



## Comparative Evaluation of Numerical and Gaussian Models for Gas Pollutants Dispersion from Industrial Flares

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### Abstract

A comparative evaluation of numerical and Gaussian models was developed for gas pollutants dispersion from industrial flares. Numerical model incorporates the finite volume method to estimate pollutants concentration from continuous sources. In this model, different profiles for wind velocity and dispersion coefficients were used depending on atmospheric stability classes. Surface roughness was also considered in numerical modeling. Pollutants concentration predicted by the presented model, were compared to those obtained by the Gaussian plume model which assumes constant wind and dispersion coefficients in vertical direction. The maximum ground level concentration agrees well in both models. However, the concentration distribution profile predicted by Gaussian model is broader than that of obtained by numerical model, due to considering effects of surface roughness in numerical model.

**Keywords:** Comparative Evaluation, Gas Pollutant, Numerical, Gaussian, Industrial Flare.

### Introduction

Flare stacks are widely used in industrial plants for the disposal of combustible vent gases which are released during continuous routine plant operations, scheduled plant maintenance periods and unscheduled or emergency venting. Flares are one of the most pollutant sources due to combustion reactions, so their modeling and monitoring are very important and should be concerned especially in oil and gas manufacturing countries.

Air dispersion models vary from simple empirical models that offer conservative estimates of pollutant concentrations to more sophisticated numerical models. In general, dispersion models may be classified as semi-empirical, empirical, numerical and physical [1].

Currently, the so-called "Gaussian Plume" model is the basic method which is used for calculating ambient air pollutant concentrations due to a point source. The major weakness of the Gaussian plume type of models is that the wind speed and dispersion coefficients are assumed to be independent of height above the ground, and hence the boundary layer flow in the first several hundred meters near the surface of the earth is not simulated [1-3].

Some attempts have been made to model pollutants dispersion of stacks and flares with numerical methods. For instance, Ragland and Dennis [2] presented a point source atmospheric diffusion model with variable wind and dispersion coefficient profiles with finite difference method. Mohebbi and Baroutioan [3] developed a three dimensional diffusion

model to predict the concentration of PM10 from Kerman Cement Plant, Iran. Kahforoushan and Fatehifar [4] created a numerical model with finite difference method to evaluate and predict of air pollutions from a gaseous flare in an oil and gas processing area. In our previous work [5] a three dimensional numerical model of gas pollutants dispersion from refinery flares with variable wind and dispersion profiles was developed. The effect of input parameters such as surface roughness, atmospheric stability classes, wind velocity, flow rate and other parameters were considered in the model.

In this work, a comparative evaluation of numerical and Gaussian models for gas pollutants dispersion from industrial flares is presented. Numerical model incorporates the finite volume method to estimate pollutant concentration from continuous sources. In this model different profiles for wind velocity and dispersion coefficients, depending on atmospheric stability classes were used. Surface roughness is also considered in the modeling. Pollutant concentrations predicted by model are compared to those predicted by the Gaussian plume model which assumes constant wind and dispersion coefficients with respect to the vertical direction.

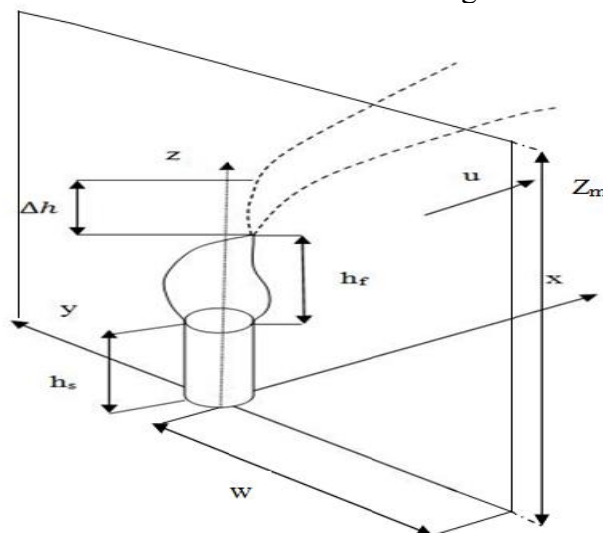
### **Modeling**

#### **Numerical Model**

The well-known advection-diffusion equation describes the transfer and diffusion of pollutants which is represented in Cartesian coordinates as:

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} = \frac{\partial}{\partial y} \left( K_y \frac{\partial C}{\partial y} \right) + \frac{\partial}{\partial z} \left( K_z \frac{\partial C}{\partial z} \right) + S + Q \quad (1)$$

$t$  is the time,  $x$  is the wind direction,  $y$  is vertical to the wind direction in the horizontal plane,  $z$  is the vertical axis,  $u$  is wind speed in direction  $x$ ,  $C$  is mean pollutant concentration,  $K_y$  and  $K_z$  are the dispersion coefficients in direction  $y$  and  $z$  respectively,  $Q$  is the chemical and photochemical reaction of pollutant and  $S$  is the emission rate. Scheme of a flare in Cartesian coordinates with symbols used in the model are shown in figure 1.



**Figure 1. Scheme of a flare in Cartesian coordinates.**



By considering the flare as a continuous point source, the steady-state assumption is applied so, unsteady state term is omitted from equation 1. The main assumptions commonly used in advection-diffusion equation are:

- 1- Diffusion in direction x is ignored, because the wind velocity is only in x direction and convection in this direction is very larger than diffusion.
- 2- In the surface layer (50 to 100 m above ground) the wind profile is considered logarithmic, for the upper layer (mixing layer) an exponential profile is considered.
- 3- The pollutants emitted from flares in the atmosphere are not reactive, so there is no any reaction between pollutants.

By applying these assumptions, the equation 1 can be written as:

$$u \frac{\partial C}{\partial x} = \frac{\partial}{\partial y} \left( K_y \frac{\partial C}{\partial y} \right) + \frac{\partial}{\partial z} \left( K_z \frac{\partial C}{\partial z} \right) + S \quad (2)$$

### ***Solution of numerical model***

The finite volume method incorporating power law scheme was used for solving equation 2, the boundary conditions are as follow:

$$\begin{aligned} \text{at } x = 0 \quad C(0, j, k) &= 0 \\ \text{at } y \rightarrow \pm w \quad \frac{\partial C}{\partial y} &= 0 \\ \text{at } z = 0 \quad \frac{\partial C}{\partial z} &= 0 \\ \text{at } z \rightarrow z_m \quad \frac{\partial C}{\partial z} &= 0 \end{aligned} \quad (3)$$

To solve equation 2 with this method the domain of problem is divided into small elements with  $\Delta x$ ,  $\Delta y$  and  $\Delta z$  dimensions. General solution of equation 2 for a element which is located at point (i,j,k) is written as follows:

$$\begin{aligned} & \left( u_w \Delta y \Delta z + \frac{k_{y_n} \Delta x \Delta z}{(\delta y)_n} + \frac{k_{y_s} \Delta x \Delta z}{(\delta y)_s} + \frac{k_{z_t} \Delta x \Delta y}{(\delta z)_t} + \frac{k_{z_b} \Delta x \Delta y}{(\delta z)_b} \right) C_P \\ &= (u_w \Delta y \Delta z) C_W + \left( \frac{k_{y_n} \Delta x \Delta z}{(\delta y)_n} \right) C_N + \left( \frac{k_{y_s} \Delta x \Delta z}{(\delta y)_s} \right) C_S + \left( \frac{k_{z_t} \Delta x \Delta y}{(\delta z)_t} \right) C_T + \left( \frac{k_{z_b} \Delta x \Delta y}{(\delta z)_b} \right) C_B \end{aligned} \quad (4)$$

In order to solve equation 2 for all elements simultaneously, a MATLAB program was written, which solves equation 2 for all elements simultaneously with using method of TDMA (TRI Diagonal Matrix Algorithm) [7]. Considered control is displayed in figure 2.

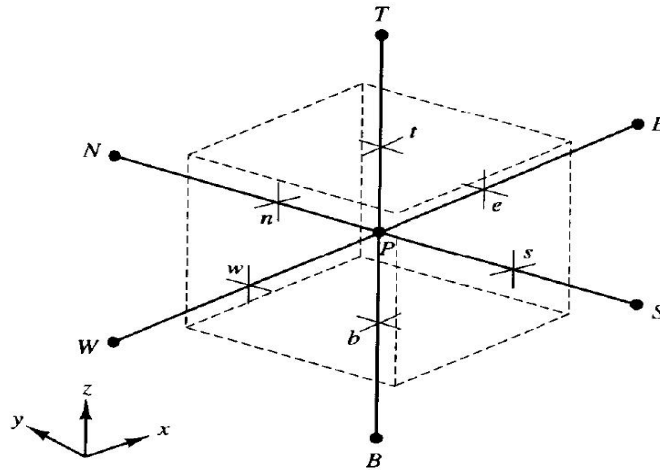


Figure 2. Selected control volume and coordinates.

### Wind Speed and Dispersion Coefficient Profiles

To obtain pollutant concentrations from equation 2, wind speed and dispersion coefficients profiles must be determined, Thus profiles and also other necessary parameters for obtaining them are discussed in following sections.

Wind speed and dispersion coefficient profiles which used in this model are summarized in table 1 [1]. Two layers are considered, the surface layer which extends up to approximately 100 m and the mixing layer which extends up to 1000 m or more.  $u_{sl}$  is wind speed at the top of the surface layer ( $Z_{sl}$ ), and  $Z_m$  is taken at the end of mixing layer. According to the table 1, a log type profile was used for wind speed within the surface layer, and in the layer ( $Z_{sl}$  to  $Z_m$ ), a linear profile was used.

In table 1,  $L$  is atmospheric parameter, with unit of length, and is calculated by:

$$L = \frac{u_*^3 C_p \rho T}{kgH} \quad (5)$$

Table 1. Dispersion coefficients and wind speed profiles for neutral atmosphere [1].

Vertical distance	Wind speed $u$	Eddy diffusivity $K_y, K_z$
$0 < z \leq z_{SL}$	$\frac{u_*}{0.4} \ln\left(\frac{z+z_0}{z_0}\right)$	$K_z = 0.4u_*z$ $K_y = 5K_z$
$Z_{SL} < z \leq z_m$	$(u_g - u_{SL})\left(\frac{z - z_{SL}}{z_m - z_{SL}}\right) + u_{SL}$	$K_z = 0.4u_*z_{SL}$ $K_y = 5K_z$



Where  $u_*$  is the mixing friction velocity,  $H$  is the net heat flux to the atmosphere,  $\rho$  is ambient air density,  $C_p$  is specific heat,  $T$  is temperature,  $k$  is Karman's constant ( $k=0.4$ ) and  $g$  is gravitational constant.  $u_*$  is calculated by following equation :

$$u_* = c_g u_g \quad (6)$$

$u_g$  is geostropic wind and is a more universal parameter, independent of terrain. The  $c_g$  is geostropic drag coefficient, a function of the Rossby surface number and  $L$ , in which Rossby surface number is calculated as:

$$R_0 = \frac{u_g}{Z_0 f} \quad (7)$$

Where  $f$  is Coriolis parameter of the earth, and  $Z_0$  is the surface roughness. Values of  $Z_0$  for different type of terrains and atmospheric stability classes are presented in Lettau [6].

### **Plume Rise**

Many equations and mathematical models have been proposed for calculating the rise of stack gas plumes [1-6]. Some of the proposed models are empirical while others have some theoretical basis. In the United States, the following equations and models for the rise of buoyant stack gas plumes have all been used to some extent: the Holland equations, the ASME equations, the TVA equation, and the Brigg's equations [1].

In this paper, all calculations are based on the Brigg's equation, this does not constitute a value judgment that Briggs's equations are more valid than the other equations which have been proposed and used. It just reflects the fact that the U.S EPA and many others have adopted Brigg's equations for use in their stack gas dispersion models.

Based upon a dimensional analysis of the variables involved as well as a theoretical analysis, Briggs developed a set of plume rise equations for bent-over, hot buoyant plumes which then correlated and compared with various field observations and data. Subsequently, Brigg modified those equations in 1971 and again in 1972. The first and most common set of Brigg's equations are 1969 version of his equations that are written as follows [1]:

$$\Delta h = 1.6F^{\frac{1}{3}}x^{\frac{2}{3}}u^{-1} \quad (8)$$

In equation 9,  $\Delta h$  [m] represents plume rise for first and transitional stages,  $x$  [m] is downwind distance from stack,  $u$  [m/s] indicates wind velocity and  $F$  [ $m^4/s^3$ ] is buoyancy parameter.

### **Flame Length**

The combusted gas plume rise from a flare stack is defined as starting at the end of the visible flame, so having defined the end or the tip of the flame as the starting point for the flare stack plume rise equations, estimating the flame length is needed to establish the vertical and horizontal location of flame tip.

An API publication [1] provides a plot of flame length as a function of the flared gas heat release obtained from large-scale, flare tests. The API correlation's line for their data can be expressed as:

$$L_f = 0.0042Q_c^{0.478} \quad (9)$$

Herein,  $L_f$  is flame length in ft and  $Q_c$  is flared gas heat release in Btu/hr.



With the Assumption that the flame is tilted  $45^\circ$  from the vertical the vertical height vector of a flare stack flame becomes:

$$h_{fv} = L(\sin 45^\circ) = 0.707 L \quad (10)$$

### **Effective Stack Height**

The plume centerline height or effective stack height ( $H_e$ ) for the gas plume is:

$$H_e = h_s + h_{fv} + \Delta h \quad (11)$$

### **Gaussian model**

The Gaussian equation for calculating concentration of pollutants at a selected point ( $x,y,z$ ) in the downwind direction from an elevated point source is as follows [1-5] :

$$C = \frac{Q}{2\pi u \sigma_y \sigma_z} \left[ -\left( \frac{y^2}{2\sigma_y^2} + \frac{(z-H)^2}{2\sigma_z^2} \right) \right] \quad (12)$$

In this equation,  $\sigma_y$  and  $\sigma_z$  are horizontal and vertical dispersion coefficients respectively,  $u$  is wind velocity at stack top,  $Q$  is emission rate (g/sec) and  $H$  is effective stack height which is calculated by equation (11). In this model, wind velocity and dispersion coefficients are constant and independent from height above ground. Dispersion coefficients were obtained from Turner equations for rural terrain and Gifford equations for urban terrain [1-3].

### **Results and Discussion**

Typical values of the applied parameters in the models are given in table 2. Surface roughness are chosen as  $Z_0=0.03m$  and  $Z_0=0.5m$  for the numerical model which these amounts are representative values for rural and urban terrains, respectively.

**Table 2. Typical values of applied parameters in numerical and Gaussian models.**

<b>He (m)</b>	<b>S(g/s)</b>	<b>Z<sub>m</sub>(m)</b>	<b>Z<sub>s1</sub>(m)</b>	<b>Mean wind velocity (m/s)</b>	<b>Δx (m)</b>	<b>Δy(m)</b>	<b>Δz(m)</b>
85	1	275	75	2	10	15	10

Ground level concentrations in different atmospheric classes and rural terrain, obtained from numerical and Gaussian models are shown in figures 3 and 4, respectively.

Maximum value of ground level concentrations of numerical model agrees well with results of Gaussian model, but because of taking account the surface roughness in numerical model, distribution profile of concentration differs from each other in two models.

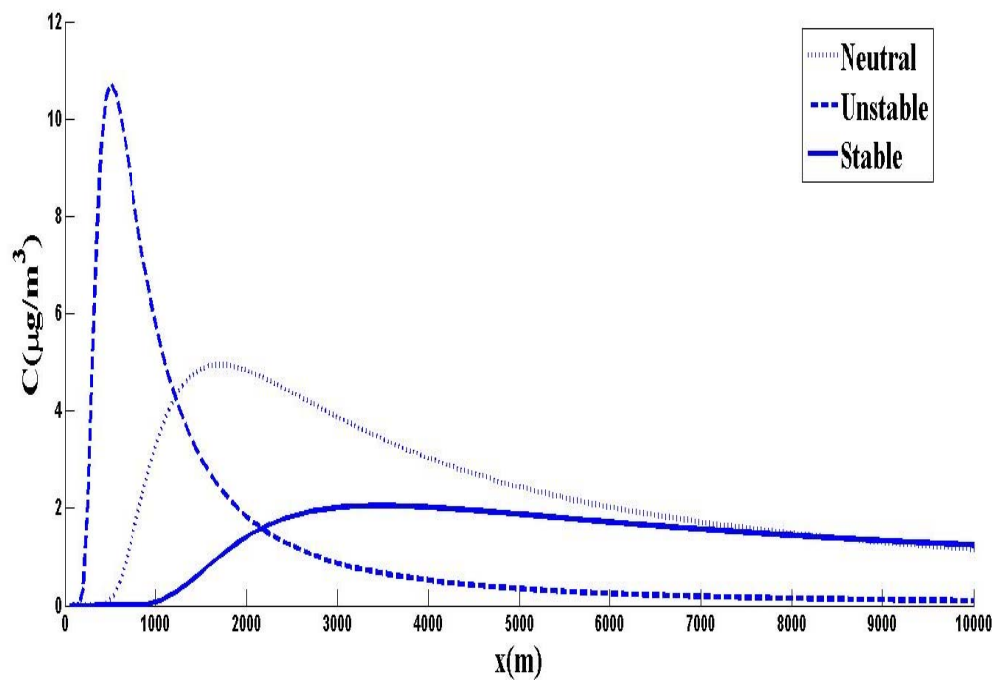


Figure 3. Ground level concentrations in different stability conditions for surface roughness parameter ( $Z_o=0.03$  m) obtained from numerical model.

In the proposed numerical model, due to considering the effect of turbulence in calculations, the maximum ground level occurs closer to the source especially in neutral and stable atmospheric conditions than Gaussian model. Moreover, the concentration profiles are narrower in numerical model which means the profiles spread faster in this model.

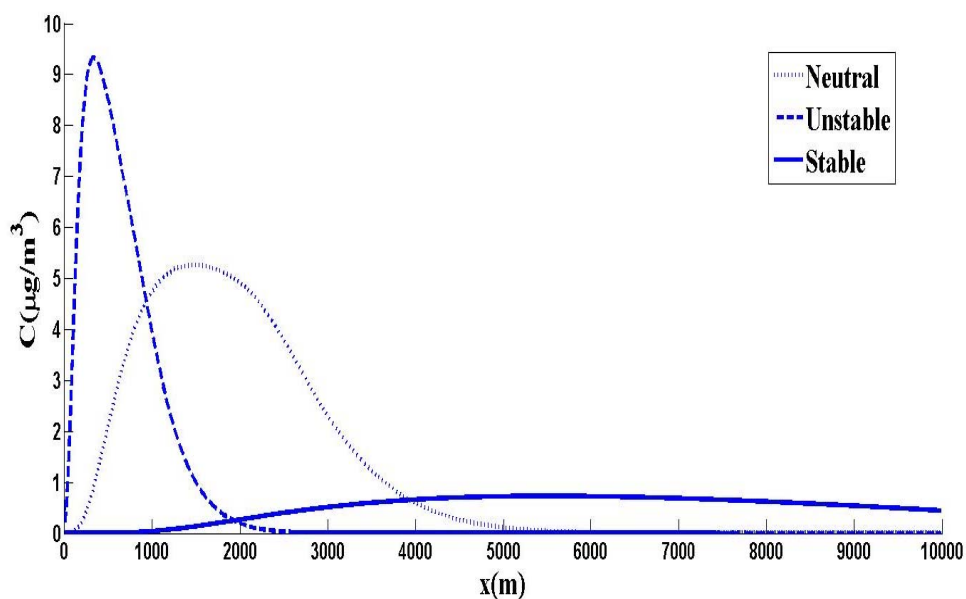


Figure 4. Ground level concentrations in different stability conditions obtained from Gaussian model with rural dispersion coefficients.



The concentration distributions in rural and urban terrains for two models are shown in figures 5 and 6. The surface roughness values of 0.03 and 0.5m were used for rural and urban terrains respectively in numerical model.

As it shown in figure 5, by increasing the surface roughness from 0.03 to 0.5m, the maximum ground level concentration reduces and shifts closer toward the flare location. However, in Gaussian model, as seen in figure 6, the maximum concentration for urban terrain shifts closer toward the source point, but its value is much larger than that of rural terrain.

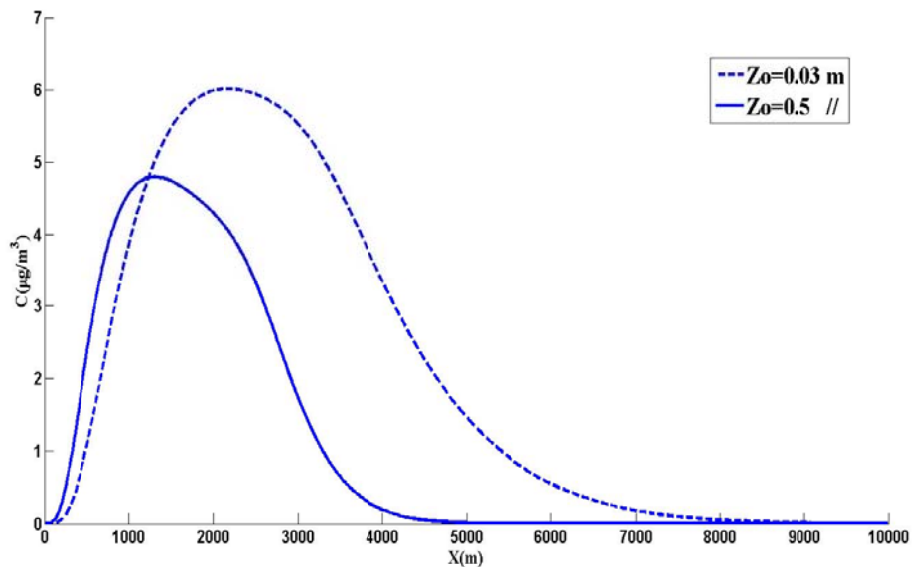


Figure 5. Ground level concentrations for two surface roughness parameters, numerical model in neutral stability conditions.

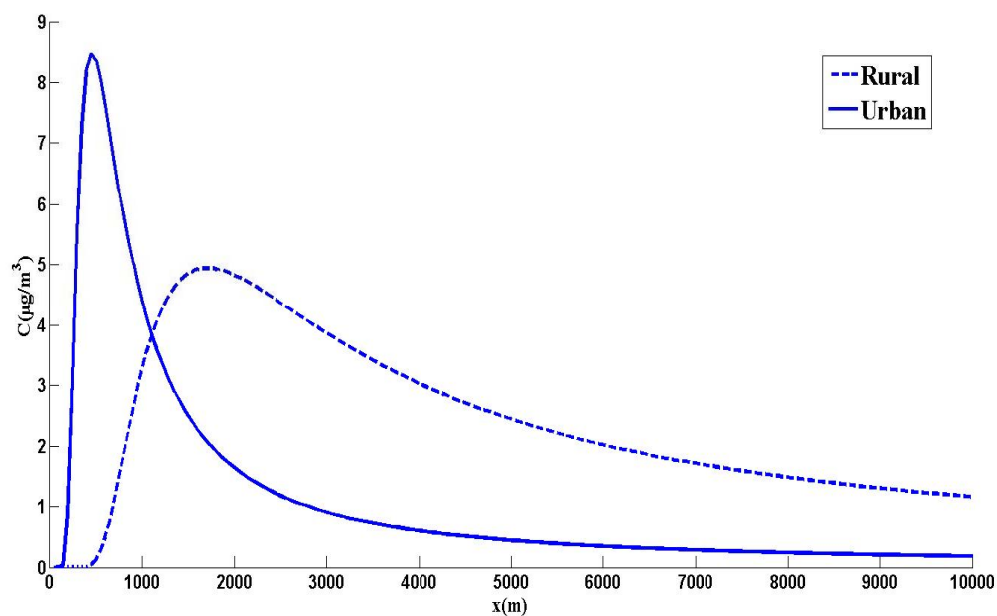


Figure 6. Ground level concentrations for urban and rural terrains, Gaussian model in neutral stability conditions.





### **Conclusions**

The maximum concentration ground level obtained from proposed numerical model agrees well with those of Gaussian model especially in neutral and stable conditions. However, the distribution of concentration profile differs significantly in both models, since the effects of surface parameters on wind and dispersion coefficients are taken account in the numerical model. By increasing the surface roughness and consequently increasing the turbulency, the maximum ground level concentration decreases and occurs at the closer position from the source in the numerical model. In the Gaussian model, although the maximum ground level concentration is closer to the source for urban terrain than rural, its value is much larger.

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