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Poster 10

MULTI-ZONE CONTAMINANT DISPERSAL ANALYSIS USING: AN ELEMENT ASSEMBLY APPROACH

J. AXLEY

National Bureau of Standards
Gaithersburg, MD
20899
U.S.A.

ABSTRACT

An *element-assembly* formulation of multi-zone contaminant dispersal analysis theory is described. In this approach a flow system is idealized as an assemblage of *mass transport elements* that model specific instances of contaminant mass transport in the flow system. Equations governing the mass transport phenomena modeled by each element are expressed in terms of contaminant concentration variables, the *nodal concentration variables*, that approximate the contaminant concentration at discrete points, the *system nodes*, in the flow system. The imposition of conservation of mass allows these element equations to be assembled to form spatially discrete but temporally continuous equations that govern the system as a whole. These *system equations* may then be solved to determine the response of the system to contaminant excitation. At its most general level this approach makes no limiting assumptions about the nature of the mass transport phenomena modeled (beyond the assumption of mass conservation) and is, therefore, not limited, in principal, to the well-mixed zone idealization, although, it includes the well-mixed multi-zone theory as a special case.

Element equations for; a) well-mixed zones, b) instantaneous flow transport (with and with out filtering), c) mass transport phenomena governed by first order kinetics, and d) mass transport phenomena governed by the one-dimensional convection diffusion equation are presented. Solution options are outlined, examples of application are presented, and the CONTAM family of programs, that provide one implementation of the theory, is briefly described.

NOMENCLATURE

A	cross-sectional area of flow passage
C	contaminant concentration expressed in terms of mass fraction
$^{\alpha}D$	dispersal coefficient for species α
g	contaminant mass generation rate associated with an element
G	direct contaminant mass generation rate at a system node
L	length of flow passage
m^e	mass of a volume of flow fluid associated with an element
P	pressure
$^{\alpha}R$	rate of kinetics process
T	temperature
t	time
$\bar{t}$	nominal transit time
$\bar{u}$	bulk (i.e., sectional average) fluid velocity
v	fluid velocity vector
w	mass transport rate
x,y,z	spacial coordinates
ϕ	upwind parameter
$^{\alpha}\gamma$	dimensionless generation rate of species α
κ	reaction rate coefficient
$^{\alpha}\eta$	filter efficiency relative to species α
ρ	mass density
τ	dimensionless time; system time constants
χ	dimensionless length

Subscripts, Superscripts and other Symbols

species index → α a ← element index
descriptive index → con x_j ← node or array element index

a,b,c,... . . specific element indices
e . . . . general element index
$\alpha,\beta,\gamma,\ldots$ . . specific species indices
α . . . . general species index
i,j,k,l,m,n . node (or array element) indices
k,n . . . . time step or iterate indices
^ . . . . . quantities modified to account for boundary conditions
~ . . . . quantities modified to account for zero "volumetric" mass terms

Vectors and Matrices

$\{C\}$ . . . . system concentration vector
$\{C^e\}$ . . . element concentration vector
$\{\Phi\}$ . . . . .(steady flow/kinetics) system eigenvectors
$\{E\}$ . . . . system excitation vector
$\{G\}$ . . . . system direct (nodal) species generation rate vector
$\{G\}$ . . . . system generation rate vector
$\{g^e\}$ . . . element-derived species generation rate vector
$[\kappa]$ . . . . kinetics rate coefficient matrix
$L^e(\{V\})$ . . transformation of vector $\{V\}$
$[M]$ . . . . system mass matrix
$[M^e]$ . . . diagonal mass matrix associated with kinetics element
$\{R\}$ . . . . kinetics rate vector
$\{R_o\}$ . . . constant component of kinetics rate vector
$[W]$ . . . . system (mass) transport rate matrix
$[Z]$ . . . . additional (hypothetical) system transformation matrix
$\{w^e\}$ . . . element mass transport rate vector
$[x^e]$ . . . . element (mass) transport matrix
$[y^e]$ . . . . element mass matrix
$[z^e]$ . . . . additional (hypothetical) element transformation matrix

INTRODUCTION

The central concern of indoor air quality analysis is the prediction of airborne contaminant dispersal in buildings. Airborne contaminants disperse throughout buildings in a complex manner that depends on the nature of airflow into, out of, and within the building system; that depends on the possibility of removal, by filtration, or generation of contaminants; and that depends on the possibility of chemical reaction, radio-chemical decay, settling, precipitation, deposition, or sorption of contaminants. More succinctly, we may say that contaminant dispersal in buildings is, in general, affected by a large variety of often very complex mass transport processes. The purpose of this paper is to present an analytical method to predict contaminant dispersal in buildings that can comprehensively and systematically account for

these complex mass transport processes.

While it is generally recognized that practical methods of contaminant dispersal analysis may be based upon either the microscopic equations of motion[1] [Davidson 87] or the well-mixed zone simplification of the macroscopic mass balance equations for flow systems[2], the application of these techniques has been largely limited to dispersal driven solely by flow mass transport processes and the possibility of combining macro and microscopic approaches has received little consideration. An element assembly formulation of the contaminant dispersal problem provides a means to not only combine the microscopic and macroscopic techniques but offers a convenient framework for the inclusion of models of the various nonflow mass transport processes that may affect the dispersal of contaminants in a building.

In this paper we shall present an element assembly formulation of the contaminant dispersal problem that generalizes the work done earlier [Axley 87, 88]. An emphasis will be placed on modeling building airflow systems, but the theory and methods developed may be applied to other flow systems as well.

The Contaminant Dispersal Model

We begin by asserting that:

> Building airflow systems may be idealized as *assemblages* of discrete *mass transport elements* that model specific instances of contaminant mass transport within the building by relating the time variation of contaminant concentration at discrete points in the building system, the *system nodes*, to the flow and nonflow processes responsible for the dispersal.

This contaminant dispersal model involves, then;

a) a spatial discretization of the domain of the airflow system (i.e., the selection and identification of the system nodes) and,

b) the discrete idealization of the mass transport processes responsible for dispersal within the system (i.e., the selection and specification of the mass transport elements).

We shall show that if element equations governing these instances of mass transport are developed within the restrictions of a certain general form then they may be directly assembled to form equations governing the dispersal of contaminants in the system as a whole. Before considering the formal development of this approach, however, it will be useful to consider the element assembly approach from the point of view of a user of this theory.

A User's View of the Element Assembly Approach

Consider the section of a hypothetical two story residence with basement shown below, Figure 1. For this building, let's say, we are concerned with the dispersal of carbon monoxide generated within the furnace of the simple forced-air heating system that serves this residence.

To model contaminant dispersal in a given building system the analyst must first become familiar with the building's airflow system (i.e., HVAC system, infiltration/exfiltration and room-to-room airflow paths) and identify any nonflow mass transport process that may significantly

[1] *Microscopic equations of motion*: differential formulations of the continuity, motion, and energy equations for fluids, (e.g., the Navier-Stokes equation or the Euler equation)

[2] *Well-mixed zone simplification of the macroscopic equations of motion:* the approach known variously as the "multi-zone", "multi-chamber", "multi-cell", or "compartments" model [Sinden 78, Sandberg 84, Walton 85], that is closely related to similar models used in the chemical engineering field [Wen 75].

affect the dispersal process. With this knowledge in mind, the analyst iteratively selects appropriate contaminant dispersal elements from the *library* of available elements and identifies system nodes to which these elements are "connected" to assemble an *idealization* of the given building airflow system.

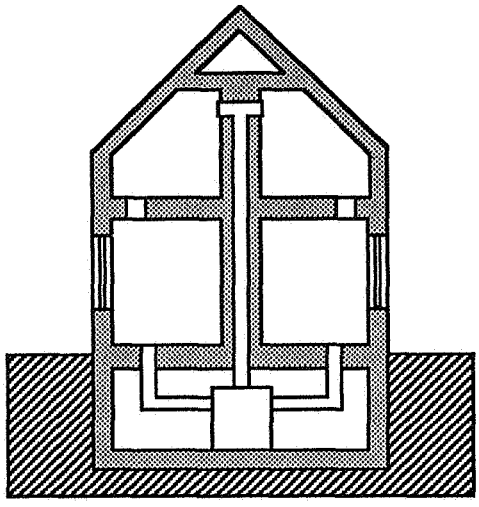

Fig. 1 Hypothetical Two Story Residence

The development of an idealization may often be formulated graphically in a direct and intuitive way. For the hypothetical problem introduced above we may select from the current library of dispersal elements shown in Figure 2.

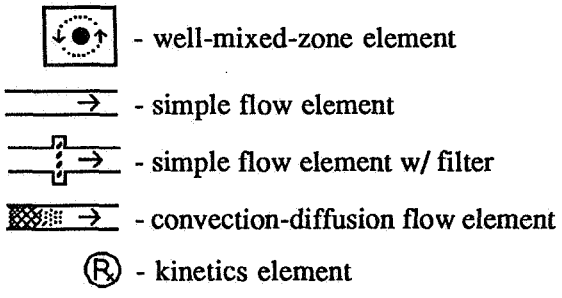

Fig. 2 Current Library of Contaminant Dispersal Elements

Figure 3 shows a possible idealization of this hypothetical building assembled graphically, and hence mathematically, from this library of elements. (The large black dots in this figure correspond to discrete points in the airflow system, the *system nodes*.)

In this example, each of the four rooms, the exterior environment, and the furnace air heating chamber have been modeled with *well-mixed-zone elements;* infiltration, exfiltration, and first-to-second story airflows have been modeled with *simple flow elements;* the HVAC duct flow paths have been modeled with *1D convection-diffusion flow elements* (in an attempt to account for flow delays in this part of the flow system) and the generation of carbon monoxide within the furnace system has been modeled with a *kinetics element*. The kinetics element makes this idealization specific to the analysis of carbon monoxide dispersal in the building system; by removing this kinetics element we would obtain an idealization appropriate for modeling the dispersal of a variety of noninteractive contaminants.

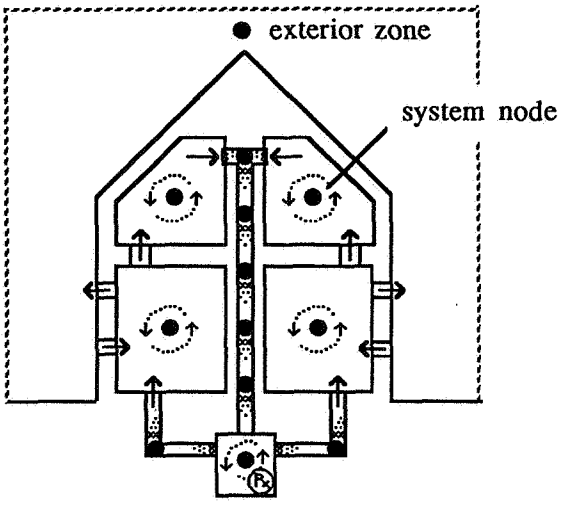

Fig. 3 Idealization of the Building Airflow System

With an idealization in hand the analyst is then in the position to consider any of several solution options, including solutions for steady state concentrations for conditions of steady contaminant generation and steady airflows, evaluation of system time constants for conditions of steady airflows, and evaluation of time histories of contaminant concentrations for various scenarios of steady or unsteady airflows with steady or unsteady contaminant generation rates.

After considering the results of the analysis the analyst may add, delete, or modify elements in an effort, for example, to mitigate an indoor contaminant hazard and then re-analyze the system to evaluate the efficacy of the proposed mitigation measure.

GENERAL FORMULATION

In this section we present a formulation of the contaminant dispersal analysis problem by element assembly that is more general than the formulations presented earlier [Axley 87, 88]. To do so, however, it is useful to repeat parts of the past presentations; the author asks the forbearance of those familiar with these earlier formulations for this repetition.

In indoor air quality analysis we may consider building airflow systems to be three dimensional fields, within which we seek to completely describe the temporal and spatial variation of the *state* of infinitesimal air parcels, providing that the concentration of contaminants within these parcels can be assumed to be uniform[3]. A parcel, here, is small relative to the scale of the components of the system but large relative to the molecular scale and its state is defined by its temperature, pressure, velocity, and contaminant concentration(s) – the *state variables* of indoor air quality analysis.

The central problem of indoor air quality analysis is, then, the determination of the spacial (x,y,z) and temporal (t) variation of contaminant species concentrations (C) within the domain of the airflow system. This analytical problem will be referred to as *contaminant dispersal analysis*.

For a single *noninteractive*[4] species, α, contaminant dispersal is driven by the air

[3] In some flow systems (e.g., chemical process flow systems) this assumption may not be appropriate; there may be a segregation of components at the micro-scale and, thus, the flow system may not be considered to be a simple continuum.

velocity field (**v**) and thus the contaminant dispersal analysis problem, for this case, may be represented, functionally, as:

$$^{\alpha}C(x,y,z,t) = {}^{\alpha}C(\,\mathbf{v}(x,y,z,t)\,) \quad ; \ldots \tag{1}$$

where the ellipses, ... , are used to indicate the geometry, initial conditions, and boundary conditions required to complete the definition of the analytical problem. To solve the contaminant dispersal problem, then, the flow field must be either specified or determined.

Two approaches to flow determination may be considered. In the first approach a nonlinear *flow analysis* problem and, in general, a coupled *thermal analysis* problem is formulated and solved, given the environmental excitation (e.g., wind, solar, and thermal excitation) acting on the building system. Alternatively, for existing buildings it may be possible to "measure" building airflows using tracer gas techniques. These techniques are based on the formulation and solution of the *inverse contaminant dispersal analysis* problem. In this presentation we will assume that building airflows are known and will not consider these related problems.

When the kinetics of contaminant reaction, settling, sorption, etc. is important, the contaminant dispersal analysis problem becomes a coupled (and, generally, nonlinear) analysis problem as (the rate of change of) each species' concentration will depend upon both species' concentrations and the airflow velocity field:

$$^{\alpha}C(x,y,z,t) = {}^{\alpha}C(\,\mathbf{v}(x,y,z,t),\ {}^{\alpha}C(x,y,z,t),\ {}^{\beta}C(x,y,z,t)\,) \quad ; \ldots \tag{2}$$

For such cases we say the contaminant is an *interactive* contaminant and describe the analytical problem as a problem of *interactive contaminant dispersal analysis.*

Basic Approach

The approach to the solution of these field problems taken here is straightforward, but involves several steps. The continuously defined state variables – the contaminant concentrations, $^{\alpha}C(x,y,z,t)$, $^{\beta}C(x,y,z,t)$, ... – are replaced by a finite set of *discrete system state variables,* $\{\mathbf{C}(t)\}$, that are meant to approximate the value of the continuous variables at discrete points – the *system nodes* – in the airflow system. Equations of a restricted, but very general form, are then defined that may be used to describe the specific mass transport processes that drive the dispersal of contaminants in the flow system. These *element equations* are defined in terms of subsets of the discrete state variables – the *discrete element state variables* $\{\mathbf{C}^{e}\}$. These element equations may be assembled to form systems of spatially discrete but temporally continuous ordinary differential equations that govern the contaminant dispersal behavior of the system as a whole.

This approach allows consideration of element models based upon both the microscopic equations of motion (e.g., using Finite Element solutions to subdomains of the flow system domain) and macroscopic mass balance equations for flow systems (i.e., the basis of the familiar well-mixed zone models) and has been contrived to be completely analogous to the approaches employed for the solution of the related flow and thermal analysis problems [Axley 86, 87].

Discrete System State Variables

We associate contaminant concentration variables with each of the system nodes and organize these discrete state variables into the *system concentration vector* which for n nodes

[4] *Noninteractive Contaminant*: a contaminant whose dispersal is not affected by kinetics of reaction, sorption, settling, or other similar or related mass transport phenomena.

is defined as:

- for the dispersal of a single species, α:

$$\{C\} \equiv \{ {}^{\alpha}C_1, {}^{\alpha}C_2, \ldots {}^{\alpha}C_n \}^T \tag{3a}$$

- for the dispersal of two species, α and β:

$$\{C\} \equiv \{ {}^{\alpha}C_1, {}^{\beta}C_1, {}^{\alpha}C_2, {}^{\beta}C_2, \ldots {}^{\alpha}C_n, {}^{\beta}C_n \}^T \tag{3b}$$

- etc.

Discrete Element State Variables

We model the mass transport processes that determine the nature of contaminant dispersal within the flow system with an *assembly* of mass transport elements. With each element "e" in the assembly we associate one or more nodes – the *element nodes* – and with each node we associate variables that define the state of the element – the *element (state) variables,* (i.e., subsets of the system variables[5]) and note their association with the system variables. Thus, for example, a contaminant dispersal element having three nodes, i, j, and k, would have the element state variables;

- for the dispersal of a single species, α:

$$\{C^e\} \equiv \{ {}^{\alpha}C_i^e, {}^{\alpha}C_j^e, {}^{\alpha}C_k^e \}^T \tag{4a}$$

- for the dispersal of two species, α and β:

$$\{C^e\} \equiv \{ {}^{\alpha}C_i^e, {}^{\beta}C_i^e, {}^{\alpha}C_j^e, {}^{\beta}C_j^e, {}^{\alpha}C_k^e, {}^{\beta}C_k^e \}^T \tag{4b}$$

- etc.

These variables will be identified as the *element concentration vectors.*

General Form of the Element Equations

We attempt to describe the *behavior* of appropriate classes of elements by equations of the general form:

$$\boxed{\{w^e\} = L^e(\{C^e\}) - \{g^e\}} \tag{5}$$

where;

$\{w^e\}$ is a vector of element contaminant mass transport rates into the element from each of the element nodes. For a three-node element with nodes, i, j, and k the elements of this vector are defined as;

- for the dispersal of a single species, α:

$$\{w^e\} \equiv \{ {}^{\alpha}w_i^e, {}^{\alpha}w_j^e, {}^{\alpha}w_k^e \}^T \tag{6a}$$

- for the dispersal of two species, α and β:

$$\{w^e\} \equiv \{ {}^{\alpha}w_i^e, {}^{\beta}w_i^e, {}^{\alpha}w_j^e, {}^{\beta}w_j^e, {}^{\alpha}w_k^e, {}^{\beta}w_k^e \}^T \tag{6b}$$

[5] As subsets of the system variables, one must distinguish, mathematically, these element variables from the system variables even though, most often, there will be no physical distinction between them.

• etc.

$L^e(\{C^e\})$ is a transformation of $\{C^e\}$ that has the form of a linear transformation and is specific to a given class of elements

$\{g^e\}$ is a vector of element-derived species generation rates.

The vector of species mass transport rates, $\{w^e\}$, for the dispersal of a single species α, may be represented diagrammatically as shown below for a hypothetical three-node flow element that links three well-mixed zone elements, Figure 4, and a single-node kinetics element associated with a single well-mixed zone element, Figure 5. The arrows indicate positive mass transport rates.

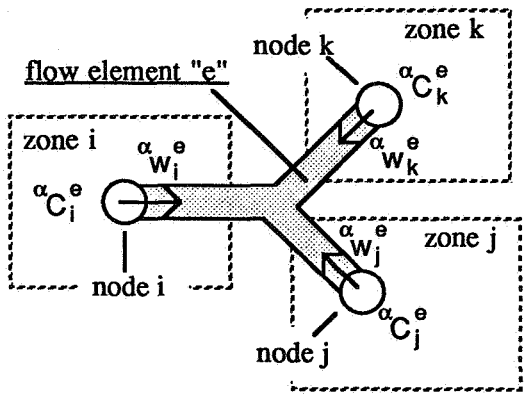

Fig. 4 Hypothetical Three-Node Flow Element

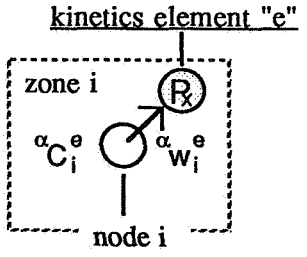

Fig. 5 Single-Node Kinetics Element

For the flow element, mass is transported physically by the airflow moving from each zone into the element; the arrows represent the positive sense of this physical transport. For kinetics elements, mass transport is somewhat more subtle as it involves a conversion of species mass from one form to another. The arrow indicating mass transport in Figure 5 is, thus, directed into the element from the zone node to indicate removal of species α by conversion, rather than physical transport.

It is important to note that it will be necessary to define the element mass transport rate vector so that there will be an element mass transport rate variable corresponding to each of the element concentration variables to account for all possibilities of mass transport.

For contaminant dispersal involving multiple species, then, a single *simple* flow element might be thought to transport each individual species from zone-to-zone while a kinetics element might be thought to transport mass, by conversion from each of the species to any or all of the other species and/or from any of the species to a noncontaminant form that is of no special interest, within the single zone associated with the kinetics element. (Inasmuch as it is difficult to represent these possible multi-species mass transport/conversion phenomena diagrammatically we shall not attempt to do so, here.)

The element transformation operator $L^e()$ is restricted to the form of a linear transformation:

$$L^e(\{C^e\}) \equiv [x^e]\{C^e\} + [y^e]\frac{d\{C^e\}}{dt} + [z^e]\frac{d^2\{C^e\}}{dt^2} + \ldots \qquad (7)$$

where;

$[x^e]$, $[y^e]$, $[z^e]$ are square transformation coefficient matrices
$[x^e]$ is the *element (mass) transport matrix*
$[y^e]$ is the *element mass matrix*

However, we admit transformation coefficient-matrices that may, in fact, vary with time and/or depend, nonlinearly, on the element concentration vector. As a practically endless variety of element equations may be formulated that have this form, the restriction to this form should not lead to any serious limitation.

System Equations

By restricting the element equations to the form of linear transformations (i.e., equations (5) and (7)) these equations may be directly *assembled* to yield the *system equations* that describe the dispersal of the contaminant species within the whole building's airflow system:

$$[W]\{C\} + [M]\frac{d\{C\}}{dt} + [Z]\frac{d^2\{C\}}{dt^2} + \ldots = \{G\} \qquad (8a)$$

where;

$$[W] = \mathop{\mathbf{A}}_{e=a,b,\ldots} [x^e]$$ the *system (mass) transport matrix* (8b)

$$[M] = \mathop{\mathbf{A}}_{e=a,b,\ldots} [y^e]$$ the *system mass matrix* (8c)

$$[Z] = \mathop{\mathbf{A}}_{e=a,b,\ldots} [z^e] \qquad (8d)$$

etc.

$$\{G\} = \{G\} + \mathop{\mathbf{A}}_{e=a,b,\ldots} \{g^e\}$$ the *system generation vector* (8e)

where $\mathbf{A}$ is the assembly operator, a generalization of the conventional summation operator, Σ. The assembly procedure is based upon the requirement that contaminant species mass must be conserved at each of the systems nodes. It may be represented formally by transformation and summation of element arrays but is practically implemented using relatively simple computational algorithms that accumulate element arrays terms in memory locations of the corresponding system array terms [Axley 87, 88].

SPECIFIC ELEMENT EQUATIONS

The element equations corresponding to the current library of contaminant dispersal elements are presented here and the basis of their development is briefly reviewed. Details relating to the development of these element equations and their use have been presented elsewhere [Axley 87, 88].

Well-Mixed Zone Element

It is often reasonable to model portions of a building airflow system as-if they are perfectly mixed zones. By definition, the concentration of contaminants is uniform within a perfectly mixed zone, thus a single variable for each contaminant species (associated with a single node

located arbitrarily within the zone) is sufficient to describe the spacial variation of contaminant concentration within a well-mixed zone. The rate of change of species mass within a well-mixed zone, or, from an element perspective, the species mass transport into the well-mixed zone "element" from the system node associated with the zone, is defined by the following element equation:

$$\{{}^{\alpha}w_i^e\} = [m^e]\left\{\frac{d{}^{\alpha}C_i^e}{dt}\right\} \qquad \textit{well-mixed zone element} \qquad (9a)$$

or, in terms of the general element transformation arrays defined above:

$$[y^e] = [m^e] \qquad \text{for:} \quad \{w^e\} \equiv \{\, {}^{\alpha}w_i^e\} \qquad (9b)$$

for species α in a well-mixed zone having a volume containing a mass of air of m^e.

Simple Flow Element

Flow through many flow passages in building airflow systems is practically instantaneous (i.e., relative to the dominant time constants of the building's dispersal system) and, therefore, may be modeled as such. The mass transport of a single species, say α, through a simple flow passage with a single inlet and outlet in which flow is assumed to be instantaneous may be described using a two-node *simple flow element.* Given the air mass flow rate $w^e(t)$ from node i to node j we may write the following element equations directly from fundamental considerations:

$$\begin{Bmatrix} {}^{\alpha}w_i^e \\ {}^{\alpha}w_j^e \end{Bmatrix} = w^e(t)\begin{bmatrix} 1 & 0 \\ -1 & 0 \end{bmatrix}\begin{Bmatrix} {}^{\alpha}C_i^e \\ {}^{\alpha}C_j^e \end{Bmatrix} \;;\; w^e(t) \geq 0 \qquad \textit{simple flow element} \qquad (10a)$$

or, in terms of the general element transformation arrays defined above:

$$[x^e] = w^e(t)\begin{bmatrix} 1 & 0 \\ -1 & 0 \end{bmatrix} \qquad \text{for:} \quad \{w^e\} \equiv \{\, {}^{\alpha}w_i^e,\ {}^{\alpha}w_j^e\}^T \qquad (10b)$$

It should be noted that the transformation matrix $[x^e]$ is seen to vary with time to account for the time variation of flow through the element. (Figure 6, below, should help to clarify the meaning of the element variables in this case.)

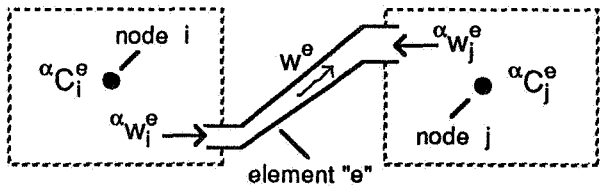

Fig. 6 Simple Contaminant Dispersal Flow Element Variables

The well-mixed, multi-zone theory presented by Sinden [78] and Sandberg [84] is completely equivalent to an element assembly approach limited to the use of well-mixed zone

and simple flow elements. Through the development of additional elements, then, we may extend the conventional multi-zone theory. We also, importantly, provide an alternative formal view of this theory that provides a deeper understanding of the qualitative character of the theory and, therefore, of contaminant dispersal in buildings in general.

Simple Flow Element with Filtration

The simple flow element equations, above, may be modified to account for the action of a filter that removes a fraction, ${}^{\alpha}\eta$, of the contaminant α as it passes through the element to yield the following element equations;

$$\begin{Bmatrix} {}^{\alpha}w_i^e \\ {}^{\alpha}w_j^e \end{Bmatrix} = w^e(t) \begin{bmatrix} 1 & 0 \\ ({}^{\alpha}\eta - 1) & 0 \end{bmatrix} \begin{Bmatrix} {}^{\alpha}C_i^e \\ {}^{\alpha}C_j^e \end{Bmatrix}$$

simple flow element w/ filtration (11a)

or, in terms of general element transformation arrays defined above:

$$[x^e] = w^e(t) \begin{bmatrix} 1 & 0 \\ ({}^{\alpha}\eta - 1) & 0 \end{bmatrix} \quad \text{for:} \quad \{w^e\} \equiv \{ {}^{\alpha}w_i^e, {}^{\alpha}w_j^e \}^T \tag{11b}$$

In this case the time variation of the transformation matrix, $[x^e]$, could be due to both the time variation of flow through the element and the time variation of the filter efficiency, ${}^{\alpha}\eta = {}^{\alpha}\eta(t)$.

1D Convection-Diffusion Flow Element

In some situations the analyst may be interested in the details of dispersal in some flow passages or may feel the noninstantaneous nature of the flow should not be ignored. If flow in these flow passages may be assumed to be practically one-dimensional (e.g., flow in portions of HVAC ducts) then the details of the convection and diffusion mass transport processes that drive the dispersal may be accounted for using assemblages of two-node *convection-diffusion elements*.

These elements may be developed using a Finite Element solution of the one-dimensional convection diffusion equation:

$$\frac{1}{Pe} \frac{\partial^2 {}^{\alpha}C}{\partial \chi^2} + {}^{\alpha}\gamma = \frac{\partial {}^{\alpha}C}{\partial \tau} + \frac{\partial {}^{\alpha}C}{\partial \chi} \tag{12a}$$

where;

$$Pe \equiv \frac{w^e L}{\rho A {}^{\alpha}D} = \frac{\bar{u} L}{{}^{\alpha}D} \quad \text{the dimensionless } \textit{Peclet Number} \tag{12b}$$

A is the cross-sectional area of the flow passage

${}^{\alpha}D$ is the dispersal coefficient for species α

L is the length of the flow passage

χ is the dimensionless length $\equiv x/L$

τ is the dimensionless time $\equiv t/\bar{t}$

${}^{\alpha}\gamma$ is the dimensionless generation rate $\equiv {}^{\alpha}gL/w^e$

${}^{\alpha}g$ is the mass generation rate of species α per unit length of flow passage

$\bar{t}$ is the nominal transit time $\equiv L/\bar{u}$

$\bar{u}$ is the bulk fluid velocity $= w^e/\rho A$

The Peclet number provides a measure of the importance of convection mass transport relative to diffusion mass transport; at one extreme Pe = 0 would correspond to a well-mixed condition and at the other Pe = ∞ would correspond to an ideal plug-flow condition.

Following the one-dimensional example discussed by Huebner and Thornton [82] element equations for a two-node flow element may be developed from equation (12) using linear shape functions (i.e., assuming species concentrations vary in a piece-wise linear manner along the flow passage) and applying either the (conventional) Galerkin method or the (upwind) Petrov-Galerkin method in the formulation of these element equations. The resulting element equations are:

$$\boxed{\{w^e\} = [[{}_c x^e] + [{}_d x^e]]\{C^e\} + [y^e]\frac{d\{C^e\}}{dt} - \{g^e\}} \quad \textit{convection-diffusion element} \qquad (13a)$$

where;

$$[{}_c x^e] = \frac{w^e}{2}\begin{bmatrix} 1 & 1 \\ -1 & -1 \end{bmatrix} + \frac{\phi\, w^e}{2}\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \qquad (13b)$$

= the *convection component* of the element mass transport matrix

ϕ = the so-called *upwind parameter*; $0 \le \phi \le 1$

$$[{}_d x^e] = \frac{\rho A\, {}^{\alpha}D}{L^e}\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \qquad (13c)$$

= the *diffusion component* of the element mass transport matrix

L^e = the length of the element (i.e., a portion of the length of the flow path)

$$[y^e] = \frac{\rho A L^e}{6}\begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix} + \frac{\phi\, \rho A L^e}{4}\begin{bmatrix} -1 & -1 \\ 1 & 1 \end{bmatrix} \qquad (13d)$$

= the *element volume mass matrix*

or

$$[y^e] \approx \frac{\rho A L^e}{2}\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \qquad (13e)$$

= the *lumped approximation* to the element volume mass matrix

$$[g^e] = \frac{{}^{\alpha}g\, L^e}{2}\begin{Bmatrix} 1 \\ 1 \end{Bmatrix} + \frac{\phi\, {}^{\alpha}g\, L^e}{2}\begin{Bmatrix} -1 \\ 1 \end{Bmatrix} \qquad (13f)$$

= the *internal generation rate vector*

for species α and fluid mass flow rate, $w^e \ge 0$, through the flow passage from node i to node j.

The use and numerical characteristics of the convection-diffusion element, the inclusion of species generation kinetics, and a comparison to the closely related *tanks-in-series* model commonly used in the chemical engineering field has been presented elsewhere [Axley 88]. Suffice it to say that this element is not for the uninitiated. Numerical solutions to the convection-diffusion equations remains a very active and controversial area of research. The inexperienced analyst is well-advised to become familiar with current literature relating to Finite Element solutions of the convection-diffusion equations before attempting to use this

element.

Two aspects of the convection-diffusion element are especially important. First, the convection-diffusion element is based upon a microscopic description of dispersal and it use provides a first example of combining macroscopic modeling techniques with microscopic techniques in a single analytical method. Secondly, from another perspective a one-dimensional flow regime may be thought to represent an imperfectly mixed zone, therefore, the convection-diffusion flow element may be considered to be an *imperfectly-mixed zone element.* The use of this element in modeling imperfectly mixed zones has yet to be explored, but it is believed it holds much promise.

Kinetics Elements

In some situations the analyst may wish to model mass transport due to chemical reaction, radiochemical decay, adsorption, absorption, settling, deposition, agglomeration, or precipitation of contaminants. The mass transport characteristics of such processes is described by the so-called *kinetics* of the process, a term borrowed from the literature of *reaction kinetics*[6].

In the present context we consider a kinetic process to involve the contaminant species α, β, ... that interact and/or are transformed in some way to form product species or phases ρ, σ, ..., as:

$$\alpha + \beta + \ldots \xrightarrow{\text{catalyst}} \rho + \sigma + \ldots \tag{14}$$

where we explicitly consider the possible affect of catalysts on the process. The product species or phases may or may not be considered to be contaminants.

In general, the rate of a given kinetic process may depend upon a variety of factors including reactant, product, and catalyst concentrations, temperature, T, pressure, P, and the detailed mechanisms of the kinetic process (i.e., the mechanisms of both chemical and physical processes that, together, govern the kinetics process) therefore, rate expressions take the general functional form of:

$$^{\alpha}R = {}^{\alpha}R(\,{}^{\alpha}C,\,{}^{\beta}C,\ldots\,{}^{\rho}C,\,{}^{\sigma}C,\ldots T,P,\ldots) \tag{15}$$

where, the rate of kinetics process may be defined in terms of the rate of change of one of the species involved in the process as:

$$^{\alpha}R \equiv \frac{d\,{}^{\alpha}C}{dt} \quad ; \textit{rate of kinetics process} \text{ in terms of species } \alpha \tag{16}$$

Rate expressions for certain general classes of chemical reactions (and presumably the kinetic processes considered here), including single-reactant, consecutive, opposing, and concurrent first order reactions [Moore 81], may take the form of linear combinations of contaminant concentrations:

$$\{R\} = -[\kappa]\{C\} + \{R_o\} \tag{17a}$$

or

[6] Reaction kinetics involves the study of the rate of change of chemical components in a single or related series of chemical reactions.

$$\begin{Bmatrix} {}^{\alpha}R \\ {}^{\beta}R \\ \vdots \\ {}^{\sigma}R \end{Bmatrix} = -\begin{bmatrix} \alpha\alpha_K & (-\alpha\beta_K) & \cdots & (-\alpha\sigma_K) \\ (-\beta\alpha_K) & \beta\beta_K & \cdots & (-\beta\sigma_K) \\ \vdots & \vdots & \ddots & \vdots \\ (-\sigma\alpha_K) & (-\sigma\beta_K) & \cdots & \sigma\sigma_K \end{bmatrix} \begin{Bmatrix} {}^{\alpha}C \\ {}^{\beta}C \\ \vdots \\ {}^{\sigma}C \end{Bmatrix} + \begin{Bmatrix} {}^{\alpha}R_o \\ {}^{\beta}R_o \\ \vdots \\ {}^{\sigma}R_o \end{Bmatrix} \tag{17b}$$

where we have included the constant component, $\{\mathbf{R}_O\}$, for completeness and recognize that, again, the rate coefficient matrix, $[\kappa]$, and the constant component vector, $\{\mathbf{R}_O\}$, will, in general, vary with temperature and pressure.

The general rate expression, equation (15), leads directly to the development of a *general kinetics element.* Limiting consideration to kinetic processes occurring within a specific well-mixed zone "e" (were it is assumed that conditions are homogeneous), associated with the system node "i" , and containing a set of contaminant species, α, β, γ, ..., we first identify the relevant element variables as:

$$\{\mathbf{C}^e\} = \{ {}^{\alpha}C_i^e, {}^{\beta}C_i^e, {}^{\gamma}C_i^e, \ldots \}^T \tag{18}$$

and

$$\{\mathbf{w}^e\} = \{ {}^{\alpha}w_i^e, {}^{\beta}w_i^e, {}^{\gamma}w_i^e, \ldots \}^T \tag{19}$$

Then from the rate definition, equation (16), and the general form of rate expressions, equation (15), we obtain the general kinetics element equations:

$$\{\mathbf{w}^e\} = -[\mathbf{M}^e]\{\mathbf{R}^e(\{\mathbf{C}^e\}, T, P)\} \tag{20a}$$

where;

$$[\mathbf{M}^e] \equiv \text{diag}\{ m^e \quad m^e \quad m^e \quad \cdots \} \tag{20b}$$

m^e = the mass of the air in the volume of the well-mixed zone "e" associated with the kinetic processes being modeled

$$\{\mathbf{R}^e(\{\mathbf{C}^e\}, T, P)\} \equiv \begin{Bmatrix} {}^{\alpha}R\,({}^{\alpha}C_i^e, {}^{\beta}C_i^e, {}^{\gamma}C_i^e, \ldots T, P) \\ {}^{\beta}R\,({}^{\alpha}C_i^e, {}^{\beta}C_i^e, {}^{\gamma}C_i^e, \ldots T, P) \\ {}^{\gamma}R\,({}^{\alpha}C_i^e, {}^{\beta}C_i^e, {}^{\gamma}C_i^e, \ldots T, P) \\ \cdots \end{Bmatrix} \tag{20c}$$

or in this case we obtain:

$$[\mathbf{x}^e] = 0 \; ; \; [\mathbf{y}^e] = 0 \; ; \; \{\mathbf{g}^e\} = [\mathbf{M}^e]\{\mathbf{R}^e(\{\mathbf{C}^e\}, T, P)\} \tag{20d}$$

an element that is defined in terms of only element-derived species generation rates.

The form of equation (20) is deceptively simple. The rate expressions defining these element-derived species generation rates depend on species concentration, in general, so that the general kinetics element introduces a nonlinear species generation contribution (i.e., a species generation rate that depends nonlinearly on the solution vector $\{\mathbf{C}\}$), which is distinctly different from the (constant or time dependent) nodal direct generation contribution. The solution of the contaminant dispersal problem involving general kinetics elements will,

therefore, generally require the application of a nonlinear solution strategy in the solution process.

Few interactive indoor contaminants have been studied in sufficient detail to completely define their kinetics, therefore, the consideration of arbitrarily nonlinear kinetics is premature at this time. For the present it is not unreasonable to attempt to approximate many kinetic processes using first order rate expressions of the form of equation (17), which when substituted into equation (20) lead to the *first order kinetics element equations*:

$$\boxed{\{w^e\} = [M^e][\kappa^e]\{C^e\} - [M^e]\{R_0^e\}}$$

first order kinetics element (21a)

or:

$$[x^e] = [M^e][\kappa^e] \; ; \; [y^e] = 0 \; ; \; \{g^e\} = [M^e]\{R_0^e\} \tag{21b}$$

where, again, one must keep in mind that the rate coefficient matrix and constant rate component will, in general, be temperature and pressure dependent.

SOLUTION OF SYSTEM EQUATIONS

System equations based upon assemblages of the specific element equations presented above will have the following form:

$$[W]\{C\} + [M]\frac{d\{C\}}{dt} = \{G\} \tag{22}$$

To complete the definition of a contaminant dispersal problem it will be necessary to modify this equation to take into account appropriate boundary conditions and, in some instances to account for system nodes having no mass associated with them. With these modifications made the analyst will, typically, consider one of three types of analyses; eigenanalysis, steady state analysis, or general dynamic analysis. These fundamental solution operations are illustrated below in Figure 7. In this section we will briefly review these operations, more complete details may be found elsewhere [Axley 87, 88].

Boundary Conditions

The analyst may wish to specify concentration at some system nodes (e.g., ambient outdoor concentrations or controlled indoor environments) and as a result a subset of the system concentration vector $\{C\}$ will be known. At all other nodes contaminant generation rates may be specified and as a result a complementary subset of the system generation vector will be known. If one makes the algebraic simplifications to equation (22) to account for these specified *boundary conditions*, which, in general, will be time varying specifications, then a reduced system of equations will result involving a subset of the system concentration vector, $[\hat{C}]$, and corresponding submatrices of the system mass and mass transport matrices, $[\hat{M}]$ and $[\hat{W}]$. This reduced system of equations will have a right hand side, the *excitation vector*, $\{\hat{E}\}$, that will include terms relating to both specified generation rates and specified concentrations.

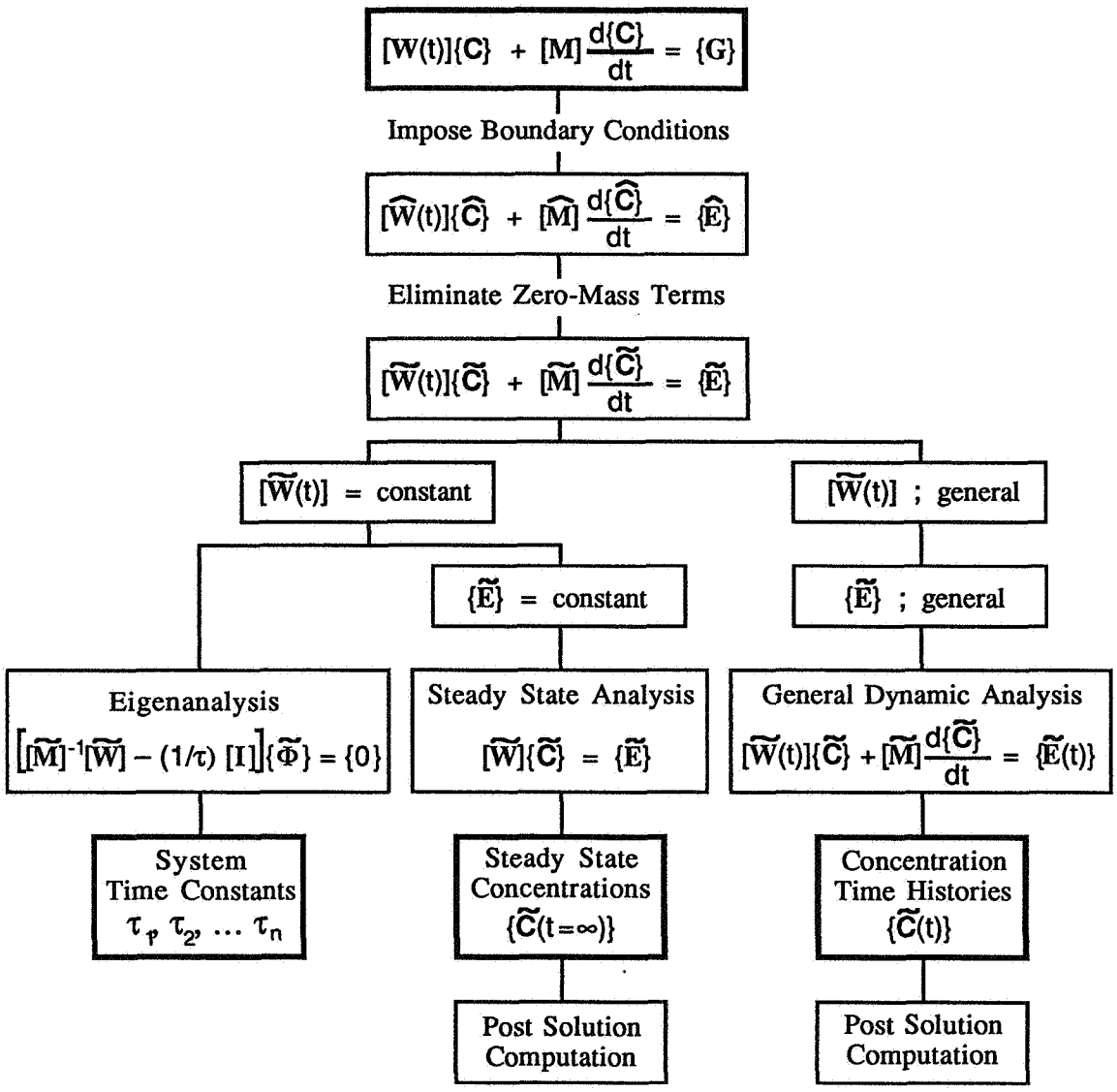

Fig. 7 Solution of System Equations

Zero-Mass Terms

In some instances the analyst may consider the mass contribution to a system node to be negligibly small (e.g., nodes in subassemblies corresponding to HVAC ductwork) and prefer to model these contributions with zero values. Zero mass terms may be accounted for algebraically resulting in a further reduction in the size of the system equations (i.e., the equation in Figure 7 with the tilde, ~, marks). This reduced set of equations will have as its unknowns the subset of the system concentration vector corresponding to those nodes having non-zero mass contributions for which contaminant generation rate time histories are specified.

Solution Options

The system equations obtained after the imposition of one or more concentration-specified boundary conditions and the elimination of zero-mass terms (i.e., the "tilde" equations in Figure 7) may then be used to solve either the eigenanalysis, steady state analysis, or general dynamic analysis problems. It may be shown that these equations will be soluble (i.e., have nonsingular system matrices) when airflow in the system idealization satisfies conservation of

total air mass flow and kinetics rate matrices are restricted to certain forms [Axley 88]. Furthermore, it may be shown that in these cases very efficient, yet numerically stable, solution methods based on LU decomposition without pivoting may be applied to the solution of these problems.

Eigenanalysis: For system idealizations involving steady flow and steady kinetics the analyst may determine the so-called system time constants using standard methods of eigenanalysis.

Steady State Analysis: For problems involving steady flow, steady kinetics, and steady excitation the system eventually will reach a condition of steady concentrations in all zones – the steady state condition. These steady state concentrations, $\{\widetilde{C}(t=\infty)\}$, may be directly determined by solving the corresponding algebraic problem. Using these steady state concentrations the analyst may also determine the steady state concentrations at those system nodes associated with zero-mass terms that were "eliminated" from consideration and determine the steady state generation rates required to maintain the concentrations specified at the remaining system nodes.

General Dynamic Analysis: For problems involving steady or unsteady flow, kinetics, and/or system excitation the analyst may solve the complete dynamic problem using a variety of direct numerical integration schemes to compute concentration time histories, $\{\widetilde{C}(t)\}$. Using these results the analyst may also determine the concentration time histories at those system nodes associated with zero-mass terms that were "eliminated" from consideration and determine the generation rates required to maintain the concentrations specified at the remaining system nodes.

IMPLEMENTATION & APPLICATION

A program, CONTAM87, has been developed at the National Bureau of Standards to provide an example of one computational implementation of the contaminant dispersal analysis theory presented above. CONTAM87 is the second member of the CONTAM series of programs [Axley 87, 88] that are being developed to provide an integrated set of computational tools for indoor air quality analysis. These tools are presented as a collection of *commands* that complete a variety of basic indoor air quality analysis operations. For example, the command FLOWELEM and its associated data defines flow element characteristics and location in a given element assembly, the command STEADY and its associated data defines and completes a steady state contaminant dispersal analysis problem, TIMECONS and its associated data defines the (steady flow/kinetics) eigenvalue problem and solves it reporting system time constants, etc. Future members of the CONTAM family will provide additional macroscopic flow analysis and inverse contaminant dispersal analysis commands, that may be used to determine airflows in building systems, and, eventually, building thermal analysis commands, based upon earlier work [Axley 86] could be added to provide a complete indoor air quality command processor language.

The programs CONTAM86 and CONTAM87 have been applied to a variety of contaminant dispersal analysis problems and have been employed to simulate new tracer gas methods for determining airflows in building systems. Here we shall present the results of three of these studies to provide some indication of the complexity of problems that may be considered.

NBS Office Building Study

Infiltration studies of a fifteen story office building are presently being conducted by members of the Indoor Air Quality and Ventilation Group at NBS. Some of these studies involve hourly injections of a commonly used tracer gas, SF_6, into the fresh air supply ports of the building HVAC system. Flows in the supply ducts were measured (with significant uncertainty) by pitot traverse, SF_6 concentration time histories were recorded, and fresh air infiltration was estimated by tracer decay. Using the airflow measurements the upper two floors of this building were idealized as shown in Figure 8.

As indicated by this idealization, fresh air was supplied to each floor through a ceiling plenum space and exhausted via an exhaust duct to the outside. In Figure 9 we compare measured SF_6 concentration time histories (measured centrally within the "space" and at the "exhaust" ports) to computed values of the 15th floor for two supply flow rates: 100% and 75% of the measured flow. In this case, the agreement between measured and computed time histories is within the uncertainty of the measured flows and validation is therefore indicated.

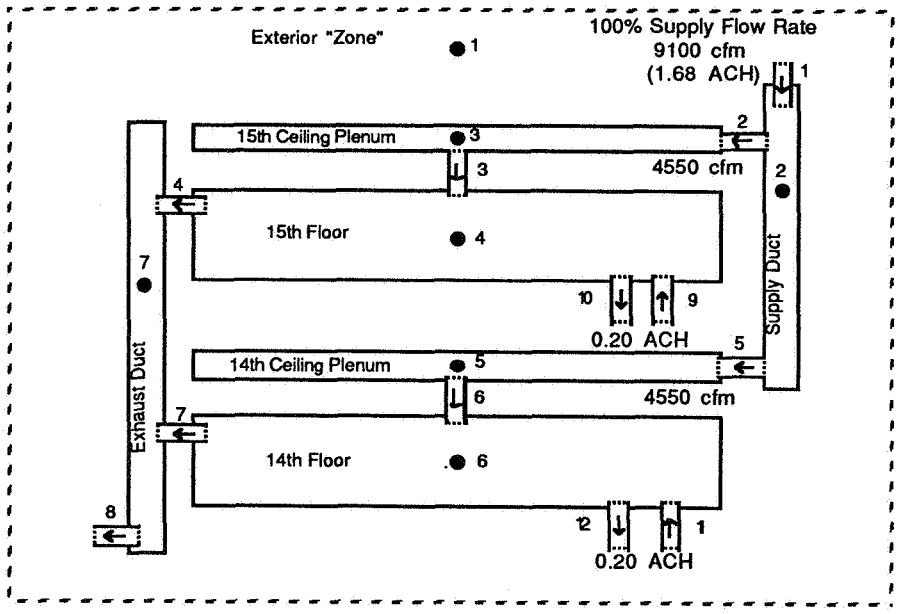

Fig. 8 Idealization of the 14th and 15th Floors of an Office Building

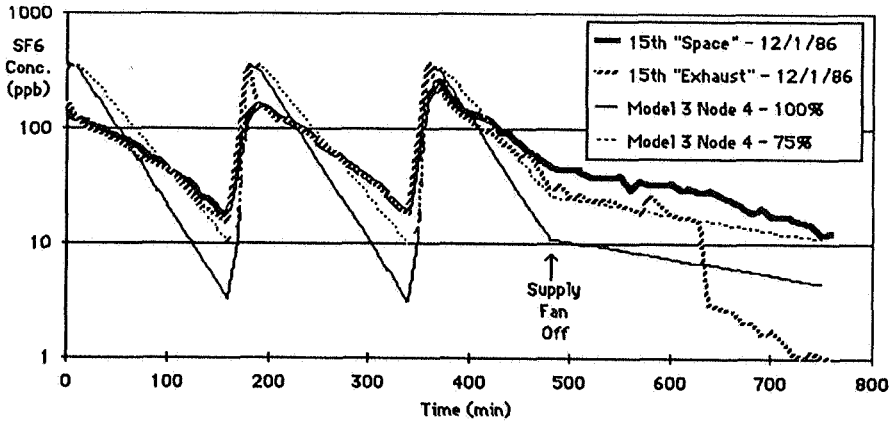

Fig. 9 Comparison of Computed and Measured Response for an Office Building

Carnegie-Mellon Townhouse Study

Borrazzo and his colleagues at Carnegie-Mellon University have conducted detailed field investigations of a two-story townhouse measuring CO, NO, and NO_2 emissions characteristics of the gas appliances within the townhouse and the dispersal of these contaminants throughout the townhouse under a variety of different weather conditions [Borrazzo 87.]. Illustrated in Figure 10 is an idealization of the townhouse and in Figure 11 the dynamic emission characteristics of the principal pollutant source; the gas range. The instantaneous emission rate, G(t), is plotted relative to the steady state value, G_{ss}. The NO_2 emission characteristics were more or less constant and are, therefore, not illustrated. NO_2 is a reactive contaminant and was modeled as so using the measured reactivity of κ=2.4 hr^{-1}.

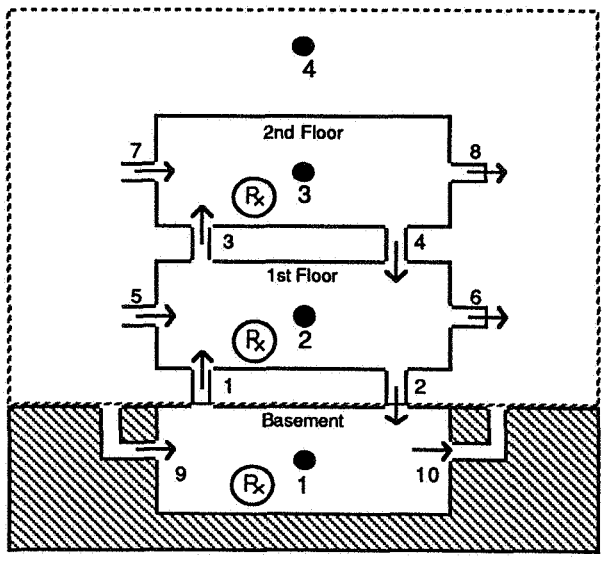

Fig.10 Townhouse Building Idealization

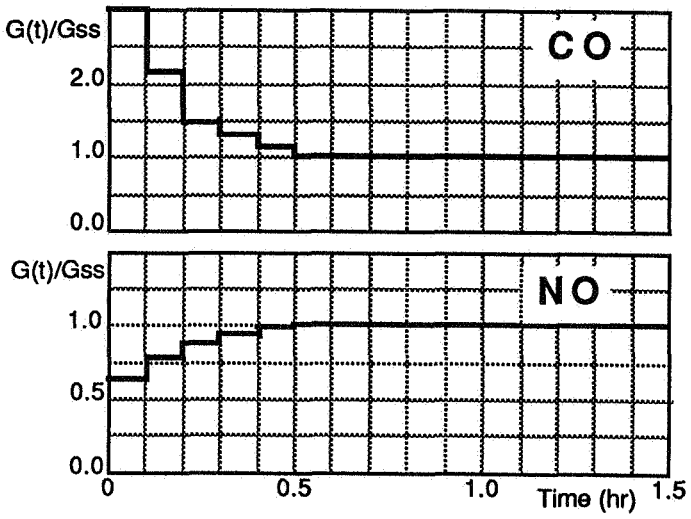

Fig. 11 Range Emission Characteristics

In Figures 11, 12 and 13 we compare computed response with measured data. The details of airflow in this building were unknown in some instances and uncertain in others so several assumptions about flow had to be made to effect the analysis. In particular, it was assumed that the measured whole-building fresh air infiltration rate of 0.21 air changes per hour (ACH) was distributed equally in all three zones, the first-to-second air exchange rate was assumed to be 7.5 ACH, the first-to-basement air exchange rate was assumed to be 0.4 ACH, and all flows were assumed to be constant.

As may be seen, the CO response was under-predicted and the NO response was over-predicted, but both are practically within the reported uncertainty of the emission characteristics (CO: 18% & NO: 6.5%).

Although, the measured NO_2 data is quite suspect, because of scatter and negative values, there appears to be some agreement between this data and the computed response. Inasmuch as this measured data was used to determine the reactivity constant the agreement here may be an artifice. The basis of determination of the reactivity, a single-zone model, and the basis of the computed response are more or less the same as the system behaves, practically, as a single-zone system. Therefore the agreement may reflect no more than this.

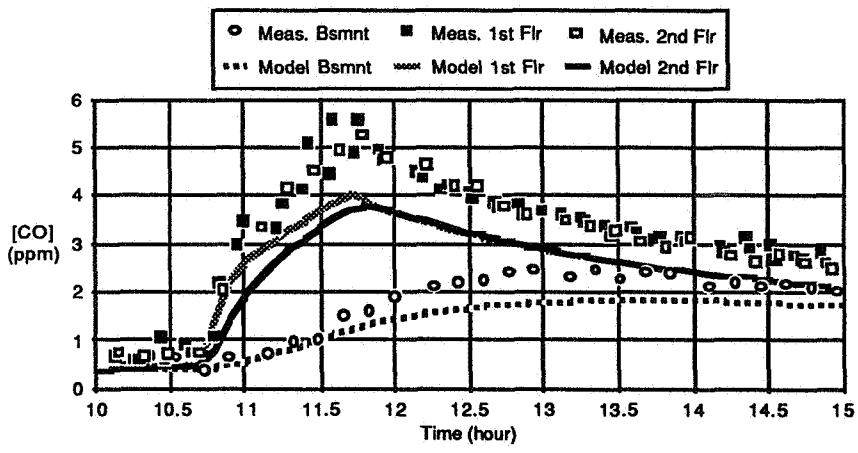

Fig. 11 Comparison of Computed and Measured CO Response

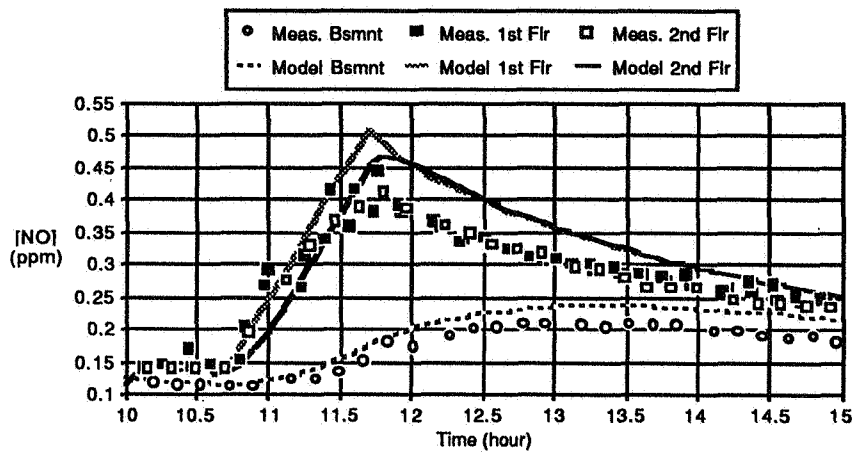

Fig. 12 Comparison of Computed and Measured NO Response

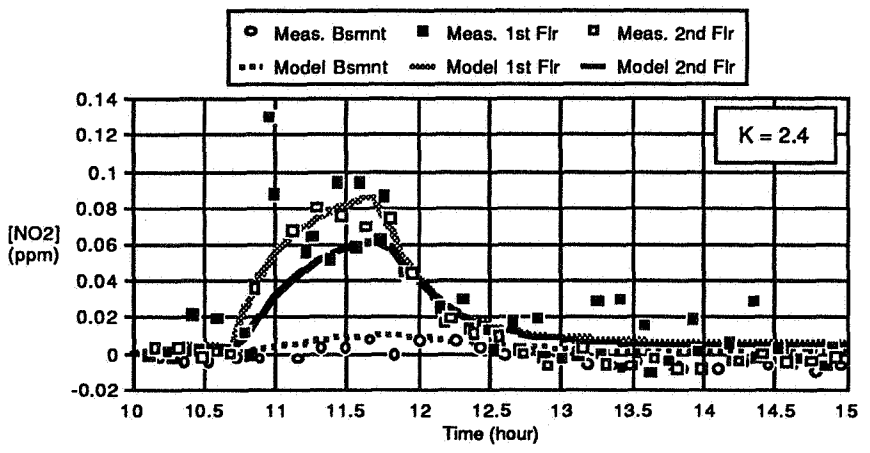

Fig. 13 Comparison of Computed and Measured NO_2 Response
(NO_2 Reactivity = 2.4 hr^{-1})

Convection -Diffusion Study

When employing the convection-diffusion flow element the analyst must take special care to assure an accurate solution has been obtained. In steady state analysis accuracy is affected by element size (i.e., the subdivision of the flow path) and the degree of upwinding chosen. Huebner and Thornton [82] show that instability may be avoided if an upwind parameter is selected satisfying the conditions;

$$\phi \geq 1 - \frac{2}{P_e^e} \; ; \; P_e^e > 2$$

$$\phi = 0 \; ; \; P_e^e \leq 2 \qquad (23)$$

where;

$$P_e^e \equiv \frac{w^e L^e}{\rho A^\alpha D} = \frac{\bar{u} L^e}{^\alpha D} \qquad \text{the } \textit{element Peclet number} \qquad (24)$$

(Note: $P_e^e = (Pe/n)$ for a flow passage idealized by an assembly of n equal-length convection-diffusion elements.) In dynamic analysis, accuracy is also affected by the integration time step selected to complete the dynamic solution and when the lumped mass approximation is employed the analyst may encounter spurious anomalies in the computed solution in some cases [Huebner 82].

Partly because of the challenge of these difficulties and partly because of the importance of the convection-diffusion equation in the area of fluid mechanics, finite element solutions of the convection-diffusion equation have become the focus of considerable research in recent years. Strategies have been put forward to improve the accuracy of the finite element approximation presented above that are, regrettably, beyond the scope of this presentation and the reader is, therefore, advised to review the current and emerging literature. The papers by Hughes and Brooks [82], Tezduyar and Ganjoo [86], and Yu and Heinrich [86] are particularly useful in this regard.

In spite of the numerical pitfalls that await the use of the convection-diffusion flow element

we shall proceed and employ these elements (with the lumped mass approximation) to compute the transport of a contaminant pulse through a length of ductwork. The conditions of this problem are illustrated in Figure 14: fluid flows through a duct of length L and radius R at a mass flow rate w^e; a contaminant is injected into the inlet stream at a rate G(t) for a short time interval introducing a pulse of contaminant of mass I into the inlet stream; the pulse is convected and dispersed as it moves along the duct. We seek to determine the concentration time history of the contaminant as it emerges from the outlet of the duct.

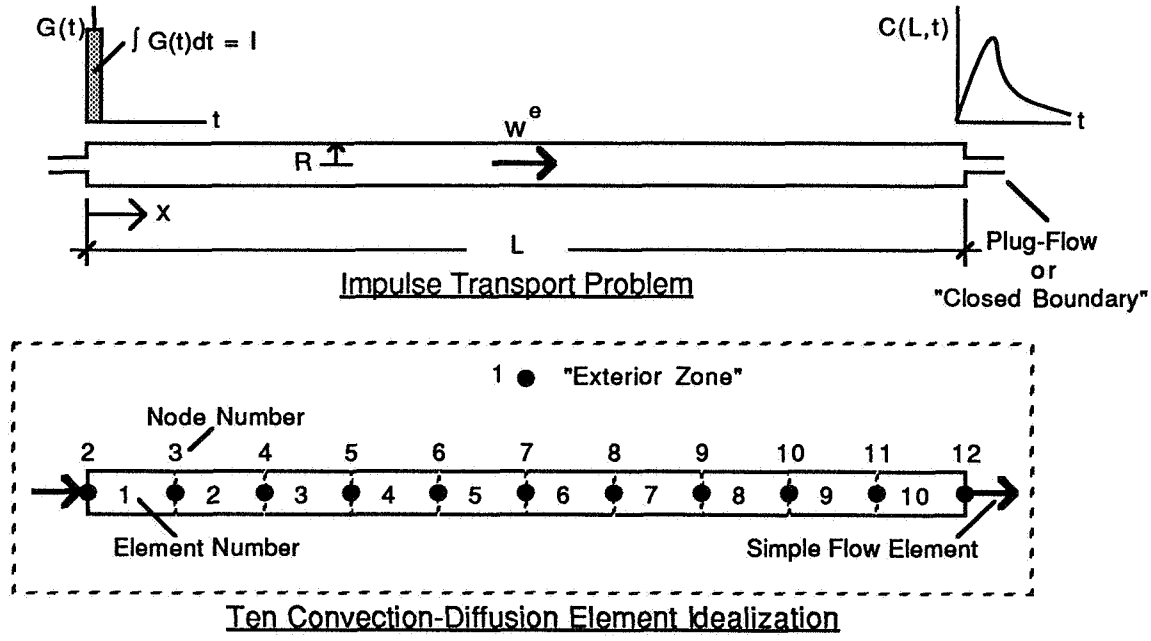

Fig. 14 The Transport of a Pulse in a Duct and the Corresponding Finite Element Idealization

The exact solution to this problem is available for an impulse, for "closed" inlet and outlet conditions, but it is expressed as an infinite sum that is practically difficult to use [Wen 75 pp. 133-137]. For Pe=0 the duct becomes a well-mixed system, the initial concentration throughout the duct becomes, simply, (I/ρAL), and the outlet concentration decays exponentially:

$$\frac{C(L,t)}{(I/\rho AL)} = e^{-t/\bar{t}} \qquad ; Pe = 0 \qquad (25)$$

For relatively large Peclet numbers the outlet concentration is well approximated by the following expression reported by Nauman and Buffham [83 pp. 101-103]:

$$\frac{C(L,t)}{(I/\rho AL)} = \sqrt{\frac{Pe}{4\pi(t/\bar{t})^3}}\, e^{\left(\frac{-Pe(1-t/\bar{t})^2}{4t/\bar{t}}\right)} \qquad ; Pe > 16 \qquad (26)$$

and for very large Peclet numbers the outlet concentration approaches a Gaussian distribution [Wen 75 p. 133]:

$$\frac{C(L,t)}{(I/\rho AL)} = \sqrt{\frac{Pe}{4\pi}}\, e^{\left(\frac{-Pe(1-t/\bar{t})^2}{4}\right)} \quad ; Pe >> 16 \qquad (27)$$

Approximate solutions to this problem were computed using a 10-element subdivision, as shown in Figure 14, and a twenty-element subdivision. The "closed" boundary condition was modeled using the simple flow element as this element models (instantaneous) plug flow conditions as required. The impulse was approximated by a pulse of finite but small duration. In all studies the upwind parameter, ϕ, was chosen to satisfy the lower bound (i.e., equality) of the stability requirement of equation (23). The results are compared below, Figure 15, to the solutions discussed above, equations (25) to (27).

It is seen that in this case the approximate, finite element solution for the low Peclet number, Pe=1, approaches the exact well-mixed solution, as expected. The approximate solution for the higher Peclet numbers has some difficulty in capturing the amplitude of the exit pulse, although, the timing and the form of the pulse appear to be well-approximated. Some part of this error may be attributed to approximating the impulse of the analytic solutions by a pulse of finite duration in the computed solutions.

Some part of the error may be attributed to the coarseness of the finite element subdivision. A comparison of the results of the 10-element and 20-element approximations for Pe=10 indicate that a convergent solution was obtained (i.e., further subdivision would not alter the solution), yet when these results are compared to the exact results reported by Wen and Fan [75 Fig. 5-8 p. 136] the amplitude appears to be underestimated by approximately 10%. This same comparison for Pe=20 indicates that a convergent solution was almost but not quite achieved. An additional subdivision would presumably reveal convergence, and the error in amplitude estimation was approximately 20%. It is interesting to note that the element Peclet numbers for these two (nearly) convergent solutions – the 10-element solution at Pe=10 and the 20-element solution at Pe=20 – are both equal to 1.0, a condition that demands no upwinding to maintain numerical stability.

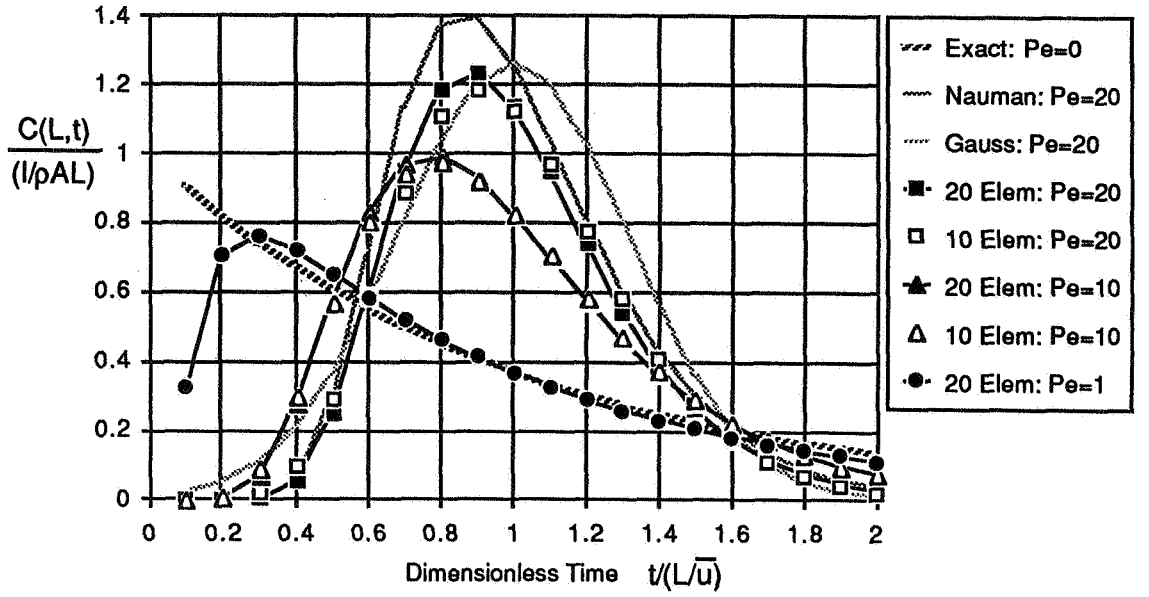

Figure 15 Comparison of Analytic Solutions with Finite Element Solutions for the Pulse Transport Problem

It may be useful to relate these nondimensional studies to more conventional units. The study for Pe=20 corresponds to studying the transport of a pulse through a circular duct of 1 m radius having a length of 10 m with a bulk flow velocity of 2 m/s (the practical minimum operational flow rate in HVAC ducts). For these conditions the dispersal coefficient may be expected to be about 1.0 m^2/s. The results reported in Figure 15 were computed using a pulse duration of 0.005 sec. The dynamic solution was computed using a time step of 0.001 second, in part to capture the short-time pulse accurately and partly to achieve a practically convergent solution.

In practical situations the inaccuracies revealed in these studies are likely to be considered very small and, thus, the convection-diffusion flow element should provide a practically useful analytical tool. Nevertheless, to minimize error the analyst is well advised to seek a convergent solution through both *mesh refinement* (i.e., repeated subdivision of the flow path), starting, perhaps, with a subdivision that results in an element Peclet number of 1.0, and *time step refinement*, starting with a time step sufficiently small to capture the dynamic variation of any excitation with reasonable accuracy, being careful to select an upwind factor so that the stability requirement of equation (23) is always satisfied. When employing convection-diffusion elements in an idealization of a building airflow system it is very likely that extremely small time steps will be required to obtain a convergent solution.

CONCLUSION

From a practical point of view, the element assembly approach is intuitively satisfying and allows consideration of systems of arbitrary complexity. From a theoretical point of view it provides a framework for the consideration of the large variety of mass transport processes that affect the dispersal of contaminants in buildings and offers additional mathematical tools to unravel the formal characteristics of whole-building dispersal models. From a research and development point of view it separates the general problem of indoor air quality analysis into two primary subproblems; element development and development of solution method. Research efforts can, thus, focus on the modeling of specific transport processes, to develop improved or new elements or, alternatively, focus on developing improved methods of solving the resulting equations while accounting for the complex coupling that may exist between the related thermal, dispersal, and flow analysis problems.

The approach has been formulated to be completely analogous and compatible with approaches based upon the Generalized Finite Element Method [Zienkiewcz 83] used to approximate solutions of the microscopic equation of motion for fluids and makes use of the numerical methods and computational strategies that have been developed to support this method and associated methods. It is expected that this compatibility will, eventually, allow the analyst to employ mixed idealizations of building airflow systems wherein a portion of the building airflow system would be modeled in detail using microscopic elements while the rest of the airflow system would be modeled using discrete or lumped parameter elements. In this way the analyst may study the details of dispersal in one area of the system, accounting for whole-system interaction, without the computational overhead of modeling the entire system microscopically. The one-dimensional convection-diffusion element presented in this paper represents the first step in this direction.

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