A boundary element model for indoor air quality simulation

David B. Carrington and Darrell W. Pepper

Department of Mechanical Engineering,
University of Nevada, Las Vegas
E-mail: swift@nye.nscee.edu

Abstract

A boundary element method (BEM) is used with a Lagrangian particle transport technique (LPT) to simulate indoor dispersion of contaminants. The BEM is used to create a simple mass-conservative velocity field within a building interior or room; the LPT employs a stochastic/random walk approach to generate a feasible dispersion pattern for contaminants released within the interior. The model provides a quick estimate of the potential dispersion pattern and flow field within a building interior. The use of the BEM and particle transport techniques permits irregular geometry, typical of interiors within buildings, to be easily simulated, and executes quickly on PCs.

1 Introduction

Emission of pollutants and their accumulation due to poor ventilation and air exchange are serious problems currently under investigation by many researchers. Major indoor air pollution problems include 1) radon gas entering buildings through cracks in the foundations, 2) environmental tobacco smoke containing inorganic gases, heavy metals, particulate, and volatile organic compounds (VOC), 3) asbestos fibers, 4) formaldehyde used in furniture, insulation, and pressed wood products, 5) lead based paints and perchlorethylene products, 6) biological pollutants from heating, ventilation, and air conditioning systems, and 7) pesticides, such as termiticides and wood preservatives.

Mathematical modeling plays an important role in helping to determine the transport and subsequent exposures attributed to exposure to hazardous material within building interiors. Although analytical models are
fast in providing order of magnitude estimates for room discharges, such approaches are very idealistic and usually quite limiting. More accurate approaches have typically required the use of multi-dimensional advection-diffusion numerical schemes; unfortunately, such methods demand much larger computational resources and are considerably slower in creating solution scenarios. New numerical techniques that fall under the category of mesh-less or meshless techniques are now appearing in the literature. These methods have been shown the detailed numerical schemes of the past – within the limitations of the types of equations being solved.

The model in this study uses the Boundary Element Method (BEM) (Tanaka [1]) and Lagrangian particle transport (LPT) (Runchal [2]), which is based on a stochastic/random walk approach for turbulent diffusion, to model velocities and concentrations within buildings and rooms. The computer model runs on PCs, and provides estimates quickly and accurately using a mesh only established on the domain boundaries. The use of BEM and LPT techniques permits irregular geometry, typical of room configurations, to be easily accommodated, and executes quickly on even low-end PCs. The BEM is one of the boundary type methods which reduces the dimensionality of a problem by one, i.e., a two-dimensional problem reduces to a line integral; a three-dimensional problem reduces to a two-dimensional surface formulation. Hence, input data processing consists only of the problem boundary geometry and boundary conditions.

In the application of the random walk model, the particle displacement in each of the coordinate directions is independently calculated using displacement algorithms. The velocity of each particle is obtained from the application of the BEM, which is used to obtain velocity components anywhere within the problem domain without the need for a nodal mesh or interpolation. A general probability distribution (correlation function) for the random component of motion due to dispersion is utilized to account for the diffusion tensor.

2 Indoor Air Quality Models

The most general models for calculating exposure to indoor air pollutants include the Environmental Protection Agency (EPA) model EXPOSURE (Sparks [3]) and National Institute of Standards and Technology (NIST) models NBSAVIS and CONTAM88. These models are based on conservation of mass, box techniques, which assume well-mixed, unidirectional flow. Although the models run on PCs, significant input data are required along with a priori knowledge of existing airflow.
EXPOSURE (Sparks [3]) uses data on source emissions, room-to-room airflow, air exchange with the outdoors, and indoor sinks to predict concentration/time profiles for all rooms. The concentration/time profiles are combined with individual activity patterns to estimate exposure. The effects of air cleaners located in either or both the central air circulating system or individual rooms on indoor air quality and exposure can be conducted. In addition, various sources can be incorporated within the model. Results of ideal test house experiments compared with model predictions are relatively good.

The NIST has developed a series of public-domain computer models for calculating air flow and contaminant dispersal in multizone buildings (Grot [4]). However, these programs require laborious preparation of input data and sophisticated building idealization to be able to model realistic building configurations. The preprocessor program NBSAVIS is used to prepare input files for airflow and indoor air quality analysis. NBSAVIS is menu driven and has the capability of editing and creating a building description and calculated the required zone and opening data for airflow and dispersion prediction. CONTAM88 is the "solver" package which integrates both the air flow and contaminant analyses into one program. Building information, leakage, fan and contaminant data are input into the preprocessor package. CONTAM88 calculates the air flows and both dynamic and steady state levels of indoor contaminants. Work is underway within the NIST to develop a 3-D model based on solution of the turbulent form of the Navier-Stokes equations using k-ε closure (Kurabuchi [5]). Approximately $10^4$ iterations are required for convergence.

3 Random Walk Approach

Particles are used to represent pollutant mass. Changes in particle position are calculated to simulate pollutant mass transport due to both advection and diffusion. The transport equation can be written in the form

$$\frac{\partial C}{\partial t} + \frac{\partial U_i C}{\partial x_i} = 0$$

where the velocity vector $U_i$ is expressed in terms of advection and "flux" diffusion as (Runchal [2])

$$U_i = \hat{U}_i + U_{f_i}$$

with $U_i$ being the true advection velocity vector and the "flux" velocity defined as
By combining the advection and diffusion terms together, a total equivalent transport velocity can be obtained. The form of the transport equation becomes identical to the equation of continuity for a general compressible fluid. The original problem of turbulent diffusion is transformed into one describing the advective changes of fluid density in a compressible fluid moving in a velocity field of total equivalent transport velocities. Mass particles are synonymous with density and follow the fluid motion in the velocity field, i.e., they are Lagrangian particles in a non-solenoidal field of total equivalent transport velocity. Their number in any location (volume) determines the concentration of pollutant for the original diffusion problem.

The probability distribution function for a three-dimensional space is (Runchal [2])

$$P_{x_i}(x_i, t) = \frac{1}{(4\pi t)^{3/2}} \exp\left\{-\frac{1}{4} \sum_{i=1}^{3} \frac{(x_i - U_i t)^2}{K_{it}} \right\}$$

where $x_i$ are the position vectors in the direction of the principal axes and $K_{12}K_{23}$ are the diagonal components of the second-order dispersion tensor in the direction of the principal axes.

The transport equation for this distribution can be written as

$$\frac{\partial P}{\partial t} + \nabla \cdot (U_i P) = \sum_{ij} (K_{ij}) \frac{\partial P}{\partial x_j}$$

where the tensor summation convention has been employed and $K_{ij}$ is a second-order dispersion tensor. The inclusion of particle decay, settling, and more complex dispersion processes involving specified turbulence correlations, can be included in eqn (5).

The problem of transport of particles by advection and dispersion commonly represented by a deterministic transport equation such as eqn (5) can also be represented simply as a series of random walks. Each of these random walks is composed of a deterministic advection component and a random component.

For example, the increment in the position vector of a particle at any time $t$ can be written as

$$U_{f_i} = -\sum_{j} \frac{K_{ij}}{C} \frac{\partial C}{\partial x_j}$$

(3)
where $D$ is a deterministic forcing function for the random component of motion. Equation (3) can be expressed simply as

$$\delta x(w, t) = \delta x_U + \delta x_D$$  \hspace{1cm} (7)

where

$$\delta x_D(w, t) = \int_{t_0}^{t} n_r \sqrt{2Kd't}$$  \hspace{1cm} (8)

where $D$ is assumed equivalent to $K$ and $n_r$ is a normally distributed random number with a mean value of zero, and a standard deviation of unity.

The integral eqn (5) can be further simplified to

$$\delta X_D = n_r \sigma$$

$$\sigma^2 = \int_{t_0}^{t} 2Kd't$$  \hspace{1cm} (9)

The variance obtained from eqn (6) is the same as that from eqn (5). Thus, eqn (3) can be written as

$$x_t - x_0 = \int_{t_0}^{t} U(x_{t'}, t')d't + n_r \{\int_{t_0}^{t} (2K(x_{t'}, t')d't\}^{1/2}$$  \hspace{1cm} (10)

For a rigorous application of the random walk method, the net particle displacement must be calculated by integration of eqn (10). However, with $U$ and $K$ as arbitrary functions of space and time, it is not always possible to obtain a closed form solution. It is generally sufficient to assume that the mean velocity and random components can be separately calculated and linearly superimposed.

For steady or quasi-steady flows, the time scale of particle motion is much smaller than the characteristic time scale of change in the mean velocity and the dispersion fields. In such a case, it is often more convenient to express $U$ and $K$ as functions of the position vector $x_t$, rather than as Lagrangian functions of time.

In the application of the random walk model, the particle displacement in each of the coordinate directions is independently calculated from the displacement algorithm, eqn (10). Before this is performed, however, the mean velocity, $U$, and the dispersion due to turbulence or other stochastic mechanisms must be specified. The velocity of any particle is obtained from the application of the BEM, which can be used to obtain velocity components anywhere within the problem domain without the need...
for a nodal mesh or interpolation. A general probability distribution or correlation function for the random component of motion due to dispersion is utilized to account for the dispersivity tensor, K.

The calculation to advance the particle configuration in time proceeds in steps, or cycles, each of which calculates the desired quantities for time $t + \Delta t$ in terms of those at time $t$. Hence,

$$x_i(t + \Delta t) = x_i(t) + U_i \Delta t$$

The velocity components are the fictitious total velocities determined for the beginning of the time interval and initial particle positions. Every particle is advanced each cycle to a new position using eqn (11). Thus, the particle traces out in time a trajectory for the pollutant mass. Boundary conditions are introduced by modifications of the fictitious total velocities. Solid boundaries are simulated by not allowing particles to be transported across the boundaries. In each cycle, the fictitious total velocity for each cell is calculated as the sum of the advection velocity and the random turbulent flux velocity. The particle positions are updated using an interpolated total velocity. The concentration per unit volume is calculated from the particle masses.

## 4 The Boundary Element Method

The BEM is one of the boundary type methods which reduces the dimensionality of a problem by one, i.e., a two-dimensional problem reduces to a line integral; a three-dimensional problem reduces to a two-dimensional surface formulation. Hence, input data processing consists only of the problem boundary geometry and boundary conditions (Brebbia [7]).

The governing equation for advection-diffusion utilizing a scalar potential can be written as

$$L[\phi] = \frac{\partial \phi}{\partial t} + \nabla \cdot (-k \nabla \phi) + (U \cdot \nabla) \phi = \rho$$

where $\phi$ denotes the source density. Assuming steady-state, the steady governing operator $L[\phi]$ and its adjoint operator $L^*[\phi]$ in which $\phi^*$ is the adjoint potential associated with $\psi$ to Green's second identity can be written as

$$\int_\Omega (L[\phi] \psi - L^*[\psi] \phi) d\Omega = \int_\Gamma - k (\frac{\partial \phi}{\partial n} \psi - \phi \frac{\partial \psi}{\partial n}) d\Gamma + \int_\Gamma U_n \phi \psi d\Gamma$$
where \( n \) is the outward normal to \( \Gamma \), and \( U_n \) is the normal component of \( U \) to \( \Gamma \) (Tanaka [1]). Equation 13 can be rewritten as

\[
c_i \phi(r_i) - \int_{\Gamma} q_n^* \phi d\Gamma = -\int_{\Gamma} \psi^* q_n d\Gamma + \int_{\Omega} \rho \psi^*
\]  

(14)

where \( c_i \) denotes a coefficient that depends on the position vector \( r_i \),

\[
\psi^*(r, r_i) = \exp\left\{-(-U \cdot r^' + |U||r^'|) / (2K)\right\} / (4\pi K |r^'|)
\]  

(15)

In two-dimensions,

\[
\psi^*(r, r_i) = K_0 \{ |U||r^'|/(2K) \} \exp\{-U \cdot r^' / (2K)\} / (2\pi K)
\]

(16)

in which \( r' = r - r_i \), \( r \) is the observation point, and \( K_0 \) is the modified Bessel function of the second kind of order zero.

A set of linear interpolation functions are used to represent the nodal potential values \( \phi \), and flux values, \( q_n^j \), which represents \( q_n \) over \( \Gamma_j \) as its centroid value. Thus,

\[
I \phi^j_{\Gamma_j} = \zeta \cdot \phi^j
\]

(17)

\[
I q_n^j_{\Gamma_j} = q_n^j
\]

(18)

where \( \phi^j \) is a set of linear interpolation functions. The matrix equivalent form of eqn (13) is

\[
[H] \{\Phi\} = [G] \{q\} + \{B\}
\]

(19)

where:

\[
[H] = h_{ij} = -\int_{\Gamma_j} q_n^j \zeta d\Gamma + c_i \delta_{ij}
\]

(20)

\[
[G] = g_{ij} = -\int_{\Gamma_j} \psi^* d\Gamma
\]

(21)

\[
\{B\} = b_i = \sum_{k=1}^{L} \int_{\Omega_k} \rho \psi^*(r, r_i) d\Omega
\]

(22)

where \( \delta_{ij} \) is the Kronecker delta, and \( \Phi \), \( q \), and \( B \) are vectors points, centroid value \( q_n \) and discretized domain integrals, respectively. The dimensions of \( \Phi \), \( q \), and \( b \) are the numbers of nodes (N), number of elements (M), and unknowns (S), respectively; matrices [H] and [G] are SxN and SxM. For Dirichlet problems, the number of unknowns S is equal to the number of elements M; for Neumann problems, S is equal to N. Simple Gaussian elimination is used to solve eqn (19).
5 Example

A simple example of the application of the BEM with Lagrangian particle transport is shown in figures. In this problem, a 2-D floor plan is first generated. Inflow/outflow is established by the boundary conditions at the right and left extreme boundaries. The geometrical description of the floor and rooms can be established from AutoCAD, or any of the other popular CAD packages. These data points are used as element/nodal values for the BEM. Figure 1 shows the potential flow lines and resulting velocity vectors throughout the series of rooms. Particles are released near the right boundary. Figure 2 shows the resulting spread of particles throughout the floor.

Figure 1. Potential flow lines and velocity vectors.

Figure 2. Particle distribution.


6 Conclusion

Indoor ventilation and air quality are simulated using the Boundary Element Method and Lagrangian particle transport. The numerical model runs on enhanced PCs. The software package provides the user with the ability to quickly evaluate history, current inventory, and location of toxic materials, as well as order of magnitude risk assessment associated with transport and diffusion.

References


