Modeling and Evaluation of Air pollution from a Gaseous Flare in an Oil and Gas Processing Area

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Abstract: Gas flaring is the one the hottest environmental issues in developing countries. Flaring of gases causes serious air pollution in oil processing area and enters many air pollutants such as NOx, CO, CO_2, SOx and total hydrocarbon into atmosphere. In this study, modeling of a typical gas flare was carried out using MATLAB. The results were compared with experimental data obtained from a gas flare in Petroleum Company in an industrial city of Nigeria. Also the effects of some parameters i.e. flare height and atmospheric conditions were studied on the dispersion pattern of pollutants.

Key-Words: - gas flares, air pollution modeling, oil processing industry

1 Introduction

Flaring is a high-temperature oxidation process used to burn combustible components, mostly hydrocarbons, of waste gases from industrial operations. Natural gas, propane, ethylene, propylene, butadiene and butane constitute over 95 percent of the waste gases flared [1]. Gas flaring is the combustion of associated gas produced with crude oil or gas fields. Gas is flared on oil and gas production installations for safety. The main reasons are lack of process or transport capacity for gas, a continuous surplus gas flow, start up, maintenance and emergency (need for pressure relief). Gases flared from refineries and petroleum productions are composed largely of low molecular weight hydrocarbons with high heating value. Waste gases containing heavy hydrocarbons such as paraffins above methane, olefins, and aromatics, cause smoke. Flares are one of most pollutant sources due to combustion reaction. So, their controlling and monitoring are concerned especially in oil and gas manufacturing country. The emissions of pollutants from flaring are either unburned fuel or by-products of the combustion process. These emissions include carbon particles (soot), unburned hydrocarbons, CO, and other partially burned and altered hydrocarbons. Also emitted are NOx and, if sulfur-containing material such as hydrogen sulfide or mercaptans is flared, sulfur dioxide. The quantities of hydrocarbon emissions generated relate to the degree of combustion [2].

Air quality modeling is an essential tool for most air pollution studies [3]. In the last decade a lot of work has been done to develop advanced Eulerian dispersion models. The classical approach of using conventional models such as Gaussian puff/plume or based on K-theory with suitable assumptions, is known to work reasonably well during most of the meteorological regimes.

The advection–diffusion equation (K-theory) has been largely applied in operational atmospheric dispersion models to predict mean concentrations of contaminants in the Planetary Boundary Layer (PBL). In principle, from this equation it is possible to obtain a theoretical model of dispersion from a continuous point source given appropriate boundary and initial conditions plus knowledge of the mean wind velocity and turbulent concentration fluxes.

The simplicity of the K-theory of turbulent diffusion has led to a widespread use of this theory as mathematical basis for simulating pollutant dispersion in the PBL [4].

In this work an Eulerian Model on the base of k-theory was used for pollution dispersion from a typical gas flare. A sensitivity analysis for some metrological and physical parameters of model is also carried out. For validation, of model, measured data from a gas flare in Petroleum Company in an industrial city of Nigeria was used [5].

2 Modeling

The modeling of dispersion of air pollutants from an industrial source can be broken down into the following steps:

1- Describing the geometry of the domain.
2-Introducing appropriate boundary conditions
3- Introducing of sources/sinks and the dispersion characteristics for the entire domain.
4- Selection of values for parameters in the model.
5- Division of the domain into cells and solution of the finite difference equations.
6- Visualization of results.

The transfer and diffusion of pollutants from point source on the basis of k-theory are described by advective–diffusive equation (Eq. (1)) [4]:

$$\frac{\partial \hat{c}_i}{\partial t} + \hat{u}_j \frac{\partial}{\partial x_j}(\hat{c}_i) = \frac{\partial}{\partial x_j}\left(K_{jj} \frac{\partial \hat{c}_i}{\partial x_j}\right) + Q_i + S_i \qquad (1)$$

Where t is the time, c_i is the mean concentration of each pollutants, u_j is the j th component of the mean fluid velocity, K_{jj} is called the eddy diffusivity, Q_i the chemical and photochemical transformation of pollution; and S_i is the rate of addition of species i at location x = (x_1, x_2, x_3) at time t. Eq. (1) is called both the mixing-length theory and the K- theory. In this equation K_{jj} is determined from empirical augments.

Let us consider the Cartesian coordinates, at constant wind velocity and turbulent diffusivities values Eq. (1) could be written in the form of Eq. (2):

$$\frac{\partial \hat{c}_i}{\partial t} + \hat{u}\frac{\partial}{\partial x}(\hat{c}_i) + \hat{v}\frac{\partial}{\partial y}(\hat{c}_i) + \hat{w}\frac{\partial}{\partial z}(\hat{c}_i) = \frac{\partial}{\partial x}\left(K_H \frac{\partial \hat{c}_i}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_H \frac{\partial \hat{c}_i}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_v \frac{\partial \hat{c}_i}{\partial z}\right) + Q_i + S_i \qquad (2)$$

Where u, v and w are the wind velocity components, K_H and K_v are the horizontal and vertical eddy diffusion coefficients. For this kind of systems, we can consider the following assumptions:

1- The initial conditions are arbitrarily set to zero. The initial conditions have been found to be important only for the initial period of simulation [6].
2- Transport by bulk motion in the x-direction exceeds diffusion in the x direction i.e. we neglect the X-axis eddy diffusion coefficients for this model.
3- The wind velocity is constant and only in x direction. In the close field, the phenomenon may have a fully three dimensional nature. But in the far field, the wind advection prevails over the horizontal diffusion. We consider far distances for that how damage is caused to the inhabitants of the environment.
4- The stack gases emitted from the industries in the atmosphere are not reactive i.e. there is no form of reaction between the pollutant.
5- There is no deposition in system [7].

Gas flare dispersion model is based on these assumptions becomes:

$$\hat{u}\frac{\partial}{\partial x}(\hat{c}_i) = \frac{\partial}{\partial y}\left(K_H \frac{\partial \hat{c}_i}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_v \frac{\partial \hat{c}_i}{\partial z}\right) \qquad (3)$$

3 Solution of Mathematical Model

We can now apply the finite difference method of solution to Eq. (3). We express first-order derivatives in terms of backward differences and second-order derivatives in terms of central differences around the point (i, j, k) using the counters i for the x-direction, j for the y-direction and k for the z-direction.

$$\left.\frac{\partial C}{\partial x}\right|_{i,j,k} = \frac{1}{\Delta x}(C_{i,j,k} - C_{i-1,j,k}) \tag{4}$$

$$\left.\frac{\partial^2 C}{\partial y^2}\right|_{i,j,k} = \frac{1}{\Delta y^2}(C_{i,j+1,k} - 2C_{i,j,k} + C_{i,j-1,k}) \tag{5}$$

$$\left.\frac{\partial^2 C}{\partial z^2}\right|_{i,j,k} = \frac{1}{\Delta z^2}(C_{i,j,k+1} - 2C_{i,j,k} + C_{i,j,k-1}) \tag{6}$$

By substitution in equation (3), we have:

$$\begin{aligned}(\Delta y^2\Delta z^2 u_k + 2\Delta x\Delta z^2 K_H + 2\Delta x\Delta y^2 K_v)C_{i,j,k} = {} & \\ \Delta y^2\Delta z^2 u_k C_{i-1,j,k} + {} & \\ \Delta x\Delta z^2 k_H (C_{i,j+1,k} + C_{i,j-1,k}) + {} & \\ \Delta x\Delta y^2 K_v (C_{i,j,k+1} + C_{i,j,k-1}) & \end{aligned} \tag{7}$$

This equation is stable and the Gauss-Sidel method is especially suitable for the solution of this problem [8].

3.1 Atmospheric Parameters

Values of wind speed and eddy diffusivity are presumed known. Wind Velocity is constant in the axial direction, but varies upward as given in the relation:

$$u_z = u_0 \left(\frac{z}{z_0}\right)^P \tag{8}$$

Where u_0 is the wind vector at z_0, and the exponent p change with atmospheric stability and surface roughness. Table 1 shows values of p for various stability categories [9]. Vertical eddy diffusivity for various stability classes are given in Table 2 [7]; where u^* is friction velocity (assumed 1.75m/s), and L is the height above the ground at which the production of turbulence by both mechanical and boundary forces is equal. L is calculated by using the equation 9. In this equation, C_p is specific heat of air, T is air temperature, k is Karman's constant (k=0.4), g is gravitational constant and H_n is net heat that enters the atmosphere. H_n for neutral atmosphere is 0, for stable atmosphere is -42 and for unstable atmosphere is 175.

$$L = -\frac{u^{*3} C_p \rho T}{k g H_n} \tag{9}$$

Table 1- Values of p for stability categories

Stability Category	Rural Exponent	Urban Exponent
A	0.07	0.1
B	0.07	0.15
C	0.10	0.20
D	0.15	0.25
E	0.35	0.25
F	0.55	0.30

A: very unstable, B: unstable, C: slightly unstable, D: neutral, E: slightly stable and F: stable

In this work three classes of atmosphere stability, neutral, stable and unstable are considered. The concentration distribution is found to be not very sensitive to the change of K_H. Thus, a value of $50 m^2/s$ is used in the model [6].

The Holand' formula was used for determining of plume rising height in stable atmosphere [10]

Table 2- vertical eddy diffusivity for various stability categories

Stability	Vertical Eddy Diffusivity	
	In surface layer, $0<z<z_{sl}$	Upper surface layer, $z_{sl}<z<z_m$
Neutral	$K_z = 0.4u_*z$	$K_z = 0.4u_*z_{sl}$
Stable	$K_z = 0.4u_*z/\left(1+\frac{5.2z}{L}\right)$	$K_z = 0.4u_*L$
Unstable	$K_z = 0.4u_*z\left(1-\frac{15z}{6L}\right)^{1/4}$	$K_z = 160u_*^2\left(1-\frac{6000u_*}{L}\right)$

$$H_e = h_s + h_{fv} + \Delta h \qquad (10)$$

$$\Delta h = \frac{v_s D}{u}\left(1.5 + 2.68\times10^{-3} PD\,\frac{(T_s - T_a)}{T_s}\right) \qquad (11)$$

Where Δh is the plume rising height, H is the effective height of flare stack, u is the wind velocity at stack height level, v_s is stack exit velocity (m/s), D is stack diameter (m), P is pressure (mbar), T_s is stack gas temperature (K) , and T_a is atmospheric temperature (K). h_{fv} is horizontal flame reach and can be calculated by fellowing equations:

$$h_{fv} = L_f(\sin 45°) = 0.707\ L_f \qquad (12)$$

$$L_f = 0.0042\ Q_c^{0.478} \qquad (13)$$

Where L_f is flame length and Q_c is burned gas heat release (Btu/hr) [9].

3.2 Boundary Conditions

For solving Eq. (7), the following initial and boundary conditions are used:

1- at x =0, $C(0,j,k)=C_0$

2- at y =0, $\frac{\partial C}{\partial y} = 0$

3-at y =W, $\frac{\partial C}{\partial y} = 0$

4- at z =0, $\frac{\partial C}{\partial z} = 0$

5- at z = mixing length , $\frac{\partial C}{\partial z} = 0$

C_0 is the initial value of each pollutant at flare position. W and mixing height are shown in Fig.1.

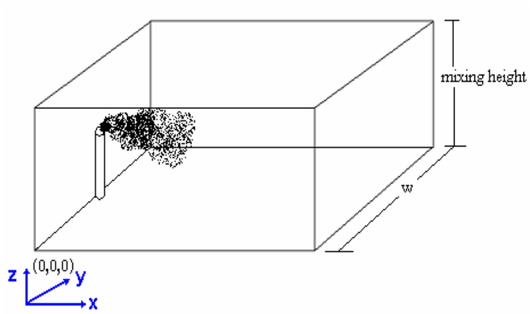

Fig.1. domain used in simulation for one flare stack

3.3 Source data

To validate the model, experimental data from analysis is carried out on pollutants discharged from a petroleum industry flare stack in Kaduna State, Nigeria was used. Pollutants were NO, CO and SO_2. Samples of air had been collected at distances of 20m, 60m, 80m and 100m away from the flare point. Experimental determinations of contaminant concentrations in selected flare in Nigeria had been yielded the concentrations of NO, SO2 and CO 96, 1120 and 14640µg/m3, respectively in 20m far from stack in ground level.

4 Computer simulation

Domain used in simulation is: X=0-5000, Y=0-1000 and Z=0-300m. The program complex has been realized on MATLAB language and consists in the following routines:

1. Enter data for concentration, emission source, final distance *x*, distance *y*, distance *z*, wind velocity, etc.
2. Set initial variables for nodes at different ground points.
3. Set concentration for different nodes at grid point using a repetition structure (do loop).

5 Results and discussion

5.1 Comparison of emission estimate with measured data

Comparison of model estimations with experimental data is carried out in atmospheric neutral stability condition. The wind speed was determined about 6 m/s. Figure 2 presents NO concentrations as functions of axial distance (40, 60, 80 and 100 m far away stack) at ground level. Mean error for NO estimation is about 5%. Figure 3 shows analysis data and model estimation for SO_2 concentration. Mean error for first 3 distances (x = 40, 60, 80m) is about 7%, but in x=100 m the error is very high. We didn't found any clear reason for this issue. If we consider CO estimations, the result are similar. The mean error is about 7% with max error in x=100 m accordance to 12%.

Generally, the model estimation are acceptable and except for SO_2 concentrations in x =100 m. The other estimations have errors less than 10%.

5.2 Analysis of parameters effect on pollutant dispersion pattern

In this study, also effect of parameters on pollutant dispersion was analyzed. For this purpose, only one pollutant i.e. SO_2 with source concentration of 1.16 mg/m^3 was considered. Various cases are presented in table 3. Figure 4 and 5 show the concentration profiles for SO_2 at ground level in flare centre line (y=0) and a height of 240m respectively. Profiles of SO_2 concentration show that atmospheric condition have high affect on pollutant distribution on ground level, so that in stable condition (case 3), was compared to other conditions, exist low value of pollutant in ground level. The worst condition is unstable mode. In this condition even increasing in height of flare stack can't affect in pollution control in ground level. Comparison of cases 1, 4 and 5 shows this result. In unstable condition, flare height is effective only in near distances (about 250m), after that due to unstable condition in atmosphere, pollution rapidly increase in ground level (case5).

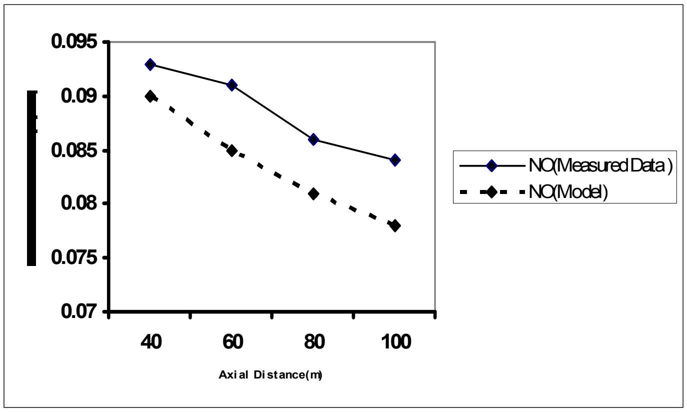

Fig.2. NO concentrations estimated by model as function of axial distance at ground level

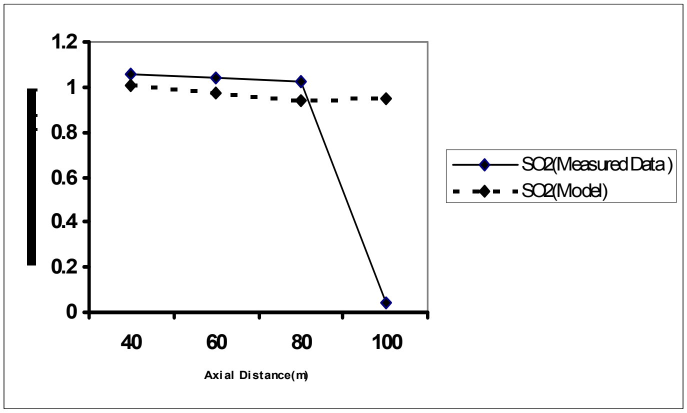

Fig.3. SO_2 concentrations estimated by model as function of axial distance at ground level

This condition is dangerous for inhabitants in environment. In Figure 5, the simulation of SO_2 concentration in centerline of flare was extended to 240 m altitude. The SO_2 concentration profile in stable condition is smooth parabolic with a maximum occurring at an axial distance of about 750m; the maximum concentration at the peak was 0.16092 mg/m^3. Also the parabolic nature of the profiles is seen for neutral condition (case 2). However, the concentrations were much larger, and the maximum concentration appears in close distances, about an axial distance of 180m with 0.42866 mg/m3 value.

Table 3. Various cases for evaluating of model parameters effect

Case No.	u_0 (m/s)	Stability condition	H_e (m)	P	K_v (m^2/S)	K_H (m^2/S)
1	3	B-C(unstable)	60	0.1	200	50
2	6	D(neutral)	60	0.15	50	50
3	8	E(stable)	60	0.35	25	50
4	3	B-C(unstable)	30	0.1	200	50
5	3	B-C(unstable)	90	0.1	200	50

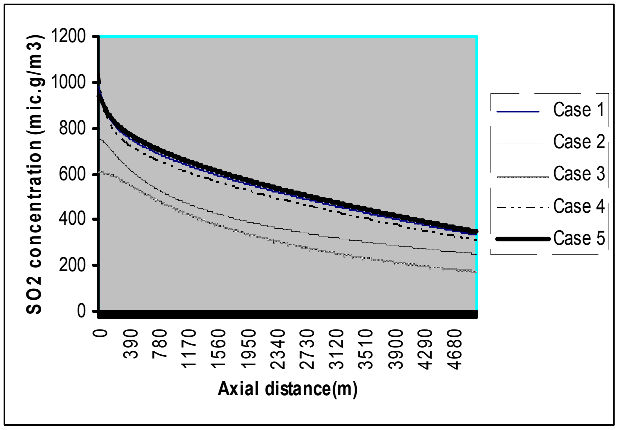

Fig.4. simulated concentration profiles of SO_2 as function of axial distance at ground level in various cases

At the same altitude and unstable conditions (see case 1, 4 and 5) SO2 concentration profile has exponential mode. This behavior could be due to turbulence in the air [4]. Although the elevated stack can emitted the pollutants in high ground levels, its effect on pollution decreasing on ground levels is not considerable, especially in unstable conditions. Thus, it has been suggested that flaring system optimization should be considered.

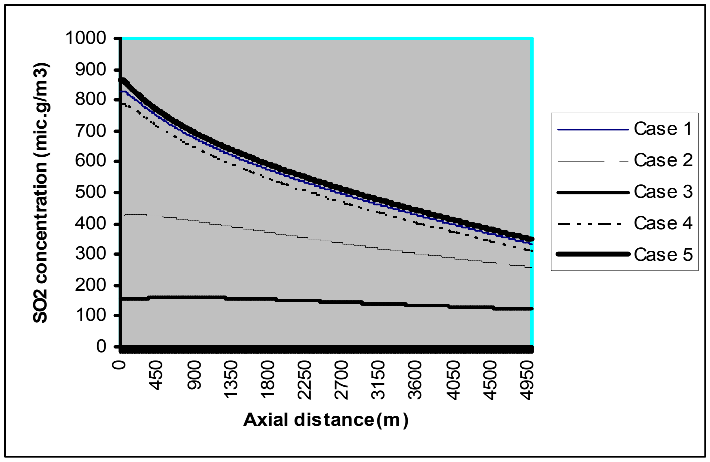

Fig.5. simulated concentration profiles of SO_2 as function of axial distance at an altitude of 240 m in various cases

6 Conclusions

In this paper, a numerical air pollution model for gas flares was developed. The model shows an acceptable agreement to real data with less than 10% average error. Also, the simulated pollutant concentration profiles in stable and neutral conditions were found to be parabolic at ground level and an altitude of 240 m.

Also pollutant concentrations became quite large at an unstable condition on the ground level. The effects of these high concentrations of the pollutants are discussed with regard to potential dangerous for people's health in polluted areas.

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References:

[1] Compilation of Air Pollutant Emission Factors, Volume 1: Stationary Point and Area Sources, Fifth edition, AP-42. Section 13.5: Industrial

Flares, *United States Environmental Protection (USEPA)*, Office of Air Quality Planning and Standards, Research Triangle Park, NC, USA, 1993.

[2] Emission Inventory Guidebook 926: Waste Incineration, Flaring in Gas and Oil Extraction, *European Environment Agency (EEA)*, 2006.

[3] Seinfeld, J. H. & Pandis, S. N., *Atmospheric Chemistry and Physics: From Air Pollution to Climate Change*, Wiley: New York, 1998.

[4] Susu, A. A., Abhulimen, E. & Adereti, B., Modeling of Air Pollution Systems with Chemical Reactions: Application to Gas Flares in Nigeria", *International Journal for Computational Methods in Engineering Science and Mechanics,* Vol.6, 2005, pp.201–213.

[5] Abdulkareem, A.S., Urban Air pollution Evaluation by Computer Simulation: A case study of petroleum refining company Nigeria, *Leonardo Journal of Sciences*, Vol.6, 2005, pp.17-28.

[6] Ku J. & Rao, S., Numerical Simulaton of Air Pollution in Urban Areas: Model Development, *Atmospheric environment*, Vol.21, 1987, pp.201-212.

[7] Fatehifar, E., Denelopment oF an optimal design of a multi-pollutant air quality monitoring network, *Ph.D. Thesis*, Shiraz University, Shiraz, Iran, 2006

[8] Constantinides, A. & Mostoufi, N., *Numerical Methods for Chemical Engineers with Matlab Applications*, Prentice Hall, Inc., 1999.

[9] Beychok, M. R., *Fundamentals of Stack Gas Dispersion*, 3'rd Edition, 1995.

[10] Peavy, H. S. et al., *Environmental Engineering*, McGraw-Hill, Inc., 1985.