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DEVELOPMENT OF A MATHEMATICAL MODEL FOR THE ASSESSMENT OF HYDROGEN SULPHIDE POLLUTANT IN AIR

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ABSTRACT

This work is aimed at developing a mathematical model to determine the concentration of Hydrogen Sulphide pollutant in air from the gas flare of a refinery. To achieve this, experimental data on concentration of Hydrogen Sulphide from Kaduna refinery and petrochemical company Nigeria were collected and the dispersion model was developed based on Gaussian distribution principle. The simulation of the model was carried out using visual basic programming. It was observed from the simulated result that the gas dispersion model developed for Hydrogen Sulphide showed a remarkable agreement with the dispersion pattern, and agrees with the experimental results with a correlation co-efficient of 0.98. Thus, the model can be used to determine the safe distance for human habitation from an industrial area and the refinery in particular.

Keywords: Mathematical Model, Pollutant, Hydrogen Sulphide

INTRODUCTION

The environment is the entire physical surrounding which include the material and other influences, which affect the growth, development and existence of all living matter. When the human population was small and its technology ability limited, its activities inflicted little damage which were repaired by the regenerative process of nature, but as population increased and became concentrated in urban areas and as man's technological capabilities increased, man was able to temporarily "dominate" nature but at the expense of his well-being and the natural environment which serves as his life support system. Man then began to realize that development couldn't be sustained if the environment is not protected and managed. There arose a new pressing challenge created by these adverse effects of depletion of planetary resources, environmental pollution and rapid population growth. Thus, there is need of understanding and controlling segment of the environment often called system to provide useful economic product for the society with little or no adverse effect on the environment. The major goals of understanding and control are complementary because effective system control requires that systems be understood and modelled. This can be achieved through mathematical modeling (The World Book Encyclopaedia, 2001). This research is aimed at developing a mathematical model to determine the concentration of Hydrogen Sulphide in the air from a typical refinery and its environs-Kaduna Refinery and Petrochemical Company (KRPC) located in northern Nigeria in order to safeguard the environment and prevent damaging effect of toxic gas on humans.

LITERATURE REVIEW

Environmental pollution is one of the most serious problems facing humanity and other life forms today. Badly polluted air can harm crops and cause life threatening illness. Some air pollutants have reduced the capacity of the atmosphere to filter out the sun's harmful ultraviolet radiation. Many scientists believe that these and other air pollutants have begun to change climates around the world (Meyers, 1992) Water and soil pollution threaten the ability of farmers to grow enough food. Ocean pollution endangers many marine organisms. Many people think of air, water and soil pollution as distinct forms of pollution. However, each of the parts of an environment – air, water, and soil- depends upon the others and upon the plants and animals living within the environment. Air pollution is the contamination of the air by such substances as fuel exhaust and smoke. It can harm the health of plant and animals and damage buildings and other structures. According to the world health organization, about one-fifth of the world's people are exposed to hazardous levels of air pollutants (Milton, 1995) Air pollution occurs when industries and vehicles release such large amounts of gas and particulates into the air such that natural processes can no longer keep the atmosphere in balance. There are two major types of air pollution (i) Outdoor air pollution (ii) Indoor air pollution.

Outdoors Air Pollution

Most of the outdoor air pollution results from the burning of fuel to power motor vehicles, heat buildings, and from industrial processes. For example, many dry cleaning plants remove dirt from clothing with the release of a chemical called perchloroethylene, a hazardous air pollutant (FEPA, 1991) One of the most common types of outdoors air pollution is smog. Smog is a brown, hazy mixture of gases and particulates. It develops when certain gases released by the combustion of gasoline and other petroleum products react with sunlight in the atmosphere. This reaction creates hundreds of harmful chemicals, which make up smog. One of the chemicals in smog is a toxic form of oxygen called ozone. Exposure to high concentrations on ozone causes headaches, eyes pain and irritation of the respiratory tract in many individuals. In some cases, ozone in the lower atmosphere can cause death (Osei, 1998) "Acid rain" is a term for rain and other precipitation that is polluted mainly by sulphuric acid and nitric acid. These acids form when gases called sulphur dioxide and nitrogen oxides react with water vapour in the air. These gases come mainly from the burning of coal, gas, and oil by cars, factories, and power plants. The acids in acid rain move through the air and water and harm the environment over large areas.

Indoors Air Pollution

This occurs when buildings with poorly designed ventilation systems trap pollutants inside. The main types of indoor pollutants are tobacco smoke, gases from stoves and furnaces, household chemicals, small fibre particles, and hazardous fumes given off by building materials including insulation, glue, and plant.

Effects of Hydrogen Sulphide

Exposure to low concentration of H_2S may cause irritation to the eyes, nose or throat. It may also cause difficulty in breathing for some asthmatics. Brief exposures can cause a loss of consciousness and possibly death. In most cases, the person appears to regain consciousness without any other effects. However, in many individuals, there may be permanent or long term effects such as headaches, poor attention span, poor memory, and poor motor functions (www. atsdr. cdc. gov/facts 114. htm) Scientists have no reports of people poisoned by ingesting hydrogen sulphide. Pigs that ate feed containing H_2S experienced diarrhoea for a few days and lost weight after about 105 days (.ref) They also have little information about what happens when the skin is exposed to H_2S, although it is known that care must be taken with the compressed liquefied product to avoid frostbite. (www. atsdr. cdc. gov/facts 114. htm)

METHODOLOGY

H_2S concentration in the air was determined by using a small monitor remote sensor commonly called the Crowcon Gasman II. Crowcon gasman II is a personal gas detector that continuously monitors the level of oxygen, H_2S or the presence of a single toxic or flammable gas in air. It is designed to be worn by individuals working in hazardous environment such as confined spaces. This will give a loud audible and bright visual alarm warning when preset concentrations of gas are exceeded. Crowcon Gasman is switched on by pressing the large bottom is an environment with clean air. The instrument tests all LCD segments, red alarm LEDs and sounder for 5 seconds before entering monitoring mode. The battery symbol and a number representing the remaining percentage of battery capacity indicate the battery condition. The instrument, which is now ready to be used, is taken to the process plant at designated areas where H_2S comes out with the fare gas. The concentration of H_2S is known by simply switching on the sensor and the gas level is shown numerically on the display. The concentration of H_2S is monitored in a particular area at regular interval of time and this should not exceed 10ppm.

Development of Mathematical Model for Hydrogen Sulphide Concentration

Mathematical modeling is a comprehensive process of representing real-world phenomena in terms of mathematical equation and extracting from them useful information for understanding and prediction (Meyers, 1992). In recent years, mathematical modeling has become a powerful tool to solve complex, interconnected and interacting phenomena arising from the rapid developments taking place in science and technology. The success in physical sciences in terms of valid mathematical models has led Scientists to extend the modeling methodology to other emerging fields of inquiry in which great studies have been made. Most discharges of H_2S to the atmosphere are from the stack, and this pollutant emission then blows downward and disperses horizontally and vertically, diluting steadily. This takes the form of a Gaussian distribution equation and is a function of wind speed and atmospheric stability. The modeling process consists of the following stages:

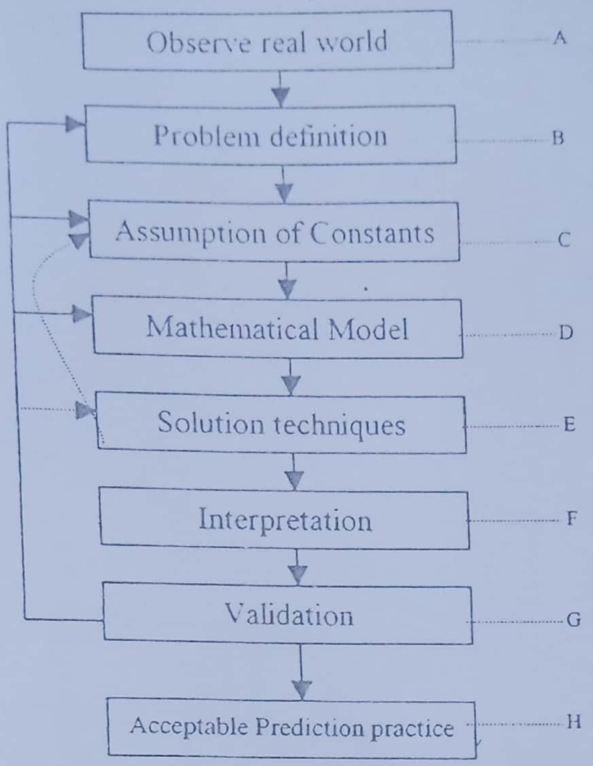


Fig1.0: Schematic of a Mathematical Procedure

Step A–B: Involves bringing out a well-defined problem from the maze of observations.
Step C: Involves sorting out the essential and significant features that need to be incorporated in the model.
Step D: Involves translating features into mathematical entities and relating them under certain simplifying but realistic assumptions and constraints. Step E and F: Involves using one or more solution techniques to obtain and interprets a solution from the viewpoint of accuracy and stability. Step G: Involves determining how closely the solution approaches the original, real-world phenomenon. If solution meets the imposed limit of acceptability, the model is considered valid and then put into practice. The following assumptions were made in developing the mathematical equation for the assessment of H_2S pollutant dispersion in air from the flare (i) A continuous and point source emissions, (ii) Downward diffusion is negligible compared to downward transport i.e. only vertical and crosswind diffusion occurs, (iii) Vertical and crosswind diffusion occur according to Gaussian distribution, (iv) The emissions rate is continuous and constant, (v) The horizontal and velocity and the main wind directions are constant,(vi)There is no deposition, washout, chemical conversion or absorption of emissions diffusing to the ground are reflected back into the plane that is, all emissions are totally conserved within the plane, (vii)There is no upper barrier to vertical diffusion and there is no crosswind diffusion barrier,(viii)Atmospheric turbulence is considered constant through out the plane travel distance, and (ix)Emissions reflected upward from the ground are distributed vertically as if released from an imaginary plane beneath the ground and are additive to the actual plane distribution. The use of d_z and d_y as constants at a given downward distanced and the assumption of an expanding conical plane, Figure 2.0 implicitly require homogenous turbulence throughout the x, y and z – dimensions of the plane. Fig. 2.0a and b Shows the schematic diagram of a continuous point-source plume and imaginary plume

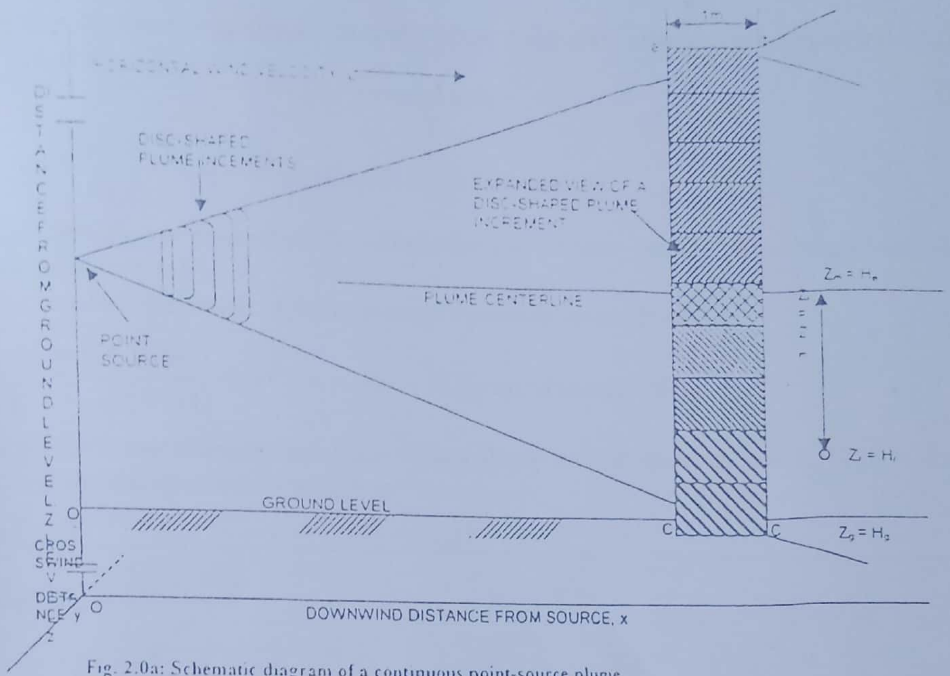


Fig. 2.0a: Schematic diagram of a continuous point-source plume

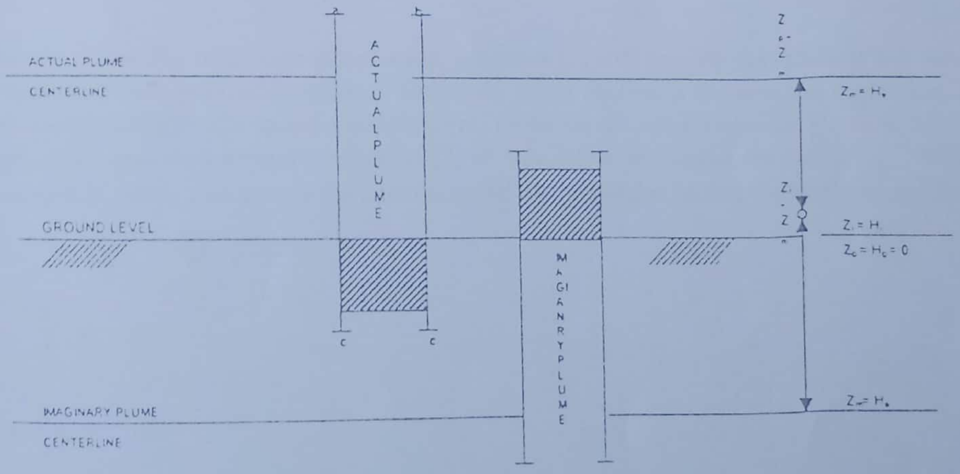


Fig_2.0b Schematic diagram of an imaginary plume concept

From Gaussian distribution (Beychok, 1995)

$$\frac{n_i}{\lambda} = \left(\frac{n_m}{\lambda}\right) e^{-(x_1-x_m)^2/2\delta^2} \text{ --------- } (1)$$

Where X_m= the mean or arithmetic average value of the class characteristic amongst the total population.

$$X_m = \frac{\Sigma[n_1(1)(x_1/\lambda)}{N} \text{ ------ (for grouped data).}$$

$$= \frac{\Sigma(n_1 X_1)}{N(\lambda)} \text{ ------- (Expressed in intervals)}$$

X_1-X_m = deviation in amount of class characteristic between members of subclass I and the mean subclass in (expressed in intervals)

σ= The standard derivation of the root mean square deviation from X_m.

$$\sigma = \sqrt{\frac{\Sigma\left[n_1(1)(X_1 - X_M)^2\right]}{\lambda^2(N-1)}} \text{ ------- (Expressed in intervals)}$$

Since all the linear characteristic scale values above are expressed as interval, λ term in equation (1) can be dispersed and the equation re-written as:

$$n_1 = (n_m) e^{-(X_1-X_m)^2/2\delta^2} \text{ --------- } (2)$$

Where: $X_m = \frac{\Sigma(N_1 X_1)}{N}$

$$\delta = \sqrt{\frac{\Sigma\left[n_1(X_1 - X_M)^2\right]}{N-1}}$$

Given the δ and X_m of a class distribution, equation (2) will provide the ration of any subclass population to the mean subclass population (n_1/n_m). However, when dealing with stack gas dispersion, it is more useful to relate the population of a specific subclass (n_1) to the total class population. Hence let (X_1 -X_m) equal to u for simplication, and then integrate equation (2) to obtain the area under the curve. ......Which is the total class population N. since that area is the summation of the rectangles having the height n_1 and the width Δu:

$$N = \sum_{-\infty}^{\infty} (n_1 \Delta u)$$

$$= \int_{-\infty}^{\infty} n_i \, dU$$

$$N = \int_{-\infty}^{\infty} n_m e^{\frac{-u^2}{2\delta^2}} du$$

$$= \int_{-\infty}^{\infty} n_m e^{\frac{-1}{2}\left(\frac{u^2}{\delta^2}\right)} du$$

$$= \int_{-\infty}^{\infty} n_m e^{\frac{-1}{2}\left(\frac{u}{\delta}\right)^2} du$$

$$= \int_{-\infty}^{\infty} n_m e^{-\left(\frac{u}{\delta\sqrt{2}}\right)^2} du$$

$$= n_m \int e^{-\left[(\delta\sqrt{2})^{-1} U\right]^2} du$$

But $\int_{-\infty}^{\infty} e^{-u^2} du = \sqrt{\pi}$ for total area under the curve of function that is symmetry about its axis (i.e. n = e^{-u^2})

$$= n_m . \delta\sqrt{2} . \sqrt{\pi} = n_m \delta \sqrt{2\pi}$$

$$N = n_m \delta (2\pi)^{\frac{1}{2}} \text{ --------- } (3)$$

Dividing equation (2) by (3) to obtain

$$\frac{n}{N} = \frac{e^{-(x_r - x_m)^2/2\delta^2}}{\delta(2\pi)^{\frac{1}{2}}} - - - - - - - - - - - - - (4)$$

Equation (4) is the Gaussian distribution equation, which can be re-arranged in form that will be used to develop stack gas dispersion model as follows.

$$n = \frac{Ne^{-(x_r - x_m)^2/2\delta^2}}{\delta(2\pi)^{\frac{1}{2}}} - - - - - - - - (5)$$

Neglecting the crosswind diffusion of the plane and looking only at the total emissions as seen by viewing the vertical dimension from a distance, and hence seeing the integrated crosswind emissions, equation (5) becomes:

$$n_r(x,z) = \frac{e^{-(z_r - z_m)^2/2\delta_z^2}}{\delta_z(2\pi)^{\frac{1}{2}}} - - - - - - - - (6)$$

Where:

N= total grams of emissions.
Z_r = any receptor location.
Z_m= location of the mean emission density (i.e. the plane centreline) in the Z-dimension.
δ_z = vertical dispersion co-efficient of the emission density in meters.
n_r (x,z) is the integrated crosswind emission density in g/m^3, seen at the receptor located at Z_r when viewing the x-z plane.

Thus, the Gaussian distribution in the vertical or Z-dimension, including up roared reflection from the ground becomes.

$$n_r(x,z) = \frac{Ne^{-(z_r - z_m{}^2/2\delta_z^2)}}{\delta_Z(2\pi)^{\frac{1}{2}}} + \frac{Ne^{-(z_r - z_m)^2/2\delta_z^2}}{\delta_z(2\pi)^{\frac{1}{2}}} - - - - - - - - (7)$$

Let N =Q/u = weight of emissions (in grams/meter) ,$Z_r - Z_m = H_r - H_e$ and
$Z_r - Z'_m = H_r - (-H_e) = H_r + H_e)$

Where:

H_e = height of plane centreline above, m and H_r = height of receptor above ground, m.
Substituting these into equation (7), it gives

$$n_r(x,z) = \frac{Q}{u\delta_z(2\pi)^{\frac{1}{2}}}\left[e^{-\frac{(H_r - H_e)^2}{2\delta_z^2}}\right] - - - - - - (8)$$

Including, the crosswind Gaussian distribution of n_r (x,z) in the Y-dimension to give,

$$n_r(x,y,z) = \frac{n_r(x,z)e^{-(y-y_m)^2/2\delta_y^2}}{\delta_y(2\pi)^{\frac{1}{2}}} - - - - - - - (9)$$

Since there is no diffusion barrier in the crosswind dimension and hence no need for another reflection term in equation (9).

The following substitution can be made into equation (9).
C=n_r (x, y, z) to conform to conversion.
Z_r = H_r to conform to conversion.
n_r (x,z) = the right-hand side of equation (8)
Y_m = 0 for the location of the mean emission density of the plume centreline in the crosswind or y-dimension. Hence:

$$C = \frac{Q}{u\delta_z\delta_{y2\pi}} e^{\frac{-y^2}{2\delta_y^2}}\left[e^{\frac{-(z_r - H_e)^2}{2\delta_z^2}} + e^{\frac{-(Z_r + H_e)^2}{2\delta_z^2}}\right] - - - - - - - - (10)$$

Let Q =ρV, substituting these into equation (10)

$$C_{H_2S} = \frac{\rho V}{U\delta_z\delta_y 2\pi} e^{-\frac{y^2}{2\delta_y^2}} \left[e^{\frac{-(Z_r - H_e)^2}{2\delta_z^2}} + e^{\frac{-(Z_r + H_e)^2}{2\delta_z^2}} \right] \text{-------}(11)$$

Where:

C = concentration of emissions in g/m^3, at any receptor located at
x meters downwind.
y meters crosswind form the centerline.
z meters above ground.

Q= source emission rate g/sec.

ρ_{H_2S} = Density of H_2S kg/m^3

V = Volume of H_2S m^3/sec.

U = Horizontal wind velocity m/sec.

δ_y =Horizontal dispersion coefficient m

δ_z = Vertical dispersion coefficient m.

H_e = Emission height or effective stack height, m

Z_r = Receptor location in the Z-dimension, m

To obtain the value of δ_y and δ_z in the equation (11), urban terrain is assumed, and Turner's version of the Pasquill co-efficient is used i.e.

$\delta = \exp[I + I(\ln x) + k(\ln x)^2]$ -----(12)

Where δ = urban dispersion co-efficient.

X = down wind distance M.

Table1.0 Pasquill stability classes

Pasquill stability class	Ambient temperature gradient (°F/1000 feet)
A-very unstable	Less than –10.4
B-unstable.	-10.4 to -9.3
C-slightly unstable.	-9.3 to –8.2
D-neutral.	-8.2 to –2.7
E-slightly stable	-2.7 to 8.2
F- stable	More than 8.2

Table 2.0 Constant I,J and K (Milton,1995)

Pasquill Stability Class	For obtaining δ_z			For obtaining δ_y		
	I	J	K	I	J	K
A	6.035	2.1097	0.2770	5.357	0.8878	-0.0076
B	4.694	1.0629	0.0136	5.058	0.9024	-0.0096
C	4.110	0.9201	-0.0020	4.651	0.9181	-0.0076
D	3.414	0.7371	-0.0316	4.230	0.9222	-0.0087
E	3.057	0.6794	-0.0430	3.922	0.9222	-0.0064
F	2.621	0.6564	-0.0340	3.533	0.9191	-0.0070

Results

Table 3.0 Values of experimental results

Month	Concentration of H_2S in air (ppm)
JANUARY	20.00
FEBUARY	29.00
MARCH	23.00
APRIL	35.00
MAY	6.00
JUNE	9.00
JULY	10.00
AUGUST	33.00
SEMPTEMBER	2.00
OCTOBER	8.00
NOVEMBER	19.00
DECEMBER	29.00

Fig. 3.0 Graph of Hydrogen Sulphide Concentration in Air for February

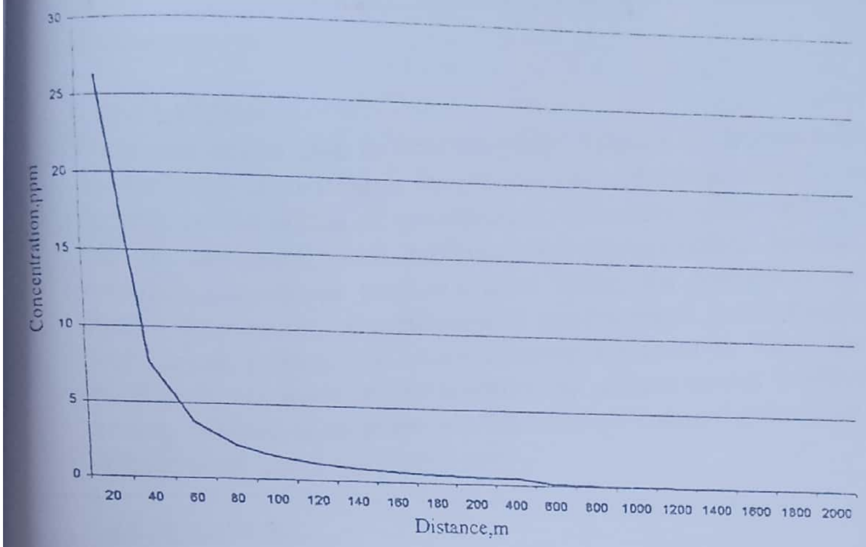
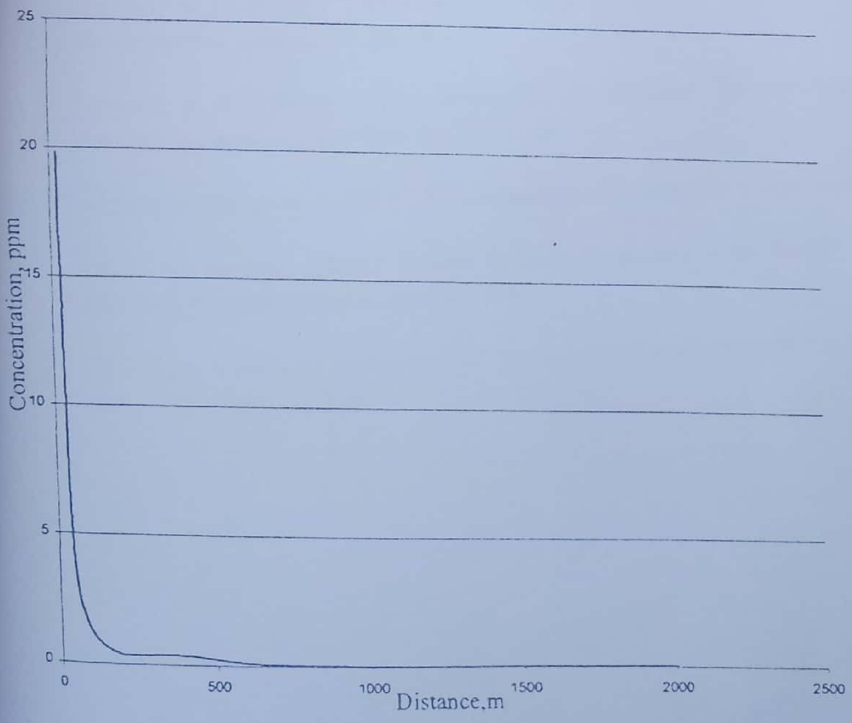


Fig.4.0 Graph of Hydrogen Sulphide concentration in Air for November



DISCUSSION OF RESULT

During the formulation of the mathematical model, Gaussian distribution principle on stack gas dispersion was applied. The model was simulated using visual Basic programming and it was observed that the model developed, showed a remarkable agreement with the dispersion pattern and quite agrees with the experimental result with a correlation co-efficient of 0.98. It was also observed that the concentration of H_2S decreases as the distance increases from the flare. Thus, confirming the validity of the model. The mathematical model developed can predict the concentration of H_2 S pollutant from gas flaring as a function of axial distance. It was observed from the simulated results Figures 3.0 and 4.0 shows that the model developed gave a remarkable agreement with the dispersion pattern and quite agrees with the experimental results with a correlation co-efficient of 0.98. The model equation that represents H_2S pollutant from gas flaring is:

$$C_{H_2S} = \frac{\rho V}{U\delta_z \delta_y 2\pi} \ell^{-\frac{y^2}{2\delta_y^2}} \left[\ell^{\frac{-(Z_r - H_e)^2}{2\delta_z^2}} + \ell^{\frac{-(Z_r - H_e)^2}{2\delta_z^2}} \right]$$

Therefore, the model equation can be used to determine the safe distance for human habitation from an industrial area.

CONCLUSION

The model can be used to determine safe distance for human habitation from an industrial area and also for the reviewing of existing or future environmental regulation by regulatory authorities. Controlling pollution depends on the efforts of governments, scientists, industrialists, and organizations. Economic development can be compatible with environmental conservation. Hence, the present problems of environmental resources degradation need not arise within the framework of sustainable development. Failure to halt further deterioration of environmental quality might jeopardize the health of large segment of the population with serious political and socio-economic implications. Thus, the Federal Environmental Protection Agency of Nigeria has made recommendation to protect human health in working places such as the refinery by setting standard of an allowable limit of H_2S concentration in air to be 10ppm.. Concentration of H_2S up to 13ppm in air is still considered safe

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