**Engineering Letters**

# A Mathematical Model of Hazardous Smoke Emission Control Considering Primary and Secondary Pollution Concentrations

Pravitra Oyjinda, Nopparat Pochai

***Abstract*— The major cause of air pollution concerns is industrial development, which has an influence on human health, human lifestyle, and the environment around an industrial zone. Air quality management assists in the control and improvement of air pollution in order to lower the quantity of numerous air contaminants. The purpose of this investigation is to examine various air pollution emission control and quality control mechanisms. Several atmospheric diffusion equations are used to solve numerous air pollution concentration indices that can represent how air pollutants disperse in the atmosphere. Primary and secondary pollutant concentrations are approximated by using the finite difference technique. Monitoring points are installed for checking the air pollutant concentration levels of sulfur dioxide ($SO_2$), sulfur trioxide ($SO_3$), and sulfuric acid ($H_2SO_4$). Suitable emission control scenarios are proposed. The approximate solutions of air pollution control simulations at each monitoring point are compared. The air quality standard is also used to compare the results of the experiments. There are suitable emission control scenarios presented. At each monitoring location, the approximate solutions of air pollution control models are compared. The proposed strategy selects a good decision-monitoring point. According to the research, an observation area should be near an industrial area. The chosen monitoring location provides the most effective overall air quality for emission control techniques around industry and residential areas. As a result, the location of collecting for each monitoring station influences the air quality of the air pollution control schedule.**

***Index Terms*— Air pollution emission control, atmospheric diffusion equation, forward time central space scheme, primary and secondary pollutants.**

## I. INTRODUCTION

Globally, air pollution is a significant problem. Industrial development causes air pollution in industrial zones. The six pollutants which are known as criteria air pollutants are particulate matter (PM), carbon monoxide (CO), sulfur dioxide ($SO_2$), nitrogen dioxide ($NO_2$), ozone ($O_3$), and lead (Pb). Air pollution which is emitted from sources has an effect on human health and the environment. Air pollutants can be classified into two groups: 1) Primary pollutants, which are air pollutants directly released from sources into the atmosphere, and 2) Secondary pollutants, which are air pollutants that occur by chemical reaction, and will react with primary pollutants or primary pollutants and existent pollutants in the atmosphere. A mathematical model is used to describe the dispersion of air pollutants, which can predict the expected impact.

In [1], a steady state two-dimensional mathematical model with mesoscale wind velocity and meteorological parameters was presented under the urban heat island effect. The source of air pollution that was emitted from the ground was the area source, and the removal mechanism was considered by the wet and dry depositions. The approximate solution was solved by using the Crank-Nicolson implicit method. In [3], the dispersion of ozone and its substrates in Riyadh, Saudi Arabia, in the summer 2012 were considered. The concentration of ozone and its substrates were analyzed by spatial distribution at 16 different locations, all urban environments. In [4], the researchers studied the atmospheric transport diffusion model. The model considered a system of delayed removal with wind velocity and diffusion coefficient. The air pollutants were emitted from an elevated source, a line source, with dry deposition on the ground. The fractional step method was employed to estimate the air pollutant concentration. In [5], the assessment of sulfur dioxide concentration was studied by developing a land-use regressive (LUR) model. Mobile monitoring was used to collect concentration data between the years 2005 and 2010 in Hamilton, Ontario, Canada. In [6], carbon dioxide was measured from an air quality monitoring (AQM) station in Yongsan, Seoul, Korea between the years 1987 and 2013. Long-term trend analysis was used to examine the concentration of carbon dioxide. From the analysis, the carbon dioxide pollutant concentration decreased from 1987 to 2013. In [7], the air pollution problem was studied by using the two-dimensional atmospheric diffusion equation. The comparison of solutions between two- and three-point sources with obstacles domain was considered. In [8], the three-dimensional atmospheric diffusion equation with different atmospheric stability classes and wind velocities from multiple point sources was proposed. The considered domain was divided into two zones, a factory zone and a residential zone. In [9], the sulfur dioxide pollutant was analyzed without obstacles by using the three-dimensional mathematical model. The concentration of pollutants in [7], [8], and [9] were

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approximated by using the fractional step method.

In [10], the researchers studied the two-dimensional advection-diffusion equation with a point source. The finite difference method was used as a research instrument. In [11], Computation Fluid Dynamic (CFD) simulations were used to study air flow and air pollutant dispersion in urban street canyons. The researchers solved the problem by developing Fluctuating Wind Boundary Condition (FWBC). The condition comparison between FWBC and Steady Wind Boundary Condition (SWBC) was investigated. In [12], a two-dimensional air pollution model with mesoscale wind velocities and eddy diffusivity profiles was presented. The researchers studied the removal mechanism of dry deposition, gravitational settling, and chemical reaction and the primary pollutant which was emitted from an area source. In [13], the two-dimensional air pollution models of primary and secondary pollutants were proposed. The researchers studied the effect of dry deposition velocity from an area source with a point source at the boundary. The Crank-Nicolson implicit method was used to calculate the solutions of [12] and [13]. In [14], the researchers studied the atmospheric diffusion equation of three-dimensional analytical solution with height-dependent wind speed and eddy diffusivities. The solutions for different boundary condition types were derived by applying Green's function concept for multiple source problems; the sources can be established everywhere in the area of interest.

In [15], the variation of sulfur dioxide pollutant emissions in China since the year 2000 was presented. The result was estimated by using a technology-based methodology specifically designed for China; then, the researchers compared the sulfur dioxide emissions with a variety of official environment statistics, ground-based measures, satellite observations, and model results of sulfur related quantities over East Asia. In [16], the mass transport model, consisting of the stream function, vorticity, and convection-diffusion equation, was considered to simulate the model for one- and two-point sources with obstacle domain. The finite element and finite difference methods were used as the numerical technique for the air pollution solution in two-dimensional space and one-dimensional time, respectively. In [17], for an air pollution model, a convection-diffusion-reaction equation, with dry deposition at the boundary and wet deposition in the source term, was proposed. The researchers analyzed the numerical solution for sulfur and nitrogen oxides, and the high order accurate time-stepping discretization scheme was applied with the Lax and Wendroff technique to solve the pollutant concentrations. In [20], the modeling and application of Atmospheric Evaluation and Research Integrated model for Spain (AERIS) were proposed. Presently, AERIS can equip the concentrations of nitrogen dioxide, ozone, sulfur dioxide, ammonia ($NH_3$), and particulate matter as a reaction to emission changes of relevant sectors in Spain. The Air Quality Modelling System (AQMS) consisted of the Weather Research and Forecast (WRF), Sparse Matrix Operator Kernel Emissions (SMOKE), and Community Multiscale Air Quality (CMAQ) models, which were used to solve the result by transfer matrices. In [21], a time dependent two-dimensional advection-diffusion model with a realistic form of different wind velocity and eddy diffusion coefficients was presented. The Crank-Nicolson implicit finite difference technique and upwind difference scheme was applied to the advection term to estimate the primary and secondary pollutant concentrations from the area source. In [22], the Campania region, Southern Italy, was used in order to consider environmental problems. The assessment of a wide and critical area under observation with different air pollution sources was proposed. In [23], a numerical simulation of three-dimensional air quality model in an area under the sky train of Bangkok Transit Systems (BTS) was studied. This consideration of air pollution problem was presented in different cases regarding the wind inflow with obstacles. The concentrations of air pollution in the tunnel were solved by using the forward time central space (FTCS) scheme. In [24], the wind current and air pollutant dispersion problem were simulated to predict the behavior of air pollution within an urban street canyon. The Computational Fluid Dynamics (CFD) techniques that were Reynolds-Averaged Navier-Stokes (RANS), Unsteady RANS (URANS), and Large Eddy Simulation (LES) were presented in order to compare the efficiency of numerical techniques. The results of the air pollution problem explained that LES was observed to produce more accurate data than RANS or URANS. In [25], a two-dimensional diffusion equation with nonlocal boundary conditions was presented. The numerical solution of the Padé schemes demonstrates that these schemes were efficient and gave accurate results.

The behavior of air pollution dispersion in the atmosphere is studied by considering the atmospheric diffusion equation. The primary pollutant sulfur dioxide and the secondary pollutants sulfur trioxide and sulfuric acid are presented. In this research, wind velocity and the diffusion coefficient are proposed as constants, and the approximate solutions for the concentrations of pollutant are solved by using the finite difference method. The purpose of this study is to examine the concentrations of sulfur dioxide, sulfur trioxide, and sulfuric acid in the multiple air pollution emission control problem. The air quality standard is also used for comparison with the results of the experiments.

## II. GOVERNING EQUATION

### A. Atmospheric Diffusion Equation

This simulation explains the dispersion behavior of air pollutants in the atmosphere. The dispersion model is used to approximate the downwind concentration of air pollutants. The three-dimensional advection-diffusion equation, which is a well-known atmospheric diffusion equation, is presented. That is

$$\frac{\partial c}{\partial t}+u\frac{\partial c}{\partial x}+v\frac{\partial c}{\partial y}+w\frac{\partial c}{\partial z}=k_x\frac{\partial^2 c}{\partial x^2}+k_y\frac{\partial^2 c}{\partial y^2}+k_z\frac{\partial^2 c}{\partial z^2}+S+R\,, \quad (1)$$

where $c=c(x,y,z,t)$ is the air pollutant concentration at $(x,y,z)$ and time $t$ (kg/m$^3$), $u$, $v$, and $w$ are the wind velocity components in x-, y-, and z-direction respectively (m/s), $k_x$, $k_y$, and $k_z$ are the diffusivity in x-, y-, and z-direction respectively (m$^2$/s), $S$ is the growth of pollutant rate due to sources (s$^{-1}$), and $R$ is the decaying of pollutant rate due to sinks (s$^{-1}$).

We assume that the advection and diffusion in the y-direction are laterally averaged. By assumption (1), all terms in y-direction can be eliminated. So, the governing equation becomes

$$\frac{\partial c}{\partial t}+u\frac{\partial c}{\partial x}+w\frac{\partial c}{\partial z}=k_x\frac{\partial^2 c}{\partial x^2}+k_z\frac{\partial^2 c}{\partial z^2}+S+R\ . \tag{2}$$

In this research, we consider the ambient air pollution near an industrial area. The air pollution in the present study can be split in two groups, primary and secondary pollutants.

### *B. Primary Pollutant Concentration Measurement Model*

Primary pollutants are air pollutants emitted directly from sources. The numerical approximate solution considers the concentration of pollutant that is sulfur dioxide. The chemical formula is $SO_2$.

#### *Sulfur Dioxide Concentration Measurement Model*

Sulfur dioxide is a major gas that is released from factory chimneys into the atmosphere. This occurs from the combustion of fuel. In this model, $c_p$ represents the concentration of sulfur dioxide. Therefore, the primary pollutant equation is

$$\frac{\partial c_p}{\partial t}+u\frac{\partial c_p}{\partial x}+w\frac{\partial c_p}{\partial z}=k_x\frac{\partial^2 c_p}{\partial x^2}+k_z\frac{\partial^2 c_p}{\partial z^2}+S_p+R_p\ , \tag{3}$$

where $S_p=q\delta(x-x_r)\delta(z-z_r)$ [9] when $q$ is the emission rate of the source (kg/s) and $\delta(\,)$ represents the Dirac's delta function and $R_p=-k_pc_p$ when $k_p$ is the first order chemical interaction rate of primary pollutant $c_p$. The cold start assumption is used for the initial condition. It follows

$$c_p(x,z,0)=0\,, \tag{4}$$

for all $x>0$ and $z>0$. The boundary conditions of sulfur dioxide assumed that

$$\frac{\partial c_p}{\partial x}(0,z,t)=0\,, \tag{5}$$

$$\frac{\partial c_p}{\partial x}(l_x,z,t)=0\,, \tag{6}$$

$$\frac{\partial c_p}{\partial z}(x,l_z,t)=0\,, \tag{7}$$

$$\frac{\partial c_p}{\partial z}(x,0,t)=v_{dp}c_p\,, \tag{8}$$

for all $t>0$ where $l_x$ is the length of the domain in x-direction, $l_z$ is the height of the inversion layer, and $v_{dp}$ is the dry deposition velocity of the primary pollutant (m/s). Sulfur dioxide deposition velocity can be referred to as diffusivity $k_z$ which is assumed to be an irreversible process.

### *C. Secondary Pollutant Concentration Measurement Model*

Secondary pollutants are air pollutants that occur in the atmosphere from a chemical interaction. There are two considered pollutants in this research. Sulfur trioxide reacts between sulfur dioxide and oxygen, and sulfuric acid is converted from sulfur dioxide, water, and oxygen. Thus, the following chemical reaction equations are

$$2SO_2+O_2\longrightarrow 2SO_3\,, \tag{9}$$

$$2SO_2+2H_2O+O_2\longrightarrow 2H_2SO_4\,. \tag{10}$$

#### *Sulfur Trioxide Concentration Measurement Model*

Sulfur trioxide is an important pollutant which can also be the agent in other pollutants. The concentration of sulfur trioxide is represented by $c_{s_1}$. Thus, the dispersion of sulfur trioxide is considered by the following equation

$$\frac{\partial c_{s_1}}{\partial t}+u\frac{\partial c_{s_1}}{\partial x}+w\frac{\partial c_{s_1}}{\partial z}=k_x\frac{\partial^2 c_{s_1}}{\partial x^2}+k_z\frac{\partial^2 c_{s_1}}{\partial z^2}+S_{s_1}\,, \tag{11}$$

where $S_{s_1}=V_gk_{s_1}c_p$ when $V_g$ is the mass ratio of secondary pollutant per the primary pollutant and $k_{s_1}$ is the first order chemical interaction rate of sulfur trioxide pollutant**.** The initial condition is assumed under the cold start assumption. That is

$$c_{s_1}(x,z,0)=0\,, \tag{12}$$

for all $x>0$ and $z>0$. Boundary conditions of sulfur trioxide supposed that

$$\frac{\partial c_{s_1}}{\partial x}(0,z,t)=0\,, \tag{13}$$

$$\frac{\partial c_{s_1}}{\partial x}(l_x,z,t)=0\,, \tag{14}$$

$$\frac{\partial c_{s_1}}{\partial z}(x,l_z,t)=0\,, \tag{15}$$

$$\frac{\partial c_{s_1}}{\partial z}(x,0,t)=v_{ds_1}c_{s_1}\,, \tag{16}$$

for all $t>0$ where $v_{ds_1}$ is the dry deposition velocity of the sulfur trioxide air pollutant (m/s).

### *D. Sulfuric Acid Concentration Measurement Model*

In this research, sulfuric acid which is one of the significant chemical compounds is the product of sulfur dioxide, water, and oxygen. We consider that $c_{s_2}$ is the concentration of sulfuric acid. So, the secondary pollutant of sulfuric acid equation is

$$\frac{\partial c_{s_2}}{\partial t}+u\frac{\partial c_{s_2}}{\partial x}+w\frac{\partial c_{s_2}}{\partial z}=k_x\frac{\partial^2 c_{s_2}}{\partial x^2}+k_z\frac{\partial^2 c_{s_2}}{\partial z^2}+S_{s_2}\,, \tag{17}$$

where $S_{s_2}=V_gk_{s_2}c_p$ when $k_{s_2}$ is the first order chemical interaction rate of sulfuric acid pollutant**.** The initial condition is similar to the condition of sulfur trioxide. That is

$$c_{s_2}(x,z,0)=0\,, \tag{18}$$

for all $x>0$ and $z>0$. Then, boundary conditions of sulfuric acid assumed that

$$\frac{\partial c_{s_2}}{\partial x}(0,z,t)=0\,, \tag{19}$$

$$\frac{\partial c_{s_2}}{\partial x}(l_x,z,t)=0\,, \tag{20}$$

$$\frac{\partial c_{s_2}}{\partial z}(x,l_z,t)=0\,, \tag{21}$$

$$\frac{\partial c_{s_2}}{\partial z}(x,0,t)=v_{ds_2}c_{s_2}\,, \tag{22}$$

for all $t>0$ where $v_{ds_2}$ is the dry deposition velocity of sulfuric acid pollutant (m/s).

Fig.1 shows the model of the air pollution emission control problem when the pollutants are emitted from a factory chimney. This research was designed to analyze the behavior and effects of primary and secondary pollutant dispersion near an industrial zone.

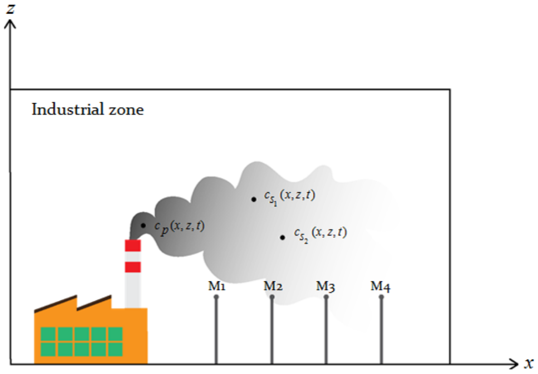

Fig. 1. Model of air pollution emission control problem

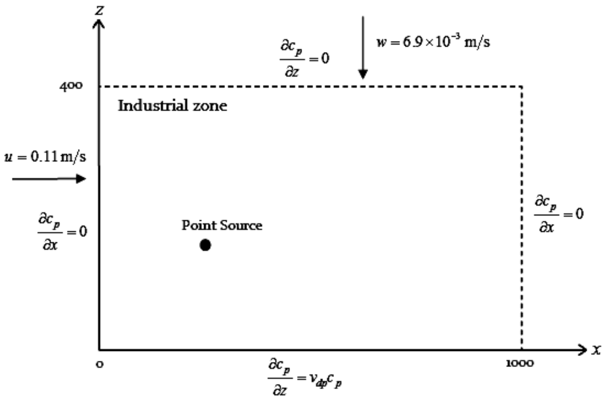

Fig. 2. Domain of sulfur dioxide approximate solutions

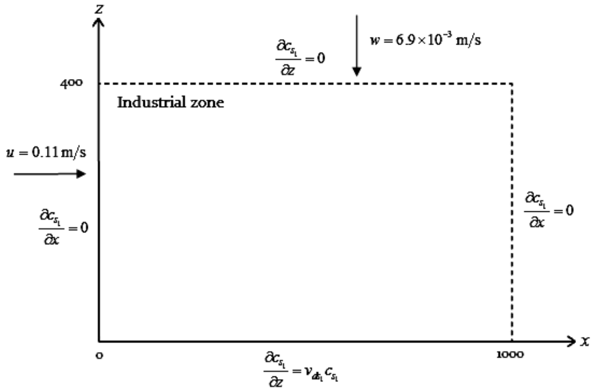

Fig. 3. Domain of sulfur trioxide approximate solutions

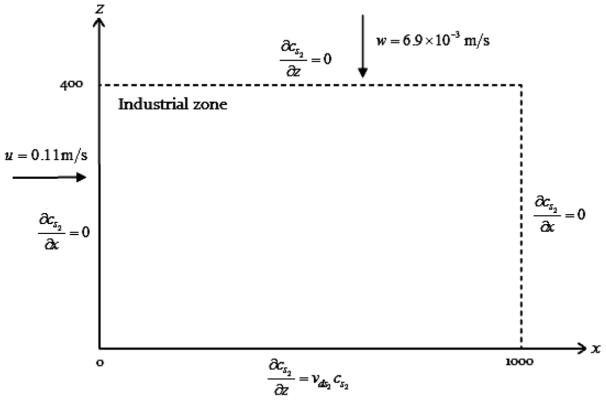

Fig. 4. Domain of sulfuric acid approximate solutions

Air quality monitoring equipment can check for three pollutants at one monitoring point. The four monitoring points are set far from the source. The monitoring points are called monitoring point no.1 (M1), monitoring point no.2 (M2), monitoring point no.3 (M3), and monitoring point no.4 (M4), at distances of 200, 300, 400, and 500 m, respectively. In Fig. 2, the domain of sulfur dioxide approximate solutions for the numerical experiment is shown. We suppose that the height of the point source is $h_{ps}$ m. The concentrated of sulfur dioxide is discharged continuously from the chimney. Figs. 3 and 4 show the domains of sulfur trioxide and sulfuric acid's approximate solutions for the numerical experiment. The concentration of sulfur trioxide and sulfuric acid is increased by the conversion of sulfur dioxide pollutant in the system. We assume that the wind and the diffusion coefficient are stable in the x- and z-directions. The sulfur dioxide, sulfur trioxide, and sulfuric acid are absorbed from the atmosphere by the removal mechanism at ground level.

### *E. Non-dimensional Form of Primary and Secondary Pollutant Concentration Measurement Models*

The transformation technique of variable is applied by converting the dimensional equation to the non-dimensional equation. The same dimensionless variable of (3), (11), and (17) are defined by $X=x/l_x$, $Z=z/l_z$, $T=t/t_{\max}$, $D_x=k_x/l_x u_{\max}$, $D_z=k_z/l_z u_{\max}$, $U=u/u_{\max}$, and $W=\beta w_{\max}/u_{\max}$ when $\beta=w/w_{\max}$. We let $c_{\max}=\max\{c_p(x,z,t)=c_{s_1}(x,z,t)=c_{s_2}(x,z,t):0\le x\le l_x, 0\le z\le l_z, 0\le t\le t_{\max}\}$, $u_{\max}=\max\{u(x,z,t):0\le x\le l_x, 0\le z\le l_z, 0\le t\le t_{\max}\}$, $w_{\max}=\max\{w(x,z,t):0\le x\le l_x, 0\le z\le l_z, 0\le t\le t_{\max}\}$ and $t_{\max}$ is a stationary time. The dimensionless forms of sulfur dioxide, sulfur trioxide, and sulfuric acid are proposed.

### *F. Non-dimensional Form of Sulfur Dioxide Concentration Measurement Model*

The dimensionless variable of sulfur dioxide concentration is defined by $C_p=c_p/c_{\max}$. When we use the relation of above variables, the dimensionless equation of sulfur dioxide can be written as

$$\begin{aligned}&\frac{1}{St}\frac{\partial C_p}{\partial T}+U\frac{\partial C_p}{\partial X}+W\frac{\partial C_p}{\partial Z}\\&=D_x\frac{\partial^2 C_p}{\partial X^2}+D_z\frac{\partial^2 C_p}{\partial Z^2}+Q\delta(X-X_r)\delta(Z-Z_r)-K_pC_p,\end{aligned} \tag{23}$$

where $l=\max\{l_x,l_z\}$ and $St=t_{\max}u_{\max}/l$.

The non-dimensional form for the initial condition of sulfur dioxide assumed that

$$C_p(X,Z,0)=0, \tag{24}$$

for all $0<X<1$ and $0<Z<1$. For the non-dimensional of boundary, it is supposed that

$$\frac{\partial C_p}{\partial X}(0,Z,T)=0, \tag{25}$$

$$\frac{\partial C_p}{\partial X}(1,Z,T)=0, \tag{26}$$

$$\frac{\partial C_p}{\partial Z}(X,1,T)=0, \qquad (27)$$

$$\frac{\partial C_p}{\partial Z}(X,0,T)=V_{dp}C_p, \qquad (28)$$

for all $T>0$.

### *G. Non-dimensional Form of Sulfur Trioxide Concentration Measurement Model*

For the secondary pollutants, we employ the same technique with the primary pollutant. Furthermore, the non-dimensional forms of sulfur trioxide and sulfuric acid are presented. From (11), we consider the dimensionless variable of sulfur trioxide concentration which is $C_{s_1}=c_{s_1}/c_{\max}$. Therefore, the non-dimensional of sulfur trioxide equation can be rearranged to give

$$\frac{1}{St}\frac{\partial C_{s_1}}{\partial T}+U\frac{\partial C_{s_1}}{\partial X}+W\frac{\partial C_{s_1}}{\partial Z}=D_x\frac{\partial^2 C_{s_1}}{\partial X^2}+D_z\frac{\partial^2 C_{s_1}}{\partial Z^2}+V_gK_{s_1}C_p. \qquad (29)$$

The non-dimensional of sulfur trioxide initial condition assumed that

$$C_{s_1}(X,Z,0)=0, \qquad (30)$$

for all $0<X<1$ and $0<Z<1$. The dimensionless form of boundary conditions assumed that

$$\frac{\partial C_{s_1}}{\partial X}(0,Z,T)=0, \qquad (31)$$

$$\frac{\partial C_{s_1}}{\partial X}(1,Z,T)=0, \qquad (32)$$

$$\frac{\partial C_{s_1}}{\partial Z}(X,1,T)=0, \qquad (33)$$

$$\frac{\partial C_{s_1}}{\partial Z}(X,0,T)=V_{ds_1}C_{s_1}, \qquad (34)$$

for all $T>0$.

### *H. Non-dimensional Form of Sulfuric Acid Concentration Measurement Model*

For (17), The dimensionless variable of sulfuric acid concentration is defined by $C_{s_2}=c_{s_2}/c_{\max}$. Thus, the non-dimensional of sulfuric acid equation is

$$\frac{1}{St}\frac{\partial C_{s_2}}{\partial T}+U\frac{\partial C_{s_2}}{\partial X}+W\frac{\partial C_{s_2}}{\partial Z}=D_x\frac{\partial^2 C_{s_2}}{\partial X^2}+D_z\frac{\partial^2 C_{s_2}}{\partial Z^2}+V_gK_{s_2}C_p. \qquad (35)$$

We assume that the initial condition of sulfuric acid is the same assumption as sulfur trioxide

$$C_{s_2}(X,Z,0)=0, \qquad (36)$$

for all $0<X<1$ and $0<Z<1$. And the non-dimensional of boundary condition assumed that

$$\frac{\partial C_{s_2}}{\partial X}(0,Z,T)=0, \qquad (37)$$

$$\frac{\partial C_{s_2}}{\partial X}(1,Z,T)=0, \qquad (38)$$

$$\frac{\partial C_{s_2}}{\partial Z}(X,1,T)=0, \qquad (39)$$

$$\frac{\partial C_{s_2}}{\partial Z}(X,0,T)=V_{ds_2}C_{s_2}, \qquad (40)$$

for all $T>0$.

## III. NUMERICAL TECHNIQUES

The air pollutant concentration model is designed to analyze the multiple air quality problems around industrial factories. The concentrations of pollutants are predicted by the approximate solution. We obtain the concentration of sulfur dioxide, sulfur trioxide, and sulfuric acid at each time $T_{n+1}$ from $T_n=n\Delta T$, $n=0,1,2,\ldots,P$ when $\Delta T$ is an increment of time. The solutions of sulfur dioxide ($SO_2$), sulfur trioxide ($SO_3$), and sulfuric acid ($H_2SO_4$) concentration at $(X,Z,T)$ are denoted by $C_p(X_i,Z_j,T_n)=C^n_{pi,j}$, $C_{s_1}(X_i,Z_j,T_n)=C^n_{s_1 i,j}$, and $C_{s_2}(X_i,Z_j,T_n)=C^n_{s_2 i,j}$ respectively. The grid spacing $\Delta X$ and $\Delta Z$ are considered by meshing the interested domain where $X_i=i\Delta X$, $i=0,1,2,\ldots,N$ and $Z_j=j\Delta Z$, $j=0,1,2,\ldots,$ M and $N\Delta X=1$, $M\Delta Z=1$. The method utilized to estimate all the solutions is the finite difference method.

### *A. Numerical Method for Primary Pollutant Model*

*Numerical Method for Sulfur Dioxide Measurement*

We use the forward time central space (FTCS) finite difference scheme for the sulfur dioxide pollutant in the non-dimensional (23). In the transient term, the method is derived by using the forward difference,

$$\frac{\partial C_p}{\partial T}=\frac{C^{n+1}_{pi,j}-C^n_{pi,j}}{\Delta T}. \qquad (41)$$

The advection and diffusion terms are considered by using the centered difference approximation. We have

$$\frac{\partial C_p}{\partial X}=\frac{C^n_{pi+1,j}-C^n_{pi-1,j}}{2\Delta X}, \qquad (42)$$

$$\frac{\partial C_p}{\partial Z}=\frac{C^n_{pi,j+1}-C^n_{pi,j-1}}{2\Delta Z}, \qquad (43)$$

$$\frac{\partial^2 C_p}{\partial X^2}=\frac{C^n_{pi+1,j}-2C^n_{pi,j}+C^n_{pi-1,j}}{(\Delta X)^2}, \qquad (44)$$

$$\frac{\partial^2 C_p}{\partial Z^2}=\frac{C^n_{pi,j+1}-2C^n_{pi,j}+C^n_{pi,j-1}}{(\Delta Z)^2}. \qquad (45)$$

We substitute (41)-(45) into (23). Then, it becomes

$$\begin{aligned}&\frac{1}{St}\left(\frac{C^{n+1}_{pi,j}-C^n_{pi,j}}{\Delta T}\right)+U\left(\frac{C^n_{pi+1,j}-C^n_{pi-1,j}}{2\Delta X}\right)+W\left(\frac{C^n_{pi,j+1}-C^n_{pi,j-1}}{2\Delta Z}\right)\\&=D_x\left(\frac{C^n_{pi+1,j}-2C^n_{pi,j}+C^n_{pi-1,j}}{(\Delta X)^2}\right)+D_z\left(\frac{C^n_{pi,j+1}-2C^n_{pi,j}+C^n_{pi,j-1}}{(\Delta Z)^2}\right)\\&+Q\delta(X-X_r)\delta(Z-Z_r)-K_pC^n_{pi,j}.\end{aligned} \qquad (46)$$

Thus, the finite difference form of sulfur dioxide equation is

$$\begin{aligned}C^{n+1}_{pi,j}&=\left(d_x-A_x\right)C^n_{pi+1,j}+\left(d_x+A_x\right)C^n_{pi-1,j}\\&+\left(1-2d_x-2d_z-St\left(\Delta T\right)K_p\right)C^n_{pi,j}+\left(d_z+A_z\right)C^n_{pi,j-1}\\&+\left(d_z-A_z\right)C^n_{pi,j+1}+St\left(\Delta T\right)Q\delta(X-X_r)\delta(Z-Z_r),\end{aligned} \qquad (47)$$

where $A_x=St(\Delta T)U/2\Delta X$, $A_z=St(\Delta T)W/2\Delta Z$, $d_x=St(\Delta T)D_x/(\Delta X)^2$, and $d_z=St(\Delta T)D_z/(\Delta Z)^2$.

### *B. Numerical Method for Secondary Pollutant Model*

For the secondary pollutants, we use the finite difference method. In addition, the forward time central space schemes for sulfur trioxide and sulfuric acid are similar to the methods for previous pollutant. The finite difference expressions are proposed.

*Numerical Method for Sulfur Trioxide Measurement*

The transient term of sulfur trioxide is substituted by using the forward difference

$$\frac{\partial C_{s_1}}{\partial T}=\frac{C^{n+1}_{s_1\,i,j}-C^{n}_{s_1\,i,j}}{\Delta T}. \tag{48}$$

Then, we use the centered difference for the advection and diffusion terms in X- and Z-direction

$$\frac{\partial C_{s_1}}{\partial X}=\frac{C^{n}_{s_1\,i+1,j}-C^{n}_{s_1\,i-1,j}}{2\Delta X}, \tag{49}$$

$$\frac{\partial C_{s_1}}{\partial Z}=\frac{C^{n}_{s_1\,i,j+1}-C^{n}_{s_1\,i,j-1}}{2\Delta Z}, \tag{50}$$

$$\frac{\partial^2 C_{s_1}}{\partial X^2}=\frac{C^{n}_{s_1\,i+1,j}-2C^{n}_{s_1\,i,j}+C^{n}_{s_1\,i-1,j}}{(\Delta X)^2}, \tag{51}$$

$$\frac{\partial^2 C_{s_1}}{\partial Z^2}=\frac{C^{n}_{s_1\,i,j+1}-2C^{n}_{s_1\,i,j}+C^{n}_{s_1\,i,j-1}}{(\Delta Z)^2}. \tag{52}$$

Equation (29) is substituted by (48)-(52). We obtain

$$\begin{aligned}&\frac{1}{St}\left(\frac{C^{n+1}_{s_1\,i,j}-C^{n}_{s_1\,i,j}}{\Delta T}\right)+U\left(\frac{C^{n}_{s_1\,i+1,j}-C^{n}_{s_1\,i-1,j}}{2\Delta X}\right)+W\left(\frac{C^{n}_{s_1\,i,j+1}-C^{n}_{s_1\,i,j-1}}{2\Delta Z}\right)\\&=D_x\left(\frac{C^{n}_{s_1\,i+1,j}-2C^{n}_{s_1\,i,j}+C^{n}_{s_1\,i-1,j}}{(\Delta X)^2}\right)+D_z\left(\frac{C^{n}_{s_1\,i,j+1}-2C^{n}_{s_1\,i,j}+C^{n}_{s_1\,i,j-1}}{(\Delta Z)^2}\right)\\&+V_gK_{s_1}C^{n}_{pi,j}.\end{aligned} \tag{53}$$

Thus, the finite difference form of the sulfur trioxide equation becomes

$$\begin{aligned}C^{n+1}_{s_1\,i,j}&=\left(d_x-A_x\right)C^{n}_{s_1\,i+1,j}+\left(d_x+A_x\right)C^{n}_{s_1\,i-1,j}\\&+\left(1-2d_x-2d_z\right)C^{n}_{s_1\,i,j}+\left(d_z+A_z\right)C^{n}_{s_1\,i,j-1}\\&+\left(d_z-A_z\right)C^{n}_{s_1\,i,j+1}+St(\Delta T)V_gK_{s_1}C^{n}_{pi,j}.\end{aligned} \tag{54}$$

### C. Numerical Method for Sulfuric Acid Measurement

Similarly, the transient term of sulfuric acid is represented as

$$\frac{\partial C_{s_2}}{\partial T}=\frac{C^{n+1}_{s_2\,i,j}-C^{n}_{s_2\,i,j}}{\Delta T}. \tag{55}$$

The advection and diffusion terms in X- and Z-direction are as follows

$$\frac{\partial C_{s_2}}{\partial X}=\frac{C^{n}_{s_2\,i+1,j}-C^{n}_{s_2\,i-1,j}}{2\Delta X}, \tag{56}$$

$$\frac{\partial C_{s_2}}{\partial Z}=\frac{C^{n}_{s_2\,i,j+1}-C^{n}_{s_2\,i,j-1}}{2\Delta Z}, \tag{57}$$

$$\frac{\partial^2 C_{s_2}}{\partial X^2}=\frac{C^{n}_{s_2\,i+1,j}-2C^{n}_{s_2\,i,j}+C^{n}_{s_2\,i-1,j}}{(\Delta X)^2}, \tag{58}$$

$$\frac{\partial^2 C_{s_2}}{\partial Z^2}=\frac{C^{n}_{s_2\,i,j+1}-2C^{n}_{s_2\,i,j}+C^{n}_{s_2\,i,j-1}}{(\Delta Z)^2}, \tag{59}$$

respectively. Equation (35) becomes

$$\begin{aligned}&\frac{1}{St}\left(\frac{C^{n+1}_{s_2\,i,j}-C^{n}_{s_2\,i,j}}{\Delta T}\right)+U\left(\frac{C^{n}_{s_2\,i+1,j}-C^{n}_{s_2\,i-1,j}}{2\Delta X}\right)+W\left(\frac{C^{n}_{s_2\,i,j+1}-C^{n}_{s_2\,i,j-1}}{2\Delta Z}\right)\\&=D_x\left(\frac{C^{n}_{s_2\,i+1,j}-2C^{n}_{s_2\,i,j}+C^{n}_{s_2\,i-1,j}}{(\Delta X)^2}\right)+D_z\left(\frac{C^{n}_{s_2\,i,j+1}-2C^{n}_{s_2\,i,j}+C^{n}_{s_2\,i,j-1}}{(\Delta Z)^2}\right)\\&+V_gK_{s_2}C^{n}_{pi,j}.\end{aligned} \tag{60}$$

Therefore, the finite difference form of the sulfuric acid can be written as

$$\begin{aligned}C^{n+1}_{s_2\,i,j}&=\left(d_x-A_x\right)C^{n}_{s_2\,i+1,j}+\left(d_x+A_x\right)C^{n}_{s_2\,i-1,j}\\&+\left(1-2d_x-2d_z\right)C^{n}_{s_2\,i,j}+\left(d_z+A_z\right)C^{n}_{s_2\,i,j-1}\\&+\left(d_z-A_z\right)C^{n}_{s_2\,i,j+1}+St(\Delta T)V_gK_{s_2}C^{n}_{pi,j}.\end{aligned} \tag{61}$$

## IV. AIR POLLUTION CONTROLLED SIMULATIONS

These experiments analyzed the dispersion conduct of air pollution for primary and secondary pollutants, and multiple air pollution emission control from an industrial factory was considered. The national ambient air quality standards (NAAQS) described in [18] were used to manage air quality control in the industrial area and nearby residential areas. Then, air quality criteria in general can be separated into two levels: 1) The primary ambient air quality standard is the standard level to protect human health, and 2) the secondary ambient air quality standard is the standard level for human well-being protection or hazard protection of animals, crops, vegetation, and buildings. In this research, we simulate two situations of decision air pollution emission control under different air quality standards. The factory discharges sulfur dioxide (SO2), while sulfur trioxide (SO3) and sulfuric acid (H2SO4) form from sulfur dioxide in the climate. Then, all air pollutants are considered at each monitoring point using the national air quality index. Air quality standards for sulfur dioxide, sulfur trioxide, and sulfuric acid, which are appropriate for these three air pollutants, are presented in Table I.

### A. Simulation: A Controlled Air Quality Standard.

Primary pollution emission is controlled by following the United States Environmental Protection Agency (USEPA) air quality standards, and secondary pollutants controlled by determining the air quality standard. The two-dimensional advection-diffusion equations (23), (29), and (35), with the interested domain 1000 m × 400 m, are considered. The proper variables for this simulation suppose that the wind velocities in the x- and z-directions are 0.11 and $6.9\times10^{-3}$ m/s, respectively. The diffusion coefficients in the x- and z-directions are 2 and 0.4 $m^2/s$, respectively, and the rate of released pollutant concentration $q$ is $2.1875\times10^{-3}$ kg/s. The height of chimney $h_{ps}$ is 50 m. This means a point source emits the sulfur dioxide at the coordinates (100,50) (m,m). The grid spacing is $\Delta x=25$ and $\Delta z=25$ m, and the time interval is $\Delta t=72$ s. In this simulation, the sulfur dioxide is released by following the empirical USEPA air quality standard, $(2/3)(6.5\times10^{-8})=4.33\times10^{-8}$ kg/m$^3$. The sulfur trioxide and sulfuric acid are accrued by the chemical interaction into the atmosphere, and the empirical air quality standards of sulfur trioxide and sulfuric acid are $(2/3)(5.45\times10^{-8})=3.63\times10^{-8}$ and $(2/3)(4.25\times10^{-8})=2.83\times10^{-8}$ kg/m$^3$, respectively. The air pollution emission operates to follow these processes. In the considered pollutants investigated, if the approximate pollutant concentration at a monitoring point is higher than the air quality standards, the chimney is shut down and waits until the concentration of sulfur dioxide, sulfur trioxide, and sulfuric acid is less than $(2/5)(6.5\times10^{-8})=2.6\times10^{-8}$, $(2/5)(5.45\times10^{-8})=2.18\times10^{-8}$, and $(2/5)(4.25\times10^{-8})=1.7\times10^{-8}$ kg/m$^3$, respectively. If the concentration of all pollutants at the monitoring point is below two fifths of the air quality standard, then the chimney is opened again to discharge the air pollution. Simulation 1 is solved by using the FTCS of sulfur dioxide (47), sulfur trioxide (54), and sulfuric acid (61) equations, with the initial and the boundary conditions (24)-(28), (30)-

(34), and (36)-(40), respectively. The numerical solutions of sulfur dioxide at all monitoring points for the decision emission control points at M1, M2, M3, and M4 are shown in Figs. 5-8. Similarly, the concentrations of sulfur trioxide and sulfuric acid which are controlled by the decision emission control points at M1, M2, M3, and M4 are shown in Figs. 9-12 and 13-16 respectively. The maximums of air pollution concentration at each monitoring point at M1, M2, M3, and M4 are presented in Table. II-V, respectively.

## V. DISCUSSION

The primary and secondary pollutant concentrations at the monitoring points are analyzed by controlling each decision monitoring point and then presented. In this research, the forward time central space scheme is used to solve sulfur dioxide (SO2), sulfur trioxide (SO3), and sulfuric acid (H2SO4) pollutant concentrations near the industrial zone. The air pollution emission control is considered at the monitoring points of M1, M2, M3, and M4. The air quality standard for sulfur dioxide, sulfur trioxide, and sulfuric acid, which is used to compare the concentration between the numerical solutions and the standards, is presented in Table. I.

The approximate solutions of the simulation are considered. For the decision emission control point at M1, Fig. 5 shows that the sulfur dioxide concentration levels at monitoring points M2-M4 are below the air quality standard level, but the concentration levels at the decision emission control point go over the standard level.

In Tables II-V and VI-IX, we choose the maximum concentration of pollutants in each case in both simulations in order to analyze the air quality for simulation. The decision on air pollution emission control at M1 shows that the quantity of sulfur dioxide and sulfuric acid at almost all monitoring points is below the standard level. On the other hand, all decision air pollution emission controls of sulfur trioxide concentration give a good quality. Table. X shows the number of standardized nodes that are controlled by M1, M2, M3, or M4. In this research, the maximum number of standardized nodes is 11 points. Overall, the concentrations at all points are below air quality standards. They do not have an effect on human health or the environment when the distance and time are increased.

Table. I. Air quality standards of $SO_2$, $SO_3$, and $H_2SO_4$ concentration measurement

| **$SO_2$** [19] ($\times 10^{-8}$) | **$SO_3$** ($\times 10^{-8}$) | **$H_2SO_4$** ($\times 10^{-8}$) |
|---|---|---|
| 6.5 | 5.45 | 4.25 |

Table. II. Maximum concentrations (kg/m$^3$) at each monitoring point when the decision emission control monitor is at M1 in the simulation

| **Monitoring Point** | **$SO_2$** ($\times 10^{-8}$) | **$SO_3$** ($\times 10^{-8}$) | **$H_2SO_4$** ($\times 10^{-8}$) |
|---|---|---|---|
| **M1** | 7.9842 | 1.0033 | 3.0096 |
| M2 | 5.7459 | 1.3139 | 3.9412 |
| M3 | 4.1085 | 1.4200 | 4.2590 |
| M4 | 3.0394 | 1.4761 | 4.4267 |

Table. III. Maximum concentrations (kg/m$^3$) at each monitoring point when the decision emission control monitor is at M2 in the simulation

| **Monitoring Point** | **$SO_2$** ($\times 10^{-8}$) | **$SO_3$** ($\times 10^{-8}$) | **$H_2SO_4$** ($\times 10^{-8}$) |
|---|---|---|---|
| M1 | 10.2178 | 1.3872 | 4.1612 |
| **M2** | 8.2383 | 1.8511 | 5.5527 |
| M3 | 6.1027 | 2.0727 | 6.2167 |
| M4 | 4.5063 | 2.1230 | 6.3668 |

Table. IV. Maximum concentrations (kg/m$^3$) at each monitoring point when the decision emission control monitor is at M3 in the simulation

| **Monitoring Point** | **$SO_2$** ($\times 10^{-8}$) | **$SO_3$** ($\times 10^{-8}$) | **$H_2SO_4$** ($\times 10^{-8}$) |
|---|---|---|---|
| M1 | 10.6290 | 1.4443 | 4.3326 |
| M2 | 9.1903 | 2.1639 | 6.4909 |
| **M3** | 7.2011 | 2.5272 | 7.5797 |
| M4 | 5.5217 | 2.6665 | 7.9966 |

Table. V. Maximum concentrations (kg/m$^3$) at each monitoring point when the decision emission control monitor is at M4 in the simulation

| **Monitoring Point** | **$SO_2$** ($\times 10^{-8}$) | **$SO_3$** ($\times 10^{-8}$) | **$H_2SO_4$** ($\times 10^{-8}$) |
|---|---|---|---|
| M1 | 10.7587 | 1.4993 | 4.4975 |
| M2 | 9.4933 | 2.2923 | 6.8760 |
| M3 | 7.6424 | 2.7455 | 8.2344 |
| **M4** | 6.0075 | 2.9620 | 8.8828 |

Table. X. Number of overall monitoring points which are under USEPA air quality standard when the different decision monitorial nodes are specified by M1, M2, M3, and M4

| **Decision Monitorial Node** | **Number of Standardized Nodes** | |
|---|---|---|
| | **Simulation 1** | **Simulation 2** |
| M1 | 9 | 11 |
| M2 | 7 | 7 |
| M3 | 5 | 5 |
| M4 | 5 | 5 |

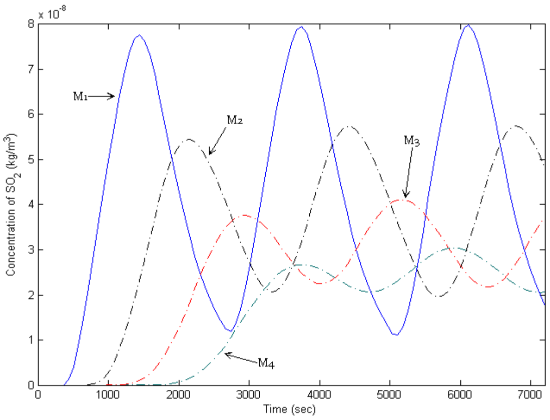

Fig. 5. Primary concentrations of $SO_2$ at monitoring points by considering decision emission control point No.1 (M1) with $SO_2$ standard in the simulation

## VI. CONCLUSION

The multiple atmospheric diffusion equations are studied by considering air pollutant concentrations near an industrial zone. The primary pollutant, sulfur dioxide (SO2), is emitted from a chimney into the atmosphere. Then, the secondary pollutants, sulfur trioxide (SO3) and sulfuric acid (H2SO4), are converted from the primary pollutants by chemical reactions. The approximate sulfur dioxide, sulfur trioxide, and sulfuric acid concentrations are calculated using the forward time central space scheme. The techniques for air pollution emission control (sulfur dioxide, sulfur trioxide, and sulfuric acid concentration) are proposed. For the purpose of identifying the appropriate emission control point, the concentrations at the monitored stations are compared to the air quality standards. According to the research, an appropriate monitoring point location is near a manufacturing plant. The selected monitoring location provides good overall air quality for emission control measures around industrial plants and residential areas. As a result, we conclude that the collecting position for each monitoring location influences air quality in the air pollution management strategy. The proposed air pollution management system could assist in reducing pollution near manufacturing sites. Other real-world situations should incorporate wind velocity in the horizontal direction, as well as humidity and rain, as pollutant sink elements in the model.

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