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A TRANSIENT NUMERICAL MODEL TO PREDICT CONTAMINANT CONCENTRATIONS IN A WORKPLACE ENVIRONMENT

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SUMMARY

Designers of ventilation systems need to understand the air movement and pollutant distribution in an indoor environment in order to meet indoor air quality objectives. A detailed analysis of ventilation system performance is even more critical if the system is designed for specific applications in which hazardous chemicals are being handled. To predict these exposures, models simulate the transient pollutant distribution in an indoor workplace. However, generation of such a prediction is not easy, particularly when the pollutant concentration is changing rapidly. Most of the air flow computer models published are steady-state models.

Goodfellow Consultants Inc. (GCI) has developed a transient model which simulates the sudden release ("puff") of a high concentration pollutant injecting into a confined space. The puff is dispersed rapidly within the air space. The model is a fully implicit model solving the finite different equations for a series of time steps in parallel. With this approach, the computational time can be minimized and the divergence problem usually associated with numerical methods can be reduced. The model calculates the pollutant distribution within the defined domain for all time steps. The time-weighted average exposures at a particular location in the defined domain can be calculated. The model has been used to calculate concentrations of contaminant in a workplace for a sudden release case. Results are compared with field measurements.

INTRODUCTION

Air movement and pollutants distribution prediction methods are widely developed by using the computation fluid dynamic techniques. A numerical model has been developed by **Goodfellow Consultants Inc. (GCI)** to simulate a transient problem of a high concentration pollutant puff injecting into a confined space. The puff is dispersed rapidly within the air space. For high pollutant concentration gradients, problems of numerical instabilities and lack of accuracy are common problems with the numerical modelling. To solve these shortcomings, GCI has attempted to model the simulation with the implicit technique which solves the finite difference equation for a series of time steps in parallel. With this approach, the computational time can be minimized and the divergence problem usually associated with numerical method can be reduced. The model calculates the pollutant distribution within the defined domain for all time steps. The time-weighted average exposures at a particular location in the defined domain can be calculated with the time-concentration curve.

THE MODEL

To simplify the complexity of this problem, the studied three-dimensional room in which the pollutant is released is reduced to a two-dimensional model. A vertical cross-sectional plane is extracted from the room for the purpose of this model. The plane is located such that it passes through the centre-line of the room, the centre-line of the pollutant source and the centre-line of the supplies and exhausts.

The simplification assumes that there is no mass transfer orthogonally to this plane. All mass transfer, as predicted by the model, will occur in this plane only. Since some dispersion from the centre-line does occur, pollutant concentrations predicted by this model are conservative.

Other assumptions which simplify this model are, as follows:

- the room is isothermal with no temperature gradients;
- the air is considered incompressible;
- density effects, between pollutant and air, are not taken into account.

The two-dimensional space is divided into NX times NY cells where NX and NY are the nodes in X and Y directions. The nodal distance in X and Y directions are denoted by Δx and Δy respectively.

POLLUTANT DISPERSION

Pollutant dispersion emanating from a specified source through the air in a room is governed by the mass transfer relationship of convection and diffusion. Convection describes the movement of the pollutant due to the bulk movement of the air while diffusion considers the movement of the pollutant through the room due to concentration gradient. Quantification of these two phenomena together can predict concentration and velocities of the pollutant movement. Diffusion effects are usually much smaller than convection effects, but should be included nevertheless due to its importance near the source, particularly when the source concentration is high.

The transient mass balance equation, as per the modified Fick's equation, can be written as (equation 1):

$$\frac{\partial C}{\partial t} - D_{AB}\left(\frac{\partial^2 C}{\partial X^2} + \frac{\partial^2 C}{\partial y^2}\right) + \left(u\frac{\partial C}{\partial X} + v\frac{\partial C}{\partial Y}\right) - R_A = 0 \qquad (1)$$

where C = pollutant concentration
D_{AB} = diffusion co-efficient
R_A = rate of pollutant generation

The stream function (Ψ) is commonly used by the fluid dynamic researchers to describe the stream flow. The definition of the stream function is

$$u = \frac{\partial \psi}{\partial y} \qquad v = -\frac{\partial \psi}{\partial x}$$

Therefore, Equation 1 may be re-written as (Equation 2):

$$\frac{C_{i,j}-C^{\circ}_{i,j}}{\Delta t} - D_{AB}\left(\frac{C_{i+1,j}-2C_{i,j}+C_{i-1,j}}{\Delta x^2}\right)$$

$$- D_{AB}\left(\frac{C_{i,j+1}-2C_{i,j}+C_{i,j-1}}{\Delta y^2}\right)$$

$$- \frac{1}{2\Delta x\Delta y}(qc_1\ C_{i,j} + qc_2\ C_{i-1,j}+qc_3\ C_{i,j}+qc_4\ C_{i,j+1}$$

$$+ qc_5\ C_{i,j} + qc_6\ C_{i+1,j}+qc_7\ C_{i,j}+qc_8\ C_{i,j-1}) - R_A = 0 \qquad (2)$$

where
$$qc_1 = \psi_{i,j+1} - \psi_{i,j} - ABS\ (\psi_{i,j+1} - \psi_{i,j})$$
$$qc_2 = \psi_{i,j+1} - \psi_{i,j} + ABS\ (\psi_{i,j+1} - \psi_{i,j})$$
$$qc_3 = \psi_{i+1,j+1} - \psi_{i,j+1} - ABS\ (\psi_{i+1,j+1} - \psi_{i,j+1})$$
$$qc_4 = \psi_{i+1,j+1} - \psi_{i,j+1} + ABS\ (\psi_{i+1,j+1} - \psi_{i,j+1})$$
$$qc_5 = \psi_{i+1,j} - \psi_{i+1,j+1} - ABS\ (\psi_{i+1,j} - \psi_{i+1,j+1})$$
$$qc_6 = \psi_{i+1,j} - \psi_{i+1,j+1} + ABS\ (\psi_{i+1,j} - \psi_{i+1,j+1})$$
$$qc_7 = \psi_{i,j} - \psi_{i+1,j} - ABS\ (\psi_{i,j} - \psi_{i+1,j})$$
$$qc_8 = \psi_{i,j} - \psi_{i+1,j} + ABS\ (\psi_{i,j} - \psi_{i+1,j})$$

Simplification enables the equation to be rewritten as follows (Equation 3):

$$(Func\ 1)\ C_{i,j} + (Func\ 2)\ C_{i+1,j} + (Func\ 3)\ C_{i-1,j} + \qquad (3)$$

$$(Func\ 4)\ C_{i,j+1} + (Func\ 5)\ C_{i,j-1} = \frac{C^{\circ}_{i,j}}{\Delta t} + R_A$$

where Func 1 =

$$\frac{1}{\Delta t} + \frac{2D_{AB}}{\Delta x^2} + \frac{2D_{AB}}{\Delta y^2} - \frac{1}{2\Delta x\Delta y}\,(qc_1 + qc_3 + qc_5 + qc_7)$$

$$\text{Func 2} = \frac{-D_{AB}}{\Delta x^2} - \frac{qc_6}{2\Delta x\Delta y}$$

$$\text{Func 3} = \frac{-D_{AB}}{\Delta x^2} - \frac{qc_2}{2\Delta x\Delta y}$$

$$\text{Func 4} = \frac{-D_{AB}}{\Delta y^2} - \frac{qc_4}{2\Delta x\Delta y}$$

$$\text{Func 5} = \frac{-D_{AB}}{\Delta y^2} - \frac{qc_8}{2\Delta x\Delta y}$$

$C_{i,j}^{*}$ = old concentration.

There is one such equation for each node resulting in NX*NY equations with NX*NY unknowns. This set of equations is then solved at each time step. The Δt value must be small enough to provide resolutions, but not too small that computer time is wasted.

STREAM FUNCTION

From above analysis, the pollutant dispersion equations can be solved if the stream functions (Ψ's) at the nodes are known. The un-steady state continuity equation gives the mechanism to solve the stream functions. The equation is (Equation 4)

$$\omega = \left(\frac{\partial^2\Psi}{\partial x^2} + \frac{\partial^2\Psi}{\partial y^2}\right) \tag{4}$$

Where ω is vorticity

The equation can be transformed into the finite difference equation as (equation 5)

$$\frac{\psi_{i+1,j} - 2\psi_{i,j} + \psi_{i-1,j}}{\Delta x^2} + \frac{\psi_{i,j+1} - 2\psi_{i,j} + \psi_{i,j-1}}{\Delta y^2} + \omega_{i,j} = 0 \tag{5}$$

where: $\psi_{i,j}$ is the stream function at node (i,j)

and: $\omega_{i,j}$ is the vorticity at node (i,j)

Equation 5 can be rewritten as (equation 6):

$$[-2\ (\Delta x^2 + \Delta y^2)]\psi_{i,j} + \Delta y^2\psi_{i+1,2} + \Delta y^2\psi_{i-1,j} + \Delta x^2\psi_{i,j+1} + \tag{6}$$

$$\Delta x_2\psi_{i,j-1} - -\omega_{i,j}$$

where: (i,j) = the node
(i + 1,j), (i - 1,j), (i,j + 1), (i,j - 1) = the adjacent nodes

VORTICITY

A new variable, vorticity, introduced in above equations can be obtained by solving the Navier-Stokes equation in the vorticity transport form as below (equation 7)

$$\frac{\partial\omega}{\partial t} + \left(u\ \frac{\partial\omega}{\partial x} + v\ \frac{\partial\omega}{\partial y}\right) - \gamma\left(\frac{\partial^2\omega}{\partial x^2} + \frac{\partial^2\omega}{\partial y^2}\right) \tag{7}$$

Equation 7 may be re-written as (Equation 8):

$$\omega_{new}=\omega_{prev}+\Delta t\ \left(\nu\left(\frac{\partial^2\omega_{new}}{\partial x^2}+\frac{\partial^2\omega_{new}}{\partial y^2}\right)-\left(u\frac{\partial\omega_{new}}{\partial x}+v\frac{\partial\omega_{new}}{\partial y}\right)\right) \tag{8}$$

New vorticities are calculated by using the vorticities from the past previous iteration. Since the concern of this equation is to solve the steady state stream functions, the value of the Δt is not critical. However, a proper value of Δt is required. If this value is too low, an answer will be found after long, laborious calculation which is not necessary. If the value is too high, convergence will not occur.

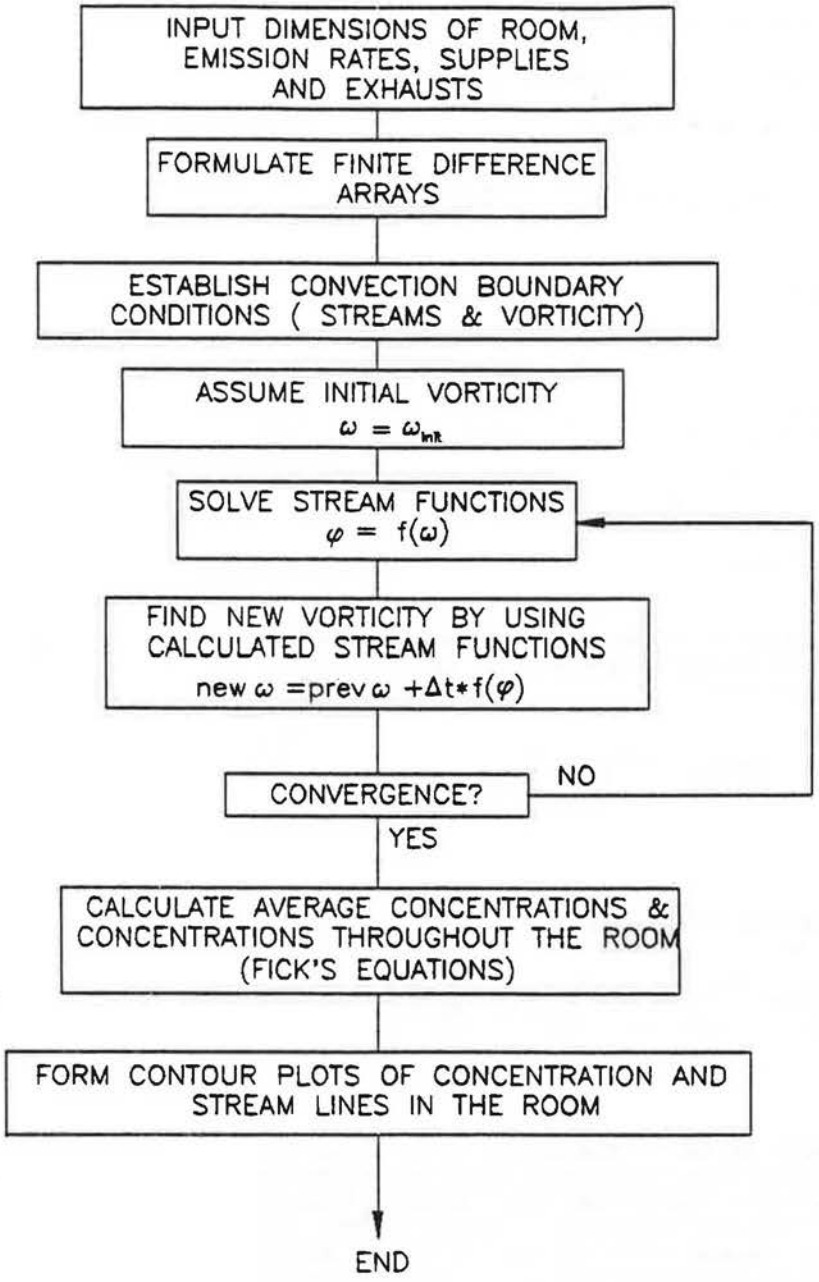


FIGURE 1 – ALGORITHM OF MODEL TECHNIQUE

To solve the equation numerically, the equation is transformed into finite difference equations and is simplified as (equation 9)

$$(\text{Func 1})\ W_{i,j} + (\text{Func 2})\ W_{i+1,j} + (\text{Func 3})\ W_{i-1,j} + (\text{Func 4})\ W_{i,j+1} + (\text{Func 5})\ W_{i,j-1} = W^*_{i,j} \tag{9}$$

where: (i, j) = the node
(i+1, j), (i-1, j), (i,j+1), (i, j-1) = the adjacent nodes.

$W_{i,j}$ = old vorticity

Func 1 =

$$1 + \Delta t \left(\frac{2\nu}{\Delta x^2} + \frac{2\nu}{\Delta y^2}\right)$$

Func 2 =

$$\Delta t \frac{[\psi_{i+1,j+1} - \psi_{i+1,j-1} + \psi_{i,j+1} - \psi_{i,j-1} + \frac{\nu}{\Delta x^2}]}{2\Delta x \Delta y}$$

Func 3 =

$$\Delta t \frac{[\psi_{i-1,j+1} - \psi_{i-1,j-1} + \psi_{i,j+1} - \psi_{i,j-1} + \frac{\nu}{\Delta x^2}]}{2\Delta x \Delta y}$$

Func 4 =

$$\Delta t \frac{[\psi_{i+1,j+1} - \psi_{i-1,j+1} + \psi_{i+1,j} - \psi_{i-1,j} + \frac{\nu}{\Delta y^2}]}{2\Delta x \Delta y}$$

Func 5 =

$$\Delta t \frac{[\psi_{i+1,j} - \psi_{i-1,j} + \psi_{i+1,j} - \psi_{i-1,j} + \frac{\nu}{\Delta y^2}]}{2\Delta x \Delta y}$$

SOLVING THE EQUATIONS

The model is written in FORTRAN 77 using structured loops and a modular format. Meaningful variable names are assigned. Every effort is made to allow for ease in debugging and understanding. The program consists of five major sections, each composed of smaller modules. Figure 1 shows a detailed algorithm of the method. The five major sections are:

- input and boundary conditions definitions;
- stream function solver;
- vorticity function solver;
- pollutant dispersion equation solver; and
- output plot

The procedure of solving the model is to develop the steady state stream functions first by using a looping approach between the continuity equation (Equation 6) and vorticity transport equations (Equation 9). Then, the steady state stream functions will be input into the modified Fick's equation (Equation 3) to solve the pollutant dispersion. This assumption is valid for the reason that the room air movement is well developed into steady state conditions before the pollutant is injected into the air space.

The technique used in the solvers is the implicit method solving the finite difference matrices for the stream function, vorticities and pollutant dispersion equations. The technique enables a value at one node to be expressed in terms of values at all of the other nodes as described in Equations 3, 6 and 9.

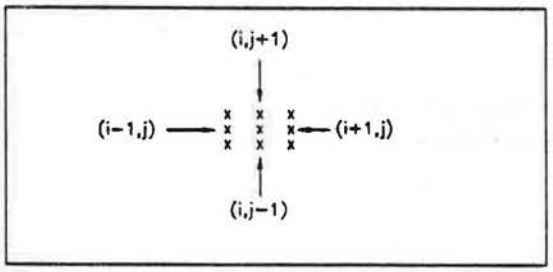


FIGURE 2 – FINITE DIFFERENCE COMPUTATIONAL STAR

FIGURE 2

This relationship forms the "computational star" as illustrated in Figure 2. There is an equation similar to above equations for each node in the defined domain. Special treatments are required for boundary nodes as there is no more node beyond the boundary. Combining all the model equations, the result is a square matrix which is NX times NY rows by NX times NY columns (NX, NY are row and column grid numbers). And the number of variables to be solved is NX times NY (i.e. for all nodes).

The general form of the matrix equation is,

$$A\ X = B$$

where: A = the square matrix of the co-efficients of the variables
X = variables matrix
B = Matrix of the right hand side of the equations

The characteristic of Matrix A is a pentadiagonal matrix -- one diagonal for each leg of the computational star for a specific node. Employing specified technique to solve pentadiagonal matrix will render the calculation faster. When the pollutant dispersion equation is solved, the number of variables in X matrix is the number of nodes times the number of time steps.

BOUNDARY CONDITIONS

As mentioned before, special treatments are required for the boundary node equations in the pentadiagonal matrix. The following section describes how the special treatments are made. Boundary conditions are assumed to be constant with time. There are three types of boundary:

- the solid wall
- the inflow/outflow
- the source

For the non-slip properties at the solid wall boundary, at each of the horizontal walls, the vertical velocity is zero and at each of the vertical walls, the horizontal velocity is zero. At the corners, both u and v are zero. Also, at the vertical walls, $\partial\Psi/\partial x$ = constant, and at the horizontal wall, $\partial\Psi/\partial y$ = constant.

In addition, the inflow at the boundaries is zero, except at the locations of supplies and exhaust where inflow equals the supply air or exhaust air velocity. Air flow is assumed to be perpendicular to the boundary.

It is also assumed that there is no diffusion across the boundaries. That is, there is no concentrations gradient at the walls. This means $\partial C/\partial x = 0$ at the vertical boundary and $\partial C/\partial y = 0$ at the horizontal boundary. Hence, nodes lying on the boundary are assigned the value for concentration of the adjacent interior node, except the boundary for the pollutant source. At the source, the concentration is assigned to be the emission concentration.

The modified boundary node equations are formulated by taking a mass balance at the boundary cell with the consideration of the above described criterions. The modified boundary equations are:

Left boundary

$$\psi_{1,j+1} - \psi_{1,j-1} = 2u_{BND}\Delta y$$

$$\omega_{1,j} = -2\,\frac{(\psi_{2,j} - \psi_{1,j})}{\Delta X^2}$$

$$C_{1,j} - C_{2,j} = 0$$

Right boundary

$$\psi_{NX,j+1} - \psi_{NX,j-1} = 2\,u_{BND}\Delta y$$

$$\omega_{NX,j} = -\,2\,\frac{(\psi_{NX-1,j} - \psi_{NX,j})}{\Delta X^2}$$

$C_{NX,j} - C_{NX-1,j} = 0$ except that at the source, (C_{NX}, source) = source strength.

Bottom Boundary

$$\psi_{i-1,1} - \psi_{i-1,1} = -2v_{BND}\Delta x$$

$$\omega_{i,1} = -2\frac{(\psi_{i,j+1} - \psi_{i,j})}{\Delta y^2}$$

$$C_{i,1} - C_{i,2} = 0$$

Top Boundary

$$\psi_{i-1,NY} - \psi_{i-1,NY} = -2\, v_{BND}\Delta x$$

$$\omega_{i,NY} = -2\frac{(\psi_{i,NY-1} - \psi_{i,NY})}{\Delta y^2}$$

$$C_{i,NY} - C_{i,NY-1} = 0$$

where: $u_{BND} = 0$ and $v_{BND} = 0$, except at inflow/outflow boundaries where u_{BND}, v_{BND} equal supply and exhaust velocities.

APPLICATION

The model has been applied to a case when a pollutant with 7500 ppm in concentration is suddenly released into a confined space. The initial pollutant concentration of the confined space is zero. The pollutant injection duration is 15 seconds. There are three supply diffusers located in the ceiling and an exhaust is also located in the same ceiling, but right above the source. The length of the room is 10.5 m and the ceiling height is 2.74m. The ceiling, floor and walls are assumed to be solid boundaries, except the locations of supplies, exhaust and source. The purpose of the study is to predict the operator's exposure to the pollutant while the operator is standing in front of the source.

The room is discretized into 101 (NY) times 26 (NY) nodes. Then, the nodal distance in x and y directions are 0.105m and 0.11m respectively.

Figure 3.0 shows schematically the controlled domain with approximate locations of supplies, exhaust and source.

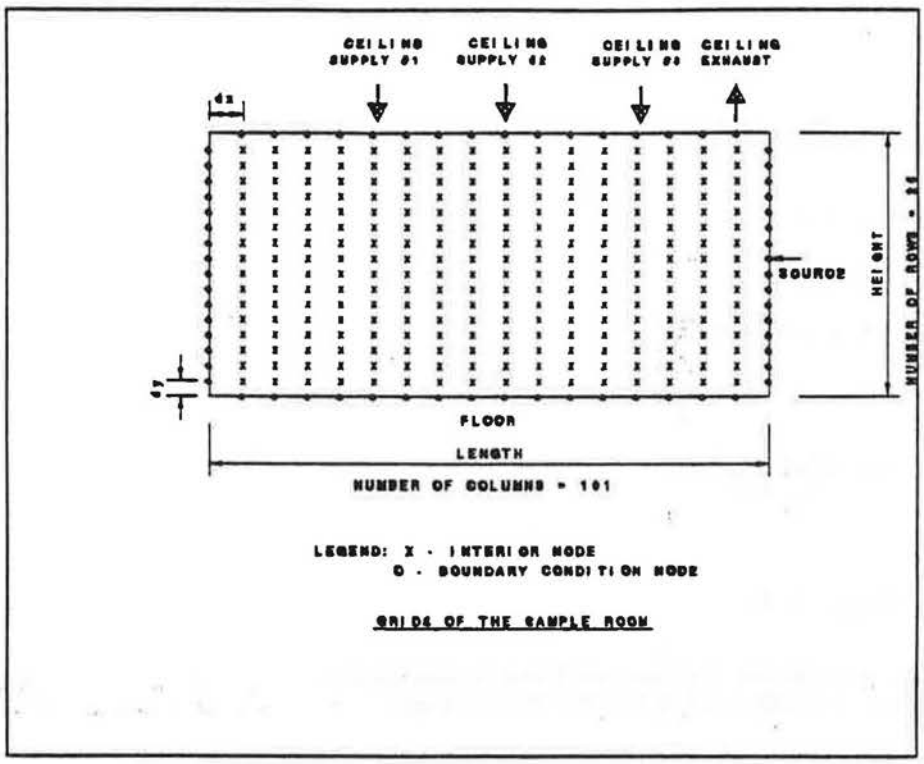


FIGURE 3

The model firstly calculates the steady-state stream functions. Figure 4.0 is the contours of stream functions representing the air flow pattern. After the stream functions have been developed, the model calculates the transient pollutant concentration profiles for all time steps. The time step difference is assigned to be 10 seconds. Therefore, 90 time steps are calculated totally. Figure 5.0 is a typical pollutant concentration contour plot of a time step. Similar contours can be plotted for each time step. The pollutant concentrations at the breathing zone of the operation for each time step can be extracted from the output data file. Figure 6.0 is the transient plot of the pollutant concentration at the location of operator. From this plot, the time weighted average can be calculated.

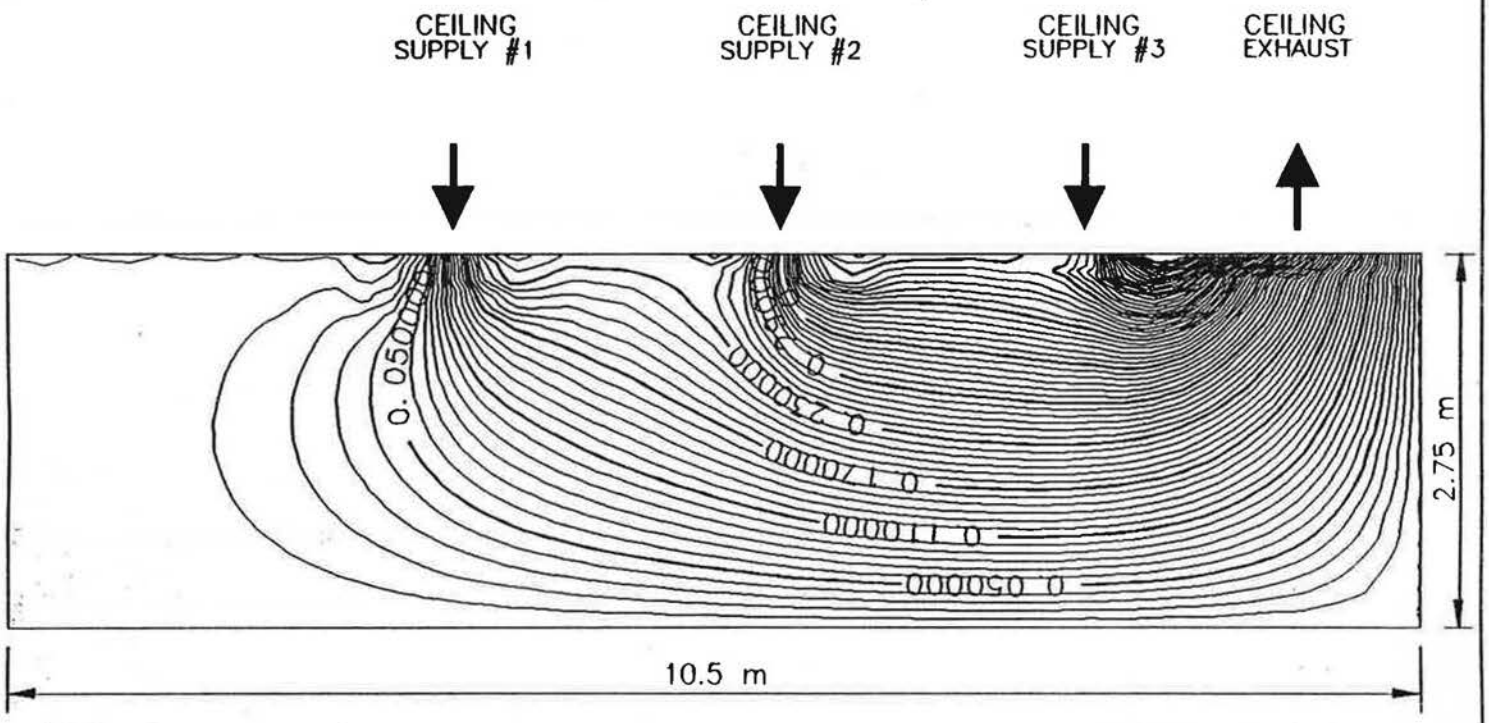


FIGURE 4 – STREAM LINE CONTOURS FOR TEST ROOM

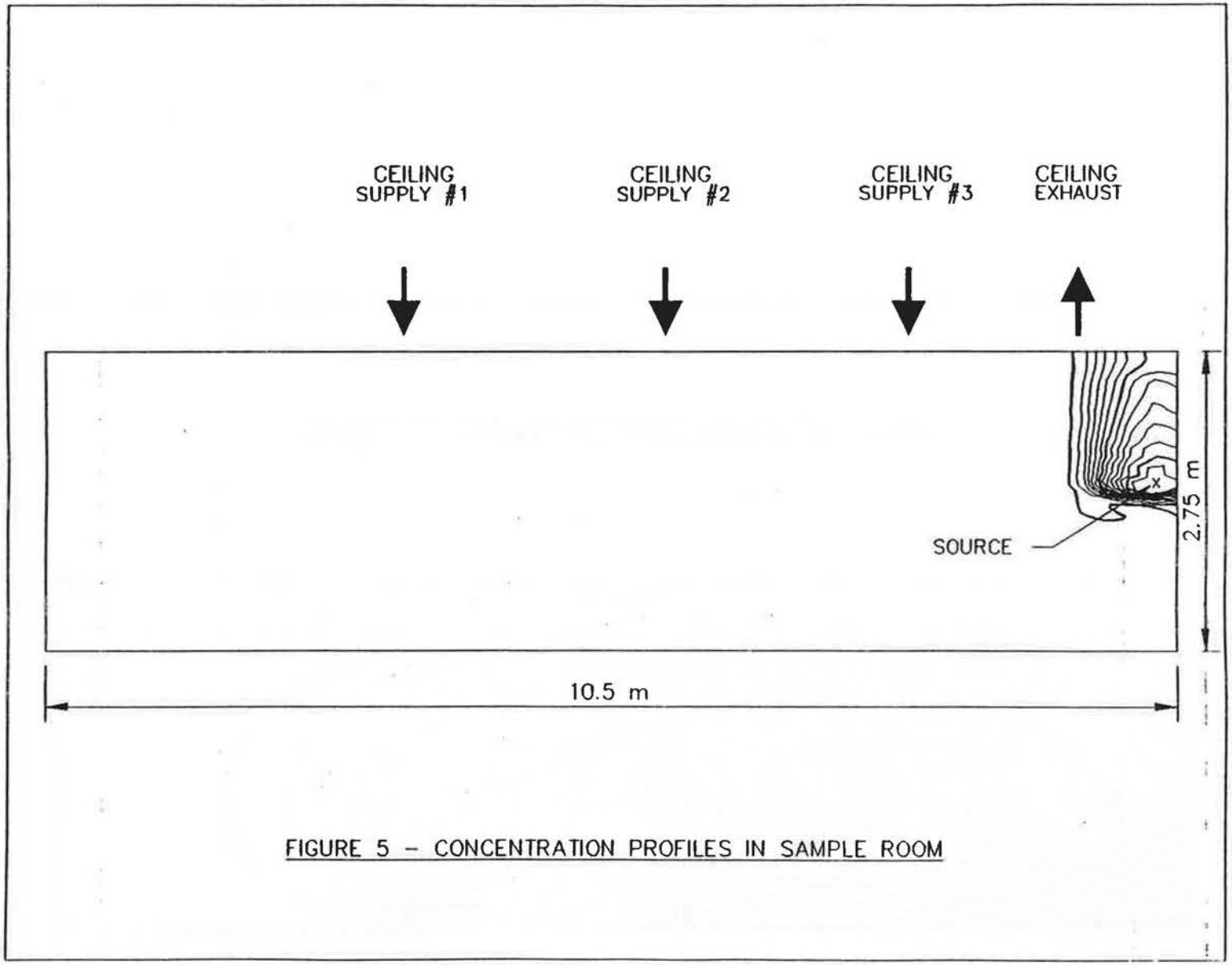
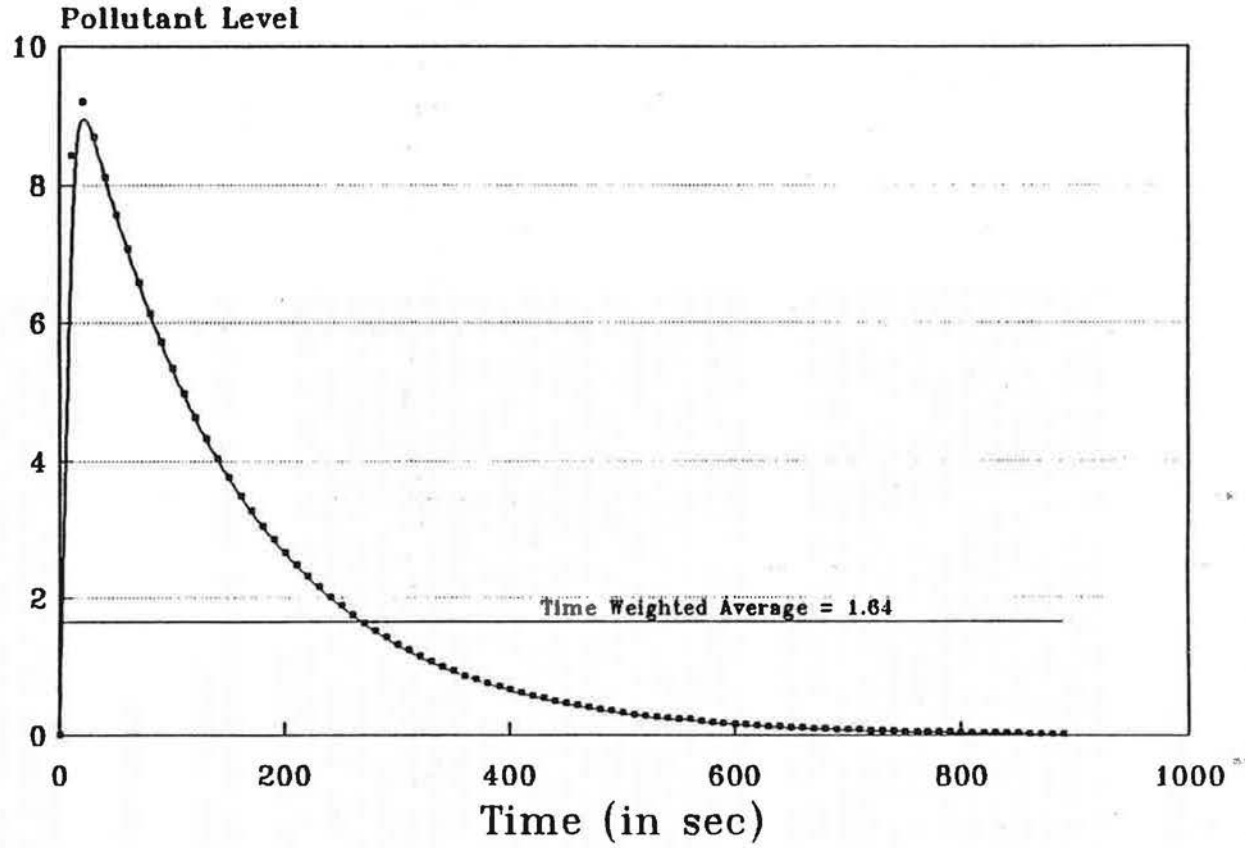


FIGURE 5 – CONCENTRATION PROFILES IN SAMPLE ROOM

FIGURE 6 – TRANSIENT POLLUTANT LEVEL
AT OPERATOR'S BREATHING ZONE



DISCUSSION

The nature of this model is the large gradients in both spatial and time domain. To maintain numerical stability, small spatial and time intervals have to be used if the model is modelled with explicit method. Small interval requires more computational time and it also leads to the uncontrolled error growth due to numerical operations. After trading off between computational time, hardware availability, programming technique and resolution requirement, an implicit method is selected. With an efficient matrix solver for the pentadiagonal matrix and the larger interval, the computation time can be reduced. Due to the computer hardware limitation, the time interval is chosen to be 10 seconds. If a more powerful machine is used, a higher resolution in time domain can be obtained.

Another consideration for the model is the computer storage requirement. With the implicit method to solve transient problems, the size of the matrix is (NX x NY x time steps) times (NX x NY x time steps). For this model, the size of the matrix is 236,340 times 236,340. This is a huge matrix. However, since the matrix is a pentadiagonal matrix, majority of the matrix elements are zero. With an effective database technique, which records only the non-zero elements, the computer storage requirements can be reduced dramatically. The model is based on vorticity - stream functions form of Navier-Stokes equation. With this form, only two variables (ω and Ψ) are used in the equations, and the pressure on the computer storage requirements can be reduced. The vorticity-stream functions method iterates between vorticity and stream function with a predefined time step. Since only the steady state stream functions are concerned, a large time step is chosen to reduce the computation time. Also, to minimize the effect of divergency that may happen between two solvers, a relaxation factor of 0.99 is used when vorticity functions are calculated.

Theoretically, divergency is not associated with an implicit method employing direct matrix solvers.

CONCLUSION

The numerical model developed by GCI allows the users to calculate the concentration profile as a function of time and position. The model has the mechanism to handle the large gradient problems which are difficult to solve. This allows the user to determine the maximum concentration and the time-weighted average (TWA).

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