Numerical Analysis of Mathematical Model for Carbon Pollution in Roads with Ventilated Embankments in Absence and Presence of Forced Convection

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Abstract- In this paper, a two-dimensional grid based numerical carbon pollution model for the estimation of carbon pollutant concentrations in roads is developed. The simulations of carbon pollutants in roads with ventilated embankments have been presented. Based on a two-dimensional advection-diffusion transport equation, the modeling system incorporates the combined influence of both model input and environmental parameters. Absence and presence of forced convection are considered, with the provision of ventilations on the walls of embankment. Boundary conditions and environmental factors are varied to achieve the desired results. Carbon concentrations is approximated by using Godunov finite volume technique. The solutions of calculated carbon pollutant concentrations at different distances, both in the horizontal and vertical directions from the source are compared. The results suggest that the advection - diffusion model is satisfactory for simulating the effect of free and forced convection on carbon concentrations in roads with ventilated embankments.

Keywords- Advection, Diffusion, Convection and Godunov Finite Volume Method

I. INTRODUCTION

I t has been estimated that 90% of urban air pollution in rapidly growing cities is attributable to motor vehicle emissions (United Nations Environmental Programme, 2011). In our earlier works from [1] and [2], we showed that carbon pollution remains a global major problem in roads that are not well designed. Simulation and optimization of gas dynamics in car's exhaust pipe presented in [3] acknowledged that emissions caused by vehicles have been a perilous issue over the last few decades. While there are many sources of air pollution in cities, including extensive open air burning of refuse and biomass as proposed in [4], industrial operations and motor vehicles play a critical role in the problem [5]. Exhaust gases, which consist of carbon, a component of particulate matter analyzed in [6] and illustrated further in [7] shows that it has adverse effects on human health. Air quality in embanked road tunnel environment can easily and immensely deteriorate if dilution of pollutants emitted from vehicles' exhausts is not enhanced. These could further be worsened by traffic congestion when the wind is still and pollutants are emitted from the vehicles when the engines are on idling mode. This coupled with daily increase in density of traffic as a result of increase in population of road users as proposed in [8], necessitates the need for greater control of emissions from combustion engines. Discussions in [9], shows that for the case of huge embankments and tunnels equipped for one-way traffic, the ventilation fans and the piston effect of moving vehicles are the principal mechanisms for transportation of exhaust gases downwind or through tunnel exit, leading to the dilution of the pollutants in the highway and in the tunnel respectively. One of the major factors that influences the acceptance of road construction and usage in Kenya is air quality, consequently, research in this area is fundamental. This study, therefore, is on influence of airflow into an embanked road on carbon pollution diffusion for a simplified road design to help appreciate reduction of both pollutants concentration and human exposure. Embankments increase turbulence and initial mixing of emitted pollutants [10]. Depending on effectiveness of the emissions' dispersion, there may be a concern whether air quality standards can be upheld. Ambient air concentrations of pollutants are frequently highest along highways as analyzed in [11], [12] and as is also evident by the black deposits of carbon pollutants on the walls of the embankments. Road embankments confine and provide means for redistribution of emissions produced by vehicles passing through road section. These levees act as topographic obstacles which cause drag and produce turbulence to compensate for the deformation of the flow field when wind flows over them as discussed in [13]. From the discussions in [14], it is shown that unless vented, closed spaces like tunnels or parking garages do not allow for free dispersion of air pollutants. To improve the situation, we incorporate forced convection and ventilation as source terms. Thus, investigation of dispersion of exhaust gases on highways, by means of mathematical modeling is vital

and less expensive in giving insight on environmental management and future economic planning.



Fig. 1: Deep unconcealed Embankment

Fig. 1 is a 2-D illustration of deep embankment constructed and towering several feet high at Pangani interchange in Kenya. The upper part is not concealed, but because of its depth, the pollutants do not flow freely out of the enclosure putting motorists' and pedestrians' lives at risk. The point marked **x** represents the point source, and we have studied how carbon particles will be dispersed from this point assuming that the wind blows across the road, enhanced by the presence of ventilations and increased wind speed. We have also looked at the boundary conditions at a, b, c and d, shown in Figure 1. In the above diagram forced convection has been incorporated by fitting suction pumps on the embankments to provide free stream to propagate advection.

II. GOVERNING EQUATIONS AND DOMAIN DESCRIPTION

Mathematical model used in this research is a combination of known 2-D advection - diffusion equation presented inform of partial differential equation (PDE) as shown in equation (1) below together with the conservation laws of mass, momentum and energy.

$$\frac{\partial c}{\partial t} + \frac{\partial}{\partial x}(uc) - \frac{\partial^2}{\partial x^2}(D_x u) - \frac{\partial^2}{\partial y^2}(D_y u) + R - S = 0$$
(1)

The PDE is given by dispersion as a sum of advection, diffusion, removal term and source term, where the first term is the rate of carbon concentration, the second term is the advection term and the third and fourth terms represent diffusion in the x - direction and y - direction respectively. The removal term refers to the boundary and environmental parameters that are expected to help in enhancing the removal of carbon particles from the road enclosure with ventilated embankments. Therefore, the PDE equation (1) derived from the mass conservation principle describes carbon pollution by vehicles on roads in the absence of forced convection (where R is omitted) and in the presence of forced convection, incorporating ventilated embankment as a parameter where: (x, y) is position of the receptor relative to the source, c = c(x, y, t)is carbon pollutant concentration at c(x,y) and time t in (kg/m^3) , *u* is wind velocity component (m/s) in the x-direction, D_x , and D_{y} are Coefficients of turbulent diffusion in x-direction and ydirection respectively in (m^2/s) which reduces degree of freedom between pollutants, *S* is source term in (sec^{-1}) which controls emission of pollutants and helps in describing the hydrodynamic equation fully and *R* is removal term or decaying of pollutant rate due to sink in (sec^{-1}) which represents changes caused by chemical reaction. In obtaining the numerical solutions in section (4), we have considered a two dimensional advection-diffusion equation (1) with a rectangular domain of interest measuring $20m \times 40ft$ illustrated by Fig. 2.



Fig. 2: Geometric Representation of Domain

Carbon particles are assumed to be continuously released at a constant rate from exhaust mounted on vehicles at a height of 5ft and at horizontal distance of 2m from the embankment. It is taken that all measurements must be made at the center of the control volume as shown in Fig. 3.



Fig. 3: Control Volume and Fluxes

The discretization will be for the p^{th} control volume. The above PDE with the conservation laws form our set of governing equations that can be described as follows:

$$\begin{cases} \frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} - D(\nabla \cdot \nabla)C + R - S = 0\\ \frac{\partial \rho \vec{V}}{\partial t} + \left[(\rho \vec{V} \cdot \nabla) \vec{V} \right] + \nabla P - \rho g + S_V = 0\\ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{V}) - S_\rho - S_D = 0\\ \frac{\partial E}{\partial t} + \nabla \cdot (E \vec{V}) + \nabla \cdot (P \vec{V}) - S_E = 0 \end{cases}$$
(2)

III. GODUNOV FINITE VOLUME METHOD

In this section, we have coupled and then reduced into weak form the advection - diffusion transport equation and conservation laws of mass, momentum and energy using Godunov Finite Volume Method (GFVM). In this discretization technique the PDEs are reduced into first order systems of equations with the highest order terms taken as source terms. The method is based on integration of the governing equations over control volume (CV) to reduce them into coupled system of algebraic equations. The amount of carbon pollutants in each cell and the fluxes across the cell are computed in mesh geometry to provide data used for analyzing the flow. Thus,

$$\int_{t_i}^{t_{i+1}} \int_{CV} \frac{\partial c}{\partial t} dV dt = \int_{t_i}^{t_{i+1}} \frac{\partial}{\partial t} [\int_{CV} c dV] dt.$$

For 2 - D,

$$\Rightarrow \int_{t_i}^{t_{i+1}} \frac{\partial}{\partial t} \left[\int_{CV} (c) dV \right] dt = \int_{xy} \left[\int_{t_i}^{t_{i+1}} \frac{\partial}{\partial t} (c) dt \right] dx dy$$
$$= \int_{xy} \left[c(t_{i+1}) - c(t_i) \right] dx dy$$
$$= \left[c(t_{i+1}) - c(t_i) \right] \delta x \delta y$$

The time interval $t_i \le t \le t_{i+1}$ at which the pollutant concentration is measured can be represented by δt . $t_{i+1} = t_i + \delta t$ $t_{i+2} = t_i + 2\delta t$ $t_{i+3} = t_i + 3\delta t$ $t = t_i + k\delta t$

where, k = time step

By induction,

$$\int_{t_i}^{t_{i+1}} \int_{CV} \frac{\partial c}{\partial t} dV dt = [c(t_i + k\delta t) - c(t_i)] \delta x \delta y$$
$$\int_t \int_y [\int_x \frac{\partial c}{\partial x} dx] dy dt = [c(x_2) - c(x_1)] \delta y \delta t$$

$$\Rightarrow [c(t_i + k\delta t) - c(t_i)]\delta x \delta y + u[c(x_2) - c(x_1)]\delta y \delta t = -R(U) + S(U)$$

$$\Rightarrow c = \frac{-R(U) + S(U)}{\delta t[k+u]}$$

Take $c = \rho \delta x \cdot \delta y \cdot 1$

$$\Rightarrow \rho = \frac{-R(U) + S(U)}{\delta t[k+u]\delta x \delta y} \tag{3}$$

Mass equation in Eulerian coordinate is:

$$\int_{CV} \{ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{V}) - S_{\rho} - S_D \} dV = 0$$

$$\Rightarrow \frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} + \frac{\partial \rho v}{\partial y} - S_{\rho} - S_D = 0$$

Momentum equation in Eulerian coordinate is:

$$\int_{CV} \{ \frac{\partial}{\partial t} (\rho \vec{V}) + [(\rho \vec{V} \cdot \nabla) \vec{V}] + \nabla P - \rho \vec{g} + \vec{S}_V \} dV = 0$$
$$\vec{V} = \begin{bmatrix} u \\ v \end{bmatrix}; \vec{g} = \begin{bmatrix} 0 \\ g \end{bmatrix}; \nabla = \begin{bmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \end{bmatrix}; \vec{S}_V = \begin{bmatrix} 0 \\ S_V \end{bmatrix}$$

We have,

$$\frac{\partial \rho v}{\partial t} + (\rho \vec{V} \cdot \nabla)v + \frac{\partial P}{\partial y} - \rho g + S_V = 0$$
$$\frac{\partial}{\partial t}(\rho u) + (\rho \vec{V} \cdot \nabla)u + \frac{\partial P}{\partial x} = 0$$
$$\Rightarrow \frac{\partial}{\partial t}(\rho u) + \rho u \frac{\partial u}{\partial x} + \rho u \frac{\partial v}{\partial y} + \frac{\partial P}{\partial x} = 0$$

And by considering steady state condition where,

$$\begin{split} [uv\frac{\partial\rho}{\partial y} + \rho v\frac{\partial u}{\partial y}] &= 0\\ \Rightarrow \rho u\frac{\partial v}{\partial y} = \frac{\partial}{\partial y}(\rho uv)\\ \frac{\partial}{\partial t}(\rho u) + \frac{\partial}{\partial x}(P + \rho uv) + \frac{\partial}{\partial y}(\rho uv) = 0 \end{split}$$

We now discretize the second part of momentum equation:

$$\frac{\partial \rho v}{\partial t} + \rho u \frac{\partial v}{\partial x} + \rho v \frac{\partial v}{\partial y} + \frac{\partial P}{\partial y} - \rho g + S_V = 0$$

And considering steady state condition,

$$\begin{aligned} [\rho v \frac{\partial u}{\partial x} + uv \frac{\partial \rho}{\partial x}] &= 0\\ \Rightarrow \rho u \frac{\partial v}{\partial x} &= \frac{\partial}{\partial x} (\rho uv)\\ \frac{\partial \rho v}{\partial t} + \frac{\partial}{\partial x} (\rho uv) + \frac{\partial}{\partial y} (\rho vv) + \frac{\partial P}{\partial y} - \rho g + S_V = 0\\ \Rightarrow \frac{\partial}{\partial t} (\rho v) + \frac{\partial}{\partial x} (\rho uv) + \frac{\partial}{\partial y} (P + \rho vv) - \rho g + S_V = 0\end{aligned}$$

Energy equation in Eulerian coordinate system is:

$$\int_{CV} \{ \frac{\partial E}{\partial t} + \nabla \cdot (E\vec{V}) - \nabla \cdot P\vec{V} - S_E \} dV = 0$$

$$\Rightarrow \frac{\partial E}{\partial t} + \nabla \cdot (E\vec{V}) = \nabla \cdot P\vec{V} + S_E$$

$$\Rightarrow \frac{\partial E}{\partial t} + \frac{\partial}{\partial x} Eu + \frac{\partial}{\partial y} Ev = -(\frac{\partial}{\partial x} Pu + \frac{\partial}{\partial y} Pv) + S_E$$

$$\Rightarrow \frac{\partial E}{\partial t} + \frac{\partial}{\partial x}u(E+P) + \frac{\partial}{\partial y}v(E+P) = S_E$$

Hence our fully discretized and coupled governing equation for each *CV* take the form below:

$$\begin{cases} \rho = \frac{-R(U) + S(U)}{\delta t[k+u]\delta x \delta y} \\ \frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} + \frac{\partial \rho v}{\partial y} = S_{\rho} + S_{D} = 0 \\ \frac{\partial}{\partial t}(\rho u) + \frac{\partial}{\partial x}(P + \rho uv) + \frac{\partial}{\partial y}(\rho uv) = 0 \\ \frac{\partial}{\partial t}(\rho v) + \frac{\partial}{\partial x}(\rho uv) + \frac{\partial}{\partial y}(P + \rho vv) = -\rho g + S_{V} \\ \frac{\partial E}{\partial t} + \frac{\partial}{\partial x}u(E + P) + \frac{\partial}{\partial y}v(E + P) = S_{E} \end{cases}$$

$$(4)$$

Thus, we express our discretized conservation laws in the form:

$$U_t + F(U)_x + G(U)_y = S(U)$$

and take $P = a^2 \rho$ hence; the last four equations of equation (4) becomes:

$$U = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ E \end{bmatrix}, F = \begin{bmatrix} \rho u \\ \rho(uu + a^2) \\ \rho uv \\ u(E + a^2\rho) \end{bmatrix}, G = \begin{bmatrix} \rho v \\ \rho uv \\ \rho(vv + a^2) \\ v(E + a^2\rho) \end{bmatrix}$$

where, *E* is the total energy per unit mass. ρu is momentum, $\rho(u^2 + a^2)$ is momentum flux in the x-direction, $\rho(v^2 + a^2)$ is momentum flux in the y-direction, ρu^2 and ρv^2 are advective fluxes in the x and y directions respectively. The products $\rho(x,t)u(x,t)$ and $\rho(y,t)v(y,t)$ give the densities of momentum in the x and y directions respectively. *U* is a column vector of conserved variables ρ , ρu , ρv and *E*. S = S(U) is a source term. Body forces such as gravity are represented in *S*. Injection of mass, momentum and energy are also included in *S*. Flux vectors F = F(U) and G = G(U) are functions of the conserved variable vector *U*, and F_x , G_y are fluxes due to convection and viscous

IV. RESULTS AND DISCUSSION

In the preceding section a computational numerical model to estimate the concentration of the carbon pollutants emitted from a point source at the point (2m, 5ft) first into a region with and secondly without advective removal mechanism and transformation process in *xy*-plane rectangular domain presenting vertical cross-section of the road tunnel is presented. Extraction mechanism presented in the domain is wind streaming at a height of 2 meters through an aperture drilled on the embankments on both the left and right side of the road. The experiment analyzes the diffusion of carbon particles from the point source and removal of carbon particles from the domain by both free and forced convection, and we have presented simulation of carbon pollution control situation using two scenarios labeled, simulation 1, and simulation 2.

A) Simulation 1: Carbon Pollution Dispersion in a Domain of Ventilated Embankment in the Absence of Forced Convection



Fig. 4: Concentration level sets of carbon pollutant after approximately 20 minutes



Fig. 5: Concentration level sets of carbon pollutant after approximately 27 minutes



Fig. 6: Concentration level sets of carbon pollutant after approximately 34 minutes



Fig. 7: Concentration level sets of carbon pollutant after approximately 41 minutes

The results of air density variation for each control volume are represented by level sets ($\rho - \rho_o$), giving the difference between densities of pure air (ρ_0) and air contaminated with with carbon particles (ρ) where $\rho > \rho_o$. These concentration levels at different times are plotted in Figure 4 to Figure 7, indicating the spread of carbon particles from the source is affected by the embankment. The concentration profiles at different distances and heights for different time lines plotted in the figures which show that the concentration of carbon particles is higher in the region close to the source point but spread out slowly. This is an indication that advection and convection are limited by presence of embankments which confine the carbon emissions from the source. The results also show that concentration of carbon pollutant is higher at ground level compared to the region above the source, which could be attributed to molecular weight of carbon particles compared to that of air affecting diffusion process. The concentration of pollutant is further seen to increase with time at different distances for given heights which may be as a result of continuous production of pollutants from the exhaust but at faster rate compared to the rate of production and this may be due to diffusion processes.

B) Simulation 2: Carbon Pollution Dispersion in a Domain of Ventilated Embankment in the Presence of Forced Convection



Fig. 8: Concentration level sets of carbon pollutant after approximately 20 minutes



Fig. 9: Concentration level sets of carbon pollutant after approximately 27 minutes



Fig. 10: Concentration level sets of carbon pollutant after approximately 34 minutes



Fig. 11: Concentration level sets of carbon pollutant after approximately 41 minutes

To demonstrate the effect of forced convection on the concentration of pollutant within roads with embankments, we have changed environmental parameter by increasing the wind speed from zero to 30m/s into the domain through a ventilation at (0,4) node by means of suction pump. The solutions show that advection and convection are improved by the presence of

forced convection. Concentration profiles at different heights and distances for different time steps are plotted as is illustrated in Fig. 8 to Fig. 11. It can be observed that the concentration of carbon particles is increased upwards and decreased downwards from the source. This can be attributed to increased convection process leading to the reduction of carbon particles in the enclosure. For higher concentration, the concentration levels are closely packed which is the case with simulation 1, while for lower concentration the concentration levels are spread out which is the case with simulation 2 and this may be due to the dominating wind effect on extraction of carbon particles. Comparing the results of simulation 1 and 2, it is seen that the rate of dilution within the region increases with time in the presence of faster extraction rate than in the absence of advection. At coordinates (15m,35ft), in the absence of forced convection, the concentration of pollution above that of pure air is $0.29g/cm^3$ while in the presence of forced convection, the concentration of pollution above that of pure air is $0.14g/cm^3$ after approximately 41 minutes. This demonstrates that forced convection has doubled the extraction rate of pollutants from the domain.

V. CONCLUSION

Time dependent two dimensional mathematical model for predicting carbon pollution in a road tunnel subjected to variation in environmental factors is presented in this paper to simulate the dispersion process of the carbon pollutants along roadway with ventilated embankments. The numerical model computes the deviation of air density (ρ - ρ_o) due to carbon emitted from a point source. In both cases it is clear that embankments confine pollutants. The dispersion mechanism plays an important role in reducing the concentration of the carbon pollutants everywhere in the region within the domain. The results indicate that there is minimal effect of free convection on the dispersion rate as the concentration of pollutants is higher at the ground level. In the case of forced convection, deviation in density of air due to pollutants is observed to be minimal.

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