1997 at site 2) as measured by AL-Rubai (1998).

Index of Agreement (IOA)

$$IOA = 1 - \frac{\sum_{i=1}^{N} (p_i - O_i)^2}{\sum_{i=1}^{N} \left(|P_i - O_{mean}| + |O_i - O_{mean}| \right)^2} \quad (2)$$

IOA is a measure of the degree to which the observed values have been accurately estimated by the model. IOA is sensitive towards differences between observed and predicted values as well as to certain changes in proportionality, and represent more consistent measure of the performance. IOA = 0 indicates no agreement, IOA = 1 indicates perfect agreement [Willmott, 1981 as cited in Awasthi et al., 2006 and Luhar et al., 2004].

Table (1) Index of Agreement (IOA) for Sites 1, and 2, Near AL – Doura Oil Refinery

Wind speed profile	Dispersion coefficients	No. of Site	Index Of Agreement (IOA)			
			SO_2	NO_2	CO	Particulates
Stability profile (Simth equation)	PGT equation	Site 1	0.84	0.66	0.68	0.61
		Site 2	0.88	0.75	0.74	0.56
	Briggs equation	Site 1	0.87	0.69	0.72	0.64
		Site 2	0.89	0.78	0.75	0.58
	Martin equation	Site 1	0.84	0.66	0.68	0.61
		Site 2	0.88	0.75	0.74	0.56
Rural profile	P-G-T equation	Site 1	0.84	0.66	0.69	0.55
		Site 2	0.88	0.76	0.76	0.57
	Briggs equation	Site 1	0.86	0.69	0.73	0.63
		Site 2	0.90	0.80	0.79	0.60
	Martin equation	Site 1	0.85	0.69	0.69	0.57
		Site 2	0.88	0.76	0.77	0.57

Source Contribution Analysis

Contribution analysis represents the contribution of a particular source to the overall concentration in a certain location (receptor point). Recognizing the source contribution information is important to many short term modelling analyses. For the designed model, contribution of each point source (stack) of the AL-Doura oil refinery to the overall maximum concentration for each pollutant are found by applying the model for the large area (14000 m × 11000 m). The designed model uses Briggs equation for dispersion coefficients in the rural area with rural wind speed profile and meteorological data reported at (15^{th}-21^{st} August 1997) and (23^{rd}-29^{th} August 1997) from AL-Rubai, 1998, with a receptor height 1.5 m. The model finds the maximum concentration within the specified period by the user.

Table (2) Maximum Hourly Concentration of the Pollutants Emitted from Multisources of AL-Doura Oil Refinery in August, 1997

day	Max. hourly concentration for SO_2 (ppm)	Max. hourly concentration for NO_2 (ppm)	Max. hourly concentration for CO (ppm)	Max. hourly concentration for Particulate (μg/ m^3) with background con.
15	0.454	0.076	1.379	45.617
16	0.474	0.089	1.751	47.682
17	0.446	0.073	1.243	45.603
18	0.474	0.079	1.391	46.319

19	0.489	0.088	1.842	47.944
20	0.473	0.076	1.589	46.312
21	0.449	0.082	1.495	46.129
23	0.482	0.083	1.586	47.479
24	0.404	0.071	1.397	44.058
25	0.433	0.073	1.375	45.084
26	0.462	0.077	1.365	46.540
27	0.474	0.085	1.556	46.953
28	0.459	0.086	1.672	46.897
29	0.481	0.085	1.627	47.924

Table (2) indicates that the maximum hourly concentration of the most pollutants had occurred in 19th August 1997. Maximum hourly concentration for SO_2 has occurred at the hour 15:00 pm, and for NO_2 has occurred at the hour 19:00 pm, and for CO has occurred at the hour 18:00 pm, and for Particulates has occurred at the hour 15:00 pm. These maximum values have resulted for the following case: meteorological data, stability class (C), north-west wind direction, and wind speed vary from (2-4) m/s.

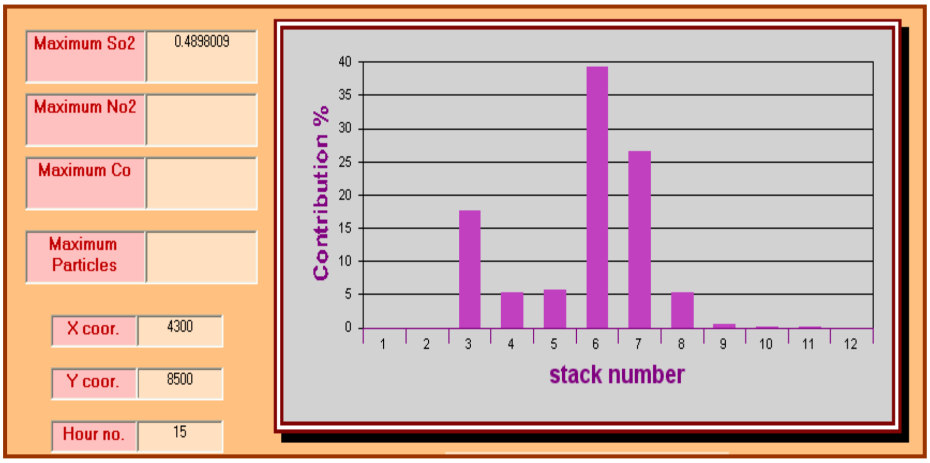


Figure (2) Contribution Analysis for SO_2 in the 19th August 1997 at a Site with Coordinates (4300, 8500) from the Origin Point

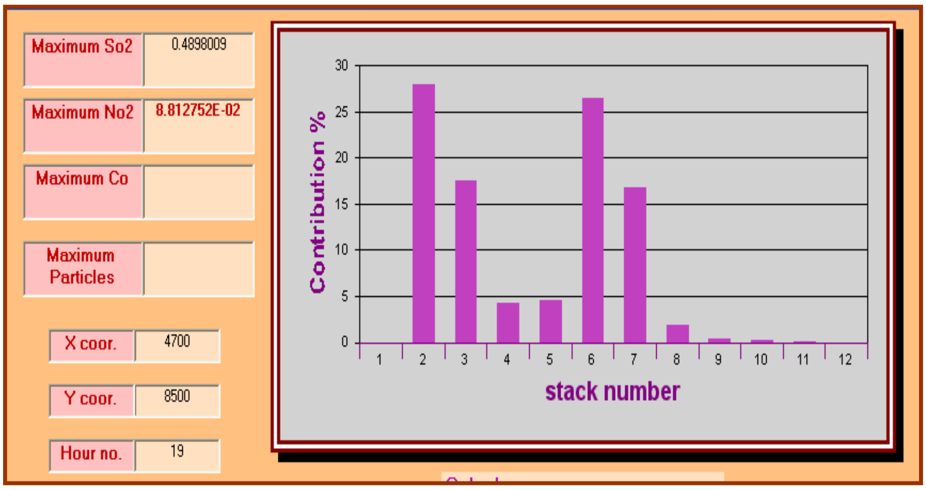


Figure (3) Contribution Analysis for NO_2 in the 19th August 1997 at a Site with Coordinates (4700, 8500) from the Origin Point

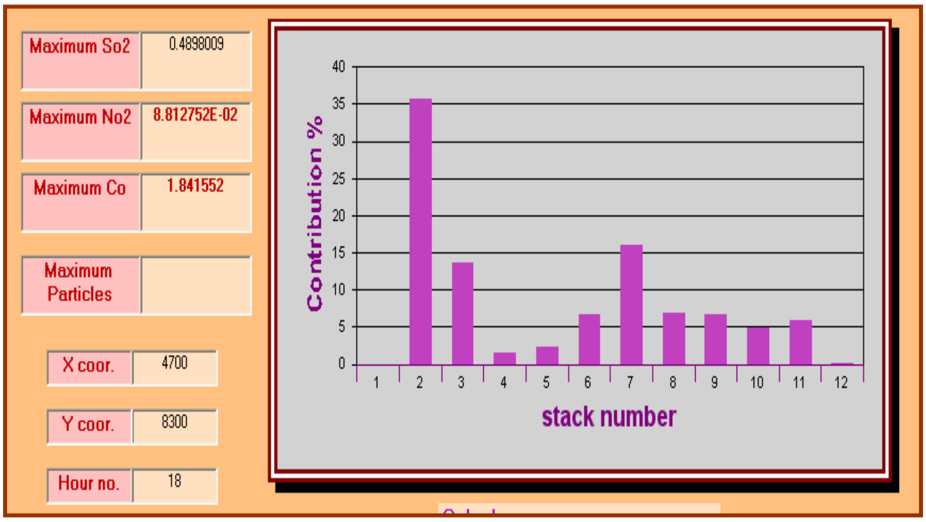


Figure (4) Contribution Analysis for CO in the 19th August 1997 at a Site with Coordinates (4700, 8300) from the Origin Point

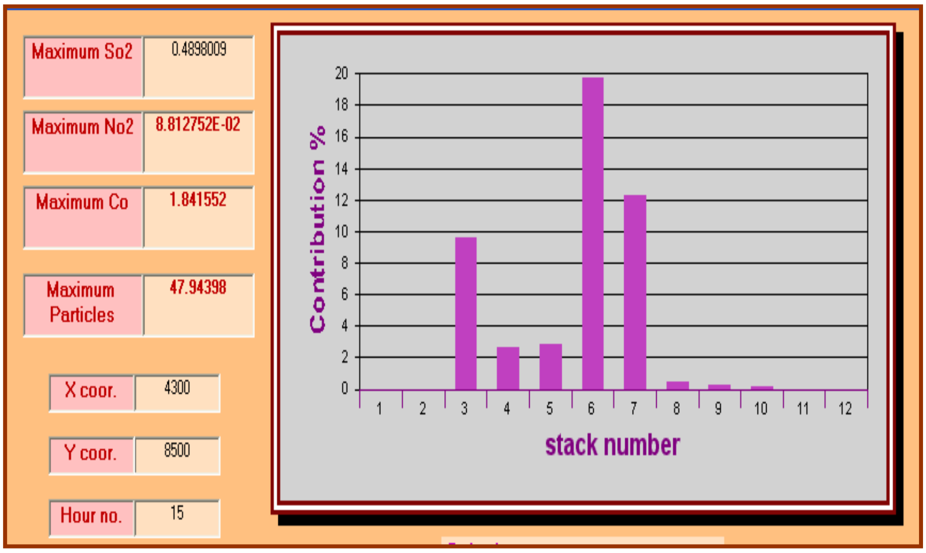


Figure (5) Contribution Analysis for Particulates with Background Concentration

in the 19th August 1997 at a Site with Coordinates (4300, 8500) from the Origin Point

TINs layer of the hourly concentrations resulted from the multisources in 19th August 1997 illustrating resulted different concentrations levels extended through the eastern south area (mostly agricultures) surrounding AL-Doura oil refinery.

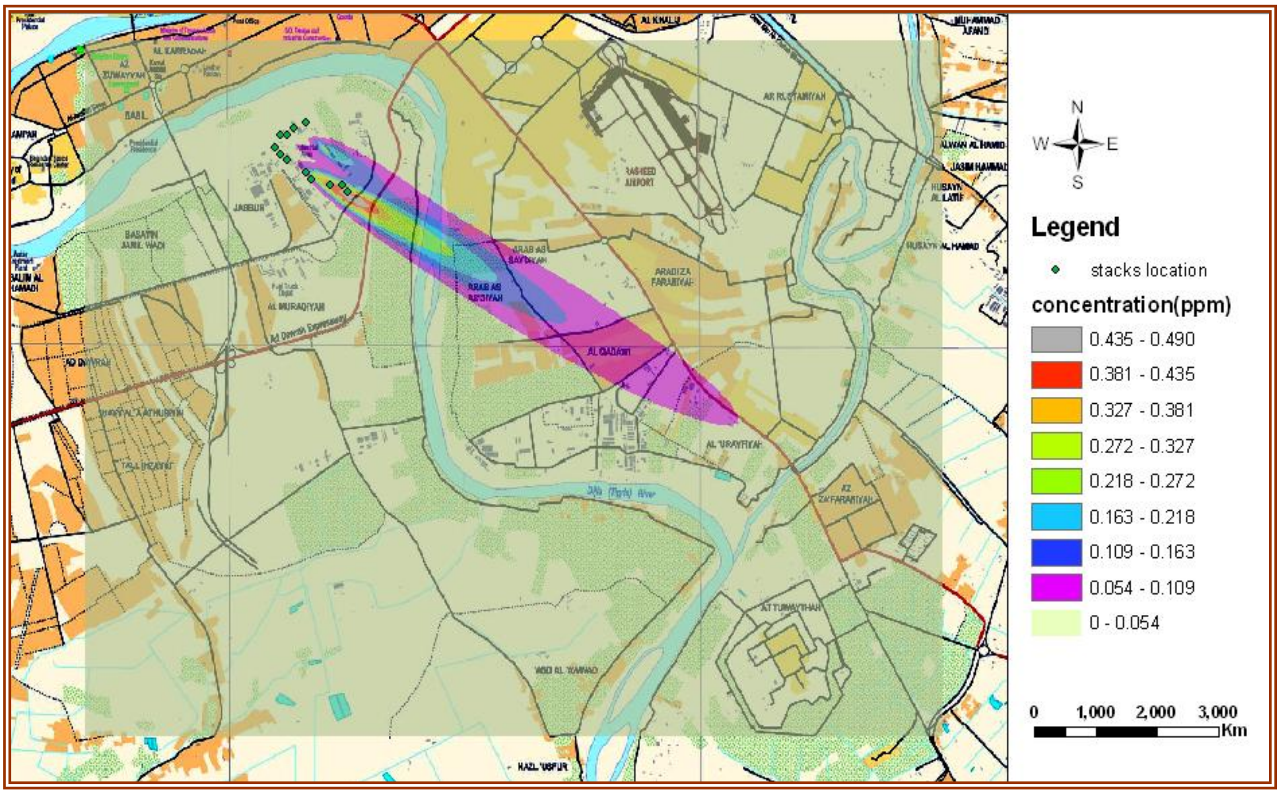


Figure (6) Contour Map for SO_2 Concentration Levels, Resulting from Stacks of AL-Doura Refinery in 19th August 1997 at 15:00 pm

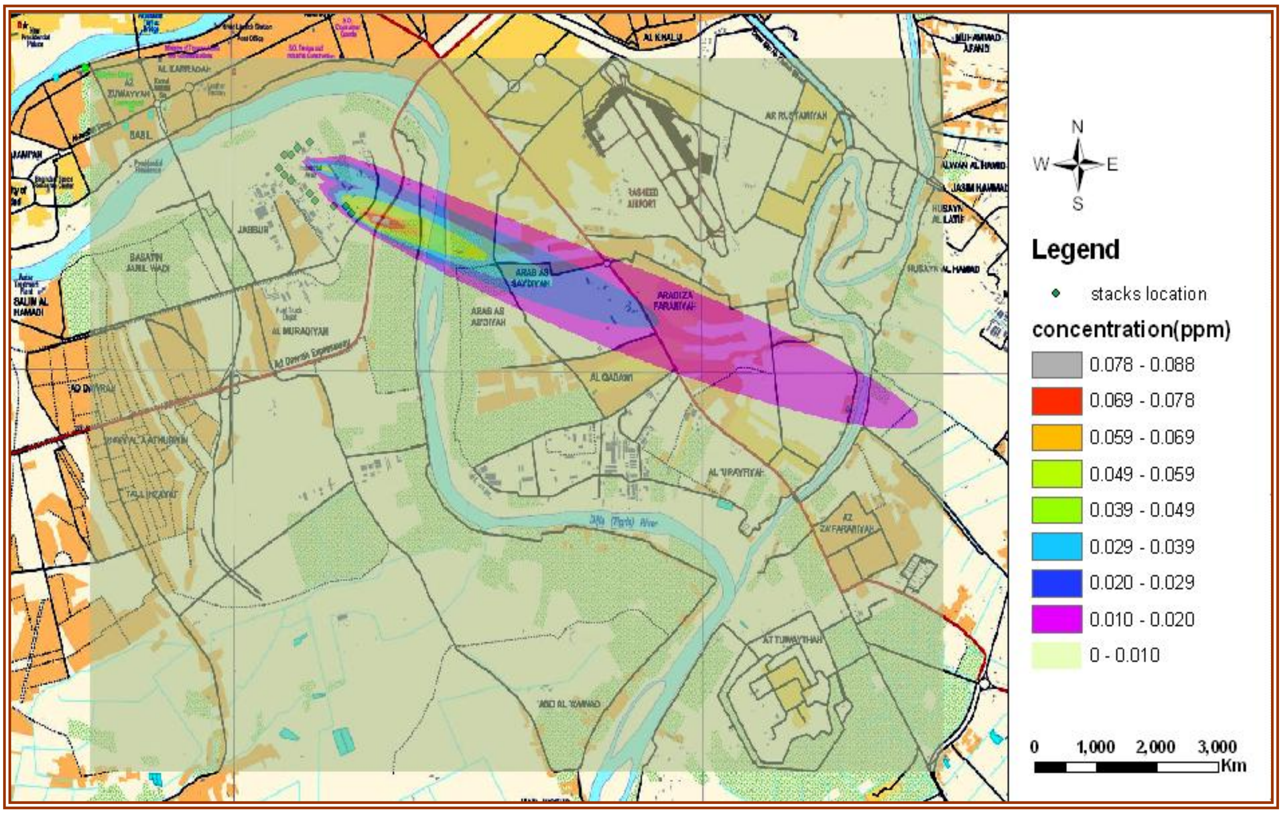


Figure (7) Contour Map for NO_2 Concentration Levels, Resulting from Stacks of AL-Doura Refinery in 19thAugust 1997at 19:00 pm

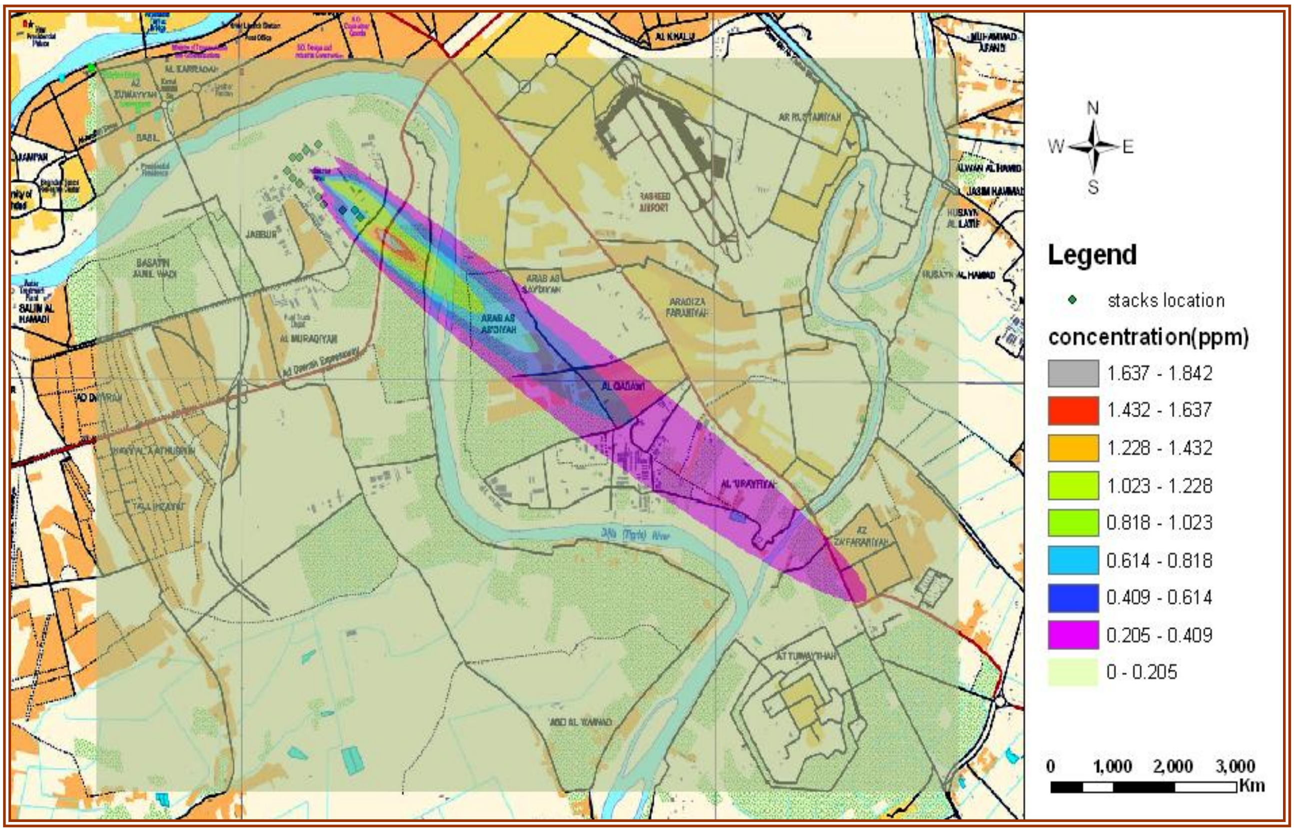


Figure (8) Contour Map for CO Concentration Levels, Resulting from Stacks of AL-Doura Oil Refinery in 19th August 1997 at 18:00 pm

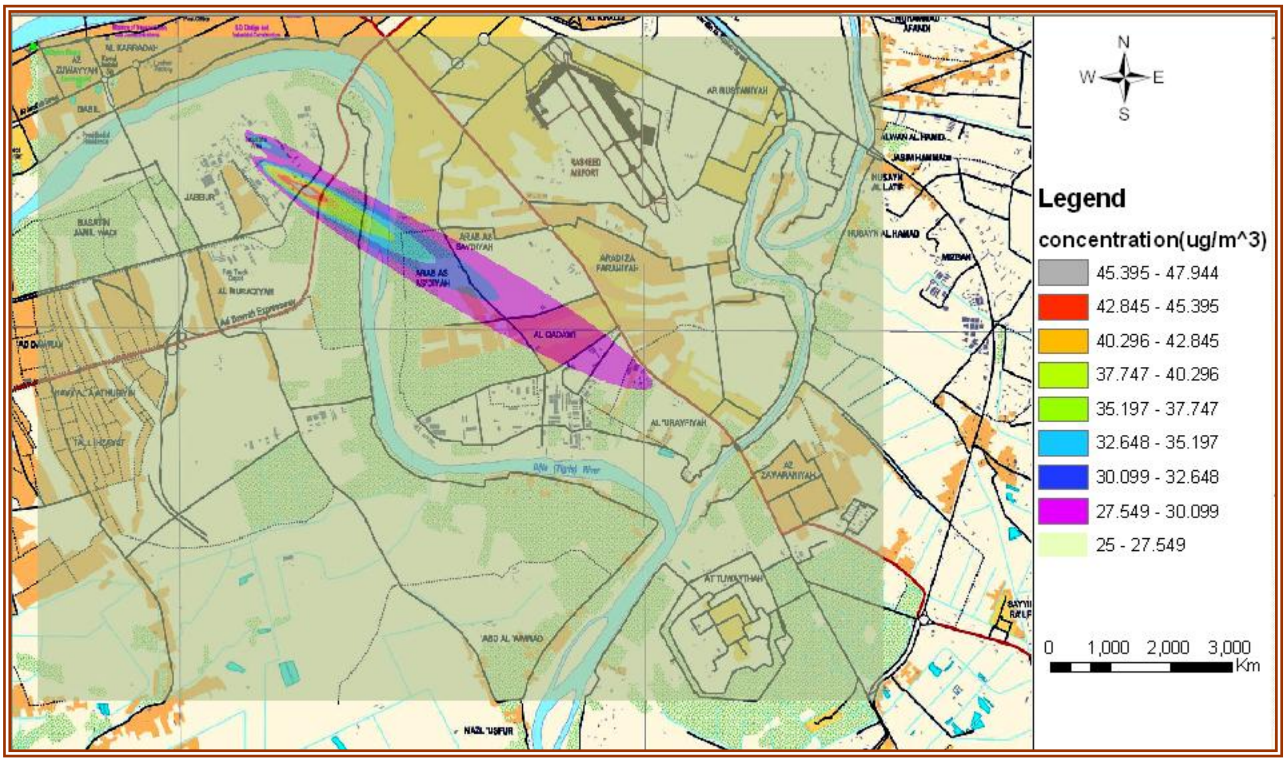


Figure (9) Contour Map for Particulates Concentration Levels with Background Concentration, Resulting from Stacks of AL-Doura Refinery in 19/8/1997at 15:00 pm

* SENSITIVITY ANALYSIS

A sensitivity analysis is the process of establishing the effect of changing the value of an input variable on the model output [Carbon, 2004]. This analysis is performed using the designed model in order to find the effect of different parameters on the dispersion of the pollutants.

The Base Case

The input data of the options of Sensitivity Analysis are selected depending on the results of the contribution analysis. This analysis indicates that, stack number 6 of the AL-Doura oil refinery is responsible for the largest contribution to the maximum hourly concentrations for SO_2, NO_2, CO and Particulates. Meteorological data which cause the maximum hourly concentration for SO_2 (higher concentration than allowable) at 19th August 1997 at hour 15:00 pm is selected for sensitivity analysis.

Sensitivity Analysis for Stability Classes

The effect of atmospheric stability on the hourly concentrations with low wind speed is shown in Figure (10).

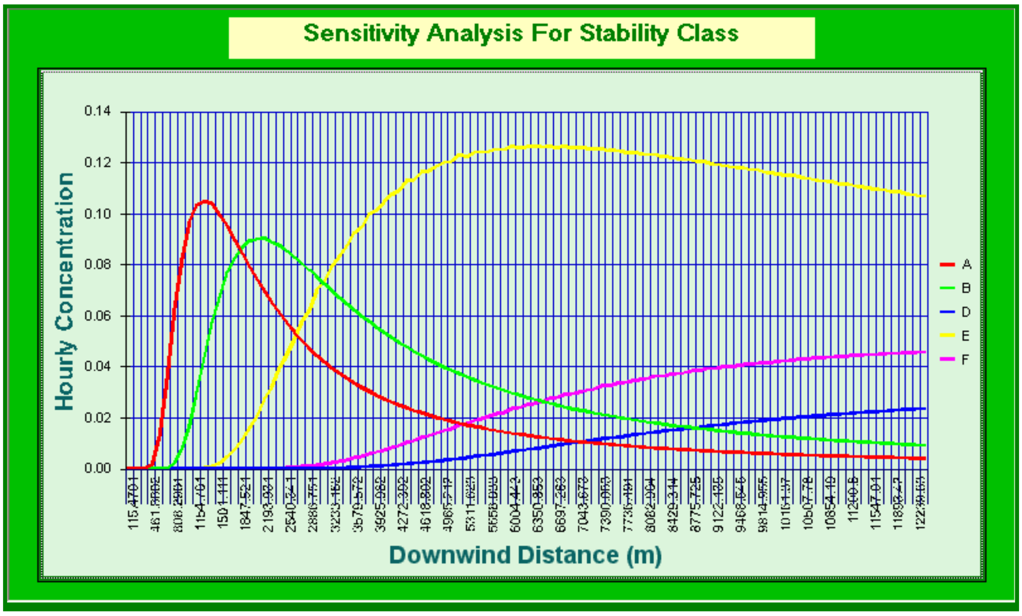


Figure (10) Sensitivity Analysis of SO_2 with Stability Classes Variation

This figure indicate that, the worst weather case condition for dispersion of pollutants with low wind speed is a winter day or an overcast night that is characterized by a slightly stable atmosphere (class E) with distance far away from the source. The other critical weather condition is sunny day (class A) with distance near from the source. Class E with wind speed equal to 0.89 m/s is considered as a critical weather case and will be named such hereafter.

Sensitivity Analysis for Wind Speed

Different values of wind speed are selected to show the influence of the wind speed with low turbulence in reducing the maximum concentration for critical weather (class E, 0.89 m/s) which represents the base case.

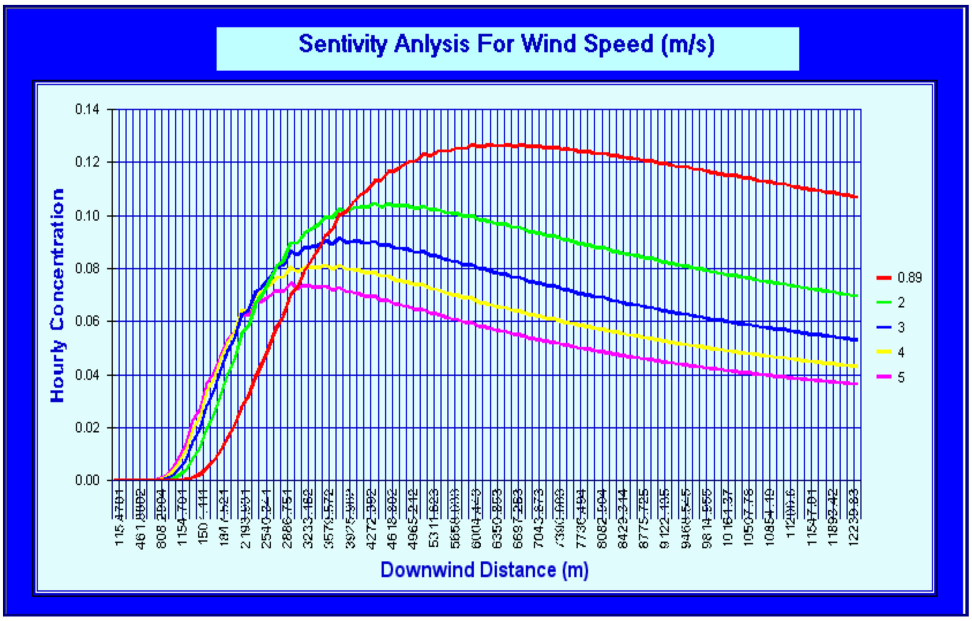


Figure (11) Sensitivity Analysis of SO_2 with Wind Speed Variation

The effects of wind speed work in two opposite directions are:
- Increasing wind speed will decrease plume rise, thus increases ground level concentrations; which are observed near from the source.
- increasing wind speed will increase mixing, thus decreasing ground level concentration ,this case is observed far away from the source.

<u>Sensitivity Analysis for Stack Properties</u>

The important parameters for the stacks represent (exit velocity (Vs), exit temperature (Ts), physical height (Hs), and emission rate (Qs)) are selected. The sensitivity analysis is done by varying one of these properties at each run in order to examine its influence of each one in reducing the concentrations of pollutants. Three cases are selected for each parameter:
- Case 1 (influence of exit velocity on the hourly concentration)
Three cases are selected, Vs1=7.4 m/s which represents the base case (stack 6), Vs2= 11.1 m/s (1.5 Vs1) and Vs3 =14.8 m/s (2 Vs1).
- Case 2 (influence of exit temperature on the hourly concentration)
Three cases are selected, Ts1 =603 k which represents the base case (stack 6), Ts1= 904.5 k (1.5 Ts1) and Ts3 =1206 k (2 Ts1).
- Case 3 (influence of physical height on the hourly concentration)
Three cases are selected, Hs1 =30 m which represents the base case (stack 6), Hs2 = 45 m (1.5 Hs1) and Hs3 =60 m (2 Hs1).
- Case 4 (influence of emission rate on the hourly concentration)
Three cases are selected for emission rate of the SO2, Qs1=198.01 g/s which represents the base case (stack 6), Qs2= 132.007 g/s (Qs1/1.5) and Qs3 =99.005 g/s (Qs1/2).

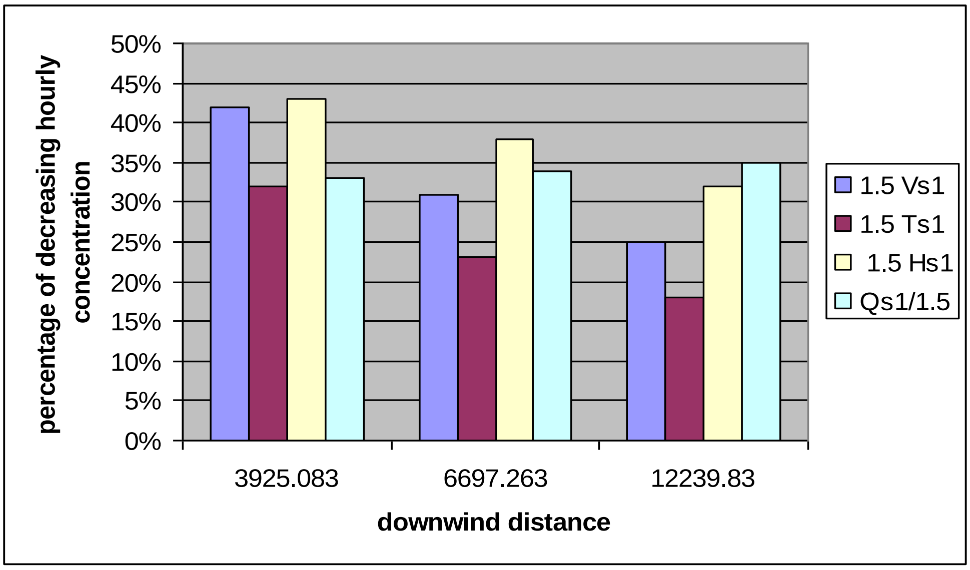


Figure (12) Sensitivity Analysis of 1.5 the Base Case for Vs1, Ts1, and Hs1 and 1/1.5 for Qs1

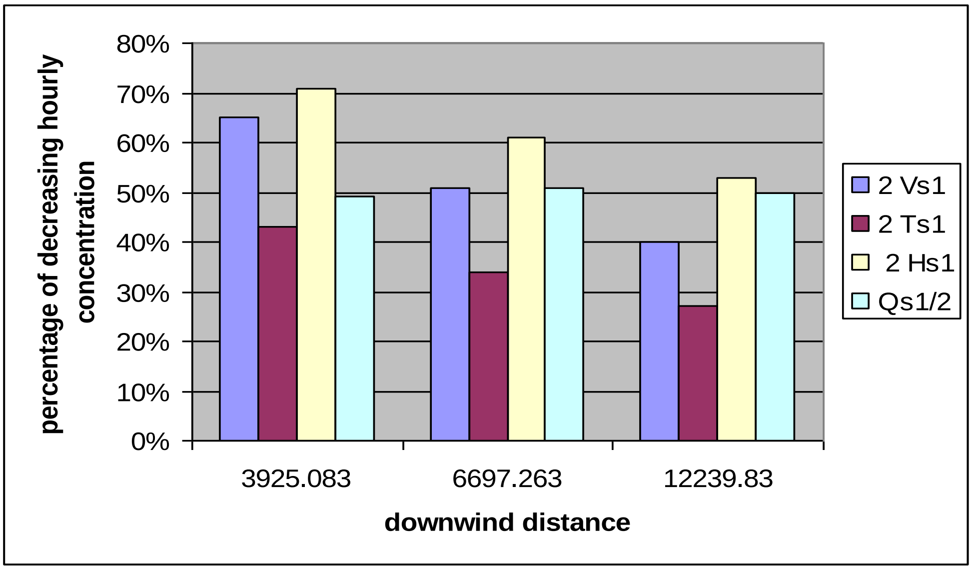


Figure (13) Sensitivity Analysis of 2 the Base Case for Vs1, Ts1, and Hs1 and 1/2 for Qs1

These Figures indicate the followings:

- Near the point source, physical height and exit velocity have higher effect on reducing hourly concentrations for the two cases of increasing these parameters by 50% and 100%.
- Far away from the source, reduction in the emission rate by a factor of 1.5 of the base case (Q/1.5) has decreased the hourly concentrations. While, if an increase in the physical height to twice of its value results in higher effect than the emission rate.

Sensitivity Analysis for Urban Area versus Rural Area

This analysis is done by taking the critical weather case (class E and wind speed is equal to 0.89 m/s) as a base case. Sensitivity analysis applies for two cases, case 1 (rural wind speed profile and Briggs dispersion coefficient for rural area) and case 2 (urban wind speed profile and Briggs dispersion coefficient for urban area).

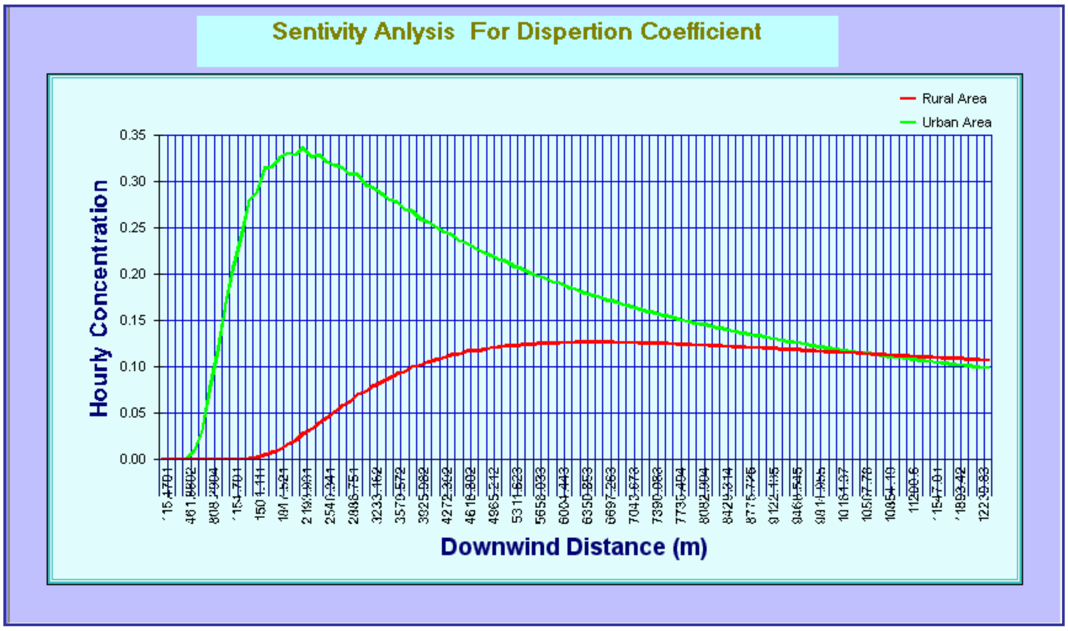


Figure (14) Sensitivity Analysis of SO_2 with Rural Versus Urban

The urban area has a large effect in increasing pollution near from source; this may be due to that, these types of area have more available sensible heat from solar surface heating and combustion sources that destabilize the surface layer of air causing mixing of the plume gases to the ground close to the source.

CONCLUSIONS

- Briggs equation for dispersion coefficients with rural wind speed profile has been found to be most suitable prediction combination for the particular sites chosen for the study; this case has yielded a large index of agreement (error- free predictions).
- The maximum hourly concentrations at the day time during period 15th -21st and 23rd -29th August 1997 for all pollutants indicate that: first maximum hourly concentrations for all pollutants happen under meteorological conditions including slightly unstable (class C) with wind speed varying from (2-10) m/s and with effects of stacks 6 and 2 of AL-Doura oil refinery. These two stacks have maximum contribution on the overall maximum concentration for the pollutant in addition to the effects of stacks 7 and 3.
- The most important observations that can be deduced from sensitivity analysis are:
  - The effect of turbulence on the reduction of concentrations of pollutants indicated that the worst case weather condition for dispersion of pollutants is characterized by a slightly stable atmosphere (class E).
  - The effect of point source properties with low wind speed and turbulence indicates that the physical height and emission rate has higher effect to reduce maximum hourly concentration of critical weather case (class E, 0.89 m/s) when increasing these parameters by 50% and 100% base case (stack 6).

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