MODIFIED MODEL FOR AIR POLLUTANTS WITH FINITE ELEMENT METHOD

NDEKWU O. B. and AGUNWAMBA J. C.
Department of Civil Engineering, Faculty of Engineering, University of Nigeria, Nsukka
Corresponding Author: NDEKWU O. B.
beneathworld@yahoo.com, onyedikachukwu.ndekwu.pg78066@unn.edu.ng

ABSTRACT
A short review paper is presented for the subject area of air quality modelling. The paper is geared towards equipping new researchers and workers with a basic appreciation for the technical aspects of their field, providing a staging point for further investigation, and highlighting useful source materials. The paper is introduced through a discussion of the practical implications regarding mathematical air quality modelling. A modified approach towards the evaluation of the fate of air pollutant along a travel route relevant to air quality monitoring is presented. Conclusion on the future/fate of pollutant transport in air quality modeling will be drawn after verification and validation.

Key words: Concentration distribution, Galerkin finite element method, half- life equation.

1.0 INTRODUCTION

The worldwide concern due to the increasing frequency of ecological disasters on our planet urged the scientific community to take action. One of the possible measures are analytical descriptions of pollution related phenomena, or simulations by effective and operational models with quantitative predictive power. The atmosphere is considered the principal vehicle by which pollutant materials are dispersed in the environment, that are either released from the productive and private sector or eventually in accidental events and thus may result in contamination of plants, animals and humans [6]. Therefore, the evaluation of airborne material transport in the Atmospheric Boundary Layer (ABL) is one of the requirements for maintenance, protection and recovery of the ecological system. In order to analyze the consequences of pollutant discharge, atmospheric dispersion models are of need, which have to be tuned using specific meteorological parameters and conditions for the considered region [2]. Moreover, they shall be subject to the local orography and shall supply with realistic information concerning environmental consequences and further help reduce impact from potential accidents such as fire events and others. Moreover, case studies by model simulations may be used to establish limits for the escape of pollutant material from specific sites into the atmosphere [3].

ISSN 2229-5518

2.0 GOVERNING EQUATION

The phenomenon of pollutant transport process in fact, has the following components: temporal variation, dispersion, convection and first order reaction or decay. These components are represented through the outlining of a differential cube [5], called control volume, and then apply the laws of physics and mathematics. In Figure 1, it is considered that the concentration (C) inside the cube is uniform because of its very small size, the x, y and z axis are analyzed which are limited by the different faces of the cube, called control surfaces.

Applying the law of conservation of mass, the variation of mass per unit of time within the control volume (mass flow rate) must be equal to the rate at which the mass enters the left side of the control volume in directions of the x, y and z axis, less the same mass that is leaving on the right side, plus differential of mass, plus the mass gains due to a point source and minus the first-order kinetics also called decay [1].

However, incorporating the half-life of the pollutant element in question into the decay constant will ensure a more accurate and realistic representative integrity of these pollutants in contaminant transport. The real approximate values of the contaminant deposition along the path of transport can actually be evaluated, instead of the use of decay constant as an assumed number. Hence, it will effectively depict the pattern of concentration fall-off of these pollutants along their path of travel. Also the actual concentration of these pollutants at various nodal points along its path can easily be computed.

ISSN 2229-5518

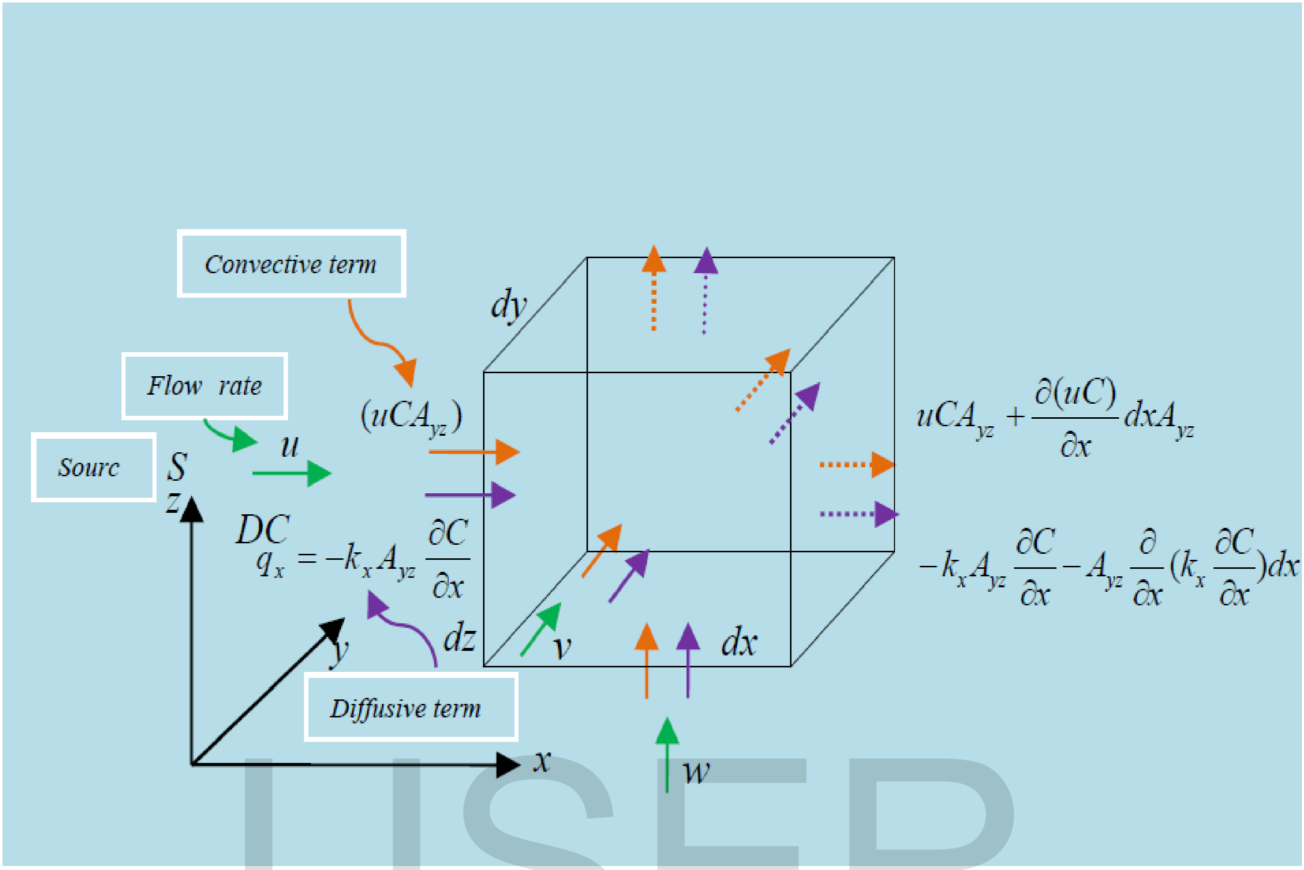

Figure 1: Diagram of the concept model for the transport of pollutants. (SOURCE: PEREZ AND PEREZ, 2016)

After applying mathematical concepts to the law of conservation of mass and make appropriate simplifications, we get to the governing equation shown below;

$$\partial c/\partial t = -u\,\partial c/\partial x - v\,\partial c/\partial y - w\,\partial c/\partial z + \partial/\partial x\left(k_x \frac{\partial c}{\partial x}\right) + \partial/\partial x\left(k_y \frac{\partial c}{\partial y}\right) + \partial/\partial x\left(k_z \frac{\partial c}{\partial z}\right) + S - DC \qquad (1)$$

Where,

u, Flow velocity of the fluid in the direction x (m/s);

v, Flow velocity of the fluid in the direction y (m/s);

w, Flow velocity of the fluid in the direction z (m/s);

C, concentration of the pollutant (CO) within the fluid (mg/lit.);

k_x, Diffusion coefficient in the direction x $(\frac{m^2}{s})$;

k_y, Diffusion coefficient in the direction$y$ ($\frac{m^2}{s}$);

k_z, Diffusion coefficient in the direction$z$ ($\frac{m^2}{s}$);

D, Decay coefficient or first order kinetics (1/S);

S, Point source of external pollution (mg/lit);

x, Length in the main flow direction (m);

y, Length in the transverse flow direction (m);

z, Length in the vertical flow direction (m);

t, Time (seg).

Considering only the longitudinal transport of pollutants (in the x direction), the equation reduces to;

$$\partial c/_{\partial t} = -u\,\partial c/_{\partial x} + \partial/_{\partial x}\left(k_x \frac{\partial c}{\partial x}\right) + S - DC$$

$$\partial c/_{\partial t} = -u\,\partial c/_{\partial x} + k_x \frac{\partial^2 c}{\partial x^2} + S - DC$$

$$\partial c/_{\partial t} + u\,\partial c/_{\partial x} + k_x \frac{\partial^2 c}{\partial x^2} + S - DC = 0 \quad (2)$$

Having this in mind, we can actually say that at steady state; $\frac{\partial c}{\partial t} = 0$

$$k_x \frac{\partial^2 c}{\partial x^2} + u\,\partial c/_{\partial x} - S + \frac{0.693}{t_{1/2}} C = 0 \quad (3)$$

Where,

$$D = K = Halflife = \frac{0.693}{t_{1/2}} \quad (4)$$

Where, C = concentration along cake height. All defined.

3.0 THE DERIVATION OF THE MODEL EQUATIONS FOR CONCENTRATION USING GALERKIN'S FINITE ELEMENT FORMATIONS

Derivation of Element Equation

The Galerkin's weighted residual method (GWRM) is the basis of the element derivation equations of the governing equation (0.0). The principle is expressed mathematically as:

$$\int_R N_\beta (\oint)\, dR = 0 \quad \beta = i; j, k, \ldots \tag{5}$$

Where N_β = shape function or approximation function.

$\oint =$ Unknown parameter and is approximated by

$\oint =$ [eli, N_j, N_R,…….] [$\varnothing p$]:

$L(\oint)$= differential equation governing $\oint$; and

R = region of interest.

Presentation and selection of approximation function as a linear N_k is chosen for that purpose and may be;

We assume a linear interpolation (basis) function as follows;

$$C = \left[\left(1 - {}^{x}/_{L}\right) \;\; {}^{x}/_{L}\right] \begin{bmatrix} c_1 \\ c_2 \end{bmatrix}$$

$$\frac{\partial c}{\partial x} = {}^{1}/_{L} \; [-1 \;\; 1] \begin{bmatrix} c_1 \\ c_2 \end{bmatrix}$$

And

$$N^T = \begin{bmatrix} 1 - {}^{x}/_{L} \\ {}^{x}/_{L} \end{bmatrix}$$

Integrating Equation (3) term by term by first substituting the interpolation functions gives;

The solution will be sought over the boundary conditions (interval) of $c_1 \leq x \leq c_\infty$

$$\int_o^L N^T \left[k_x \frac{\partial^2 c}{\partial x^2} + u \,{}^{\partial c}\!/_{\partial x} - S + \frac{0.693}{t_{1/2}} C \right] dx = 0 \tag{6}$$

3.1 Element Formation with Linear Shape Function.

Term 1:

$$k_x \int_O^L N^T \frac{\partial^2 c}{\partial x^2} dx = k_x N^T \frac{\partial c}{\partial x}\Big|_O^L - \int_O^L \frac{dN^T}{\partial x}\frac{\partial c}{\partial x} dx$$

Note: $\frac{\partial N^T}{\partial X} = \frac{\partial}{\partial X}\begin{bmatrix} 1 - x/L \\ x/L \end{bmatrix} = \frac{1}{L}\begin{bmatrix} -1 \\ 1 \end{bmatrix}$

The first term to the right of equality becomes zero as no values of ${}^{\partial c}\!/_{\partial x}$ is specified. Thus;

$$k_x \int_O^L N^T \frac{\partial^2 c}{\partial x^2} dx = -k_x \int_O^L \frac{dN^T}{\partial x}\frac{\partial c}{\partial x} dx$$

$$= -k_x \int_O^L \begin{bmatrix} 1 - x/L \\ x/L \end{bmatrix} {}^1\!/_L \,[-1 \;\; 1] \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} dx$$

$$= \frac{-k_x}{L}\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}\begin{bmatrix} c_1 \\ c_2 \end{bmatrix} \tag{7}$$

Term 2:

$$\int_O^L N^T u \frac{\partial c}{\partial x} dx = u \int_O^L N^T \frac{\partial c}{\partial x} dx$$

$$= u \int_O^L \begin{bmatrix} [1 - x/L] \\ x/L \end{bmatrix} {}^1\!/_L \,[-1 \;\; 1] \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} dx$$

$$= \frac{u}{L}\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}\begin{bmatrix} c_1 \\ c_2 \end{bmatrix} \tag{8}$$

Term (3):

$$\int_O^L N^T \frac{0.693}{t_{1/2}}\, Cdx = \frac{0.693}{t_{1/2}} \int_O^L N^T CdX = \frac{wL}{2}\begin{bmatrix}1\\1\end{bmatrix}$$

$$= \frac{0.693}{t_{1/2}} \int_O^L \begin{bmatrix}(1-x/L)\\ x/L\end{bmatrix}\begin{bmatrix}(1-x/L) & x/L\end{bmatrix}\begin{bmatrix}c_1\\c_2\end{bmatrix} dx$$

$$= \frac{0.693L}{6t_{1/2}}\begin{bmatrix}2 & 1\\1 & 2\end{bmatrix}\begin{bmatrix}c_1\\c_2\end{bmatrix} \quad (9)$$

(Term 4):

$$-\int_O^L N^T Sdx = -S\int_O^L \begin{bmatrix}(1-x/L)\\ x/L\end{bmatrix} dx = \frac{-SL}{2}\begin{bmatrix}1\\1\end{bmatrix} \quad (10)$$

Combining each of the evaluation terms yields the following element equations:

$$\frac{-k_x}{L}\begin{bmatrix}1 & -1\\-1 & 1\end{bmatrix}\begin{bmatrix}c_1\\c_2\end{bmatrix} + \frac{u}{L}\begin{bmatrix}1 & -1\\-1 & 1\end{bmatrix}\begin{bmatrix}c_1\\c_2\end{bmatrix} + \frac{0.693L}{6t_{1/2}}\begin{bmatrix}2 & 1\\1 & 2\end{bmatrix}\begin{bmatrix}c_1\\c_2\end{bmatrix} = \frac{SL}{2}\begin{bmatrix}1\\1\end{bmatrix} \quad (11)$$

Alternatively, the conductivity matrices to the left of equation (11) can be combined as.

$$\begin{bmatrix}-D_1 + D_2 + 2D_3 & D_1 - D_2 + D_3\\ D_1 - D_2 + D_3 & -D_1 + D_2 + 2D_3\end{bmatrix}\begin{bmatrix}c_1\\c_2\end{bmatrix}$$

$$= \frac{SL}{2}\begin{bmatrix}1\\1\end{bmatrix} \quad (12)$$

Or

[D] {c} = {v}

Where $D_1 = K_x/L, D_2 = u/L, D_3 = 0.693L/6t_{1/2}$ and [D] = Conductivity matrix.

3.2 ASSEMBLE ELEMENT EQUATIONS INTO GLOBAL EQUATIONS.

We assume a one-dimensional stretch, divided into four elements with five nodes (linear option) as shown in Figure (2) below we have;

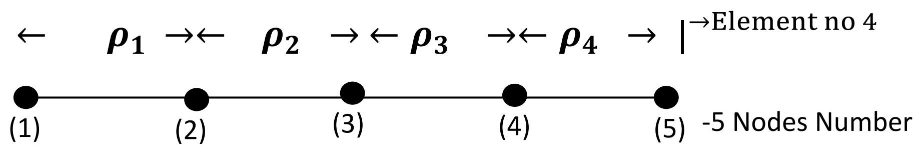

Figure 2: Discritized one-dimensional linear stretch for linear option

The element assemblage for linear option (Equation 12) results as follows;

$$\begin{bmatrix} -D_1+D_2+2D_3 & -D_1-D_2+D_3 & 00000000 & 00000 & 00000 \\ -D_1+D_2+D_3 & -2D_1+2D_2+4D_3 & D_1-D_2+D_3 & 00000 & 00000 \\ 0000000000 & -D_1+D_2+D_3 & -2D_1+2D_2+4D_3 & D_1-D_2+D_3 & 00000 \\ 0000000000 & 000000000 & D_1-D_2+D_3 & -2D_1+2D_2+4D_3 & D_1-D_2+D_3 \\ 0000000000 & 000000000 & 00000000 & D_1-D_2+D_3 & -D_1+D_2-2D_3 \end{bmatrix} \begin{bmatrix} C1 \\ C2 \\ C3 \\ C4 \\ C5 \end{bmatrix}$$

$$= \frac{SL}{2} \begin{bmatrix} 1 \\ 2 \\ 2 \\ 2 \\ 1 \end{bmatrix} \qquad (13)$$

REFERENCE

[1] Bird, R.B., Stewart, W.E. and Lightfoot, E.N. (1964). Fenómenos de transporte. Barcelona, España: Ed. Reverté,.

[2] Costa, C.P., Tirabassi, T., Vilhena, M.T. and Moreira, D.M. (2011). A general formulation for pollutant dispersion in the atmosphere. J. Eng. Math., Published online. Doi 10.1007/s10665 011-9495-z.

[3] Moreira, D.M., Vilhena, M.T., Tirabassi, T., Buske, D., Costa, C.P. (2010). Comparison between analytical models to simulate pollutant dispersion in the atmosphere. Int. J. Env. And Waste Management, Vol. 6, page numbers (327-344).

[4] Perez, A.V. and Perez, N. (2016). Simulation with the finite element method of air pollution with carbon monoxide in the City of Arequipa (Peru). In Proceedings of the 24th International Conference on Modelling, Monitoring and Management of Air Pollution (AIR 2016) PT2 23-33.

[5] Seinfeld J.H., Spyros N. (1998). Pandis, Journal of Atmospheric Chemistry.

[6] Wortmann, S.; Vilhena, M. T.; Moreira, D. M. and Buske, D. (2005). A new analytical approach to simulate the pollutant dispersion in the PBL. Atmos. Environ., Vol. 39, page numbers (2171-2178).