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RESEARCH ARTICLE

SENSITIVITY ANALYSIS OF POLLUTANT DISPERSION FROM PETROLEUM REFINING PROCESS USING ADVECTION DIFFUSION EQUATION: A MATHEMATICAL MODELING APPROACH

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ABSTRACT

Air pollution is one of the most serious environmental problems in urban areas due to rapid development and starting of new industries. This salient hazard affects the human health and economy of the country. Mathematical models can be considered as one approach to identify the controlling measures of air pollution. These models consist of parameters which fluctuate with respect to external factors such as climate. Hence it is significant to recognize the dynamic behavior of air pollution model with respect to parameters. The two dimensional advection-diffusion equation is used to simulate the pollutant concentrations. Sensitivity equations are derived considering the variation of pollutant concentration with respect to parameters. Model equation and the sensitivity system are solved simultaneously using finite difference approximation. According to the study, the variation of pollutant concentration with respect to the parameters wind velocity and the diffusion coefficient are significant. When the velocity of wind doubled, it reduces the concentration of the pollutant in the ground level. But this pollutant air deposited in the highest places of the domain. These results reveal that considering different climatic periods and different zones, model parameters get dissimilar values. Hence, modifying air quality model season wise and area wise is important.

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INTRODUCTION

Air pollution is now becoming a worldwide problem and it is the world's largest single environmental health risk. According to the available records seven million people died annually as a result of air pollution exposure and it is the one in eight of total global deaths (WHO, 2014). This issue seriously immerged in Sri Lanka with no difference in other countries. Recent researches (G. D'Amato *et al*., 2010; Zannetti, 2003) reveal that rapid urbanization, industrialization, population density and traffic density have been warned the quality of air. The main ambient pollutants are Carbon Dioxide (CO_2), Carbon Monoxide (CO), Nitrogen Oxides (NO), Sulphur Oxides (SO) and Lead (Pb). This salient hazard has a reflective effect on the economy, well-being, health and life chances of human of the country. The records available in Sri Lanka reveal that air pollution causes a 7 percent increase in daily mortality, 30–35 percent in bronchitis and other respiratory diseases. Therefore understanding of pollutant dispersion patterns is needed and it is an essential task now a day. Mathematical models can be considered as a useful tool to understand dynamic behavior of pollutant dispersion and its control measures of air pollution. The air quality models consist of several parameters which vary with respect to external variables such as climate factors and human behavior. To study the controllability of the air pollution, it is necessary requirement that we need to have a good understanding about the sensitivity of air quality model with respect to parameters and includes those facts in to the mathematical model. There are two basic methods have been used to measure the sensitivity of the air quality model with respect to parameters. The first one is the direct (Hindmarsh and Serban, 2011) or forward method. In this simple technique, the sensitivity equations are derived from the model equations and solved simultaneously with the model equation. This method is very efficient for computing sensitivities of many functions with respect to few parameters. The second method is based on the Green's function or adjoint method (Duffy, 2009; Petzold and Li, 2004), in which the sensitivity coefficients are

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computed from integrals of the Green's function of sensitivity equations derived from the model equations. This method is efficient for computing sensitivities when it required finding the sensitivity of a few functions with respect to many parameters.

In this study, the sensitivity of pollutant dispersion model with respect to parameters is considered. For this purpose direct sensitivity analysis is applied to the pollutant dispersion model which is developed considering the oil refinery process in Sapugaskanda, Sri Lanka. Sapugaskanda is situated in the western part of the country which is a suburb area in Colombo. This refinery situated very nearer to the sea. Sapugaskanda has 11 refinery stacks and it emits Carbon Dioxide (CO_2), Nitrogen Dioxide (NO_2) and Sulphur Dioxides (SO_2) as the main pollutants.

Mathematical Model

The transport and diffusion of pollutant is described by the two dimensional *advection-diffusion* (Griebel *et al*., 1998) equation.

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

where C^S is the pollutant concentration of substance S, λ_s is a diffusion coefficient of substance S, $\vec{u}$ is wind velocity, t is the time and Q is the relevant source term of substance S. This equation is solved numerically subject to the initial and boundary conditions. As boundary conditions (Fatehifar *et al*., 2007) Dirichlet condition $(C|_{\Gamma_1} = 0)$ is applied along the boundary segment Γ_1, which the pollutant is being injected. For the other remaining boundaries Γ_2 homogeneous Neumann condition $\left((\partial C/\partial n)|_{\Gamma_2} = 0\right)$, means normal derivative of the boundary segment Γ_2 should vanish) are imposed. Initially assume that the pollutant concentration of the domain is zero.
Position of the refinery, height and the width of the selected domain are illustrated in Figure 1. The selected domain is considered as a staggered grid.

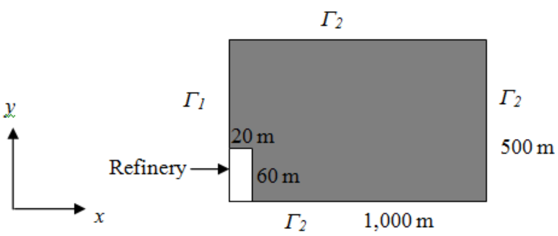

Figure 1. Selected domain for the simulation

For simplicity several assumptions are made. Namely, 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 is desirable to consider a large scale experiment in a scaled down and more manageable settings. Therefore, dimensionless variables are considered as follows:

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

where c_0, u_0 and L are scalar constants. Recasting equation (1) in the variables (2) leads to the equation

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

Dropping * this can be written in the following form

$$\frac{\partial C^S}{\partial t} + \vec{u}.\nabla C^S = \frac{\lambda_S}{u_0 L}\Delta C^S + \frac{Q(C^S)\,L}{u_0 c_0}. \tag{4}$$

Sensitivity Equation

The sensitivity of a model output to a parameter can be calculated as a partial derivative of the output with respect to the parameter p:

$$\frac{\partial\,(\text{model output})}{\partial\,(\text{model parameter})},$$

and it is called as the sensitivity coefficient (Perera, 2009; Yang *et al*., 1998) of the model. Usually model has several parameters, but we are interested in sensitivity with respect to single parameter at once. Therefore, we can treat one parameter after another while preserving the remaining ones fixed. Thus, imagine that the following theory depends only one parameter. Consider the boundary value problem,

$$\frac{\partial C}{\partial t} = f(t, c, c_x, c_y, c_{xx}, c_{yy}, p), \tag{5}$$

where p denote the parameter. Here c_x and c_y denote the first order partial derivatives with respect to x and y. Similarly c_{xx} and c_{yy} denote the second order partial derivatives with respect to x and y. When parameter p is replaced in (5) by $q = p + \; p$ another solution can be obtained, which is denoted by

$$\frac{\partial \hat{C}}{\partial t} = f(t, \hat{c}, \hat{c}_x, \hat{c}_y, \hat{c}_{xx}, \hat{c}_{yy}, q). \tag{6}$$

Now subtract (6) from (5) and apply Taylor series we get

$$\begin{aligned}\frac{\partial \hat{C}}{\partial t} - \frac{\partial C}{\partial t} &= f(t, \hat{c}, \hat{c}_x, \hat{c}_y, \hat{c}_{xx}, \hat{c}_{yy}, q) - f(t, c, c_x, c_y, c_{xx}, c_{yy}, p) \\ &= \frac{\partial f}{\partial C}(\hat{C} - C) + \frac{\partial f}{\partial C_x}(\hat{C}_x - C_x) + \frac{\partial f}{\partial C_y}(\hat{C}_y - C_y) + \frac{\partial f}{\partial C_{xx}}(\hat{C}_{xx} - C_{xx}) \\ &\quad + \frac{\partial f}{\partial C_{yy}}(\hat{C}_{yy} - C_{yy}) + \frac{\partial f}{\partial p}(q - p) + \textit{higher order terms}.\end{aligned}$$

Now introducing the sensitivity variable

$\sigma = \dfrac{\hat{C} - C}{q - p} = \dfrac{\partial C}{\partial p}$, and neglecting higher order terms, sensitivity equation can be obtained as

$$\frac{\partial\sigma}{\partial t}=\frac{\partial f}{\partial C}\sigma+\frac{\partial f}{\partial C_x}\sigma_x+\frac{\partial f}{\partial C_y}\sigma_y+\frac{\partial f}{\partial C_{xx}}\sigma_{xx}+\frac{\partial f}{\partial C_{yy}}\sigma_{yy}+\frac{\partial f}{\partial p}. \quad (7)$$

We consider the sensitivity of pollutant dispersion model with respect to parameters. Wind velocity and the diffusion coefficient are considered as the model parameters and obtained the sensitivity system for $\sigma_1 = \partial C/\partial u$ and $\sigma_2 = \partial C/\partial \lambda$ respectively. The selected initial and boundary condition are as follows:

Initial Condition: $\sigma = 0$

Boundary Conditions: $\sigma|_{\Gamma_1} = 0$, boundary where the pollutant is being injected and $(\partial\sigma/\partial n)|_{\Gamma_2} = 0$, remaining boundaries

Numerical Method

Both systems (4 and 7) are solved numerically using finite difference approximation. The equations are discretized at the grid points considering a staggered arrangement and replace the first and second order partial derivatives. Expressed the derivatives using the counters *i* for the *x*-direction, *j* for the *y*-direction and thus the discrete terms of the equation (4) are given by:

$$\begin{aligned}
\left[\frac{\partial C^S}{\partial t}\right]_{i,j}^{(n+1)} &= \frac{1}{\delta t}\left(C_{i,j}^{S(n+1)} \quad C_{i,j}^{S(n)}\right),\\
\left[\frac{\partial C^S}{\partial y}\right]_{i,j} &= \frac{1}{2\delta y}\left(C_{i,j+1}^{S} \quad C_{i,j-1}^{S}\right),\\
\left[\frac{\partial C^S}{\partial x}\right]_{i,j} &= \frac{1}{2\delta x}\left(C_{i+1,j}^{S} \quad C_{i-1,j}^{S}\right), \qquad (8)\\
\left[\frac{\partial^2 C^S}{\partial x^2}\right]_{i,j} &= \frac{1}{\delta x^2}\left(C_{i+1,j}^{S} \quad 2C_{i,j}^{S}+C_{i-1,j}^{S}\right),\\
\left[\frac{\partial^2 C^S}{\partial y^2}\right]_{i,j} &= \frac{1}{\delta y^2}\left(C_{i,j+1}^{S} \quad 2C_{i,j}^{S}+C_{i,j-1}^{S}\right),
\end{aligned}$$

where the subscript (*n*) denote the time level. Similarly we can approximate the derivatives of σ as (8). Only difference is replacing *C* by σ. The two dimensional steady state values are obtained as the solutions. For this purpose, a C program is written and MATLAB program is applied to visualize the results. Simulations are carried out considering a 1,000m width and 500m height domain. The stability condition (Griebel *et al*., 1998) for the (4) is:

$$\delta t = \frac{C_0 L}{2\lambda}\left(\frac{1}{\delta x^2}+\frac{1}{\delta y^2}\right)^{-1}. \qquad (9)$$

The Algorithm

The simulation algorithm of pollutant dispersion from petroleum refinery process can be described as follows:

1. Select climate data, stack characteristics and the domain details.
2. Assign the initial and boundary values for *C* and σ.
3. Calculate exact place of pollutant entrance to the atmosphere. The term *Q* is considered at the grid points where the oil refinery is positioned. This term is zero for all other cells.

4. Choose δt, δx and δy according to (9).

While $t < t_{max}$

Compute $C^{(n+1)}$ and $\sigma^{(n+1)}$ simultaneously.
$t := t + \delta t$

5. Obtain the two dimensional steady state solutions.

6. Visualize the result graphically using MATLAB.

RESULTS AND DISCUSSION

Figure 1 to Figure 5 show the pollutant concentration change with time considering the dispersion of CO_2. In Figures 1 to 3, the height is the same but the distances are different. In the Figures 1, Figures 4 and Figures 5, the distance is the same but the heights are different. The wind velocity increases the saturation time of the pollutant concentration decreases. When going inside the domain, the saturation time of the pollutant concentration increases. Similarly, when going up, the saturation time of the pollutant concentration increases. Figure 6 shows the effect of wind velocity on pollutant dispersion considering CO_2 in steady state. According to the Figure 6 the pollution concentration decreases when the wind velocity increases. That is wind speed is inversely proportional to the pollutant dispersion. Pollutants go far away from the refinery region and decrease the concentration of the pollutants. Figure 7 and Figure 8 shows the steady state vertical and horizontal pollutant concentration distribution of CO_2 at the end of the domain with different wind velocity. According to the graphs pollutants go far away from the refinery region and increase the upper levels concentration when the wind speed increases.

Figure 9 shows the effect on the CO_2 concentration in steady state due to wind velocity in a particular place (the distance is 125m away from the refinery and the height is 125m). Figure 10 shows the effect of wind on pollutants dispersion. For this purpose defined an arbitrary threshold value for the concentration and identify the effect of pollutant dispersion. In this case threshold value is equal to 82.345g/m^3. According to the Figure 10, pollutant dispersion increases when the wind velocity increases. Figure 11 to Figure 13 show the sensitivity of pollutant dispersion with respect to the wind velocity. The results are obtained in steady state. It can be noticed that the variation of pollutant with respect to the wind velocity is significant. Figure 14 to Figure 16 represent the sensitivity of pollutant dispersion of CO_2 with respect to the parameter dispersion coefficient in steady state. Looking at Figure 14 to Figure 16 can be seen that the variation of pollutant dispersion with respect to the dispersion coefficient is significant. According to the graph when the diffusion coefficient increases the pollutant dispersion also increases. Lower the dispersion coefficient yields lower pollution dispersion.

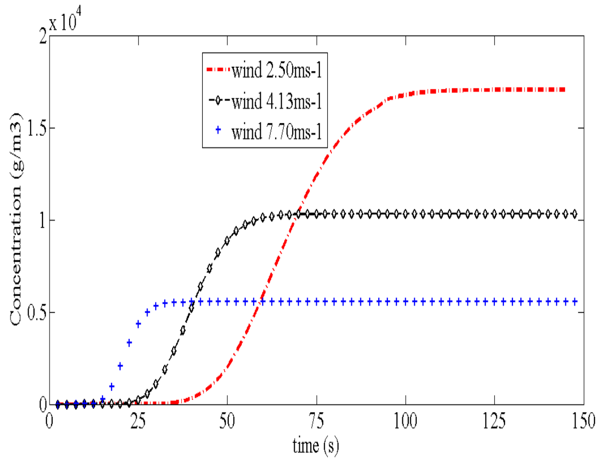

Figure 1. Pollutant concentration vs time, distance = 150m and height = 150m

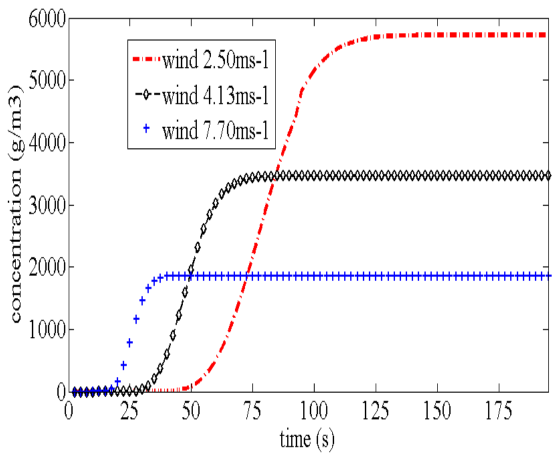

Figure 2. Pollutant concentration vs time, distance = 200m and height = 150m

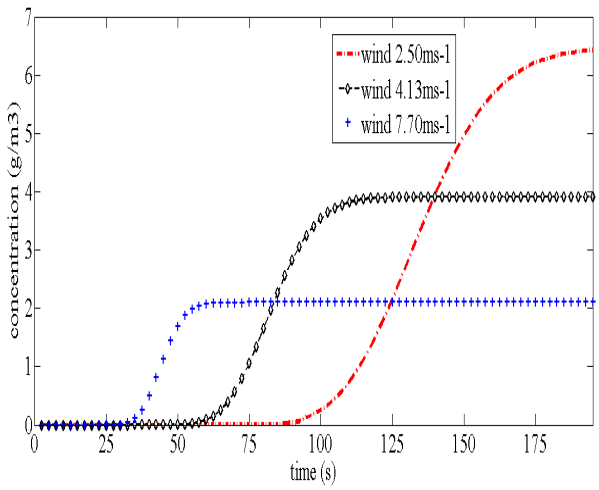

Figure 3. Pollutant concentration vs time, distance = 400m and height = 150m

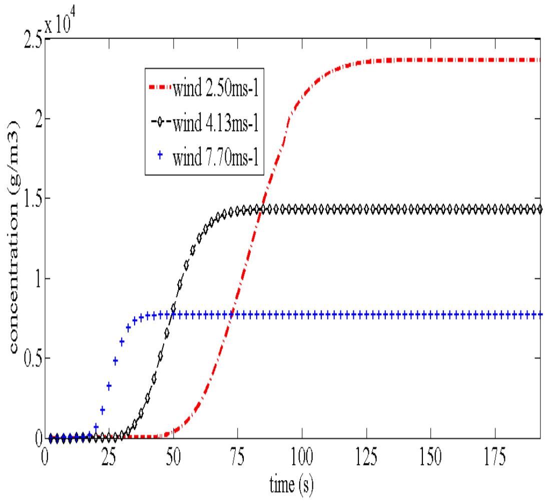

Figure 4. Pollutant concentration vs time, distance = 150m and height = 200m

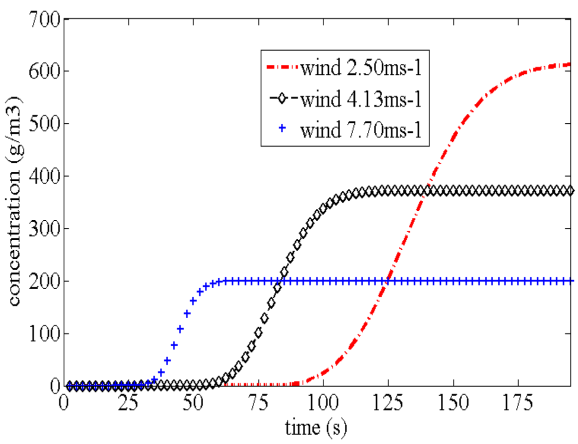

Figure 5. Pollutant concentration vs time, distance = 150m and height = 400m

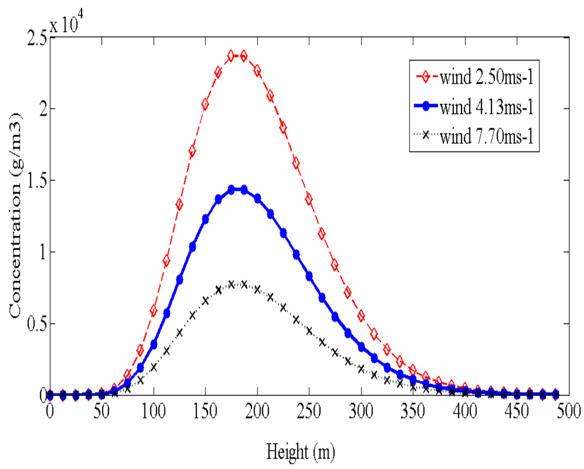

Figure 6. CO_2 concentration distribution at distance = 150m, wind speed 4.46ms^{-1}, 6.38ms^{-1} and 7.07 ms^{-1}

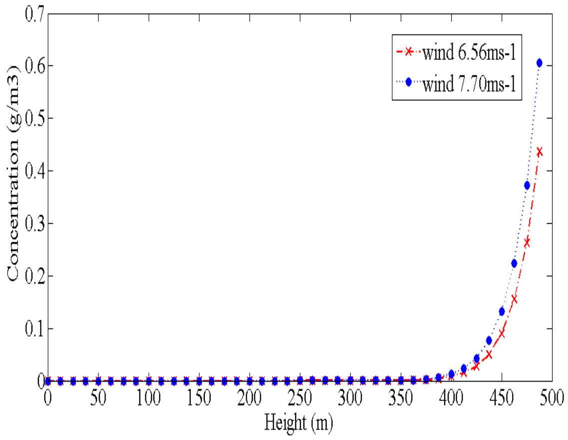

Figure 7. CO_2 concentration distribution at distance = 1,000m, wind speed 6.56ms^{-1} and 7.70ms^{-1}

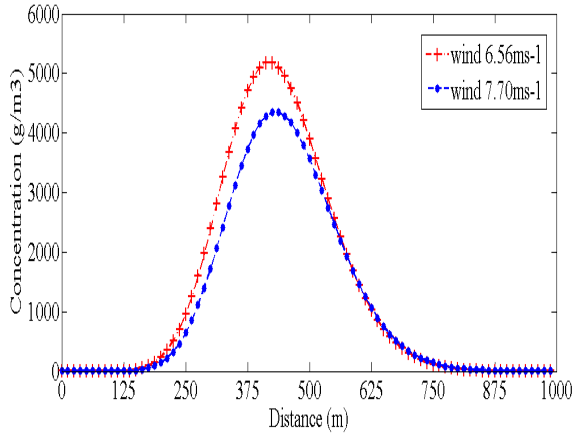

Figure 8. CO_2 concentration distribution at height = 500m, wind speed 6.56ms^{-1} and 7.70ms^{-1}

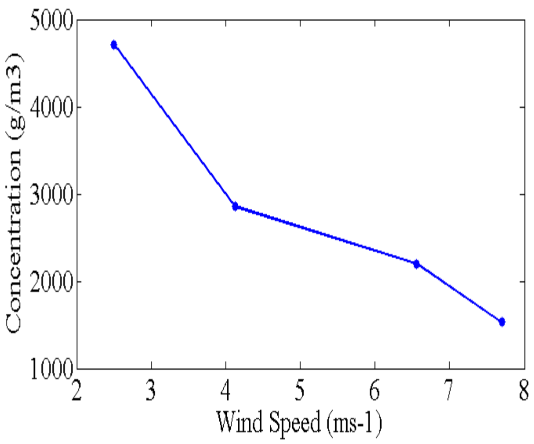

Figure 9. Effect of wind velocity on steady state pollutant concentration in a particular place, distance = 150m and height = 150m

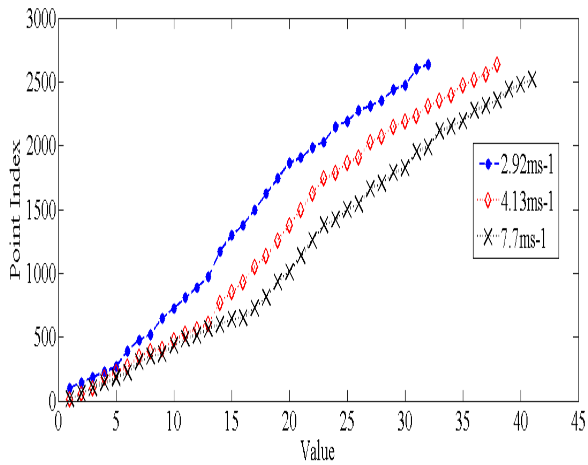

Figure 10. Effect of wind velocity on steady state pollutant dispersion considering and arbitrary threshold value

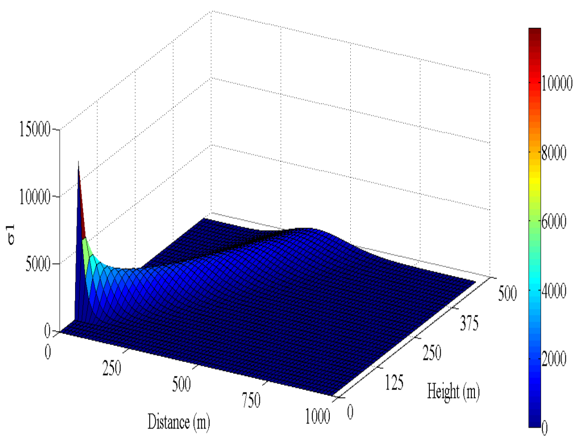

Figure 11. The steady state gradient of concentration with respect to the parameter wind velocity

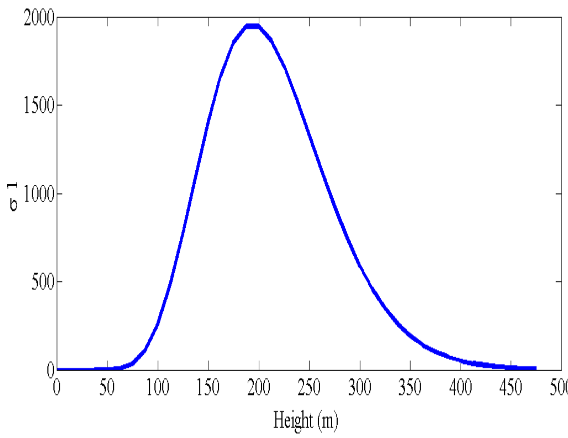

Figure 12. The steady state gradient of concentration with respect to the parameter wind velocity, distance = 150m

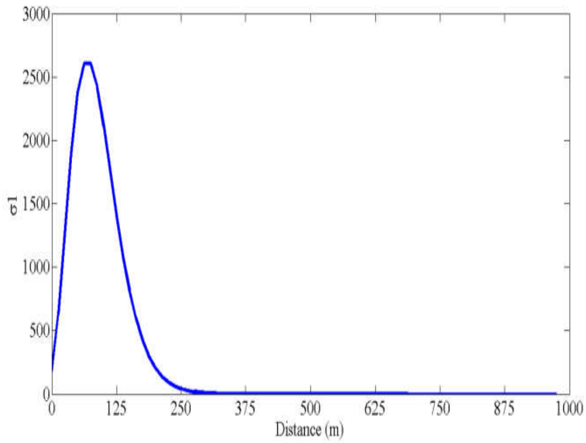

Figure 13. The steady state gradient of concentration with respect to the parameter wind velocity, height = 150m

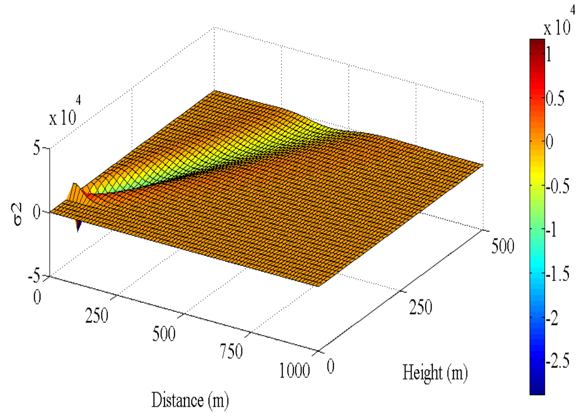

Figure 14. The steady state gradient of concentration with respect to the parameter diffusion coefficient

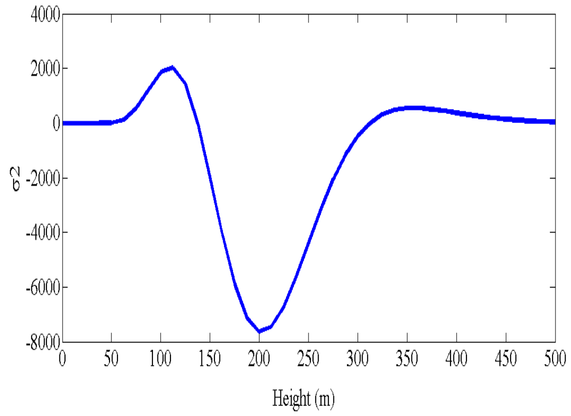

Figure 15. The steady state gradient of concentration with respect to the parameter diffusion coefficient, distance = 150m

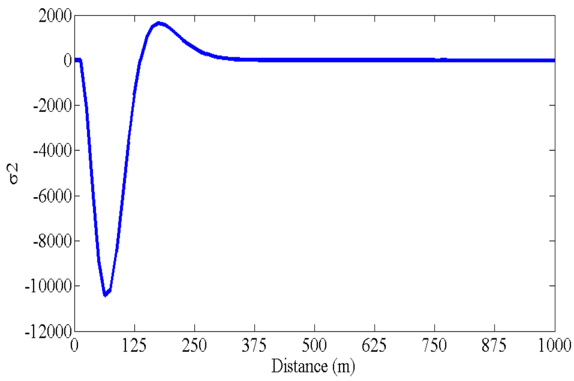

Figure 16. The steady state gradient of concentration with respect to the parameter diffusion coefficient, height = 150m

Conclusion

In this study, the sensitivity of pollutant dispersion model with respect to parameters is presented. Simulations are carried out considering the petroleum refinery process which is in Sapugaskanda, Sri Lanka. Wind velocity and diffusion coefficient are considered as the parameters. For solving the mathematical model, finite difference method is used and a C program is written. The model equation and the sensitivity system are solved simultaneously. The results show that the dispersion of pollutants with respect to parameters is significant. The pollution dispersion depends on climatic factors. The climate of Sri Lanka is led by the Southwest and Northeast monsoons regional scale wind regimes. So the meteorological conditions such as wind velocity, air temperature and rainfall depend on these seasons. Pollution concentration decreases when the wind velocity increases and pollutant go far away from the stack region. When the velocity of wind doubled, it will dilute the absorption of the pollutant by 50%. But this pollutant air deposits in the highest places of the domain. Therefore, impact area is increased. The dispersion of pollutants is proportional to the diffusion coefficient. Therefore, considering various climatic seasons and different areas, model parameters get different values. Therefore, in future we have to modify air quality model season wise and area wise. In other words, we need to identify these dynamical behaviors and do parameter estimation before implementing any kind of central activities.

REFERENCES

D'Amato, G., Cecchi, L., D'Amato, M. and Liccardi, G. 2010. Urban air pollution and climate change as environmental risk factors of respiratory allergy: an update. *Journal of Investigational Allergology and Clinical Immunology*, 20(2): 95-102.

Duffy, A. C. 2009. An introduction to gradient computation by the discrete adjoint method. Technical report, Florida State University.

Fatehifar, E., Elkamel, A., Taheri, M., Anderson, W. A. and Abdul-Wahab, S. A,. 2007. Modeling and simulation of multi pollutant dispersion from a network of refinery stack using a multiple cell approach. *Environ Eng Sci*., 24:795-811.

Griebel, M., Dornseifer, T. and Neunhoeffer, T. 1998. Numerical simulation in fluid dynamics: a practical introduction. SIAM.

Hindmarsh, A.C. and Serban, R. 2011. Example programs for CVODE v2.7.0. Technical report, LLNL, UCRL-SM-208110.

Perera, S. S. N. 2000. Sensitivity of dengue fever transmission model with respect to parameters. *JSc- EUSL*, 6:101-112.

Petzold, L. and Li, S. 2004. Adjoint sensitivity analysis for time-dependent partial differential equations with adaptive mesh refinement. *Journal of Computational Physics*, 198:310-325.

WHO, 2014. 7 million premature deaths annually linked to air pollution. World Health Organization. Available: http://www.who.int/mediacentre/news/releases/2014/air-llution/en/ (Accessed September 4, 2014).

Yang, Y. J., Wilkinson, J. G. and Russell, A. G. 1998. Fast sensitivity analysis of three dimensional photochemical models. *Air pollution modeling and its application VII*, 107-114.

Zannetti, P. 2003. Air quality modeling, theories, methodologies, computational techniques and available databases and software. *Enviro Comp Institute and Waste Management Association*, USA.

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