Abstract—A mathematical model is applied to understand the distribution of air pollutants by formulating a 2D advection-diffusion equation with time dependent. It is necessary to simulate air pollution distribution to find out whether the pollutants are more concentrated at ground level or near the source of emission under particular atmospheric conditions such as stable or unstable condition. This is done by considering wind profile, eddy diffusivity and temperature as parameters in the model. The explicit finite difference method is used to solve the mathematical model and visualized by a computer program we developed using lazarus software. The results show that atmospheric parameters largely affect the distribution of pollutants and the level of concentration of pollutants. That is, the change in concentration of pollutants is dependent on the atmospheric condition.

Index Terms—Advection, Air Pollution, Diffusion, Modeling.

I. INTRODUCTION

Air pollution has been one of the major environmental problems facing governments and world leaders for decades. The pollution problem affects human life and its surrounding environment and sometimes pollutants can travel to areas very far from the source of emission thereby affecting living organisms in that area. One of the ways to understand how pollutants disperse in the atmosphere is through mathematical simulation and [1] stated that simulation of air pollution is useful in providing information about the spread of pollutants in an area, the scale and level of pollution and estimation.

Modelling and simulation of air pollution distribution is to observe the effects meteorological factors such as wind, temperature, humidity, pressure, etc. have on the dispersal of pollutants. Reference [2] did a study on air pollution dispersion using a steady state two-dimensional mathematical model. They considered mesoscale wind which is generated by urban surface together with friction from buildings create a local wind called mesoscale wind. It is considered that the mean wind speed changes with increasing height and the mesoscale wind which is a function that depends on temperature. Diffusion takes place alongside advection and this reduces the concentration of the pollutants by turbulence. It is assumed that the mean concentration of pollutants is constant along the y – direction, thus reducing it to a two dimensional problem. In the physical processes, advection carries the pollutants in the x – direction and transports them as far as the wind blows. The mixture of the mean wind and the heat from the Earth’s surface together with friction from buildings create a local wind called mesoscale wind. It is considered that the mean wind speed changes with increasing height and the mesoscale wind which is a function that depends on temperature. Diffusion takes place alongside advection and this reduces the concentration of the pollutants by turbulence. It is assumed that the mean concentration of pollutants is constant along the y – direction, thus reducing it to a two dimensional problem. In the physical processes, advection carries the pollutants in the x – direction and transports them as far as the wind blows. The mixture of the mean wind and the heat from the Earth’s surface together with friction from buildings create a local wind called mesoscale wind. It is considered that the mean wind speed changes with increasing height and the mesoscale wind which is a function that depends on temperature. Diffusion takes place alongside advection and this reduces the concentration of the pollutants by turbulence. It is assumed that the mean concentration of pollutants is constant along the y – direction, thus reducing it to a two dimensional problem. In the physical processes, advection carries the pollutants in the x – direction and transports them as far as the wind blows. The mixture of the mean wind and the heat from the Earth’s surface together with friction from buildings create a local wind called mesoscale wind. It is considered that the mean wind speed changes with increasing height and the mesoscale wind which is a function that depends on temperature. Diffusion takes place alongside advection and this reduces the concentration of the pollutants by turbulence. It is assumed that the mean concentration of pollutants is constant along the y – direction, thus reducing it to a two dimensional problem.
that influences the distribution of pollutants as it affects turbulence. Therefore, the change in temperature \( T \) with time would be as follows:

\[
\frac{\partial T}{\partial t} = Q_x \frac{\partial^2 T}{\partial x^2} + Q_z \frac{\partial^2 T}{\partial z^2} \tag{4}
\]

where \( Q_x, Q_z \) are the heat diffusion rate in the \( x \) and \( z \) directions respectively.

III. METHOD OF SOLUTION

A. Domain

The objective is to analyze the pollutants concentration in a given two-dimensional domain \((x, z)\) at time \( t \) by developing a program using Lazarus software. Eq. (3) and Eq. (4) would be solved numerically by explicit finite difference scheme to obtain the solution.

To apply the finite difference scheme, the domain \((x, z)\) is subdivided into a set of similar rectangles of sides \( \Delta x \) and \( \Delta z \), by equally spaced grid lines, parallel to the \( z \)-axis, determined by \( x = i \Delta x, i = 0,1,2,...,M \) and parallel to \( x \)-axis, determined by \( z = j \Delta z, j = 0,1,2,...,N \). Hence, the domain of interest belongs \( M \times N \) grids and the intersection of grid lines (grid points) determine the concentration of pollutants \( C \) and also the temperature \( T \). The entire grid would be computed with time difference \( \Delta t \). The concentration \( C \) at a grid point \((i, j)\) with time \( n \) is denoted by \( C_{i,j}^n \) and the temperature \( T \) at a grid point \((i, j)\) with time \( n \) is denoted by \( T_{i,j}^n \).

B. Initial and Boundary Condition

Before the system is run, the initial value is needed to set the system up. At the initial time \( t = 0 \), temperature \( T_0 \) is set in the domain. The boundary for the domain is taken and it is assumed that at the beginning when \( t = 0 \), there is pollution emission \( C_0 \) at some point in the domain. Thus, \( C(x, z, 0) = C_0 \) at \( t = 0 \) for \( 0 < x < M \) and \( 0 < z < N \) (\( M \) – horizontal and \( N \) – vertical grid points) and where \( C_0 \) is the pollutants concentration at position \((x, z)\) at \( t = 0 \).

As a boundary value problem, the boundary condition is needed to control the system, with \( C = C_0 \), where the value of the solution at the boundary is known.

C. Meteorological Parameters

Meteorological parameters have an influence on air pollutants distribution. Wind can transport the pollutants far away from the source of emission and the diffusivity determines the rate at which pollutants diffuse. These parameters are dependent on the intensity of turbulence which is influenced by atmospheric stability. In reality, to solve the Eq. (3) the variable wind velocity and the eddy diffusivity are considered to be functions of vertical distance, as suggested by [5]:

\[
u = Ur \left( \frac{z}{z_r} \right)^\alpha
\]

\[
K_z = K_r \left( \frac{z}{z_r} \right)^\beta
\]

where \( Ur \) and \( K_r \) are the measured wind speed \((m/s)\) and vertical diffusivity at a reference height \( z_r \) (m), \( \alpha \) and \( \beta \) are the constants depending on the atmospheric stability and surface roughness.

The mathematical forms of mesoscale wind in the horizontal and vertical directions as suggested by [6] are:

\[
u_x = -ax \left( \frac{z}{z_r} \right)^\alpha
\]

\[
u_z = \frac{a z}{\alpha + 1} \left( \frac{z}{z_r} \right)^\alpha
\]

where \( a \) is a proportionality constant \((s^3)\).

In the realistic form, temperature affects turbulence which then affects the mesoscale wind. Therefore, the mathematical form of the mesoscale wind in the vertical direction becomes

\[
\nu_z = \frac{a z}{\alpha + 1} \left( \frac{z}{z_r} \right)^\alpha + \frac{T - \min T}{\max T - \min T}
\]

D. Numerical Solution

The solution of Eq. (3) and Eq. (4) would be found numerically by explicit finite difference scheme. The explicit finite difference scheme implies that:

\[
\frac{\partial C}{\partial t} = \frac{C_{i,j}^{n+1} - C_{i,j}^n}{\Delta t}
\]

The central difference scheme is used for the advection and diffusion terms; the first derivative is as follows:

\[
\frac{\partial C}{\partial x} = \frac{C_{i+1,j}^n - C_{i-1,j}^n}{2\Delta x}
\]

And the second derivative would be

\[
\frac{\partial^2 C}{\partial x^2} = \frac{C_{i+1,j}^n - 2C_{i,j}^n + C_{i-1,j}^n}{\Delta x^2}
\]

The approximations (5), (6) and (7) are applied to Eq. (3) and (4). Substituting the approximations into Eq. (3) results in the equation below:

\[
\frac{C_{i,j}^{n+1} - C_{i,j}^n}{\Delta t} + U \frac{C_{i+1,j}^n - C_{i-1,j}^n}{2\Delta x} + W \frac{C_{i,j+1}^n - C_{i,j-1}^n}{2\Delta z} = \frac{K_z}{\Delta z^2} \frac{C_{i,j+1}^n - 2C_{i,j}^n + C_{i,j-1}^n}{\Delta z^2} + \frac{K_x}{\Delta x^2} \frac{C_{i+1,j}^n - 2C_{i,j}^n + C_{i-1,j}^n}{\Delta x^2} - \lambda (C_{i,j}^n + C_{i,j+1}^n)
\]
Rearranging Eq. (8) in the finite difference form, \( c_{i,j}^{n+1} \) is obtained as:

\[
c_{i,j}^{n+1} = a_1 c_{i,j}^n - a_2 (c_{i+1,j}^n - c_{i-1,j}^n) - a_3 (c_{i,j+1}^n - c_{i,j-1}^n) + a_4 (c_{i+1,j+1}^n - 2c_{i,j}^n + c_{i-1,j+1}^n)
\]

where

\[
a_1 = \frac{1 - \lambda \Delta t}{1 + \lambda \Delta t}
\]

\[
a_2 = \frac{\Delta t^2}{2 \lambda \Delta \xi}
\]

\[
a_3 = \frac{1 + \lambda \Delta t}{\Delta \xi^2}
\]

\[
a_4 = \frac{1 + \lambda \Delta t}{\Delta \xi^2}
\]

It may be noted that explicit finite difference scheme requires a stability condition. Therefore \( a_1, a_2, a_3, a_4 \) and \( a_5 \) have to be less than 0.25.

The second derivative is applied to the spatial dimensions and then approximations (5) and (7) would be substituted into Eq. (4), it would be:

\[
\frac{T_{i,j}^n - T_{i,j}^{n-1}}{\Delta t} = Q_x \frac{T_{i+1,j}^n - 2T_{i,j}^n + T_{i-1,j}^n}{\Delta \xi^2} + Q_z \frac{T_{i,j+1}^n - 2T_{i,j}^n + T_{i,j-1}^n}{\Delta \zeta^2}
\]

Rearranging Eq. (10) gives:

\[
T_{i,j}^n = \frac{Q_x}{\Delta \xi^2} T_{i+1,j}^n + \frac{Q_z}{\Delta \zeta^2} T_{i,j+1}^n + \frac{Q_x}{\Delta \xi^2} T_{i-1,j}^n + \frac{Q_z}{\Delta \zeta^2} T_{i,j-1}^n + \frac{2Q_x}{\Delta \xi^2} T_{i,j}^{n-1} + \frac{2Q_z}{\Delta \zeta^2} T_{i,j}^{n-1}
\]

\[
- \frac{2Q_x}{\Delta \xi^2} T_{i+1,j}^{n-1} - \frac{2Q_z}{\Delta \zeta^2} T_{i,j+1}^{n-1} + \frac{Q_x}{\Delta \xi^2} T_{i-1,j}^{n-1} + \frac{Q_z}{\Delta \zeta^2} T_{i,j-1}^{n-1}
\]

Eq. (9) and (10) can be computed for each \( i = 1, 2, 3, \ldots M \) and \( j = 1, 2, 3, \ldots N \) which is true for interior grid points. At the boundary grid points, the boundary conditions are needed for discretization. Therefore,

\[
c_{0,j}^{n} = c_{0,j}^{n}; T_{0,j}^{n} = T_0
\]

For \( j = 0, 1, 2, \ldots, N \) and \( n = 1, 2, 3, \ldots \). Similarly, the boundary condition for the last \( x - \) axis can be written as:

\[
c_{i,0}^{n} = c_{i,0}^{n}; T_{i,0}^{n} = T_0
\]

For \( i = M; j = 0, 1, 2, \ldots, N \) and \( n = 1, 2, 3, \ldots \). While for the vertical grid, the boundary conditions are:

\[
c_{i,0}^{n} = c_{i,0}^{n}; T_{i,0}^{n} = T_0
\]

For \( i = 0, 1, 2, \ldots, M \) and \( n = 1, 2, 3, \ldots \).

For \( j = N; i = 0, 1, 2, \ldots, M \) and \( n = 1, 2, 3, \ldots \). As stated earlier, the wind component and eddy diffusivity are functions of vertical distance. Therefore, the function of the large-scale wind becomes \( U = u + u_x \), hence

\[
U[i, j] = Ur \left( \frac{j}{z_r} \right)^\alpha + \left( -a(i) \left( \frac{j}{z_r} \right)^\alpha \right)
\]

and the function for the mesoscale wind which is dependent on the change of temperature becomes

\[
W_t[j] = \left( \frac{\alpha(j)}{\alpha + 1} \left( \frac{j}{z_r} \right)^\alpha \right) \left( \frac{T_{i,j} - \min T}{\max T - \min T} \right)
\]

For eddy diffusivity,

\[
K_z[j] = K_r \left( \frac{j}{z_r} \right)^\beta
\]

All these parameters are counted from \( i = 1, 2, 3, \ldots M \) and \( j = 1, 2, 3, \ldots N \), which is the same in the downwind \( (x) \) direction with \( j \) becoming \( i \).

IV. RESULT AND DISCUSSION

This study is to analyze the distribution of pollutants under the influence of large-scale wind, mesoscale wind and eddy diffusivity. The meteorological parameters defined in Eq. (12), (13) and (14) have some unknown parameters which are \( Ur, a, K_r, z_r, \alpha, \beta \) and therefore for the computation of air pollutant concentration, these input parameters are required. The range of values for some of the parameters are as follows:

\( Ur = -50 \) to \( 50 \) m/s, \( K_r = 0 \) to \( 5 \) m/s², \( a = -1 \) to \( 1 \) s⁻¹, \( z_r = 10 \) m. The values of other unknown parameters \( \alpha \) and \( \beta \) are taken according to the stability conditions of the atmosphere and surface roughness as described in some previous studies which is shown in table 1 [7], with these values of \( \alpha \) (table 1) corresponding to different stability classes, the value of \( \beta \) can be obtained as \( \beta = 1 - \alpha \), based on Schmidt’s conjugate power law [8].

<table>
<thead>
<tr>
<th>Stability</th>
<th>( \alpha )</th>
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<tbody>
<tr>
<td>Case I</td>
<td>Unstable</td>
</tr>
<tr>
<td>Case II</td>
<td>Neutral</td>
</tr>
<tr>
<td>Case III</td>
<td>Stable</td>
</tr>
</tbody>
</table>

It is assumed that pollutants are emitted at a constant rate in a uniformly distributed domain. The area extends up to 500 m downwind and 500 m in the vertical direction. The initial concentration and temperature are taken to be \( C_0 = 1 \) and \( T_0 = 27^\circ C \) and it is assumed that the range of heat diffusion \( Q_z = Q_z \) from 0 to 5 m/s². The removal of
pollutants is assumed to be taking place by either dry deposition or wet deposition processes. The value for the removal parameter $\lambda = 10^{-6}$ s$^{-1}$ is assumed to be constant in all atmospheric conditions.

A numerical method based on explicit scheme requires solutions to be within their range of validity. This analysis is done for $M = 100$ and $N = 100$ independent grids.

To be able to gain insight clearly on air pollutants distribution under the effect of meteorological parameters like large-scale wind, mesoscale wind, eddy diffusivity and heat diffusion for unstable, neutral and stable atmospheric conditions, the computed concentration values have been analyzed and displayed graphically in Figs. 2a, 2b, 2c and 3a, 3b, 3c.

Fig. 1. Air pollution simulation interface.

Figure 1. shows the user interface for the program developed using Lazarus programming software. From the program, the atmospheric conditions can be selected along with the initial values for the concentration and temperature all in their respective units. Arbitrary points are chosen from the plane on the left by changing the X and Z label. The system is initialized by using the slider for each of the parameters in the model. When the program is run, the pollutants are seen as the white smog shown in figure 1 and the corresponding graph is plotted which shows the decrease or increase in the level of concentration of pollutants by varying any of the parameters in the model.

Fig. 2a. Unstable atmospheric condition.

Fig. 2b. Neutral atmospheric condition.

Fig. 2c. Stable atmospheric condition.

An arbitrary point is chosen in order to be able to measure the change in concentration whenever any of the parameters is varied. The program is run by selecting an atmospheric condition and the system is initialized by choosing initial values for the various parameters.

Figs. 2a, 2b, 2c show the distribution of pollutants in an unstable, neutral and stable atmospheric conditions. The simulation was done with a large-scale wind of $10m/s$, a proportional constant (turbulence) of $0.1m/s^2$, a diffusion rate of $3.5m/s^2$ and a heat diffusion rate of $3m/s^2$. The concentration of pollutants either increase or decrease as the parameters are varied in any of the atmospheric conditions.

Fig. 3a. Unstable atmospheric condition.

Fig. 3b. Neutral atmospheric condition.

Fig. 3c. Stable atmospheric condition.
Figure 3a, 3b, 3c show the change in the level of concentration of pollutants when the parameters are varied. The simulation starts with the same values used in fig 2a, 2b and 2c. As time went on, the large-scale wind is changed to 22 m/s, the proportional constant used was 0.2 m/s², the diffusion rate was increased to 3.8 m/s² and the heat diffusion was increased to 4 m/s². It can be seen that, a change in the various parameters resulted in a corresponding change in the level of concentration in each of the atmospheric conditions.

V. CONCLUSION

The distribution of pollutants under meteorological factors like wind, turbulence, the rate of diffusion and heat diffusion has been studied. Other factors can be topography (terrain), such as mountain, valleys and the physical and chemical properties of pollutants. However, this research is focused on some meteorological factors as mentioned earlier. The amount and the type of pollutants that are emitted into the atmosphere play a role in determining the degree of air pollution in that area. Once pollutants are released into the atmosphere, the weather (meteorological factors) largely determines how well they disperse. Turbulence mixes pollutants into the surrounding air. Wind speed also contributes to how quickly pollutants are carried away from the source of emission. When the rate of diffusion increases, pollutants tend to diffuse faster.

The advection diffusion used in this research explains the distribution of pollutants in the atmosphere. Advection is responsible for carrying the pollutants by wind from the source of emission and diffusion is responsible for the transport of pollutants from a higher concentration to a low concentration in a particular area.

From the results, it could be seen that the distribution of pollutants in the atmosphere depends largely on atmospheric parameters and an increase or decrease in any of them results in a corresponding increase or decrease in the level of concentration of pollutants in the atmosphere. The change in concentration of pollutants in the atmosphere is dependent on the atmospheric condition at a particular point in time as these parameters change in each of the conditions.

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Ulfah S has obtained a B.Sc degree (2012) in mathematics education from the University of Muhammadiyah Prof. DR. Hamka, Jakarta, Indonesia. She is currently an M.Sc. student in Applied Mathematics under the supervision of Dr. Sonporn Chuai-Aree at the Prince of Songkla University, Pattani Campus, Thailand.

Chuai-Aree S has obtained an M.Sc. degree (2000) and Ph.D. degree (2009) from University of Heidelberg, Heidelberg, Germany. Presently he is working as a lecturer in the Department of Mathematics and Computer Science at Prince of Songkla University, Pattani Campus, Thailand. He is also the deputy director of the Office of Academic Resources, Prince of Songkla University, Pattani Campus, Thailand; Director of Pattani Bay Watch (PBWatch.NET) Project: Project for participatory natural disaster monitoring and management (http://www.pbwatch.net) and a member of the committee of Borijak Project supporting the scholarship for junior high school students in North-East Thailand.