



# Prediction of Carbon Monoxide Concentration Due to Vehicular Emission Using Roe-Riemann Solver

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**Abstract-** The Roe-Riemann solver, a finite volume difference method which has a great stability for prediction of fluid flow was developed for the prediction of carbon monoxide due to vehicular emission for input source strength emitted at a given value. Time, distance, air velocity and pollutant speed were the parameters considered in developing the dispersion model, which predicts the concentration profile for dispersion. The simulation of the model was carried out using the parameters (time, distance, air velocity and pollutant speed) to show the effect of air velocity and pollutant speed on concentration profile at various axial wind height/distance above ground level. From the results obtained, it shows that as the air velocity, pollutant speed and axial height/distance above ground level increases [(0.5m/s-2.5m/s), (2.50m/s-3.00m/s), (1m-11m)] respectively. The concentration of pollutant decreases from 0.98mol/m<sup>3</sup> to 0.82mol/m<sup>3</sup> due to dispersion of pollutant. It was observed that there is a great dispersion of pollutant concentration at high air velocity, pollutant speed and axial height/distance above ground level.

**Keywords-** Carbon Monoxide; Roe-Riemann solver; Vehicular emission.

## I. INTRODUCTION

The large majority of today's cars and trucks travel by using internal combustion engines that burn gasoline or other fossil fuels. The process of burning gasoline to power cars and trucks contributes to air pollution by releasing a variety of emissions such as oxides of sulphur, oxides of nitrogen, carbon monoxide, carbon dioxide, particulate matter, etc., into the atmosphere. Emissions that are released directly into the atmosphere from the tailpipes of cars and trucks are the primary source of vehicular pollution. But motor vehicles also pollute the air during the processes of manufacturing, refueling and from the emissions associated with oil refining and distribution of the fuel they burn.

Carbon monoxide being one of the major pollutants associated with motor vehicles is a very dangerous gas. Cars and trucks are the source of nearly two-thirds of this pollutant. When inhaled, it blocks the transport of oxygen to the brain, heart, and other vital organs in the human body. New born

children and people with chronic illnesses are especially susceptible to the effects of carbon monoxide. The effect of pollution in the atmosphere to the society in general, especially in the long term is very costly. Illness and premature death due wholly or in part to air pollution places a great burden upon the society by way of increased costs of medical treatment through the loss of labour. In addition, air pollution adversely affects solids, water, wildlife, weather, climate and transportation as well as reducing economic values and personal effort and wellbeing [1]. In urban environment that has low assimilative capacity, vehicular emission is of great concern. The emission reacts forming various species in various meteorological conditions interfering with man's activities. Vehicular emission in typical urban center constitute over 60% of total population emission compared to industries, power plants, refuse disposal, space heating, etc. [2].

Vehicular emission is the byproducts of burning automobile fuels. There are four basic types of vehicular emissions, namely; Hydrocarbon, carbon monoxide, oxides of nitrogen and particulates. The three basic sources of vehicular emission are; engine crankcase blow by fumes (20%), fuel vapour (20%), and engine exhaust gases (60%) [3]. The major emissions from the burning of diesel are sulphur dioxide (SO<sub>2</sub>), lead (Pb), etc. Vehicular emissions are control in two ways; Tailpipe emission control and evaporative emission control. The Tailpipe emission control are ways of reducing the emission of exhaust gases, such as hydrocarbon (HC), NO<sub>x</sub>, CO, CO<sub>2</sub> and particulates. Tailpipe emission can be controlled by increasing engine efficiency, increasing vehicle efficiency, increasing driving efficiency, and cleaning up the emission. The evaporative emissions control are ways of reducing emissions due evaporated fuel such as gas tank venting, ruining losses and refueling losses. These can be control by capturing vented vapour and reducing refueling losses.

There is a need for effective measures to mitigate the adverse impacts of motor vehicles use, the living environment in the cities of the developing world will continue to deteriorate and become increasingly unbearable if nothing is done to combat this great menace. Thus, in order to characterize the variation of these pollutants in space and time, there is need for

monitoring. Air monitoring alone is expensive, time consuming and requires skilled manpower and sophisticated equipment. It is therefore necessary to develop and simulate models which must be flexible enough to determine the concentration with the changes in the source, concentration and meteorological conditions. Basically, models have a degree of control and capacity for exploring virtual realities beyond those available to us through field and laboratory experiments, particularly when dealing with atmospheric phenomenon. The Roe-Riemann solver provides a very nice scheme for calculating solution of time dependent problems in one dimension. But once a dimensional Riemann solver is constructed for a particular system of equation, it is easy to extend it to multiple dimensions. The simplest multidimensional Riemann solver treats each other of the directions dimensionally as if it were a set of one dimensional problem.

## II. DEVELOPMENT OF MODEL

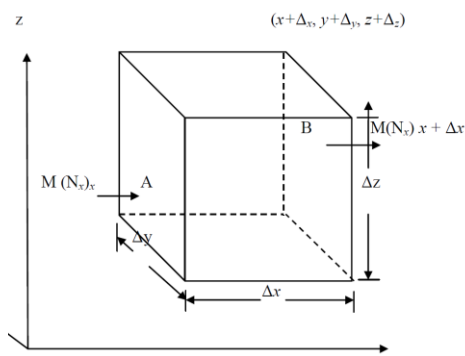


Figure 1. Region of elemental volume in space.

For a small volume element  $\Delta x$ ,  $\Delta y$ ,  $\Delta z$ , fixed in space as shown in Figure 1. A material balance based on continuity equation can be developed. The mathematical model for the prediction of carbon monoxide due to vehicular emission is based on this continuity equation.

$$(\text{Rate of mass input}) - (\text{Rate of mass output}) + (\text{Net rate of amount of mass introduced by the source strength}) = (\text{Rate of accumulation}) \quad (1)$$

The mass flow rate of pollutants into the three (3) phases with a common corner at A is

$$M[(N_x)\Delta y\Delta z + (N_y)\Delta x\Delta z + (N_z)\Delta x\Delta y] \quad (2)$$

Where,  $N_x$  is the flux in x-direction ( $\text{mol/m}^2\text{s}$ );  $(N_x)X$  is the value at location x;  $M$  is the molecular weight of the pollutant CO ( $\text{g/mol}$ ).

Similarly, the mass rate of flow out of the three (3) phases with a common corner B is:

$$M[(N_x)_{x+\Delta x}\Delta y\Delta z + (N_y)_{y+\Delta y}\Delta x\Delta z + (N_z)_{z+\Delta z}\Delta x\Delta y] \quad (3)$$

The total pollutant in the element is  $\Delta x$ ,  $\Delta y$ ,  $\Delta z$  and density,  $\rho$ , has a rate of accumulation as:

$$\Delta x\Delta y\Delta z \frac{\delta \rho}{\delta t} \quad (4)$$

Where,  $\rho$  is the density of carbon monoxide in ( $\text{g/m}^3$ ).

The net rate of amount of mass introduced by source strength is given as

$$\Delta x\Delta y\Delta z q \quad (5)$$

Where,  $q$  is the source strength in ( $\text{g/m}^3\text{s}$ ).

The overall expression for the element is obtained when equations (2) through (5) is substituted into equation (1). And is given as;

$$\frac{\delta(MN_x)}{\delta x} + \frac{\delta(MNy)}{\delta y} + \frac{\delta(MNz)}{\delta z} + \frac{\delta \rho}{\delta t} = q \quad (6)$$

Note that the flux ( $N_x$ ) for the pollutant, CO is made of two parts namely; the one resulting from the bulk of the fluid pollutant CO motion and the one resulting from diffusion of CO. This implies that flux  $N$  is given as;

$$N = K + J \quad (7)$$

Where,  $K$  is the bulk motion of CO and  $J$  is the diffusion motion of CO.

If the pollutant is in the same direction as that of the wind, equation (7) in terms of masses in the x-direction is expressed as;

$$MN_x = U_x \rho m + V_x \rho + MJ_x \quad (8)$$

However, when the pollutant is in the opposite direction to that of the wind, and the direction of the wind as positive x-direction and the pollutant negative x-direction, in terms of masses and in the x-direction, equation (7) gives;

$$MN_x = U_x \rho m - V_x \rho + MJ_x \quad (9)$$

Where,  $\rho m$  is the density of the mixture of air and the pollutant as the pollutant mixed with the air, thus changing the density of air ( $\text{g/m}^3$ );  $\rho$  is the density of the pollutant which is constant ( $\text{g/m}^3$ );  $U_x$  is the velocity of wind in x-direction ( $\text{m/s}$ );  $V_x$  is the velocity of pollutant in x-direction ( $\text{m/s}$ ).

Now, since  $\rho m$  is the density of the mixture of air and the pollutant mixed with the air, thus changing the density of air. It can be represented through the following general relationship;

$$p = \frac{PM}{RT} \quad (10)$$

$$\rho m = \frac{M_{air} P_{air}}{RT} + \frac{M P_{CO}}{RT} \quad (11)$$

Where,  $\frac{M_{air} P_{air}}{RT} = \frac{M_{air}(P_T - P_{CO})}{RT}$ ; is the density of air ( $\text{g/m}^3$ );  $\frac{M P_{CO}}{RT}$  is the density of carbon monoxide ( $\text{g/m}^3$ );  $P_{air} = P_T - P_{CO}$  is Partial pressure of air (atm);  $P_T$  = Total pressure of mixture of air and CO (atm);  $P_{CO}$  = Pressure of carbon monoxide (atm);  $M$  = molecular weight of CO ( $\text{g/mol}$ );  $M_{air}$  = molecular weight of air ( $\text{g/mol}$ );  $R$  = gas constant ( $\text{atm.cm}^3/\text{mol.k}$ );  $T$  is

the Temperature of which a sample of dry air would have density as the mixture (k).  
Using a partial differential method, the diffusion flux,  $J_x$  is given as;

$$J_x = -\Delta \frac{\delta c}{\delta x} \quad (12)$$

Differentiating equation (9) gives;

$$\frac{\delta MNx}{\delta x} = \rho m \frac{\delta Ux}{\delta x} + U_x \frac{\delta \rho m}{\delta x} + \rho \frac{\delta Vx}{\delta x} + V_x \frac{\delta \rho}{\delta x} + M \frac{\delta Jx}{\delta x} \quad (13)$$

Since  $\frac{\delta MNx}{\delta x}$  has been obtained in the equation (13), then equation (6) can be written in three (3) dimensional forms as:

$$\rho m \left[ \frac{\delta Ux}{\delta x} + \frac{\delta Uy}{\delta y} + \frac{\delta Uz}{\delta z} \right] + \left[ Ux \frac{\delta \rho m}{\delta x} + Uy \frac{\delta \rho m}{\delta y} + Uz \frac{\delta \rho m}{\delta z} \right] + \left[ Vx \frac{\delta \rho}{\delta x} + Vy \frac{\delta \rho}{\delta y} + Vz \frac{\delta \rho}{\delta z} \right] + M \left[ \frac{\delta Jx}{\delta x} + \frac{\delta Jy}{\delta y} + \frac{\delta Jz}{\delta z} \right] + \frac{\delta \rho m}{\delta t} = q \quad (14)$$

Similarly, equation (9) becomes;

$$\rho m \left[ \frac{\delta Ux}{\delta x} + \frac{\delta Uy}{\delta y} + \frac{\delta Uz}{\delta z} \right] + \left[ Ux \frac{\delta \rho m}{\delta x} + Uy \frac{\delta \rho m}{\delta y} + Uz \frac{\delta \rho m}{\delta z} \right] + \rho \left[ \frac{\delta Vx}{\delta x} + \frac{\delta Vy}{\delta y} + \frac{\delta Vz}{\delta z} \right] + \left[ Vx \frac{\delta \rho}{\delta x} + Vy \frac{\delta \rho}{\delta y} + Vz \frac{\delta \rho}{\delta z} \right] - MD \left[ \frac{\delta^2 c}{\delta x^2} + \frac{\delta^2 c}{\delta y^2} + \frac{\delta^2 c}{\delta z^2} \right] + \frac{\delta \rho m}{\delta t} = q \quad (15)$$

Applying the equation of continuity,

$\frac{\delta Ux}{\delta x} + \frac{\delta Uy}{\delta y} + \frac{\delta Uz}{\delta z}$  and  $\frac{\delta Vx}{\delta x} + \frac{\delta Vy}{\delta y} + \frac{\delta Vz}{\delta z}$  tends to zero, then equation (15) becomes;

$$\frac{\delta c}{\delta t} = - \left[ Ux \frac{\delta c}{\delta x} + Uy \frac{\delta c}{\delta y} + Uz \frac{\delta c}{\delta z} \right] - \left[ Vx \frac{\delta c}{\delta x} + Vy \frac{\delta c}{\delta y} + Vz \frac{\delta c}{\delta z} \right] + \Delta \left[ \frac{\delta^2 c}{\delta x^2} + \frac{\delta^2 c}{\delta y^2} + \frac{\delta^2 c}{\delta z^2} \right] + q \quad (16)$$

The variables  $U_x$ ,  $U_y$ ,  $U_z$ ,  $V_x$ ,  $V_y$ ,  $V_z$ , and  $c$  can each be described as the sum of the mean and a turbulent composition as follows;

$$U_x = \bar{U}_x + U'_x, U_y = \bar{U}_y + U'_y, U_z = \bar{U}_z + U'_z \quad (17)$$

$$V_x = \bar{V}_x + V'_x, V_y = \bar{V}_y + V'_y, V_z = \bar{V}_z + V'_z \quad (18)$$

$$C = \bar{C} + C' \quad (19)$$

Where  $U_x$  and  $V_x$  are the instantaneous measurement of the east and west component velocities;  $\bar{U}_x$  and  $V'_x$  are the deviation of  $U$  and  $V$  from the mean.

Substituting (17) through (19) into (16) and assuming an incompressible, non-divergent atmosphere as assumption for the most scales of motion affecting vehicles emission produced. The expression becomes;

$$\frac{\delta c}{\delta t} = - \left[ \frac{\delta Ux\bar{C}}{\delta x} + \frac{\delta Uy\bar{C}}{\delta y} + \frac{\delta Uz\bar{C}}{\delta z} \right] - \left[ \frac{\delta Vx\bar{C}}{\delta x} + \frac{\delta Vy\bar{C}}{\delta y} + \frac{\delta Vz\bar{C}}{\delta z} \right] - \left[ \frac{\delta Ux'c'}{\delta x} + \frac{\delta Uy'c'}{\delta y} + \frac{\delta Uz'c'}{\delta z} \right] + \left[ \frac{\delta Vx'c'}{\delta x} + \frac{\delta Vy'c'}{\delta y} + \frac{\delta Vz'c'}{\delta z} \right] + x \frac{\delta^2 c}{\delta x^2} + \Delta y \frac{\delta^2 c}{\delta y^2} + \Delta z \frac{\delta^2 c}{\delta z^2} + q \quad (20)$$

The term on the left hand side describe the change of concentration with time. The first two terms in the bracket on

the right hand side describes the change due to mean motion (transport), the second two terms in the brackets describe the changes due to turbulent (dispersion) and the third term with the derivative of concentration square describes the molecular diffusion. The Reynolds's number of molecular diffusion is small compared to that of turbulent diffusion thus, we can ignore the molecular diffusion term in equation (20) above to zero.

$$\Delta x \frac{\delta^2 c}{\delta x^2} + \Delta y \frac{\delta^2 c}{\delta y^2} + \Delta z \frac{\delta^2 c}{\delta z^2} = 0 \quad (21)$$

The turbulence fluxes ( $V'_x C'$ ,  $V'_y C'$ ,  $V'_z C'$ ) defined as the mass of pollutant deposition per unit area per unit time due to turbulence are difficult to measure directly, then

$$\frac{\delta V'_x C'}{\delta x} + \frac{\delta V'_y C'}{\delta y} + \frac{\delta V'_z C'}{\delta z} = 0 \quad (22)$$

It is common therefore to assume that turbulence is proportional to the gradient of the mean concentration.

$$U'_x C' = -Kx \left( \frac{\delta c}{\delta x} \right) \quad (23)$$

$$U'_y C' = -Ky \left( \frac{\delta c}{\delta x} \right) \quad (24)$$

$$U'_z C' = -Kz \left( \frac{\delta c}{\delta x} \right) \quad (25)$$

Where,  $Kz$  is proportionality constant called the eddy diffusion. By further assuming that the eddy diffusivity values  $Kx$ ,  $Ky$ , and  $Kz$  are invariant along their respective axis, an assumption often made to simplify the calculation, but not necessarily physically realistic, this expression can be simplified to the parabola form as:

$$\frac{\delta c}{\delta t} = Kx \frac{\delta^2 \bar{c}}{\delta x^2} + Ky \frac{\delta^2 \bar{c}}{\delta y^2} + Kz \frac{\delta^2 \bar{c}}{\delta z^2} - \left[ \frac{\bar{U}_x \delta \bar{C}}{\delta x} + \frac{\bar{U}_y \delta \bar{C}}{\delta y} + \frac{\bar{U}_z \delta \bar{C}}{\delta z} \right] - \left[ \frac{\bar{V}_x \delta \bar{C}}{\delta x} + \frac{\bar{V}_y \delta \bar{C}}{\delta y} + \frac{\bar{V}_z \delta \bar{C}}{\delta z} \right] + q \quad (26)$$

For continuous source strength of pollutant, the emission of the pollutant source strength ( $q$ ) remains constant. This means that the source strength ( $q$ ) of pollutant e.g. carbon monoxide from car exhaust gas to the atmosphere is considered not increasing with time;

$$\frac{\delta c}{\delta t} = Kx \frac{\delta^2 \bar{c}}{\delta x^2} + Ky \frac{\delta^2 \bar{c}}{\delta y^2} + Kz \frac{\delta^2 \bar{c}}{\delta z^2} - \left[ \frac{\bar{U}_x \delta \bar{C}}{\delta x} + \frac{\bar{U}_y \delta \bar{C}}{\delta y} + \frac{\bar{U}_z \delta \bar{C}}{\delta z} \right] - \left[ \frac{\bar{V}_x \delta \bar{C}}{\delta x} + \frac{\bar{V}_y \delta \bar{C}}{\delta y} + \frac{\bar{V}_z \delta \bar{C}}{\delta z} \right] + q \quad (27)$$

When pollutant is released intermittently, with the source strength ( $q$ ) of the pollutant remaining constant, the expression becomes

$$\frac{\delta c}{\delta t} = Kx \frac{\delta^2 \bar{c}}{\delta x^2} + Ky \frac{\delta^2 \bar{c}}{\delta y^2} + Kz \frac{\delta^2 \bar{c}}{\delta z^2} - \left[ \frac{\bar{U}_x \delta \bar{C}}{\delta x} + \frac{\bar{U}_y \delta \bar{C}}{\delta y} + \frac{\bar{U}_z \delta \bar{C}}{\delta z} \right] - \left[ \frac{\bar{V}_x \delta \bar{C}}{\delta x} + \frac{\bar{V}_y \delta \bar{C}}{\delta y} + \frac{\bar{V}_z \delta \bar{C}}{\delta z} \right] + q \quad (28)$$

When the velocity of the pollutant is zero (i.e.  $V_n=0$ ), thus the model equation becomes;

$$\frac{\delta c}{\delta t} = Kx \frac{\delta^2 \bar{c}}{\delta x^2} - Ky \frac{\delta^2 \bar{c}}{\delta y^2} - Kz \frac{\delta^2 \bar{c}}{\delta z^2} - \left[ \frac{\bar{U}_x \delta \bar{C}}{\delta x} + \frac{\bar{U}_y \delta \bar{C}}{\delta y} + \frac{\bar{U}_z \delta \bar{C}}{\delta z} \right] + q \quad (29)$$

### A. Roe-Riemann Application To Equation

There are various approximate methods of numerical solution available for solving model equation. The major ones among the numerical solution methods are Crank Nicholson method [4], explicit finite difference scheme, implicit finite difference scheme, finite volume scheme, etc. This present work will use Roe-Riemann solver which is based on finite volume scheme.

The discretization of the system of equations can be written in vector form. Assuming fluxing in x-direction, equation (28) becomes:

$$\frac{\delta c}{\delta t} + \frac{\bar{u}_x \delta \bar{c}}{\delta x} + \frac{\bar{v}_x \delta \bar{c}}{\delta x} - \frac{kx \delta^2 \bar{c}}{\delta x^2} = q \quad (30)$$

The numerical approximation to equation (28) begins by dividing space into cell with edges at  $X_{i+1/2}$  and uniform width  $\Delta x$ , although this restriction can be relaxed. Integration  $C(x,t)$  over a spatial cell and dividing by  $\Delta x$ , we get space average data in cell (1) and time (t).

The general Roe-Riemann equation in one dimension along x-direction is given as;

$$\frac{\delta U}{\delta t} + \frac{\delta AU}{\delta x} = S(u) \quad (31)$$

Where,

$$U_i(t) = \frac{1}{\Delta x} \int_{x-1/2}^{x+1/2} U(x,t) \delta x \quad (32)$$

Integrating over cell (1) gives;

$$\frac{\delta U_i}{\delta t} + \frac{AU_{i-1/2} - AU_{i+1/2}}{\Delta x} = S_i \quad (33)$$

Where,  $U_i(t)$  is a vector of the spatial averages at time (t);  $S(u)$  is source vector;  $AU_{i-1/2}$  is the flux of each of the moment in the x-direction;  $AU$  is flux (rate of flow of state (u) across an interface);  $U_i$  is cell state;  $U_{i+1/2}$  is intercell state;  $U(x,t)$  is vector state of variable.

Since

$$AU = F \quad (34)$$

$$\frac{\delta AU}{\delta U} + \frac{\delta F}{\delta U} \quad (35)$$

$$A = \frac{\delta F}{\delta U} \quad (36)$$

$$A_x = \frac{\delta F_x}{\delta U(x)} \quad (37)$$

Similarly equation 35 becomes:

$$\frac{\delta(AU)_x}{\delta U} = \frac{\delta F_x}{\delta U} \quad (38)$$

By re-arranging equation (28) in 3-dimensional form we have;

$$Ut + Fx + Fy + Fz = S \quad (39)$$

Where,

$$U = \begin{pmatrix} C \\ 0 \end{pmatrix} \quad (40)$$

$$Fx = \begin{pmatrix} Ux C + \frac{Vx C}{0} - \delta/\delta x Kx C \end{pmatrix} \quad (41)$$

$$Fy = \begin{pmatrix} Uy C + \frac{Vy C}{0} - \delta/\delta y Ky C \end{pmatrix} \quad (42)$$

$$Fz = \begin{pmatrix} Uz C + \frac{Vz C}{0} - \delta/\delta z Kz C \end{pmatrix} \quad (43)$$

$$S = \begin{pmatrix} q \\ 0 \end{pmatrix} \quad (44)$$

The Jacobian matrix A in equation (37) in 3-dimensional form can be computed as;

$$Ax = \frac{\delta F_x}{\delta t} = \begin{pmatrix} Ux + Vx \\ 0 \end{pmatrix} \quad (45)$$

$$Ay = \frac{\delta F_y}{\delta t} = \begin{pmatrix} Uy + Vy \\ 0 \end{pmatrix} \quad (46)$$

$$Az = \frac{\delta F_z}{\delta t} = \begin{pmatrix} Uz + Vz \\ 0 \end{pmatrix} \quad (47)$$

The Eigen values of equation (45), (46) and (47) in 3-dimension is given as:

$$\lambda_x = Ux + Vx \quad (48)$$

$$\lambda_y = Uy + Vy \quad (49)$$

$$\lambda_z = Uz + Vz \quad (50)$$

We have determined an approximate value which must satisfy the flux (F).

$$F = AU = \sum \bar{\alpha}_x \bar{e}_x \bar{\lambda}_x \quad (51)$$

Where,  $\bar{e}_n$  is the Eigen vector,  $\Delta C = \bar{\alpha}$  (change in concentration),  $\Delta C.V = \bar{\alpha} \lambda$

The use of summation will not affect any changes in flux, therefore;

$$\Delta F = \Delta C \lambda_x \bar{e}_x \quad (52)$$

$$\Delta F = \Delta C \lambda_x \text{ i.e } \bar{e}_x = 1 \text{ for unit vector}$$

For a unidirectional system, the flux at the cell interface is given by,

$$A_x U_{i+1/2} = 1/2 [A_x U_i + A_x U_{i+1}] - 1/2 \sum \bar{\alpha}_x \bar{\lambda}_x \bar{e}_x \quad (53)$$

The flux  $F_{i \pm 1/2}$  in one dimension can be computed as:

$$F_{i \pm 1/2} = 1/2 [F_{i+1} + F_i] - 1/2 \sum \bar{\alpha}_n \bar{\lambda}_n \bar{e}_n \quad (54)$$

Using  $i, j, k$  for the direction of  $x, y, z$  respectively, the flux at the cell interface in three dimensional forms can be written respectively as:

$$F_{i \pm 1/2} = 1/2 [F_{i+1} + F_i] - 1/2 \sum \bar{\alpha}_{xn} \bar{\lambda}_{xn} \bar{e}_{xn} \quad (55)$$

$$F_{j \pm 1/2} = 1/2 [F_{j+1} + F_j] - 1/2 \sum \bar{\alpha}_{yn} \bar{\lambda}_{yn} \bar{e}_{yn} \quad (56)$$

$$F_{k \pm 1/2} = 1/2 [F_{k+1} + F_k] - 1/2 \sum \bar{\alpha}_{zn} \bar{\lambda}_{zn} \bar{e}_{zn} \quad (57)$$

Substituting equation (52) into the equation of (55) gives:

$$F_{i \pm 1/2} = 1/2 [F_{i+1} + F_i] - 1/2 \Delta F_{i \pm 1/2} \quad (58)$$

Where,  $\Delta F_{i \pm 1/2}$ , change in flux between the grid point  $i$  and  $i + 1/2$  is computed by (Figure 2)

$$\Delta F_{i+1/2} = \frac{\Delta F}{2} \quad (59)$$

Within the finite volume scheme, the simplest way to incorporate source term (i.e. source strength) into numerical method is to add on a point wise approximate of each cell. The resulting Riemann scheme is incorporate with the source term can be written in three dimensions in the form of equation below;

$$U_{i+1,j,k}^n = U_{ijk}^n - \frac{\Delta t}{\Delta x} (F_{i+1/2,j,k} - F_{i-1/2,j,k}) - \frac{\Delta t}{\Delta y} (F_{i,j+1/2,k} - F_{i,j-1/2,k}) - \frac{\Delta t}{\Delta z} (F_{i,j,k+1/2} - F_{i,j,k-1/2}) + \Delta t q_{i+1}^n \quad (60)$$

For a unidirectional system, (i.e one dimension axis), the above discretized model solving equation reduces to the form of

$$U_{i+1}^n = U_i^n - \frac{\Delta t}{\Delta x} (F_{i+1/2} + F_{i-1/2}) + \Delta t q_{i+1}^n \quad (61)$$

Equation (61) is the general model solving equation known as Roe-Riemann solver equation. Rewriting equation (51) in terms of concentration, we have;

$$C_{i+1}^n = C_i^n - \frac{\Delta t}{\Delta x} (F_{i+1/2} + F_{i-1/2}) + \Delta t q_{i+1}^n \quad (62)$$

Equation (62) is the general developed model Roe-Riemann solver equation for determining the concentration of carbon monoxide, CO emitted from motor vehicles.

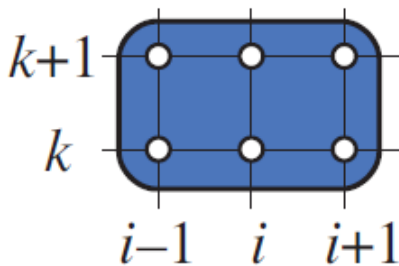


Figure 2. Crank-Nicolson computational Molecules.

Where,

$i, j$  = equal cell location in grid

$n$  = time level

$i+1$  = nest grid point

$C_{i,j}^n$  = concentration at the node  $i, j$ .

$C_{i+1,j}^n$  = concentration at the node  $i+1, j$ .

$F_{i,j}$  = flux in the cell grid node  $i, j$ .

$F_{i+1,j}$  = flux in the cell grid node  $i+1, j$ .

$F_{i-1,j}$  = flux in the cell grid node  $i-1, j$ .

$F_{i,j+1}$  = flux in the cell grid node  $i, j+1$ .

$F_{i,j-1}$  = flux in the cell grid node  $i, j-1$ .

The boundary Conditions are as follows

1.  $C(X_0, Y_0, Z_0, t) > 0$   
For  $t \geq 0, X_0 = 0, Y_0 = 0, Z_0 = 0$   
or  $C(i, j, k)$  for  $t \geq 0, I = 0, j = 0, k = 0$
2.  $q(i, j, k) > 0$   
for all  $i \geq 0, j \geq 0, k \geq 0, t \geq 0$

### B. Assumptions

Some of the assumptions used include: a constant car speed is assumed; density of air is constant at 30°C; emission of carbon monoxide is constant at constant car speed; diffusion coefficient of carbon monoxide/air system is constant at atmospheric pressure and temperature; A unit-directional transport of carbon monoxide in air is assumed; Velocity of air is constant at a given height in the atmosphere; Assuming the variation in concentration is determined over 10 equal spatial of both time and distance.

### C. Data Used In Calculation

- Velocity of air (U); range of value of velocity (0.5m/s – 2.5m/s) was considered so as to show the effect of change in wind velocity to concentration distribution. This is based on the assumption that we have calm and light velocity in the environment considered.
- Density of air; a value of 1.16kg/m<sup>3</sup> applies for condition of atmospheric temperature and pressure (1atm 30°C).
- Velocity of carbon monoxide existing depends on the vehicle operating condition. Values range from 2.3m/s to 3.0m/s is considered in the conditions. The basis of the consideration of two stroke engine cars operating at a speed of 25km/hr, (6.94m/s) and temperature and pressure of 2300k and 1000kpa to 2250kpa, the correlation was given by Metghalachi and Keck [5].
- Source strength (q); it could also be called the generation term. It is obtained under the condition of constant car speed of 25km/hr and emission factor of 56.89km. A range of 0.00458g/m<sup>3</sup>s to 0.0103g/m<sup>3</sup>s applies for 2300k temperature for a pressure range of 1000 – 2250KPa. The basis is the consideration of stroke engine operating at the condition stated earlier.
- Diffusion coefficient (K); for purpose up to about 10 atmosphere or even higher, the diffusion coefficient for a binary mixture of gases, A and B may be estimated from Fuller, Schettler and Girding relation [6].  
$$K_{AB} = \frac{1.0 \times 10^{-7} \times T^{1.75} \times \left[ \frac{1}{M_A} + \frac{1}{M_B} \right]^{\frac{1}{2}}}{P[(\Sigma V_A)^{0.33} + (\Sigma V_B)^{0.33}]^2}$$
- A value of  $K_{AB} = 2.05 \times 10^{-5} \text{m}^2/\text{s}$  applies for the carbon monoxide/air system. This is based on the diffusion coefficient of carbon monoxide/air system is constant at atmospheric temperature and pressure.

### D. Numerical Simulation Input Data

From the assumptions stated above and source of data used in the calculation (i.e the numerical simulation input data) are

generated at equal intervals and tabulated as shown in Table 1 below.

Table 1. Numerical simulation input data

Height (m)	Velocity of Air U (m/s)	Velocity of CO V (m/s)	Source Strength q (mol/m <sup>3</sup> s)
1	0.50	2.50	0.000164
2	0.70	2.55	0.000186
3	0.90	2.60	0.000208
4	1.10	2.65	0.000231
5	1.30	2.70	0.000253
6	1.50	2.70	0.000275
7	1.70	2.75	0.000297
8	1.90	2.80	0.000320
9	2.10	2.85	0.000342
10	2.30	2.90	0.000364
11	2.50	3.00	0.000368

From Literature, based on the correlation given by Metghalachi and Keck [7, 8], the numerical simulations were carried out at ground level. The concentrations were determined as function of axial distance 10m for a simulation time of 10seconds. The simulation results were presented in Table 2.

### III. RESULTS

The results of the numerical solution of the model are shown in Table 2 below.

Table 2. Manually and computed simulation result

Height above the ground and axial distance (m)	Velocity of Air U (m/s)	Velocity of CO V (m/s)	Source Strength q (mol/m <sup>3</sup> s)	Conc. of CO mol/m <sup>3</sup>
1	0.50	2.50	0.000164	0.98
2	0.70	2.55	0.000186	0.95
3	0.90	2.60	0.000208	0.94
4	1.10	2.65	0.000231	0.92
5	1.30	2.70	0.000253	0.90
6	1.50	2.70	0.000275	0.89
7	1.70	2.75	0.000297	0.87
8	1.90	2.80	0.000320	0.86
9	2.10	2.85	0.000342	0.85
10	2.30	2.90	0.000364	0.84
11	2.50	3.00	0.000368	0.82

### IV. DISCUSSION

#### A. Effects of Air Velocity

The plots of concentration against velocity of air and axial distance/height above the ground level are shown in Figure 3 and Figure 4. The concentration profiles for all the components exhibit exponential distribution. The exponential nature of the profile shows that there is a considerable decrease from 0.98mol/m<sup>3</sup> to 0.82mol/m<sup>3</sup> in the concentration of pollutant as it is being dispersed above the ground level. As the height above the ground level increases from 1m to 11m, the air velocity also increases from 0.5m/s to 2.5m/s, thus, leading to a decrease from 0.98mol/m<sup>3</sup> to 0.82mol/m<sup>3</sup> in pollutant concentration [7]. This shows that there is better pollution dispersion as air velocity increases from 0.5m/s to 2.5m/s, thus diluting the pollutant. Also, it was observed that at the same height above the ground level, but at different air velocities, the pollutant concentration shows an inverse relation with velocity.

Considering Figure 3 and Figure 4, and taking the horizontal axis of Figure 4 as the axial wind distance, as the air velocity increases from 0.50m/s to 2.50m/s, the pollutant concentration decreases from 0.98mol/m<sup>3</sup> to 0.82mol/m<sup>3</sup> along the axial wind distance as a result of better dispersion of the pollutant which leads to its dilution. Also, at the same axial wind distance, higher concentration of pollutant occurred at a low air velocity than at a higher velocity. It thus shows that the higher the air velocity, the more the pollutant is being dispersed and the lower the pollutants concentration.

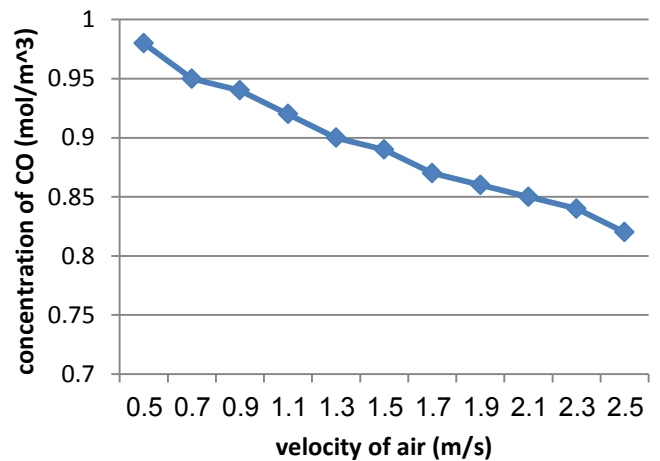


Figure 3. Effect of air velocity on CO concentration



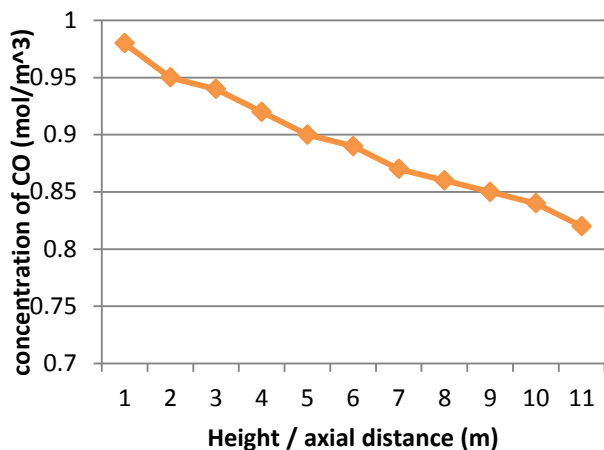


Figure 4. Height/axial distance effect on Concentration of CO

### B. Effects of pollutant speed

Figure 5 illustrates the effect of pollutant speed. The concentration profile for Figure 5 is similar to Figure 3 as they both exhibit exponential distribution profile. This implies that as the pollutant speed increases from 2.50m/s to 3.00m/s, there is a considerable decrease from 0.98mol/m<sup>3</sup> to 0.82mol/m<sup>3</sup> in pollutant concentration as the height above the ground level increases from 1m to 11m as a result of dilution of pollutant as it rises up [9]. At the same height above the ground level but at different pollutant speed, the concentration is inversely proportional to the pollutant speed. Also, at the same speed but at different height above the ground level, the pollutant concentration decreased with height.

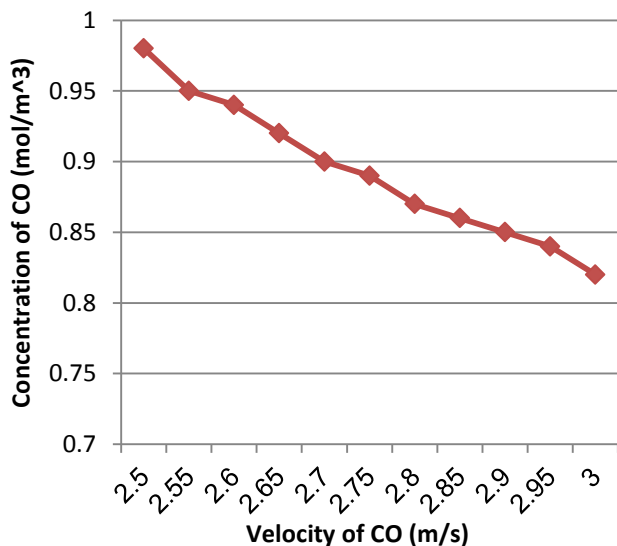


Figure 5. Effects of pollutant speed on concentration of CO

## V. CONCLUSION

The prediction of carbon monoxide concentration due to vehicular emissions as a function of some physical parameters such as velocity of air, velocity of pollutant, height above the ground level/axial distance and source strength was achieved using the mathematical model generated from Roe-Riemann based on the continuity equation. The results obtained shows that increase in air velocity from 0.50m/s to 2.50m/s decreases the concentration of pollutant from 0.98mol/m<sup>3</sup> to 0.82mol/m<sup>3</sup> as the axial wind distance and height above the ground level increases from 1m – 11m. Increase in pollutant speed from 2.50m/s to 3.00m/s decreases the concentration of pollutant from 0.98mol/m<sup>3</sup> to 0.82mol/m<sup>3</sup> as the axial wind distance and height above the ground level increases.

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