MODELING OF AIR POLLUTION DUE TO CARBON MONOXIDE EMISSION FROM VEHICLE EXHAUST

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ABSTRACT

Carbon monoxide (CO) is an important air pollutant because of its severe health effects at high concentration. It is an odourless, colourless, tasteless and non-irritating but potentially lethal gas produced from incomplete combustion of liquid, solid and gaseous fuel. In urban centres, the primary source of CO is vehicle exhaust emission from incomplete combustion. Previous studies have shown that a small number of high emitting vehicles are responsible for the majority of the CO emission in most urban areas. In this paper, a mathematical model has been developed using the time-dependent advection-diffusion equation of air pollution to predict the concentration of CO emission from vehicle exhaust into the atmosphere as time increases indefinitely. The mathematical model is solved using numerical methods based on the Crank-Nicolson finite difference scheme. The result shows that as CO flows in the x; y; z-axes (considering a 3-dimensional space) with respect to time, diffusion occurs and CO decays in the atmosphere.

INTRODUCTION

Air pollution has been an ongoing problem in many countries of the world. Highway traffic is a major source of air pollution. CO is one of the most common and widely distributed air pollutant gases. This gas can be lethal to human beings within minutes of high concentration exceeding 12800 parts per million (ppm) (Davis and Cornwell 1998; Sadullah *et al.*, 2003). In cities, as much as 95 percent of all CO emission comes from motor vehicle exhausts (U.S. EPA, 1999). Other sources of CO include industrial process, non-transportation fuel combustion and natural sources such as wild fire.

The easiest available study of CO data was done by Colucci and Bageman (1969), who compared CO concentration in Detroit, New York and Los Angeles and found that Los Angeles' high levels are related to frequent atmospheric temperature inversion and lower wind speed. Many CO models have been developed to forecast its concentration and health effect. Several efforts have been made for the development of model of point source and line source, since observational studies show that the wind speed and eddy diffusivity vary with vertical height above the ground (Stull, 1998). The concentration of contaminant released into the air may therefore be described by the time dependent advection - diffusion equation, which is a second order partial differential equation of the parabolic case (Stockie, 2011). Efforts have been exerted on the task of searching analytical solutions for the advection-diffusion equation in order to simulate the pollutant dispersion in the atmospheric boundary layer (ABL). Analytic solutions of the advection-diffusion equation are usually obtained just for stationary conditions and by making strong assumptions about the eddy diffusivity coefficients (K) and wind speed profiles (U). They are assumed as constant throughout the whole ABL or follow a power law (van Ulden, 1978; Pasqual and Smith, 1983; Seinfeld, 1986; Tirabassi, *et a*l., 1986; Sharan*et al*., 1996). Moriera, *et al*., (2015) presented a solution of the advection-diffusion equation based on the Laplace transform considering the ABL as a multilayer system. Analytic solution of the advection - diffusion equation with wind speed and vertical eddy diffusivity both as power function of vertical height, bounded by the ABL as well are known for point and line source (Seinfeld, 1986; Lin and Hildemann, 1996). The advection-diffusion equation has also been solved analytically with wind speed as a function of height and eddy diffusivity as a function of downwind distance from the source (Sharan and Modani, 2006).

Sharan and Kumar (2009) formulated the advection-diffusion equation considering the wind speed as a function of vertical height and eddy diffusivity as a function of both vertical height and downward distance applicable only for point source release in reaction to boundary conditions. However, Dirichlet (total absorption), Neumann (total reaction) and mixed boundary conditions are applied in the solution of the advection – diffusion equation. More recently, Daniela Buske, *et al* (2012) presented the general steady three-dimensional solution of the advection-diffusion equation considering a vertically inhomogeneous atmospheric boundary layer for arbitrary vertical profiles of wind and eddy-diffusion coefficients.

Since exact analytic solutions cannot generally be found, it is often necessary to resort to numerical methods to find approximate solutions of the advection - diffusion equation, in order to investigate the prediction of the model. E. Sousa (2003) studied the condition that ensured stability for various schemes for the advection - diffusion equation, while A. C. Hindmarsh*et a*l. (1984) examined the stability criteria for the multi dimensional advection-diffusion equation. M. Dehghan (2004) defines and calculates the stability for several numerical methods e.g. Forward in Time, Central in Space, Forward in Time, Backward in Space; Lax - Wendroff; Backward in Time, Central in Space; and Crank-Nicolson methods for the three dimensional advection - diffusion equation and compares the numerical and analytical solutions. S. Choo-in (2001) used a Box model to determine the pollutants in the street tunnel of Thailand.Fadugba, *et al*, (2013) have proved the Crank- Nicolson method to be unconditionally stable and to have higher order of accuracy than most other methods in solving parabolic partial differential equations.

MODEL FORMULATION

The key to studying air pollution models of this type is to employ the concept of Partial Differential Equation of a parabolic case that describes the pollutant's concentration per unit time. The time dependent advection-diffusion equation of air pollutant is needed to model carbon monoxide concentration requires the transport equation, the flux law and the law of conservation of mass.

$$\frac{\partial C}{\partial t} + U\frac{\partial C}{\partial x} = D\frac{\partial^2 C}{\partial x^2} \quad . \quad . \quad . \quad . \quad .. \qquad (1)$$

Equation (1) is the time dependent advection-diffusion equation in one dimensional space. For a 3-dimensional space;

$$\frac{\partial C}{\partial t} = \sum_{i=1}^{3}\left(-U_i\frac{\partial C}{\partial x_i} + D_i\frac{\partial^2 C}{\partial {x_i}^2}\right) \qquad (2)$$

i.e.
$$\frac{\partial C}{\partial t} = -U\frac{\partial C}{\partial x} + D_x\frac{\partial^2 C}{\partial x^2} - V\frac{\partial C}{\partial y} + D_y\frac{\partial^2 C}{\partial y^2} - W\frac{\partial C}{\partial z} + D_z\frac{\partial^2 C}{\partial z^2} \qquad (3)$$

where we have defined$x_i = (x, y, z)$, $U_i = (U, V, W)$, $D_i = (D_x, D_y, D_z)$.

Equation (3) is employed in modeling air pollution concentration and is required in modeling the concentration of carbon monoxide emission. Thus, the mathematical model of the concentration of air pollution due to carbon monoxide emission from vehicle exhaust into the atmosphere is given by

$$\frac{\partial C}{\partial t} = -U\nabla C + D\nabla^2 C - RC \qquad (4)$$

Where C is the concentration of carbon monoxide, RC is the difference between the source and sink of carbon monoxide in the atmosphere, U is the wind speed, D is the diffusion coefficient, and the other operators have their usual meaning.

Equation (4) is the equation for uniform flow (i.e., the change in wind speed $\nabla U = 0$). It can be modified for turbulent flow in the atmosphere by expressing the wind speed as the sum of mean and turbulence components. In that case equation (4) becomes

$$\frac{\partial C}{\partial t} = -(U\nabla C + C\nabla U) + D\nabla^2 C - RC \qquad (5)$$

Applying the averaging and local closure procedures in which the K – theory is used to reduce equation (5) to a first order equation, results in

$$\frac{\partial C}{\partial t} + U\nabla C = \nabla K \nabla C - RC \qquad (6)$$

where K is the diffusion coefficient, the K tensor is diagonal, molecular diffusion is negligible and $C(x, y, z, t)$ represents the concentration of carbon monoxide.

Method of solution

Equation (6) can be solved analytically or numerically if input data U, K and RC are provided with initial and boundary conditions. Applying the numerical method based on the Crank – Nicolson finite difference scheme to obtain the solution at different atmospheric boundary conditions and the K – theory, equation (6) becomes;

$$\frac{\partial C}{\partial t} + U\frac{\partial C}{\partial x} + V\frac{\partial C}{\partial y} + w\frac{\partial C}{\partial z} = \frac{\partial}{\partial x}\left(K_x \frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y \frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_z \frac{\partial C}{\partial z}\right) - RC. \qquad (7)$$

Where K_x, K_y and K_z are eddy diffusivities along x, y and z directions respectively.

The following assumptions are made in the solution of equation (7).

i. The vertical velocity component (w) is neglected in comparison to the horizontal (u and v)
ii. The $x-axis$ is oriented in the direction of mean wind (i.e. $u = U \; and \; v = 0$)
iii. The lateral flux of carbon monoxide along the cross wind direction is assumed to be small, i.e. $V\frac{\partial C}{\partial y}$ and $\frac{\partial}{\partial y}\left(K_y \frac{\partial C}{\partial y}\right) \to 0$
iv. Horizontal advection is greater than horizontal diffusion for not too small values of wind velocity, i.e., downwind diffusion is neglected in comparison to transport due to wind speed. i.e., $U\frac{\partial C}{\partial x} >> \frac{\partial}{\partial y}\left(K_x \frac{\partial C}{\partial x}\right)$.

Application of these conditions reduces equation (7) to

$$\frac{\partial C}{\partial t} + U\frac{\partial C}{\partial x} = \frac{\partial}{\partial z}\left(K_z \frac{\partial C}{\partial z}\right) - RC \qquad (8)$$

$$\Rightarrow \frac{\partial C}{\partial t} + U\frac{\partial C}{\partial x} = K_z \frac{\partial^2 C}{\partial z^2} - RC \qquad (.9)$$

To solve (9), we apply the initial and boundary conditions (the mixed boundary conditions) in which h is the height of the vehicle exhaust from the ground. Thus

$$C(x, y, z, t) = 0 \text{ at } z = h$$

$$K_z \frac{\partial C(x, y, z, t)}{\partial z} = 0 \text{ at } z = h$$

We apply the numerical method based on the Crank – Nicolson finite difference scheme to solve equation (9). The dependent variable C is a function of independent variables x, y, z, t, where i represents the position of x and z and m represents time. The derivatives of equation (9) are replaced by the arithmetic average of its finite difference approximation at the mth and $(m+1)th$ time step and the change in x and z at the $(i-1)th$, ith and $(i+1)th$ position.

Define

$$\frac{\partial C}{\partial t} = \frac{C_i^{m+1} - C_i^m}{\Delta t} \qquad (10)$$

$$\frac{\partial C}{\partial x}=\frac{1}{2}\left(\frac{C_{i+1}^{m+1}-C_{i-1}^{m+1}}{2\Delta x}+\frac{C_{i+1}^{m}-C_{i-1}^{m}}{2\Delta x}\right)$$

$$U\frac{\partial C}{\partial x}=\frac{U}{4\Delta x}\left(C_{i+1}^{m+1}-C_{i-1}^{m+1}+C_{i+1}^{m}-C_{i-1}^{m}\right) \quad (11)$$

$$\frac{\partial^2 C}{\partial z^2}=\frac{1}{2}\left(\frac{C_{i+1}^{m+1}-2C_{i}^{m+1}+C_{i-1}^{m+1}}{(\Delta x)^2}+\frac{C_{i+1}^{m}-2C_{i}^{m}+C_{i-1}^{m}}{2\Delta x}\right)$$

$$K_z\frac{\partial^2 C}{\partial z^2}=\frac{K_z}{2(\Delta z)^2}\left(C_{i+1}^{m+1}-2C_{i}^{m+1}+C_{i=1}^{m1}+C_{i+1}^{m}-2C_{i}^{m}+C_{i-1}^{m}\right) \quad (12)$$

$$C=\frac{1}{2}\left(C_{i}^{m+1}-C_{i}^{m}\right)$$

$$RC=\frac{R}{2}\left(C_{i}^{m+1}-C_{i}^{m}\right) \quad (13)$$

Substituting the above equations into (9) and multiplying through by Δt gives

$$C_{i}^{m+1}-C_{i}^{m}+\frac{U\Delta t}{4\Delta x}\left(C_{i+1}^{m+1}-C_{i-1}^{m+1}+C_{i+1}^{m}-C_{i-1}^{m}\right)=$$
$$\frac{K_z\Delta t}{2(\Delta z)^2}\left(C_{i+1}^{m+1}-2C_{i}^{m+1}+C_{i=1}^{m+1}+C_{i+1}^{m}-2C_{i}^{m}+C_{i-1}^{m}\right)-\frac{R\Delta t}{2}\left(C_{i}^{m+1}-C_{i}^{m}\right) \quad (14)$$

Let $\lambda=\frac{K_z\Delta t}{2(\Delta z)^2},\ \alpha=\frac{U\Delta t}{4\Delta x},\ \beta=\frac{R\Delta t}{2}.$

Substituting α, β and λ into equation (14), we obtain

$$C_{i}^{m+1}-C_{i}^{m}+\alpha\left(C_{i+1}^{m+1}-C_{i-1}^{m+1}+C_{i+1}^{m}-C_{i-1}^{m}\right)=$$
$$\lambda\left(C_{i+1}^{m+1}-2C_{i}^{m+1}+C_{i=1}^{m+1}+C_{i+1}^{m}-2C_{i}^{m}+C_{i-1}^{m}\right)-\beta\left(C_{i}^{m+1}-C_{i}^{m}\right) \quad (15)$$

Simplifying further we obtain

$$-C_{i}^{m}(1-2\lambda+\beta)+C_{i}^{m+1}(1+2\lambda+\beta)-C_{i-1}^{m}(\alpha+\lambda)-C_{i-1}^{m}(\alpha+\lambda)$$
$$+C_{i+1}^{m}(\alpha-\lambda)+C_{i+1}^{m}(\alpha-\lambda)=0 \quad (16)$$

Let $A=1+2\lambda-\beta, B=1+2\lambda+\beta, D=\alpha+\lambda, E=\alpha-\lambda$; substituting A, B, D and E into (16) yields

$$-AC_{i}^{m}+BC_{i}^{m+1}-DC_{i-1}^{m}-DC_{i-1}^{m+1}+EC_{i+1}^{m}+EC_{i+1}^{m+1}=0 \quad (17)$$

Applying the boundary conditions to (17), that is,

$$C(x,y,z,t)=0 \text{ at } z=0 \text{ and } K_z\frac{\partial C(x,y,z,t)}{\partial z}=0 \text{ at } z=h.$$

But $C=\frac{1}{2}\left(C_{i}^{m+1}-C_{i}^{m}\right)$ and $K_z\frac{\partial^2 C}{\partial z^2}=\frac{K_z}{2(\Delta z)^2}\left(C_{i+1}^{m+1}-2C_{i}^{m+1}+C_{i=1}^{m+1}+C_{i+1}^{m}-2C_{i}^{m}+C_{i-1}^{m}\right)$

Let $\chi=\frac{K_z}{2(\Delta z)^2}$

So that at $z=0, \frac{1}{2}\left(C_{i}^{m+1}-C_{i}^{m}\right)=0$ i.e., $BC_{i}^{m+1}-AC_{i}^{m}=0$ (18)

Also at $z=h$, $\chi\left(C_{i+1}^{m+1}-2C_{i}^{m+1}+C_{i=1}^{m+1}+C_{i+1}^{m}-2C_{i}^{m}+C_{i-1}^{m}\right)=0$

$$\Rightarrow -DC_{i-1}^{m}-DC_{i-1}^{m+1}+EC_{i+1}^{m}+EC_{i+1}^{m+1}=0 \quad (19)$$

From (18) and (19),

$$\Rightarrow BC_i^{m+1} - AC_i^m \equiv \frac{1}{2}\left(C_i^{m+1} - C_i^m\right) \equiv C(x, y, z) \equiv 0 \qquad (20)$$

Therefore $C(x, y, z) \to 0$ as $x, y, z \to \pm\infty$ and $t \to \infty$

The result in equation (20) shows that as CO moves in the x, y, z axes with respect to time, diffusion occurs and CO decays in the atmosphere.

RESULT AND DISCUSSION

The mathematical modeling equation (6) to predict the concentration of carbon monoxide emission from motor vehicle exhaust into the atmosphere with respect to time was built from the advection-diffusion equation for air pollutants. The equation was solved using the Crank-Nicolson finite difference scheme. It is observed that the concentration of carbon monoxide, $C(x, y, z)$, reduces as it flows in the atmosphere over a period of time due to wind speed and turbulence.

CONCLUSION

In developed and developing countries, traffic emissions are major contributors to poor urban air quality. A number of recent applications have been specifically developed to assess the contribution of traffic to air pollution. The common approach has been to consider traffic as exogenous information that has loose or no connection with land-use activities. The increasing use of automobiles and the consequent increase in the ambient air pollution necessitates modeling the concentration of carbon monoxide emission from motor vehicle exhaust, which is a point source model. The model despite a few limitations on its prediction and assumptions can be used for both regulatory process and for developing clean air strategies. The model is employed for the prediction of long-term average concentration of carbon monoxide in the atmosphere. It demands various boundary conditions, assumptions and development of formulation with physical conditions.

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