Numerical Computations of Three-dimensional Air-Quality Model with Variations on Atmospheric Stability Classes and Wind Velocities using Fractional Step Method

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Abstract—**The air pollutants emitted from industrial plants are considered one of the major causes of the typical air pollution problem. A mathematical model for describing the dispersion of the air pollutants released from the source into the atmosphere is examined. A numerical approximation using the three dimensional fractional step method is applied based on the discretization of the time dependent atmospheric advection-diffusion equation. The diffusion coefficients are supplied by the meteorological station. The concentration of the pollutants at the source is assumed to be a δ-function, which gives rise to a steady emission rate of pollutants. The resulting model is solved for the test problem with the range of parameters in the Pasquill's stability classes. In this research, the effects of the variations of atmospheric stability classes and wind velocities on the three-dimensional air-quality models are observed. The fractional step method is used to solve the dispersion model. This paper proposes a fractional step method so as to make the model simpler without any significant loss of computational efficiency. The results obtained indicate that the proposed experimental variations of the atmospheric stability classes and wind velocities do affect the air quality around the industrial areas.**

Keywords: Finite differences, Atmospheric diffusion equations, Air-quality model, Fractional step method

1 Introduction

Air pollution is an important environmental problem since pollutants ultimately become dispersed throughout the entire atmosphere. The air pollution is taken into account as a critical concern more in big cities and industrialized regions. The high concentrations of gases and particles from coal combustion and, more recently, motor vehicles have produced severe loss of air quantity and significant health effects in urban areas. In industrial areas, sources that emit high above the ground through stacks, such as power plants or industrial sources, can cause problems, especially under unstable meteorological conditions producing portions of the plume to reach the ground in high concentrations.

The polluted air causes harmful effects on human health, property, aesthetics, and the global climate. Although the air pollution laws mostly concerned with human health protection are constituted in many industrialized countries, the air quality control is still a crucial aspect worldwide. We can measure the air-quality by measuring the quantity concentration of the air pollutant in the atmosphere from many difference sources. A quantitative assessment of the air pollution in the atmosphere from any position at times can be implemented by monitoring them from the stations locating at places. Most stations are installed on the places suspected to have a great deal of pollution such as urban, in-bound, awful traffic places and industrial areas. In reality, all of these monitoring systems are definitely depend on the allot budget while in mathematical simulation, the pollutant concentration can be predicted from anywhere at any time using the air-quality model and the atmospheric diffusion equations. The equations will show the disperse concentration of the air pollutant in horizontal and vertical angles as the time passes by and reflect with meteorological conditions. After that, the results will be calculated by some numerical methods.

In [3], they develop a land-use regression model for sulfur dioxide air pollution concentrations. They also make use of mobile monitoring data collected in Hamilton, Ontario, Canada, from the year 2005 through 2010. The observed SO_2 concentrations are regressed against a comprehensive set of land use and transportation variables. Land use and transportation variables are assessed as the amount of each characteristic within the buffers of 50, 100, 200, 400, 800, and 1600 m around the pollution observation sites. In [4], they describe the design and application of the Atmospheric Evaluation and Research Integrated model for Spain (AERIS). Currently, AERIS can provide concentration profiles of NO2, O3, SO2, NH3, PM,

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as a response to emission variations of relevant sectors in Spain. Results are calculated using transfer matrices based on an air quality modelling system (AQMS) composed by the WRF (meteorology), SMOKE (emissions) and CMAQ (atmospheric-chemical processes) models. In [6], they use the finite difference method in the air pollution model of two dimensional spaces with single-point source. In [7], the air pollution problem in three dimensional spaces with multiple sources are presented. The initial conditions in the domains are assumed to be zero everywhere without obstacles. In [8] and [9], the air pollution in two dimensional spaces with obstacles domain are also studied. In [14], they address the limitations of these existing studies, by developing Fluctuating Wind Boundary Conditions (FWBC). In [2], they propose first and second order positive numerical methods for the advection equation. They consider the direct discretization of the model problem and comment on its superiority to the so called method of lines. They investigate the accuracy, stability and positivity properties of the direct discretization.

The source of the air pollutant is the main key leading to emission inventories. The smoke discharged from industrial plants is a principle reason of the air pollution problem. In this research, the effects of the variations of atmospheric stability classes and wind velocities on the three-dimensional air-quality models are examined. The fractional step method is also used in solving the smoke dispersion model.

2 The Governing Equation

2.1 Air-Quality Model

We introduced the well-known atmospheric diffusion equation

$$\frac{\partial c}{\partial t} + v_x\frac{\partial c}{\partial x} + v_y\frac{\partial c}{\partial y} + v_z\frac{\partial c}{\partial z} = k_x\frac{\partial^2 c}{\partial x^2} + k_y\frac{\partial^2 c}{\partial y^2} + \frac{\partial}{\partial z}\left(k_z\frac{\partial c}{\partial z}\right) + s, \qquad (1)$$

where $c = c(x,y,z,t)$ is the air pollutant concentration (kg/m^3), k_x, k_y and k_z are diffusion coefficients (m^2/s), v_x, v_y and v_z are the flow velocities (m/sec) in $x-$, $y-$, and z-directions, respectively, s is the rate of change of substance concentration due to the sources (sec^{-1}), for all $(x,y,z) \in \Gamma = \{(x,y,z) \in \mathbb{R}^3 : x_E \le x \le x_W, y_S \le y \le y_N, 0 \le z \le h_{Top}\}$, for all time $0 < t \le \mathcal{T}$, and h_{Top} is the hight of inversion layer base.

Assuming that the horizontal advection dominates the horizontal diffusion by the wind and the vertical diffusion dominates the vertical advection by the wind. Consequently, the horizontal advection in $y-$direction is negligible. We have a cross section along the $y-$axis at the plane of obstacle. With their above assumptions, so Eq.(1) becomes

$$\frac{\partial c}{\partial t} + v_x\frac{\partial c}{\partial x} = k_x\frac{\partial^2 c}{\partial x^2} + k_y\frac{\partial^2 c}{\partial y^2} + \frac{\partial}{\partial z}\left(k_z\frac{\partial c}{\partial z}\right) + s, \quad (2)$$

where $v_x = u$. The classic formula k_z used by Shir and Shieh [15] has modified in the following way:

$$k_z[z, S(t)] = k_D[S(t)]z \exp\left\{-\rho[S(t)]\frac{z}{h_{Top}}\right\} \quad (3)$$

where $k_D[S(t)]$ is obtained as follows:

$$k_D[S(t)] = z_R^{-1}k_z[z_R, S(t)] \exp\left\{\rho[S(t)]\frac{z_R}{h_{Top}}\right\}. \quad (4)$$

By the assumption as [6], [7] and [9], the initial condition is taken to be zero concentration of air pollutant everywhere in the domain by cold start technique. We can obtain that

$$c(x,y,z,0) = 0, \quad (5)$$

for all $(x,y,z) \in \Gamma$. The boundary conditions on the east-, west-, south- and north-edges of domain are assumed as,

$$c(x_E,y,z,t) = c(x_W,y,z,t) = 0, \quad (6)$$

$$c(x,y_S,z,t) = c(x,y_N,z,t) = 0. \quad (7)$$

The boundary conditions on the ground and the inversion layer are also assumed as,

$$\frac{\partial c}{\partial z}(x,y,0,t) = \frac{\partial c}{\partial z}(x,y,h_{Top},t) = 0. \quad (8)$$

2.2 Nondimensionalize of Air-Quality Model

We can obtain the nondimensional form of the atmospheric diffusion equation Eq.(2) by changing all variables as follow [7],

$$\frac{\partial C}{\partial T} + U\frac{\partial C}{\partial X} = K_X\frac{\partial^2 C}{\partial X^2} + K_Y\frac{\partial^2 C}{\partial Y^2} + \frac{\partial}{\partial Z}\left(K_Z\frac{\partial C}{\partial Z}\right) + S(X,Y,Z,T), \quad (9)$$

where $X = x/h_s$, $Y = y/h_s$, $Z = z/h_s$, $Z_s = z_s/h_s$, $U(Z) = v_x/\bar{u}$, where $\bar{u} = v_x(z = h_s)$, $T = t\bar{k}_z/h_s^2$, $Q = qh_s^2/\bar{k}_z$, $K_x = K_y = k_x/\bar{k}_z$, $K_z = k_z[Z,S(t)]/\bar{k}_z$, $C = h_s^3c$, $\bar{k}_z = k_z(z = h_s)$, for all $(X,Y,Z) \in \Omega = \{(X,Y,Z) \in \mathbb{R}^3 : 0 \le X \le L_x, 0 \le y \le L_y, 0 \le z \le H_{Top}\}$, and H_{Top} is the height of the inversion layer. We can also obtain the initial condition,

$$C(X,Y,Z,0) = 0. \quad (10)$$

The boundary conditions of the east-west layers, south-north layers and bottom-top layers are also become,

$$C(0,Y,Z,T) = C(L_x,Y,Z,T) = 0, \quad (11)$$

$$C(X,0,Z,T) = C(X,L_y,Z,T) = 0, \tag{12}$$

$$\frac{\partial C}{\partial Z}(X,Y,0,T) = 0, \tag{13}$$

$$\frac{\partial C}{\partial Z}(X,Y,H_{Top},T) = 0, \tag{14}$$

respectively.

3 Numerical Technique: fractional step method

We will introduce the fractional step method of [19] in the nondimensional form of the atmospheric diffusion equation Eqs.(9-14). The Eq.(9) is separated into 3 stages by using the fractional step technique. In each time step of T-directions is discretized from T_n to T_{n+1} with the time increment ΔT. To obtain the nondimensional concentration C at time T_{n+1} from its value at a base T. Each of equations is solved numerically over a fraction of each time step as following.

3.1 Emission Stage

The contribution of the source term of nondimensional air pollutant is expressed as follows

$$S(X,Y,Z,T) = \sum_{r=1}^{N} Q_r \delta(X-X_r)\delta(Y-Y_r)\delta(Z-Z_0), \tag{15}$$

for all $(X,Y,Z) \in \Omega$, where $\delta(\ )$ stands for Dirac's delta function, Q_r is the emission rate of the r^{th} source and X_r, Y_r are the coordinates of the r^{th} source.

3.2 Advection Stage

By taking the Carlson's method [18] devised a finite difference scheme which is unconditionally stable to solve a one-dimensional advection equation in X-direction, we can obtain

$$\frac{\partial C''}{\partial T} = -U(Z)\frac{\partial C''}{\partial X}, \tag{16}$$

for all $0 \le X \le L_x$. In our computations, we assume that the wind velocity is positive.

3.3 Diffusion Stage

By taking the Crank-Nicolson method [1], [16] to solve a one-dimensional diffusion equation in Z-direction. The Crank-Nicolson method gives an unconditionally stable for any choice of θ satisfying $1/2 \le \theta \le 1$. In our computations, we choose $\theta = 1/2$. It follows that the Crank-Nicolson method for diffusion equation in $X-$, $Y-$ and $Z-$ directions becomes

$$\frac{\partial C'''}{\partial T} = K_X \frac{\partial^2 C'''}{\partial X^2}, \tag{17}$$

$$\frac{\partial C^{(4)}}{\partial T} = K_Y \frac{\partial^2 C^{(4)}}{\partial Y^2}, \tag{18}$$

$$\frac{\partial C^{(5)}}{\partial T} = \frac{\partial}{\partial Z}\left(K_Z \frac{\partial C^{(5)}}{\partial Z}\right). \tag{19}$$

In succession, the auxiliary terms in each stage are denoted by prime ($'$) that is C', C'', C''', $C^{(4)}$ and $C^{(5)}$ respectively.

4 Effects of Variation on Atmospheric Stability Classes

The boundary layer thickness and the wind speed profile are functions of the atmospheric stability and the surface roughness. Hence the exponent $\alpha(S(t))$ must vary in relation to the stability characteristics of the atmosphere and the surface roughness. The useful atmospheric stability $S(t)$ was classified according to Pasquill's class [17] categories ranging from A (strong instability) to F (extreme stability) on the basis of wind and cloudiness data supplied by the meteorological station at level z_R and $\alpha(S(t))$ are given functions of stability that reported in Table 1.

Table 1: The wind and diffusion parameters of Pasquill's stability classes [17]

$S(t)$	$\alpha(S(t))$	$\rho(S(t))$	$k_z[z_R, S(t)]$ (m^2/s)	$k_x(S(t)) = k_y(S(t))$ (m^2/s)
A	0.05	6	45.0	250.0
B	0.1	6	15.0	100.0
C	0.2	4	6.0	30.0
D	0.3	4	2.0	10.0
E	0.4	2	0.4	3.0
F	0.5	2	0.2	1.0

4.1 Numerical Experiment 1 (A constant wind and diffusion coefficients)

A three dimensional atmospheric diffusion equation Eq.(2) with nonzero different coefficients U, K_x, K_y and K_z is tested by a theoretical solution of [5],

$$C = \frac{Q}{4\pi\sqrt{K_x K_y K_z}\sqrt{\frac{X^2}{K_x}+\frac{Y^2}{K_y}+\frac{Z^2}{K_z}}} \times \exp\left[\frac{U}{2\sqrt{K_x}}\left(\frac{X}{\sqrt{K_x}} - \sqrt{\frac{X^2}{K_x}+\frac{Y^2}{K_y}+\frac{Z^2}{K_z}}\right)\right]. \tag{20}$$

The concentrations were taken with $\Delta X = 1$, $\Delta Y = 2$, $\Delta Z = 0.1$, $\Delta T = 0.25$, and computed with 512 time steps. The wind and diffusion coefficients are constants, assumed to be $U = 1$ and $K_x = K_y = 5$, $K_z = 1$. The numerical results are obtained by the numerical techniques Eqs.(15)-(19), they are shown in Table 2 and Fig. 1. The accurate of the numerical scheme are illustrated in Fig. 2 and Fig. 3.

4.2 Numerical experiment 2

The considered domain is assumed to be 1.5 x 0.7 km^2 as an industrial area that based on a rectangular

Table 2: The numerical solution along the $X-$axis (fixed Y = 2 and Z = 1) $\Delta T = 0.25$ with constant wind and diffusion coefficients

T, X	$X = 0$	$X = 25$	$X = 50$	$X = 75$	$X = 100$
$8\Delta T$	0.0065	2.2761E-08	0.0000	0.0000	0.0000
$16\Delta T$	0.0086	4.5723E-06	1.4000E-13	0.0000	0.0000
$32\Delta T$	0.0103	0.0001	1.1144E-08	0.0000	0.0000
$64\Delta T$	0.0113	0.0009	1.0976E-05	6.7577E-09	1.9000E-13
$128\Delta T$	0.0113	0.0009	1.0976E-05	6.7577E-09	1.9000E-13
$256\Delta T$	0.0113	0.0009	1.0976E-05	6.7577E-09	1.9000E-13
$512\Delta T$	0.0113	0.0009	1.0976E-05	6.7577E-09	1.9000E-13

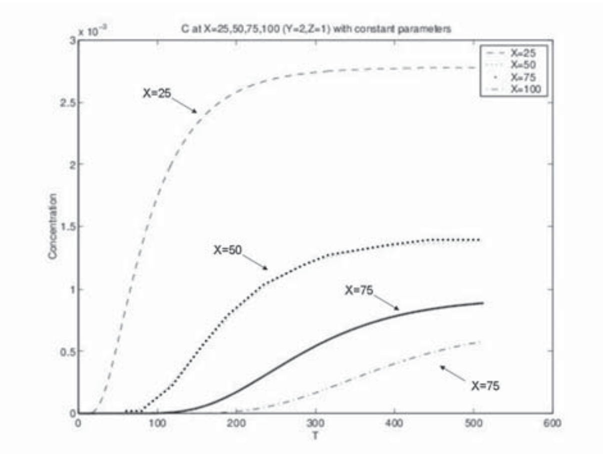


Figure 1: The computed air pollutant concentration at $X = 25, 50, 75, 100$ fixed $Z = 1, Y = 2$, at different T.

as Fig.4(a). We assume that the domain contains 3 buildings as the obstacles that to separate the area into 2 zones: an factory zone and an residential zone, respectively. We also assume that the buildings are standing as shown in Fig.5. The buildings have a three-dimensional dimension: 45 x 90 x 21 m^3 that standing on the ground on the base. The sources of air pollutant are assumed only at the level $z = h_s = 15$ m so as to represent chimneys above the ground. We also assume that the uniform line sources are lie along the $X-$axis with the total emission rate 350 gram/sec.
The atmospheric diffusion Eq.(2) in the three-dimensional space with appropriate parameter values for the tropical area were taken from Pasquill stability reference classes [17]. The atmospheric Pasquill stability classes on the cases of most unstable: (i) Class A (highly unstable) (ii) Class B (normal unstable) and (iii) Class C (slightly unstable) are investigated.
By using the numerical techniques Eqs.(15)-(19), we can obtain the dimensional approximate concentration of air pollutant in the XY-plane for each hight levels. The dimensional air pollutant concentrations at the level of height 3 meters above the ground with difference time step are illustrated in contour graphs by Fig.5, 6 and 7.
The approximated concentrations of air pollutant by the diffusion coefficients of Class A,B and C are differences on height levels are 3 and 15 meters above ground around an factory zone and an residential zone are shown in

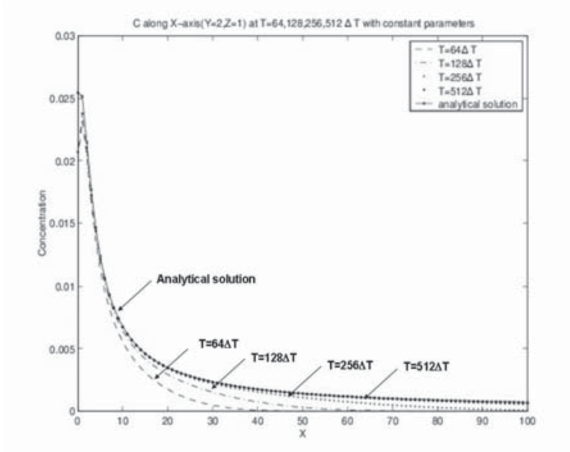


Figure 2: The analytical and numerical solution along X-axis for fixed $Z = 1, Y = 2$ at different T.

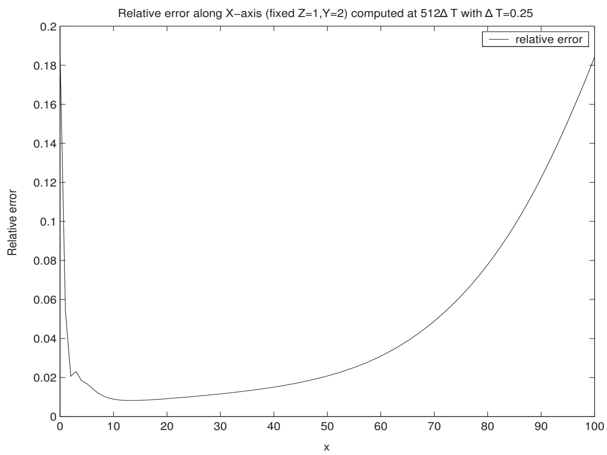


Figure 3: The relative error at $T = 512\Delta T$.

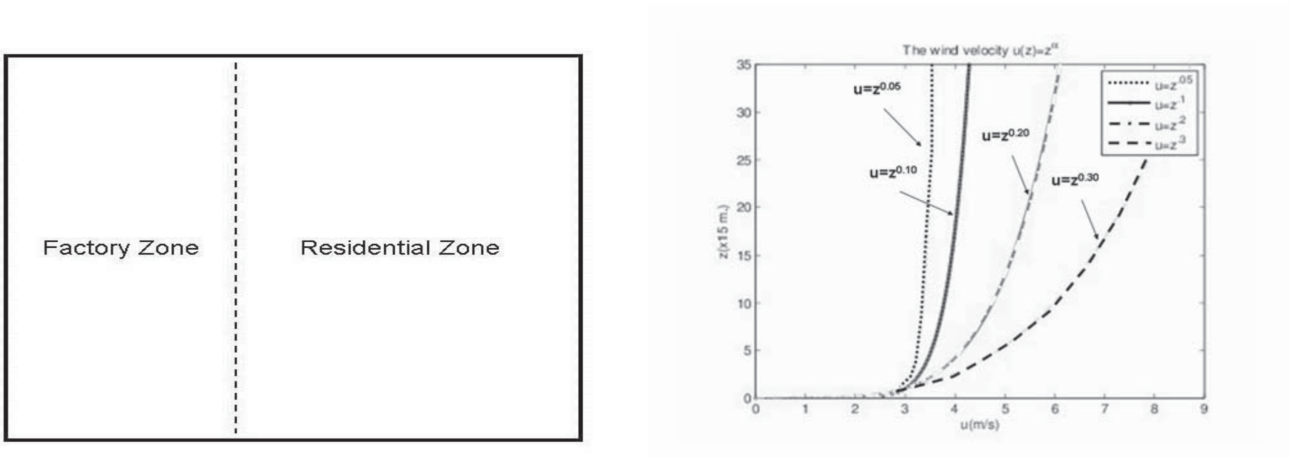
Table 3 and Table 4, respectively.

5 Effects of Variation on Wind Velocities

In this section, the atmospheric diffusion equation Eq.(2) in three-dimensional space with appropriate parameter values for the tropical area by the Pasquill stability reference class A (highest unstable) will be considered. The considered domain is also assume to be an area 1.50x0.70 km^2 as Fig.8. We assuming that the area contains a big obstacle building as a rectangle prism with dimension 150x150x60 m^3. The diffusion coefficient is $\bar{k}_z = 45$ m^2/sec and the unit velocity is $\bar{u} = 3$ m/sec that are corresponding to the supported data of the Pasquill stability class A so as to turn out that Reynolds number Re=1. In our computation, the sources are assumed at $z = h_s = 15$ m as a chimney above the ground.

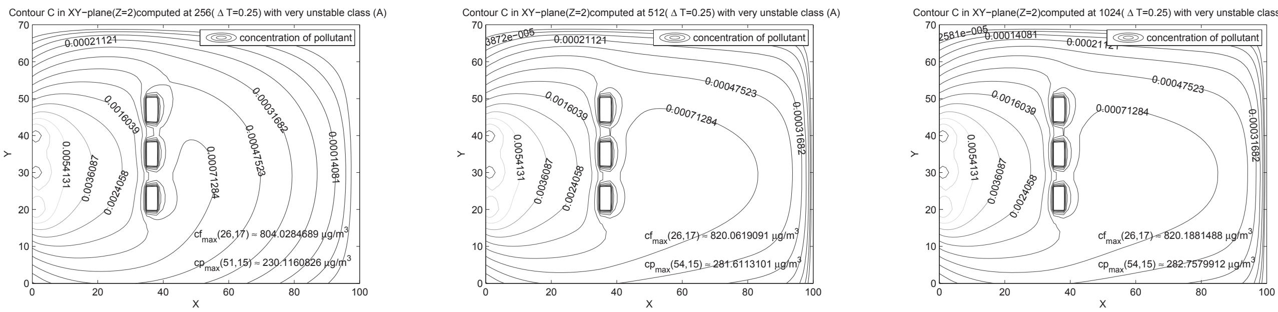
5.1 Numerical experiment 3

In this experiment, we also using Eqs.(15)-(19) with the uniform line sources along the $X-$axis with the total



(a) (b)

Figure 4: (a) A considered domain (b) The wind velocities



(a) (b) (c)

Figure 5: The computed concentration of air pollutant in XY -plane (height 3 m) with class A (highest unstable) at (a) $256\Delta T$. (b) $512\Delta T$ and (c) $1024\Delta T$

Table 3: The computed concentration of air pollutant around a factory zone (fixed $y = 220$)m at $512\Delta T$.

x (m)	300	375	450	600	675
class A :					
$z = 3$	0.8599	0.7134	0.5466	0.1356	0.2513
$z = 15$	0.8470	0.7065	0.5493	0.1676	0.2598
class B :					
$z = 3$	2.3577	1.9285	1.4418	0.3671	0.6683
$z = 15$	2.3210	1.9108	1.4544	0.4543	0.6927
class C :					
$z = 3$	5.1715	4.2177	3.1995	0.8252	1.5095
$z = 15$	5.0866	4.1762	3.2255	1.0180	1.5594

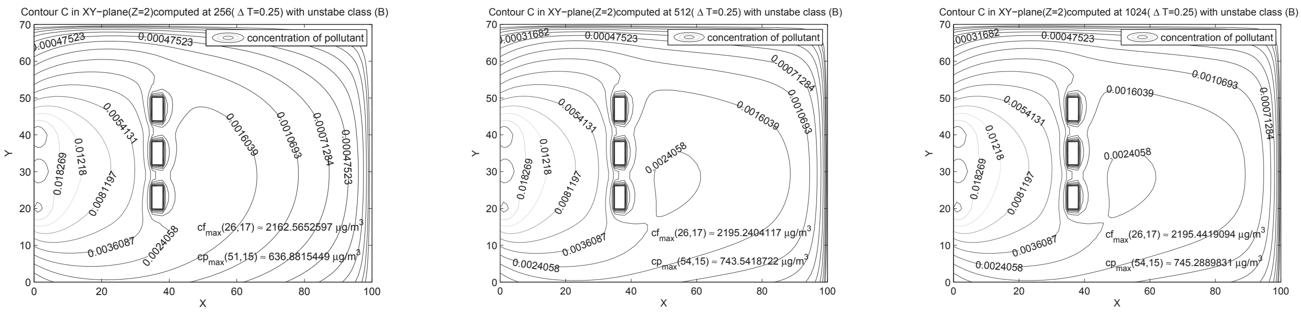
Table 4: The computed concentration of air pollutant around an residential zone (fixed $y = 180$ m) at $512\Delta T$.

x (m)	750	900	1050	1200	1350
class A :					
$z = 3$	0.2683	0.2509	0.2262	0.1996	0.1584
$z = 15$	0.2699	0.2510	0.2261	0.1995	0.1585
class B :					
$z = 3$	7.1284	6.6363	5.9533	5.2161	4.0283
$z = 15$	7.1823	6.6428	5.9527	5.2163	4.0371
class C :					
$z = 3$	1.5686	1.4677	1.3337	1.2010	0.9926
$z = 15$	1.5783	1.4685	1.3333	1.2011	0.9965

emission rate 320 gram/sec comparing between 2 and 3 release points of air pollutant sources with a constant wind velocity $U = 1$ to obtain air pollutant concentration for each zones. The computed air pollutant concentration on the ground 0 m and the height 65 m are shown in Fig.8 and Fig.9, respectively.

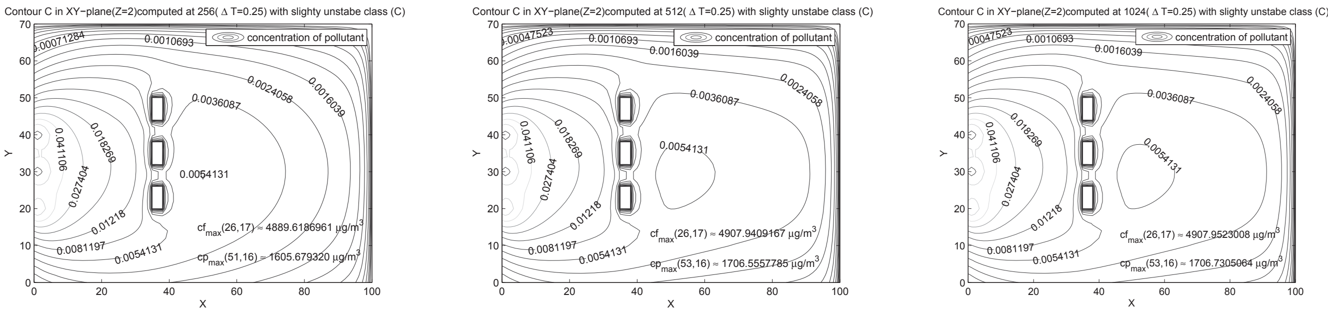
5.2 Numerical experiment 4

In this experiment, we also using the numerical techniques Eqs.(15)-(19), we will consider the interested cases when the wind velocities are difference. We will propose the affect of the variation of them in x-direction so as to obtain the velocity in z-direction as show in Table 5. We can obtain the comparison of difference wind velocities as shown in Fig.4(b).



(a) (b) (c)

Figure 6: The computed concentration of air pollutant in XY -plane (height 3 m) with class B (normal unstable) at (a) $256\Delta T$. (b) $512\Delta T$ and (c) $1024\Delta T$



(a) (b) (c)

Figure 7: The computed concentration of air pollutant in XY -plane (height 3 m) with class C (slightly unstable) at (a) $256\Delta T$. (b) $512\Delta T$ and (c) $1024\Delta T$

Table 5: The considered wind velocities

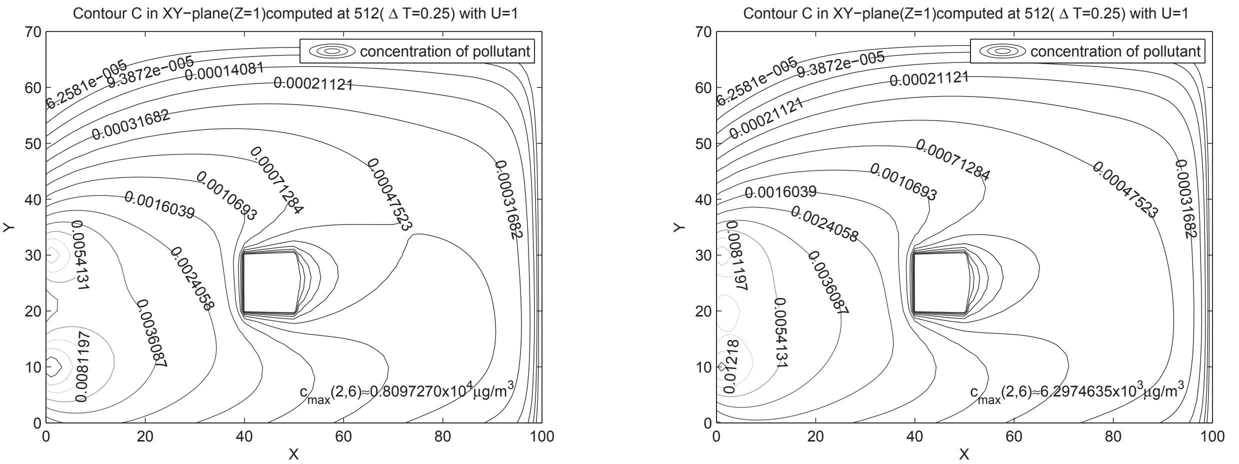
$\alpha(t)$	Wind velocities	$u = \bar{u} \cdot Z^{\alpha}$ (m/s)
	z=5 m	z=65 m
0.0500	3.0000	3.2514
0.1000	3.0000	3.5239
0.2000	3.0000	4.1392
0.3000	3.0000	4.8620

Next, we assume that the non-uniform line sources with the total emission rate 500 gram/sec with difference nondimensional wind velocities$U = Z^{0.30}$, $U = Z^{0.20}$, $U = Z^{0.10}$ and $U = Z^{0.05}$ are released by 4 point sources around a factory zone into the atmosphere in our domain. The computed air pollutant concentrations on the ground layer (height 5 m) and the release layer (height 65 m) for each cases of wind velocities are illustrated in Fig.10 and Fig.11, respectively.

6 Discussion

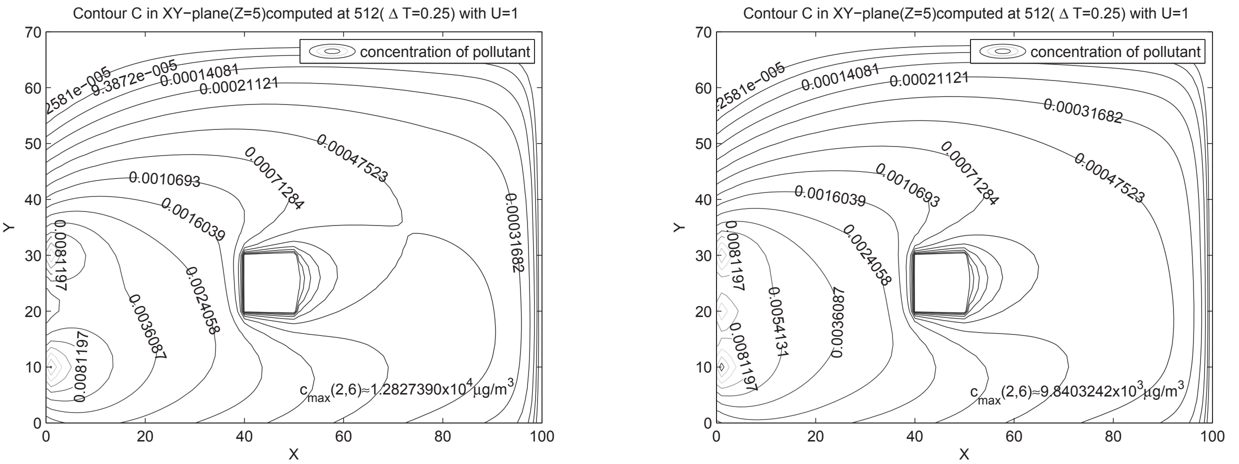
We can see that the contour graph in each class of atmospheric stability are shown that the concentration behavior by the time 5, 10 and 20 minutes passed. It much change from 5 to 10 minutes and a bit change at time 10 and 20 minutes passed. From Fig.5, 6, 7 and Tables 3-4, the contour graph in each class of atmospheric stability is shown with the concentration behavior after 5, 10, and 20 minutes. It changes considerably from after 5 to after 10 minutes and the change declines from after 10 to 20 minutes. Therefore, the computational time would be theoretically at $512\Delta T$. We can see that the maximum air-quality levels are going to increase by varying the stabilities class A, class B, and class C, respectively. By the comparison of different atmospheric stability classes, the results soundly agree with the real situation.

Fig.8 and Fig.9 show that the maximum concentrations of the pollutant at the same point in the three sources case are less than those of the two sources case. They are compared at the same level of Z and thus can lead to a conclusion that the number of sources does affect the air pollutant concentration. Furthermore, both Fig.10 and Fig.11 illustrate that the maximum concentrations measured at the same position on the same plane of Z will decrease as the wind velocities increase. Consequently, the wind velocities affect the air pollutant concentration as well.



(a) (b)

Figure 8: The computed concentration of air pollutant along XY plane on the ground layer (height 5 m) which is uniform line source along $x-$axis (a) 2 point sources and (b) 3 point sources



(a) (b)

Figure 9: The computed concentration of air pollutant along XY plane on the discharging level (height 65 m) which is uniform line source along $x-$axis (a) 2 point sources and (b) 3 point sources

7 Conclusion

The concentrations of the pollutant in the control area with obstacle domain are calculated. The computed results are approximated by the fractional step method using the MATLAB code, with respected to the transformed atmospheric diffusion equation. The pollutant concentration at the sources is larger than that at any point in the domain. Also, the pollutant concentration decreases as the point measured moves away from the source at later time. This paper proposes a fractional step method so as to make it simpler without any significant loss of the computational efficiency. The results obtained indicate that the proposed experimental variation of the atmospheric stability classes and wind velocities does affect the air-quality in industrial areas.

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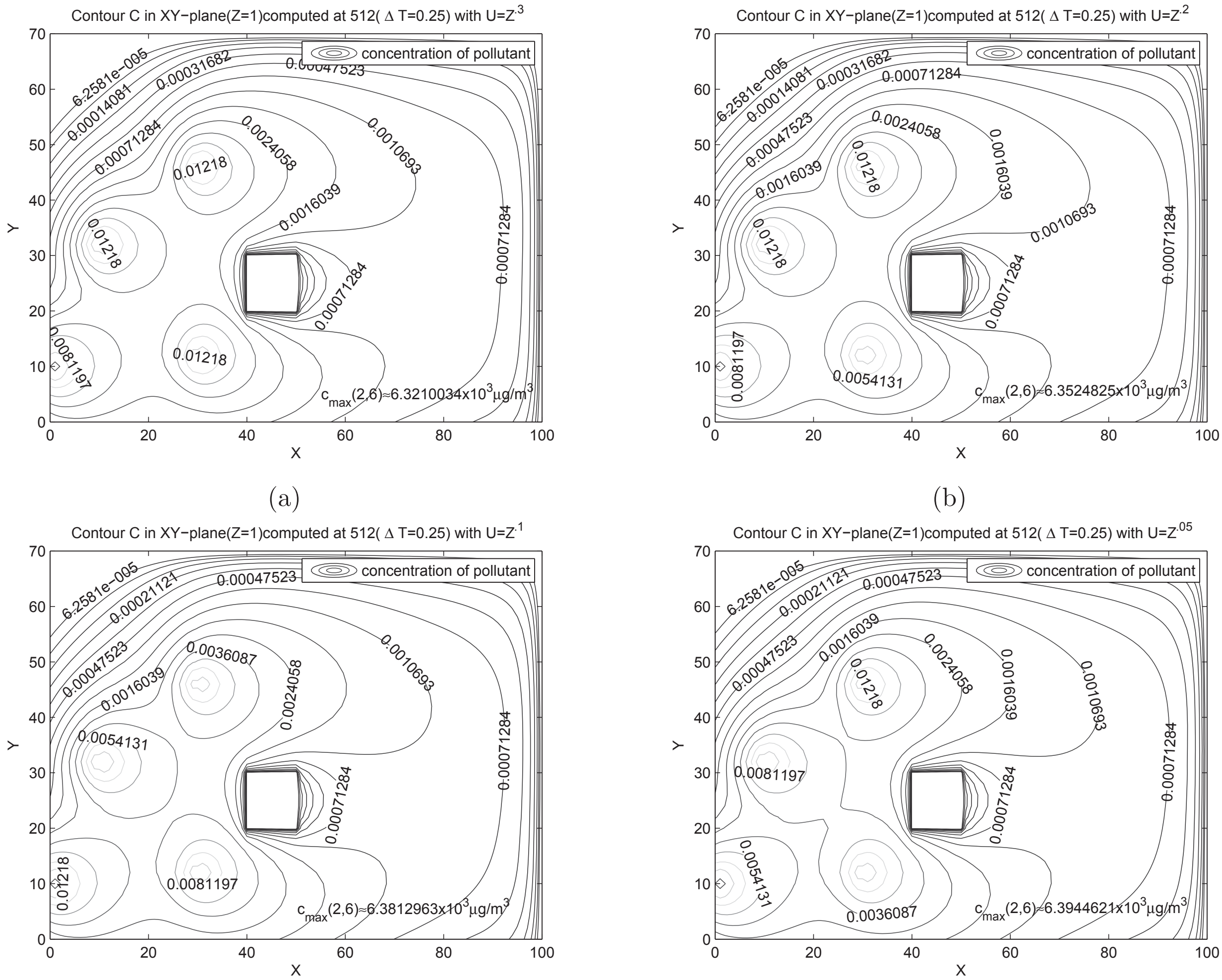

(a) (b) (c) (d)

Figure 10: The computed concentration of air pollutant along XY plane on the ground layer (height 5 m) when the wind velocities are varied (a) $U = Z^{.3}$, (b) $U = Z^{.2}$, (c) $U = Z^{.1}$ and (d) $U = Z^{.05}$.

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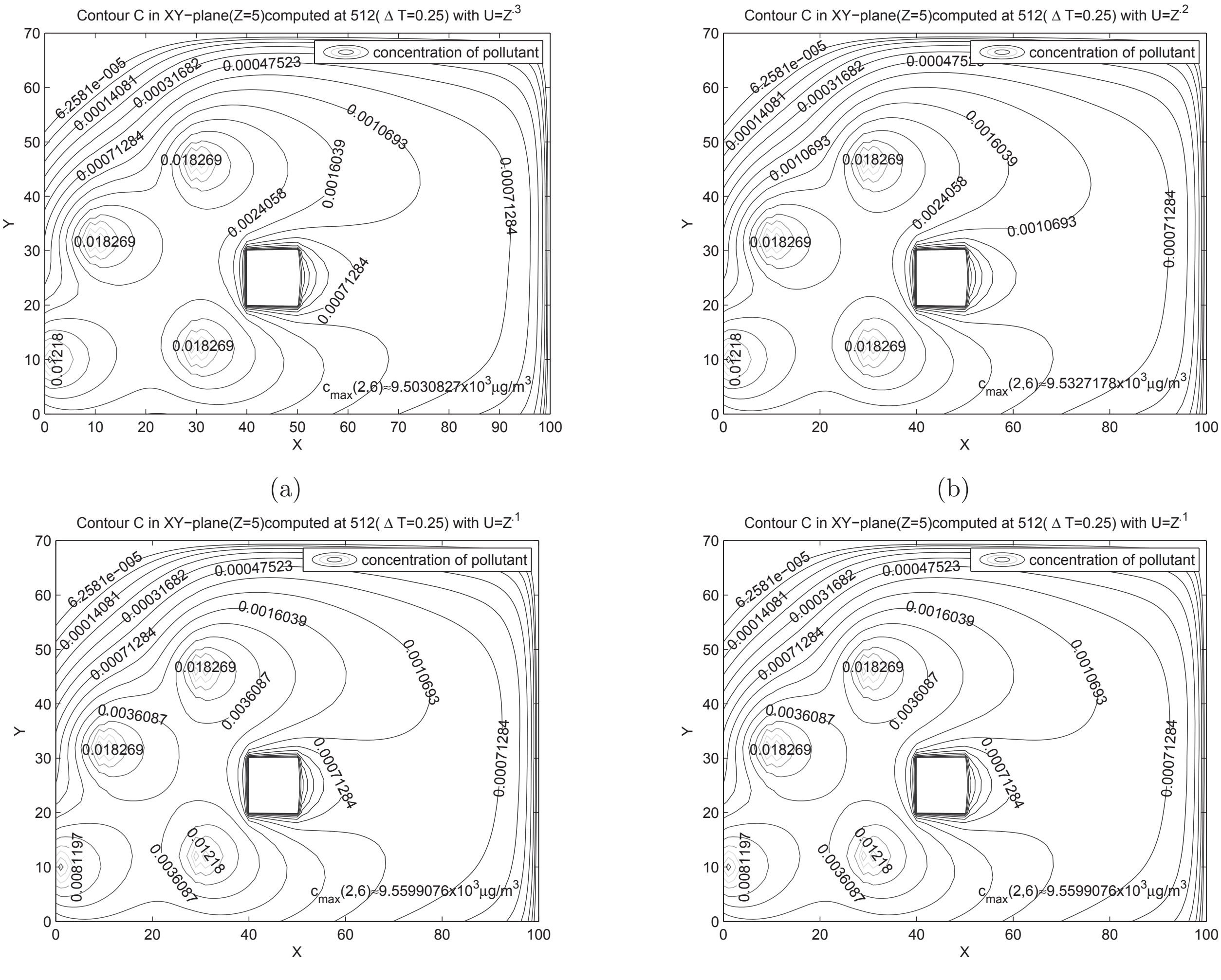

(a) (b) (c) (d)

Figure 11: The computed concentration of air pollutant along XY plane on the discharging layer (height 65 m) when the wind velocities are varied (a) $U = Z^{.3}$, (b) $U = Z^{.2}$, (c) $U = Z^{.1}$ and (d) $U = Z^{.05}$.

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