Modeling Pollutant Dispersion from Petroleum Refining Process in Sri Lanka

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Abstract

Air pollution is a major problem in Sri Lanka due to rapid urbanization and development of industries. In Sri Lanka, the quality of air has a profound impact on the economy. The most obvious of these impacts is related to health problems associated with poor air quality and the corresponding cost of medical care and treatment. Over the last 15 years, the demand for petroleum products has risen at an annual average rate of about 5%. Therefore it is important to build air quality models, which are mathematical descriptions of the concentration of pollutants.

In this study the dispersion of air pollutants of petroleum refinery process in Sapugaskanda, Sri Lanka was modeled using two dimensional advection-diffusion equations. The finite difference method was used to solve the problem. The pollutant dispersion of Carbon Dioxide, Nitrogen Dioxide and Sulphur Dioxides was studied. The effects of parameters such as wind velocity and stack height were investigated. Simulation was carried out using a C program. A MATLAB program was applied to visualize the result. According to the study, dispersion pattern of pollutants showed that the extent of diffusion is dependent of meteorological conditions such as wind speed and source characteristics.

Keywords: simulation, pollutants dispersion, mathematical modeling, diffusion

Introduction

Air pollution is now becoming a critical issue in both developed and developing countries. This issue has been seriously emerged in Sri Lanka with no difference in other Asian countries. Sri Lanka is witnessing a significant increase in the level of ambient air pollution due to urbanization and increasing levels of industrialization. The main ambient pollutants are being identified as Carbon Dioxide (CO2), Carbon Monoxide (CO), Nitrogen Oxides (NO), Sulphur Dioxides (SO2) and Lead (Pb). Those kinds of pollutants come from the vehicles exhausts, industrial emissions, petroleum refinery process and thermal power plants. In Sri Lanka, quality of the air has profound impacts on the economy as well. The most obvious of these impacts is related to health problems (Nandasena, Wickremasinghe, & Sathiakumar, 2012) associated with poor air quality and the corresponding cost of medical care and treatments. Therefore it is important to build and use air quality models, which are mathematical descriptions in concentration of mixture of ambient pollutants. Over the last 15 years, the demand for petroleum products has risen at an annual average rate of about 5% (Ministry of Petroleum Industries, 2014). The current annul requirement of crude oil in the country stands at around 2 Million MT.

Air quality modeling experts have made significant progress in recent years in developing new methods to meet the challenges of simulating long-range pollutant transport. Simulation of pollutant dispersion using a Gaussian model (Abdulkareem, 2005; Melli & Runca, 1979; Zannetti, 2003) has been explained in many applications. This model is commonly applied due to its straightforwardness, ease of use and results gained by it seem to be reasonable. However some studies have shown some weak points like the effect of wind velocity is not included, no chemical reactions, time independent and no gravitational fallout. The flow around the obstacles such as buildings, trees and other natural roughness elements influence the dispersion of pollutants. Gaussian model is not capable to represent the flow around the obstacles. Therefore it is important to build air quality models based on computational fluid dynamics (Al-Adwani, 2007; Ibrehem & Talib, 2012; Madala, Satyanarayana & Prasad, 2012) which include those effects are good alternative to represent complex systems.

This paper presents a study of pollution dispersion from Sapugaskanda petroleum refinery stacks in Sri Lanka. Sapugaskanda is situated in Western Sri Lanka which is a suburb area in Colombo the capital city. Refinery is located much closer to the sea. The main harbor is also located in Colombo. Refinery has 11 stacks and gaseous pollutants like Carbon Dioxide (CO2), Nitrogen Oxide (NO) and Sulphur Dioxides (SO2) are present in their emissions. During March to November wind comes from sea side (South West direction) and it takes the polluted air towards the country side. Once the pollutants are generated, they get transported in the atmosphere by movement of air. In general, their movement is governed by a host of factors including meteorological conditions, and the nature of the pollutant.

The objective of this study is to identify pollutant dispersion from petroleum refinery stacks. First, pollutant dispersion from a stack was considered. The advection-diffusion equation was used. The domain was considered as a staggered grid. Then the equation was discredited.

Finally, the concentration of pollutant was simulated at the grid points. For this purpose, a C program (Griebel, Dornseifer, & Neunhoeffer, 1998) was written and MATLAB program was applied for visualizing the results. The program was then modified in order to simulate multiple refinery stacks. The effects of meteorological parameters such as wind and temperature and stack characteristic on pollutant dispersion were discussed.

Mathematical Modeling

The concentration CS of each pollutant substance S, satisfies its own advection-diffusion (Griebel, Dornseifer, & Neunhoeffer, 1998) equation of the form,

$$\frac{\partial C^S}{\partial t} + \vec{u}.\nabla C^S = \lambda_S \Delta C^S + Q(C^S) \, , \qquad (1)$$

where λ is a diffusion coefficient, $\vec{u}$ is wind velocity and Q is a source term. The adjective transport of the substance is described by the term $\vec{u}.\nabla C,$ and the uniform diffusive spreading in all directions, by the term $\lambda \Delta C$. As boundary conditions (Fatehifar, Elkamel, Taheri, Anderson, & Abdul-Wahab, 2007) Dirichlet condition ($C|\Gamma 1=0$) along the boundary segment Γ1, which the pollutant is being injected and homogeneous Neumann condition (($\partial C/\partial n)|\ \Gamma 2=0$), means normal derivative of the boundary segment Γ2 should vanish) along the remaining boundary Γ2, were imposed.
For simplicity several assumptions were made. They are, there are no pollutant reactions in the system, wind comes in South West direction from the sea side towards the country and no gravitational forces.
It was desirable to consider a large scale experiment in a scaled down and more manageable settings. Therefore dimensionless variables were considered as follows:

$$C^* := \frac{C}{c_0}, \quad \vec{x}^* := \frac{\vec{x}}{L}, \quad \vec{u}^* := \frac{\vec{u}}{u_0}, \quad t^* := \frac{tu_0}{L} \, , \qquad (2)$$

where c0, u0, and L are scalar constants. Recasting equation (1) in the variables (2) leads to the equation

$$\frac{\partial C^{*S}}{\partial t^*} + \vec{u}^* . \nabla C^{*S} = \frac{\lambda_S}{u_0 L} \Delta C^{*S} + \frac{Q(C^S)\, L}{u_0 c_0} \, . \qquad (3)$$

Position of the refinery, height and the width of the selected domain are illustrated in Fig. 1. The selected domain was considered as a staggered grid.

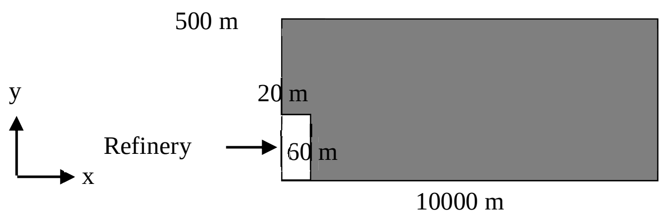

Figure 4: Selected domain for the simulation.

The finite difference method was used to solve the mathematical model numerically. Equation was discretized considering a staggered arrangement. Expressed the derivatives using the counters i for the x-direction, j for the y-direction and thus the discrete terms of the equation (3) are given by:

$$\left[\frac{\partial C^{*S}}{\partial t^*}\right]_{i,j}^{(n+1)} = \frac{1}{\delta}\left(C_{i,j}^{*S(n+1)} - C_{i,j}^{*S(n)} \right) \, , \qquad (4)$$

$$\left[\frac{\partial C^{*s}}{\partial x^{*}}\right]_{i,j} = \frac{1}{2\delta x}\left(C^{*s}_{i+1,j} - C^{*s}_{i-1,j}\right), \quad (5)$$

$$\left[\frac{\partial C^{*s}}{\partial y^{*}}\right]_{i,j} = \frac{1}{2\delta y}\left(C^{*s}_{i,j+1} - C^{*s}_{i,j-1}\right), \quad (6)$$

$$\left[\frac{\partial^2 C^{*s}}{\partial x^{*2}}\right]_{i,j} = \frac{1}{\delta x^2}\left(C^{*s}_{i+1,j} - 2C^{*s}_{i,j} + C^{*s}_{i-1,j}\right), \quad (7)$$

$$\left[\frac{\partial^2 C^{*s}}{\partial y^{*2}}\right]_{i,j} = \frac{1}{\delta y^2}\left(C^{*s}_{i,j+1} - 2C^{*s}_{i,j} + C^{*s}_{i,j-1}\right). \quad (8)$$

Here, values of wind speed and diffusion coefficient are presumed known. The stability condition (Griebel, Dornseifer, & Neunhoeffer, 1998) for the system is:

$$\delta t < \frac{c_0 L}{2\lambda}\left(\frac{1}{\delta x^2} + \frac{1}{\delta y^2}\right)^{-1}. \quad (9)$$

Wind Velocity

The wind profile power law was used to adjust the wind speed at different height. The wind profile power law relationship is:

$$u = u_r\left(\frac{y}{y_r}\right)^{\alpha}, \quad (10)$$

where u is the wind speed at height y, and ur is the known wind speed at a reference height yr. The exponent (α) is an empirically derived coefficient that varies dependent upon the stability of the atmosphere. For stable conditions, α is approximately 1/7 (Zannetti, 2003).

Plume Rise

The effective stack height H is not only the physical stacks' height hs but include also the plume rise δh,

$$H = hs + \delta h. \quad (11)$$

Plume rise is actually calculated as the distance to the imaginary centerline of the plume rather than to the upper or lower edge of the plume. Therefore the stack height (Zannetti, 2003) used in the calculations must be the effective stack height. Holland's equation is used for prediction of plume rise.

$$\delta h = \frac{v_s D}{u}\left(1.5 + 2.68\times 10^{-3} PD\frac{(T_s - T_a)}{T_s}\right). \quad (12)$$

Where, vs is stack exit velocity (ms-1), D is stack diameter (m), u is wind velocity (ms-1) measured or calculated at the height hs, P is pressure (mbar), Ts is stack gas temperature (K) and Ta is atmospheric temperature (K). In order to get the better predictions modify Holland's equation (Fatehifar, Elkamel, Taheri, Anderson, & Abdul-Wahab, 2007) was used. The modified Holland's equations are shown below:

$$\Delta h = \begin{cases} \delta h(\text{Holland Eq.}) - 32.42 + 0.8576\, hs, & hs < 35, \\ \delta h(\text{Holland Eq.}) - 10.1527 + 0.3135\, hs, & 35 \le hs < 80, \\ \delta h(\text{Holland Eq.}) + 12.39 + 0.17\, hs, & 80 \le hs. \end{cases} \quad (13)$$

The Algorithm

The pollutant dispersion from one refinery stack was considered first. The simulation process is broken down to the following steps.

The inputs to the C program were selected as meteorological data, stack characteristics and the domain details.

Calculated δh and exact place of pollutant entrance to the atmosphere.

The term Q was considered at the grid points where the stacks are positioned. This term is zero for all other cells.

Simulated the concentration of each pollutant at grid points.

The two dimensional steady state solutions were obtained for simplicity.

The results are visualized graphically using MATLAB.

The program was then modified in order to incorporate the simulation of pollutant dispersion from a multiple stacks. The only difference was the inclusion of multiple Q terms.

Results and Discussion

The effects of meteorological conditions such as wind velocity, air temperature and dispersion coefficient on pollutant dispersion were obtained. Fig. 2 shows the effect of wind velocity on pollutant dispersion and Fig. 3 shows the effect of wind velocity on ground level concentration. According to the Fig. 2 and Fig. 3 pollution dispersion decreases when the wind velocity increases. Pollutants go far away from the stack region and increase the upper levels concentration. Looking at Fig. 4, it can be seen that the effect of stack height on pollution dispersion. If we increased the height of the stack, pollutants go far away from the stack and decrease the ground level concentration. Fig. 5 illustrates the maximum concentration distribution of CO2 from a one stack with distance.

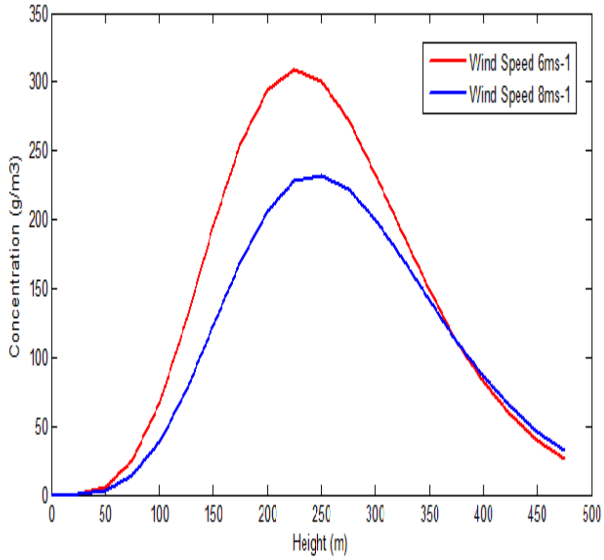

Figure 2: CO_2 concentration distribution

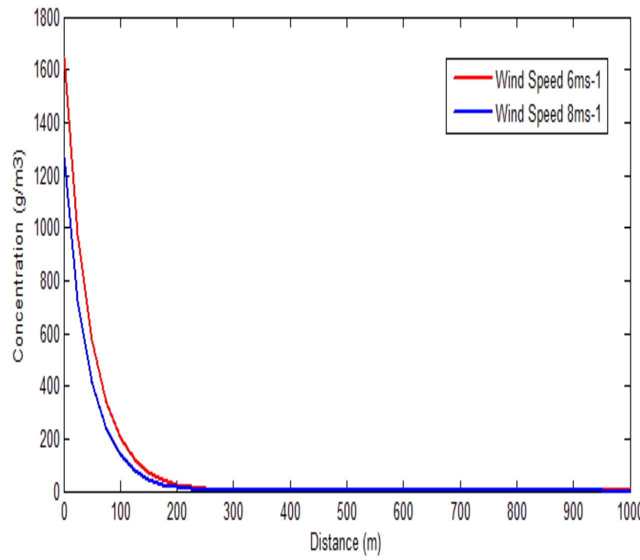

Figure 3: CO_2 concentration distribution at ground level, wind speed 6ms-1 and 8ms-1.

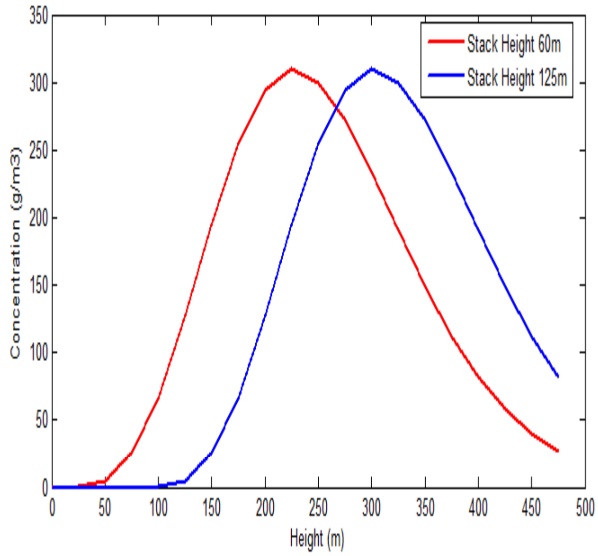

Figure 4: CO_2 concentration distribution at distance = 300m, stack height 60m and 125m.

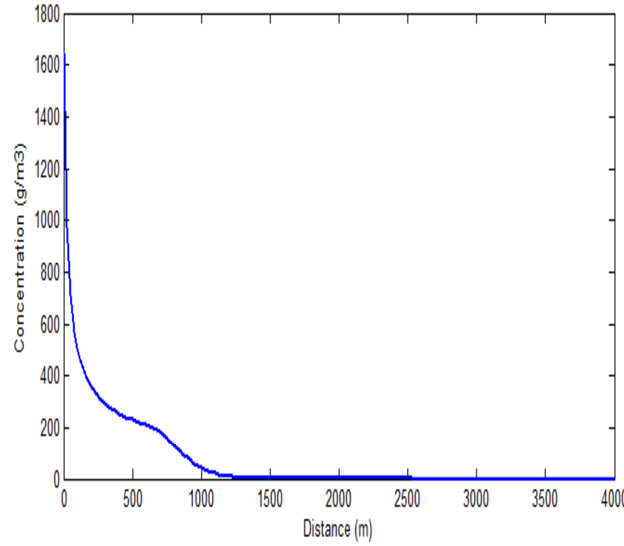

Figure 5: Maximum CO2 concentration distribution vs. distance.

Figures 6 to 11 shows the contour plots and the surface plots of pollutants considering all the stacks in the area.

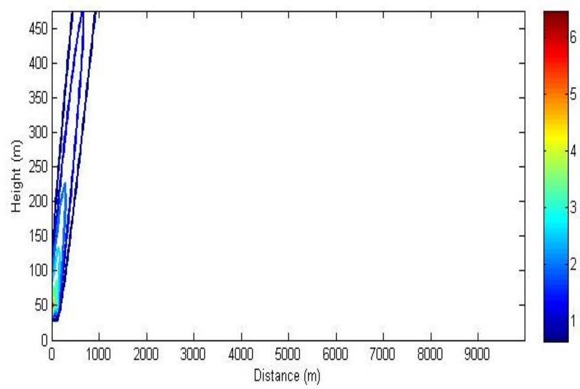

Figure 6: Contour plot of CO2 considering all the stacks.

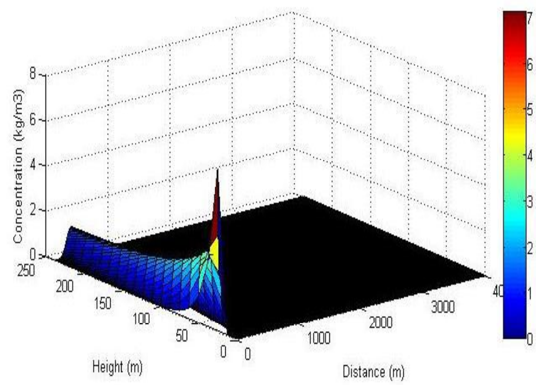

Figure 7: CO_2 concentration distribution considering all the stacks.

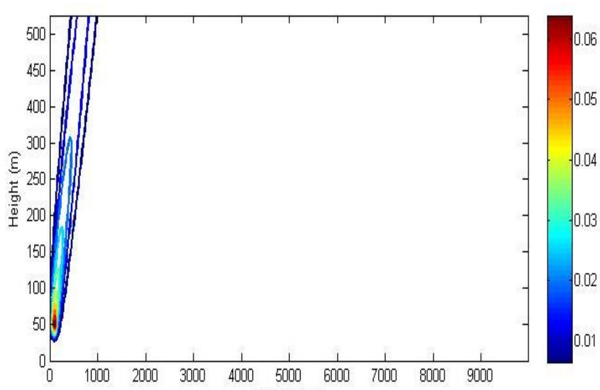

Figure 8: Contour plot of SO_2 considering all the stacks.

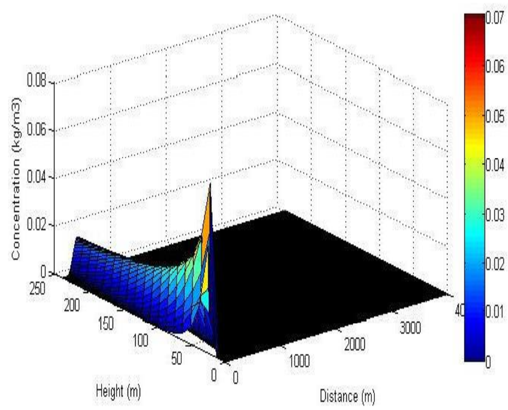

Figure 9: SO_2 concentration distribution considering all the stacks.

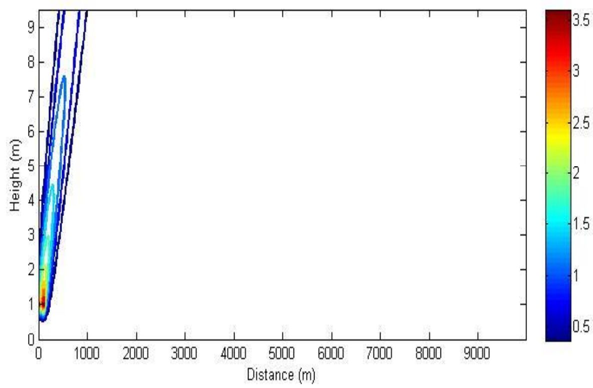

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Figure 10: Contour plot of NO_2 considering all the stacks.

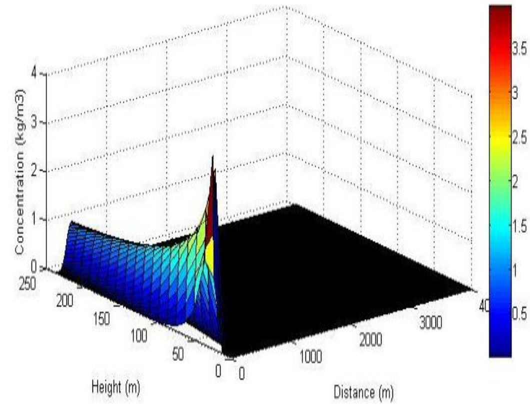

Figure 11: NO_2 concentration distribution considering all the stacks.

Conclusions

In this study, a two dimensional simulation of pollutant dispersion from Sapugaskanda petroleum refinery process were presented. For solving mathematical model, finite difference method was used and a C program was written. The effects of different meteorological parameters such as wind velocity on pollutant dispersion, height of the stack were analyzed. The results show that the dispersion of pollutants is inversely proportional to the wind velocity. Also the source characteristics were studied. Increasing the stack height pollutants go to the upper atmospheric layer and dispersion takes place over a large area and it decreases the ground level concentration. This type of simple model has many limitations. The effect of gravitation, effect of Beyoncé forces, effects of wind velocity change in the domain were not considered.
Therefore in future we would implement a more advance mathematical model considering the mass transfer, heat transfer and momentum changes with free boundary conditions.

References

Abdulkareem, AS 2005, 'Urban Air Pollution Evaluation in Computer Simulation: A Case Study of Petroleum Refining Company Nigeria', *Leonardo Journal of Sciences,* vol. 6, pp.17-28.

Al-Adwani, S 2007, 'A Hybrid Neural Network- Mathematic al Programming Approach to Design an Air Quality Monitoring Network for an Industrial Complex', A Thesis Submitted in partial fulfillment of the Requirements of University of Waterloo for the Master of Applied Science in Chemical Engineering. Canada: University of Waterloo.

Fatehifar, E, Elkamel, A, Taheri, M, Anderson, W. A & Abdul-Wahab, SA 2007, 'Modeling and Simulation of Multi Pollutant Dispersion from a Network of Refinery Stack Using a Multiple Cell Approach', *ENVIRON ENG SCI*, vol. 24, pp. 795-811.

Griebel, M, Dornseifer, T & Neunhoeffer, T 1998, 'Numerical Simulation in Fluid Dynamics: a Practical Introduction', *SIAM*.

Ibrehem, AS & Talib, N 2012, 'A Mathematical Model for Measuring Air Pollution of Power Plant', *Journal of Purity, Utility Reaction and Environment,* vol. 1(3), pp. 142-152.

Madala, S, Satyanarayana, ANV & Prasad VK 2012, 'Micro-Scale Dispersion of Air Pollutants Over an Urban Setup in a Coastal Region', *Open Journal of Air Pollution.* [online] 1. pp.51-58. Available from: http://www.SciRP.org/journal/ojap. [Accessed: 2 February 2014].

Melli, P & Runca, E 1979, 'Gaussian Plume Model Parameters for Ground-Level and Elevated Sources Derived from the Atmospheric Diffusion Equation in a Neutral Case', *Journal of Applied Meteorology*, vol. 18, pp. 1216-1221.

Ministry of Petroleum Industries 2014, 'Facts and Figures (Statistics), Petroleum Scenario', Retrieved from the Ministry of Petroleum Industries website: http://www.petroleummin.gov.lk.

Nandasena, S, Wickremasinghe, AR & Sathiakumar, N 2012, 'Air Pollution and Public Health in Developing Countries: Is Sri Lanka Different?', *Journal of the College of Community Physicians of Sri Lanka*. vol. 17(1), pp. 21-42.

Zannetti, P 2003, 'Air Quality Modeling: Theories, Methodologies, Computational Techniques, and Available Databases and Software', USA: EnviroComp Institute and Air & Waste Management Association.