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Multi-Zone Dispersal Analysis by Element Assembly*

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An element-assembly formulation of multi-zone contaminant dispersal theory that is not limited to the well-mixed zone idealization is described. In this approach flow systems are idealized as assemblages of elements that model specific instances of contaminant mass transport within a system. A general form and specific examples of element equations are presented. The process of assembling these element equations to form system equations and the qualitative character of the resulting system equations is discussed. Solutions options are outlined, examples of application are presented, and one implementation of the theory, the CONTAM family of programs developed at NBS, is briefly described.

NOMENCLATURE

A	cross-sectional area of flow passage
C	contaminant concentration expressed in terms of mass fraction
aD	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
am	stoichiometric mass of species α involved in kinetics process
P	pressure
R	radius
Re	Reynolds number
aR	rate of kinetics process
T	temperature
t	time
\bar{t}	nominal transit time
δt	numerical integration time step
\bar{u}	bulk (i.e. sectional average) fluid velocity
\mathbf{v}	fluid velocity vector
w	mass transport rate
x, y, z	spatial coordinates
ϕ	upwind parameter
$^a\gamma$	dimensionless generation rate of species α
κ	reaction rate coefficient
$^a\eta$	filter efficiency relative to species α
ρ	mass density
τ	dimensionless time; system time constants
θ	stability factor; integration parameter
μ	flow fluid viscosity
χ	dimensionless length

Subscripts, superscripts and other symbols

species index $\rightarrow \alpha$ γ^e — element index
descriptive index \rightarrow con a j — node or array element index
 α $\chi_{(k)}$ — the " k th" iterate
con $\chi_{(n)}$ — the " n th" time step

a, b, c, \dots	specific element indices
e	general element index
$\alpha, \beta, \gamma, \dots$	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
\sim	quantities modified to account for boundary conditions
\sim	quantities modified to account for zero "volumetric" mass terms; intermediate values

Vectors and matrices

$[B]$	element-to-system-variables Boolean transformation matrix
$\{C\}, \{C^e\}$	system concentration vector
$\{C^e\}$	element concentration vector
$\{\Phi\}$	(steady flow/kinetics) system eigenvectors
$\{E\}, \{E^e\}$	system excitation vector
$\{G\}$	system direct (nodal) species generation rate vector
$\{G^e\}$	system generation rate vector
$\{g^e\}$	element-derived species generation rate vector
$[K]$	kinetics rate coefficient matrix
$L'(\{V\})$	transformation of vector $\{V\}$
$[M], [M^e]$	system mass matrix
$[M^e]$	diagonal mass matrix associated with kinetics element
$\{R\}$	kinetics rate vector
$\{R_0\}$	constant component of kinetics rate vector
$[W], [W^e]$	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 an air flow 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, radiochemical decay, settling, or sorption of contaminants.

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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 procedure to predict contaminant dispersal in buildings that comprehensively and systematically accounts 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] or the well-mixed zone simplification of the macroscopic mass balance equations for flow systems,† 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.

In this paper we shall present an element assembly formulation of the contaminant dispersal problem that generalizes the work done earlier [6, 7, 8]. In this earlier work an element assembly formulation of the macroscopic approach based upon the usual well-mixed zone simplification was presented. The formulation presented here makes no limiting assumption at the global (i.e. system-wide) level about the nature of the mass transport processes being modeled and is, therefore, not limited by the well-mixed zone simplification. The well-mixed zone macroscopic approach is, however, included as a special case. Consequently, the present formulation provides a means to combine microscopic and macroscopic approaches and offers a framework for the inclusion of a practically unlimited variety of models for both flow and nonflow mass transport processes that may affect the dispersal of contaminants in buildings.

The well-mixed zone simplification of the previous approach becomes, in the present formulation, simply a new class of contaminant dispersal element. In addition two new classes of contaminant dispersal elements are introduced; the kinetics element that may be used to model mass transport processes governed by kinetic theory and a one dimensional convection-diffusion element that may be used to model the microscopic details of dispersal in one dimensional flow regimes. An emphasis will be placed on modeling building air flow systems, but the theory and methods developed may be applied to other flow systems as well.

The contaminant dispersal model

We begin by asserting the following.

Building air flow 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 contami-

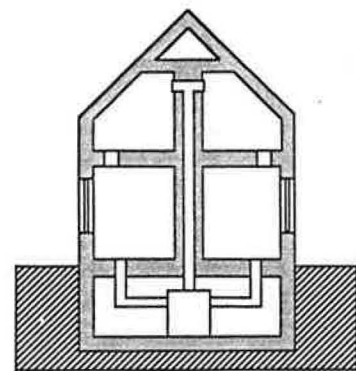


Fig. 1. Hypothetical two storey residence.

nant concentration at discrete points in the building system, the *system nodes*, to the flow and non-flow processes responsible for the dispersal.

The contaminant dispersal model involves, then, a spatial discretization of the domain of the air flow system (i.e. the selection and identification of the system nodes) and 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

With a knowledge of the air flow paths and the mass transport phenomena governing the dispersal the analyst selects from the *library* of available elements to assemble an idealization of a given building system. The development of an idealization may often be formulated graphically in a rather direct and very intuitive way. In Fig. 1 we show a hypothetical section of a two storey residence; Fig. 2 shows the current *library* of dispersal elements, and Fig. 3 shows a possible idealization of the hypothetical building assembled graphically, and hence mathematically, from the current library of elements. (The large black dots in this figure correspond to discrete points in the air flow system, the *system nodes*.)

In this example, each of the four rooms, the exterior

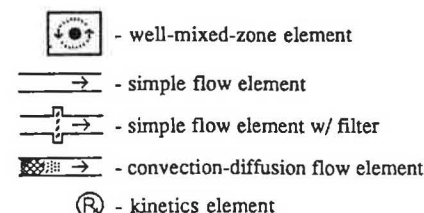


Fig. 2. Current library of contaminant dispersal elements.

* Microscopic equations of motion: the differential formulation of the continuity, motion, and energy equations for fluids.

† 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 [2, 3, 4], that is closely related to similar models used in the chemical engineering field [5].

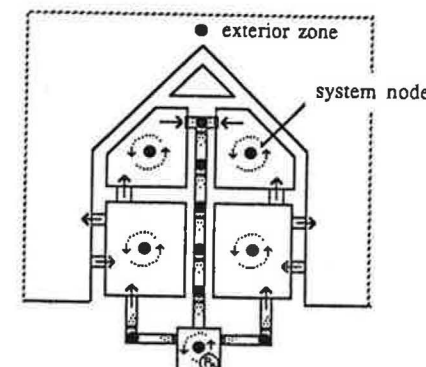


Fig. 3. Idealization of the building air flow system.

environment, and the furnace air heating chamber have been modeled with *well-mixed zone elements*; infiltration, exfiltration, and first-to-second storey air flows have been modeled with *simple flow elements*; the HVAC duct flow paths have been modeled with 1-D *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*. Thus, this idealization would be appropriate for the analysis of carbon monoxide dispersal in the building system.

With the 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 air flows, evaluation of system time constants for conditions of steady air flows, and evaluation of time histories of contaminant concentrations for various scenarios of steady or unsteady air flows with steady or unsteady contaminant generation rates.

After considering the results of the analysis the analyst may add, delete, or modify elements to, from, or of the assembly, in an effort, for example, to mitigate any indoor contaminant hazard and reanalyse the system to evaluate the efficacy of the mitigation measure.

GENERAL FORMULATION

In indoor air quality analysis we may consider building air flow 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.* 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,

* 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.

† Non-interactive contaminant: a contaminant whose dispersal is not affected by kinetics of reaction, sorption, settling, or other similar or related mass transport phenomena.

then, the determination of the spatial (x, y, z) and temporal (t) variation of contaminant species concentrations within the domain of the air flow system. This analytical problem will be referred to as *contaminant dispersal analysis*.

For a single *non-interactive*† species, α , contaminant dispersal is driven by the air velocity field and thus the contaminant dispersal analysis problem, for this case, may be represented, functionally, as:

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

where the ellipses, \dots , 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 non-linear *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 [6, 7]. Alternatively, for existing buildings it may be possible to "measure" building air flows 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 air flows 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, non-linear) analysis problem as (the rate of change of) each species' concentration will depend upon both species' concentrations and the air flow velocity field:

$${}^{\alpha}C(x, y, z, t) = {}^{\alpha}C(v(x, y, z, t),$$

$${}^{\alpha}C(x, y, z, t), {}^{\beta}C(x, y, z, t)); \dots \quad (2)$$

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 general formulation to the solution to these field problems taken here is straightforward, but involves several steps. The continuously defined state variables—the contaminant(s) concentrations, ${}^{\alpha}C(x, y, z, t)$, ${}^{\beta}C(x, y, z, t)$, \dots —are replaced by a finite set of *discrete system state variables*, $\{C(t)\}$, that are meant to approximate the value of the continuous variables at discrete points—the *system nodes*—in the air flow 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* $\{C^e\}$. It is then shown that 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 by first establishing formal relationships between the discrete system state variables and the discrete element state variables

and then demanding the conservation of contaminant species mass at each of the system nodes.

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 [6, 7, 9].

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 vectors* which for n nodes are defined as:

for the dispersal of a single species, α :

$$\{C\} \equiv \{^{\alpha}C_1, ^{\alpha}C_2, \dots, ^{\alpha}C_n\}^T; \quad (3a)$$

for the dispersal of two species, α and β :

$$\{C\} \equiv \{^{\alpha}C_1, ^{\beta}C_1, ^{\alpha}C_2, ^{\beta}C_2, \dots, ^{\alpha}C_n, ^{\beta}C_n\}^T; \quad (3b)$$

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*) 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 :

$$\{C^e\} \equiv \{^{\alpha}C_i^e, ^{\alpha}C_j^e, ^{\alpha}C_k^e\}^T; \quad (4a)$$

for the dispersal of two species, α and β :

$$\{C^e\} \equiv \{^{\alpha}C_i^e, ^{\beta}C_i^e, ^{\alpha}C_j^e, ^{\beta}C_j^e, ^{\alpha}C_k^e, ^{\beta}C_k^e\}^T; \quad (4b)$$

etc.

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

General form of the element equations

We attempt to describe the *behavior* of an element by equations of the general form:

$$\{w^e\} = L^e(\{C^e\}) - \{g^e\}, \quad (5)$$

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:

*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.

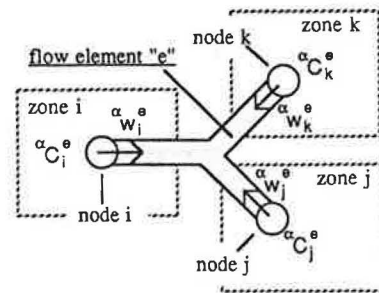


Fig. 4. Hypothetical three-node flow element.

for the dispersal of a single species, α :

$$\{w^e\} \equiv \{^{\alpha}w_i^e, ^{\alpha}w_j^e, ^{\alpha}w_k^e\}^T; \quad (6a)$$

for the dispersal of two species, α and β :

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

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 above for a hypothetical three node flow element that links three well-mixed zone elements, Fig. 4, and a single-node kinetics element associated with a single well-mixed zone element, Fig. 5. The arrows indicate positive mass transport rates.

For the flow element, mass is transported physically by the air flow 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 Fig. 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 has no special interest,

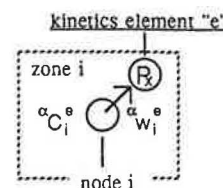


Fig. 5. Single-node kinetics element.

within the single zone associated with the kinetics element.

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

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

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

There exists a one-to-one correspondence between an element's concentration variables and the system's concentration variables that may be described by a simple Boolean transformation:

$$\{C^e\} = [B^e]\{C\}, \quad (8)$$

where $[B^e]$ is an $m \times n$ Boolean Transformation matrix (i.e. consisting of only ones and zeros) for an m -node element within an n -node system idealization.

The Boolean transformation is simply a means to express the equality of each of the element concentration variables with its associated system concentration variable within the framework of concise vector notation; it defines the relation between the (larger) vector of system concentration variables and the (smaller) vector of a specific elements concentration variables, a subset of the system variables.

This same Boolean transformation matrix may be used to transform the vector element mass transport rates, $\{w^e\}$, into a "system-sized" vector of mass transport rates for element "e", $\{W^e\}$, defined as:

$$\{W^e\} \equiv [B^e]^T\{w^e\}. \quad (9)$$

This vector $\{W^e\}$ will have the same number of elements as the system concentration vector $\{C\}$. It represents the net species mass transport rate from each of the system nodes into a specific element "e". Therefore, the sum of these vectors for all elements in the system assemblage will equal a vector describing the total mass transport from the system nodes into all elements combined:

$$\sum_{e=a,b,\dots} \{W^e\} = \left\{ \begin{array}{l} \text{total species} \\ \text{mass transport} \\ \text{from each node} \\ \text{into connected elements} \\ \text{at each node} \end{array} \right\}, \quad (10)$$

which, if mass is to be conserved, must equal any species mass generated directly at each of the systems nodes or:

$$\sum_{e=a,b,\dots} \{W^e\} = \{G\}, \quad (11)$$

where $\{G\}$ is the *direct species generation rate vector*, defined:

for a single species, α , as:

$$\{G\} \equiv \{^{\alpha}G_1, ^{\alpha}G_2, \dots, ^{\alpha}G_n\}^T; \quad (12a)$$

for two species, α and β , as:

$$\{G\} \equiv \{^{\alpha}G_1, ^{\beta}G_1, ^{\alpha}G_2, ^{\beta}G_2, \dots, ^{\alpha}G_n, ^{\beta}G_n\}^T; \quad (12b)$$

etc.

$^{\alpha}G_i$ the direct mass generation rate of species α at node i .

Substituting the transformation relations, Equations (8) and (9), along with the general form of the element equations, Equation (5), into the species mass conservation relation, Equation (11), we obtain the final result:

$$[W]\{C\} + [M]\frac{d\{C\}}{dt} + [Z]\frac{d^2\{C\}}{dt^2} + \dots = \{G\}, \quad (13a)$$

where:

$$[W] = \sum_{e=a,b,\dots} [B^e]^T[x^e][B^e], \quad \text{the system (mass) transport matrix}; \quad (13b)$$

$$[M] = \sum_{e=a,b,\dots} [B^e]^T[y^e][B^e], \quad \text{the system mass matrix}; \quad (13c)$$

$$[Z] = \sum_{e=a,b,\dots} [B^e]^T[z^e][B^e]; \quad (13d)$$

etc.

$$\{G\} = \{G\} + \sum_{e=a,b,\dots} [B^e]^T\{g^e\}, \quad \text{the system generator vector.} \quad (13e)$$

The assembly operator

The summation and Boolean transformation of element matrices, contained in the expressions above, is an operation that recurs frequently in Finite Element and related discrete modeling literature and, therefore, has come to be defined as a standard operation—the *assembly operation*—designated by the symbol \mathcal{A} , the so-called *assembly operator*, where:

for element vector assembly:

$$\mathcal{A}\{v^e\} \equiv \sum_{e=a,b,\dots} [B^e]^T\{v^e\}, \quad (14a)$$

for element matrix assembly:

$$\mathcal{A}[m^e] \equiv \sum_{e=a,b,\dots} [B^e]^T[m^e][B^e]. \quad (14b)$$

The assembly operator is a generalization of the conventional summation operator, Σ , and equal to the summation operator when the Boolean transformation matrices equal the identity matrix.

The assembly operation is important, theoretically, in that it provides the necessary formal definition of the assembly process required for subsequent mathematical analysis. It does not, however, define an efficient numerical procedure for assembling the element arrays needed to form the system equations for practical contaminant dispersal analysis—the indicated Boolean transfor-

mations involve multiplications by either zero or one and, therefore, need not be actually implemented. Practically, then, the assembly operation is carried out using relatively simple algorithms that accumulate element array terms within system array memory locations according to the physical connectivity of each element. The "LM Algorithm" presented by Bathe [10] provides an example of one possible algorithm.

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 [6, 7, 8].

Well-mixed zone element

It may be reasonable to model portions of a building air flow system as if they were 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 spatial 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 zone, is defined by the following element equation:

$$\{w_i^e\} = [m^e] \left\{ \frac{d^2 C_i^e}{dt} \right\}, \quad (15a)$$

for species α in a well-mixed zone having a volume containing a mass of air of m^e . In this case, then, the element equations are defined in terms of a 1×1 element mass matrix that is simply equal to the mass of the volume of air in the well-mixed zone:

$$[y^e] = [m^e]. \quad (15b)$$

Simple flow element

Flow through many flow passages in building air flow systems is practically instantaneous (i.e. relative to the dominant time constants of the building 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:

$$\begin{Bmatrix} w_i^e \\ w_j^e \end{Bmatrix} = w^e(t) \begin{bmatrix} 1 & 0 \\ -1 & 0 \end{bmatrix} \begin{Bmatrix} C_i^e \\ C_j^e \end{Bmatrix}; \quad w^e(t) \geq 0, \quad (16a)$$

or, in this case we have:

$$[x^e] = w^e(t) \begin{bmatrix} 1 & 0 \\ -1 & 0 \end{bmatrix}; \quad [y^e] = [0]; \quad \{g^e\} = \{0\}, \quad (16b)$$

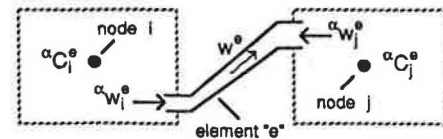


Fig. 6. Simple contaminant dispersal flow element variables.

$$\{w^e\} \equiv \{w_i^e, w_j^e\}^T. \quad (16c)$$

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, above, should help to clarify the meaning of the element variables in this case.)

The simple flow element may also be thought to provide a model of *plug flow* flow passages (i.e. having one-directional uniform flow velocity profiles), as instantaneous flow and instantaneous plug flow are equivalent. A more meaningful plug flow element should, reasonably, account for flow delay along the flow passage (i.e. should model the non-instantaneous aspect of flow), thus we shall make the distinction, here, between a simple instantaneous flow element and a simple non-instantaneous plug flow element (that has yet to be developed).

The multi-chamber theory presented by Sinden [2] and Sandberg [3] 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, however, we extend significantly the conventional multi-chamber theory. We also provide an alternative formal view of this theory that provides a deeper understanding of the qualitative character of theory and, therefore, of contaminant dispersal in buildings.

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, η , of the contaminant as it passes through the element to yield the following element equations;

$$\begin{Bmatrix} w_i^e \\ w_j^e \end{Bmatrix} = w^e(t) \begin{bmatrix} 1 & 0 \\ (\eta-1) & 0 \end{bmatrix} \begin{Bmatrix} C_i^e \\ C_j^e \end{Bmatrix}; \quad w^e(t) \geq 0, \quad (17a)$$

or, in this case we have:

$$[x^e] = w^e(t) \begin{bmatrix} 1 & 0 \\ (\eta-1) & 0 \end{bmatrix} \quad [y^e] = [0]; \quad \{g^e\} = \{0\}. \quad (17b)$$

In this case the time variation of the first 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, $\eta = \eta(t)$.

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. longer 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:

$$\frac{1}{Pe} \frac{\partial^2 C}{\partial \chi^2} + \gamma = \frac{\partial C}{\partial \tau} + \frac{\partial C}{\partial \chi}, \quad (18a)$$

where:

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

$\alpha^e D$ 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 $\equiv t/\bar{t}$; γ is the dimensionless generation rate $\equiv gL/w^e$; \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 $Pe = \infty$ would correspond to an ideal plug-flow condition.

The convection-diffusion process depends critically on the dispersal coefficient. A complete discussion of this coefficient is well beyond the scope of this paper; the reader is, therefore, directed to the discussion provided by Naumann and Buffham [11] and Wen and Fan [5]. For flow situations that might be expected to be encountered in building air flow systems (e.g. turbulent, isothermal, flow in relatively long passages) the correlation developed by Taylor [see 5] is likely to be useful:

$$\alpha^e D \approx \beta D \approx \dots \approx 2\bar{u}R \times \left(\frac{3.0 \times 10^7}{Re^{2.1}} + \frac{1.35}{Re^{0.125}} \right); \quad Re > 2000 \quad (19)$$

where: R is the flow passage radius; $Re \equiv 2\rho\bar{u}R/\mu$; the Reynolds number; μ is the flow fluid viscosity.

Following the one dimensional example discussed by Huebner and Thornton [12], element equations for a two-node flow element may be developed from Equation (18) 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:

$$\{w^e\} = [[x^e] + [y^e]] \{C^e\} + [y^e] \frac{d\{C^e\}}{dt} - \{g^e\}, \quad (20a)$$

where:

$$[x^e] = \frac{w^e}{2} \begin{bmatrix} 1 & 1 \\ -1 & -1 \end{bmatrix} + \frac{\phi w^e}{2} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix};$$

$w^e \geq 0$, the convection component of the element mass transport matrix; (20b)

ϕ the so-called upwind parameter; $0 \leq \phi \leq 1$;

$$[y^e] = \frac{\rho A^e D}{L^e} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}, \quad \text{the diffusion component of the element mass transport matrix; (20c)}$$

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

$$[y^e] = \frac{\rho A L^e}{6} \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix} + \frac{\phi \rho A L^e}{4} \begin{bmatrix} -1 & -1 \\ 1 & 1 \end{bmatrix}, \quad \text{the element volume mass matrix; (20d)}$$

or

$$[y^e] \approx \frac{\rho A L^e}{2} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad \text{the lumped approximation to the element volume mass matrix; (20e)}$$

$$\{g^e\} = \frac{gL^e}{2} \begin{Bmatrix} 1 \\ 1 \end{Bmatrix} + \frac{\phi gL^e}{2} \begin{Bmatrix} -1 \\ 1 \end{Bmatrix}, \quad \text{the internal generation rate vector (20f)}$$

for species α and fluid mass flow rate, w^e , 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 [8]. 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 (i.e. it is based on partial differential mass balance relations) and its use provides a first example of combining macroscopic modeling methods (i.e. the well-mixed zone and simple flow elements) with microscopic methods in a single analytical procedure. 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, 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*. (Reaction kinetics involves the study of the rate of change of chemical components in a single or related series of chemical reactions).

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

$$\alpha + \beta + \dots \xrightarrow{\text{catalyst}} \rho + \sigma + \dots, \quad (21)$$

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.

Given the rate of change of a selected component's concentration, say α , is defined as:

$$^{\alpha}R \equiv \frac{d^{\alpha}C}{dt}; \text{rate of kinetics process of species } \alpha \quad (22)$$

and the stoichiometry of the process, expressed in terms of relative masses, $^{\alpha}m, ^{\beta}m, \dots$, of reactants and products as:

$$^{\alpha}m + ^{\beta}m + \dots \xrightarrow{\text{catalyst}} ^{\rho}m + ^{\sigma}m + \dots, \quad (23)$$

the rate of change of the other components' concentrations may be related to that of the selected component's, by consideration of the conservation of mass, as:

$$^{\alpha}R = \left(\frac{^{\beta}m}{^{\alpha}m}\right)^{\beta}R = \dots = -\left(\frac{^{\rho}m}{^{\alpha}m}\right)^{\rho}R = -\left(\frac{^{\sigma}m}{^{\alpha}m}\right)^{\sigma}R, \quad (24)$$

thus, the rate of a given kinetic process may be described in terms of the rate of change of concentration of any one of the reactants or products.

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:

$$^{\alpha}R = ^{\alpha}R(^{\alpha}C, ^{\beta}C, \dots, ^{\rho}C, ^{\sigma}C, \dots, T, P, \dots). \quad (25)$$

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 [13], often take the form of linear combinations of contaminant concentrations:

$$\{R\} = -[k]\{C\} + \{R_0\}, \quad (26a)$$

or:

$$\begin{Bmatrix} ^{\alpha}R \\ ^{\beta}R \\ \vdots \\ ^{\sigma}R \end{Bmatrix} = - \begin{bmatrix} ^{\alpha\alpha}k & ^{\alpha\beta}k & \dots & ^{\alpha\sigma}k \\ ^{\beta\alpha}k & ^{\beta\beta}k & \dots & ^{\beta\sigma}k \\ \vdots & \vdots & \ddots & \vdots \\ ^{\sigma\alpha}k & ^{\sigma\beta}k & \dots & ^{\sigma\sigma}k \end{bmatrix} \begin{Bmatrix} ^{\alpha}C \\ ^{\beta}C \\ \vdots \\ ^{\sigma}C \end{Bmatrix} + \begin{Bmatrix} ^{\alpha}R_0 \\ ^{\beta}R_0 \\ \vdots \\ ^{\sigma}R_0 \end{Bmatrix}, \quad (26b)$$

where we have included the constant component, $\{R_0\}$, for completeness and recognize that, again, the rate coefficient matrix, $[k]$, and the constant component

vector, $\{R_0\}$, will, in general, vary with temperature and pressure.

It may also be possible to linearize other non-linear rate expressions by employing a Taylor's expansion about some state of concentration to obtain an approximate rate expression expressed as the sum of a series of first order rate expressions that, together with Equation (24), may be used to form a linearized system of first order rate expressions of the form of Equation (26). One could then, conceivably, employ this linearization strategy, within an appropriate nonlinear solution method, to account for arbitrarily complex kinetics.

The general rate expression, Equation (25), 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, $\alpha, \beta, \gamma, \dots$, we first identify the relevant element variables as:

$$\{C^e\} = \{^{\alpha}C_i^e, ^{\beta}C_i^e, ^{\gamma}C_i^e, \dots\}^T, \quad (27)$$

and:

$$\{w^e\} = \{^{\alpha}w_i^e, ^{\beta}w_i^e, ^{\gamma}w_i^e, \dots\}^T. \quad (28)$$

Then from the rate definition, Equation (22), and the general form of rate expressions, Equation (25), we obtain the general kinetics element equations:

$$\{w^e\} = -[M^e]\{R^e(\{C^e\}, T, P)\}, \quad (29a)$$

where:

$$[M^e] \equiv \begin{bmatrix} m^e & 0 & 0 & \dots \\ 0 & m^e & 0 & \dots \\ 0 & 0 & m^e & \dots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix}; \quad (29b)$$

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

$$\{R^e(\{C^e\}, T, P)\}$$

$$\equiv \begin{Bmatrix} ^{\alpha}R(^{\alpha}C_i^e, ^{\beta}C_i^e, ^{\gamma}C_i^e, \dots, T, P) \\ ^{\beta}R(^{\alpha}C_i^e, ^{\beta}C_i^e, ^{\gamma}C_i^e, \dots, T, P) \\ ^{\gamma}R(^{\alpha}C_i^e, ^{\beta}C_i^e, ^{\gamma}C_i^e, \dots, T, P) \\ \vdots \end{Bmatrix}, \quad (29c)$$

or in this case we obtain:

$$\{x^e\} = 0; \quad \{y^e\} = 0; \quad \{g^e\} = [M^e]\{R^e(\{C^e\}, T, P)\}, \quad (29d)$$

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

The form of Equation (29) 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 *non-linear* species generation contribution (i.e. a species generation rate that depends nonlinearly on the solution vector $\{C\}$), 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 non-linear 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 (26), which when substituted into Equation (29) lead to the *first order kinetics element equations*:

$$\{w^e\} = [M^e][k^e]\{C^e\} - [M^e]\{R_0^e\}, \quad (30a)$$

or:

$$\{x^e\} = [M^e][k^e]; \quad \{y^e\} = 0; \quad \{g^e\} = [M^e]\{R_0^e\}, \quad (30b)$$

where, again, one must keep in mind that the rate coefficient matrix and constant rate component will, in general, be temperature and pressure dependent. (Özkaynak *et al.* present such system equations for a single-zone model including simplified NO_x chemical kinetics [14].)

The kinetics elements are unique in that they are necessarily associated with well-mixed zone elements, as presented here. With this association established they may be assembled, however, in the usual manner (i.e. by Equations (13a)–(13e)) to account for their contribution to the system equations.

SOLUTION OF SYSTEM EQUATIONS

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

$$[W]\{C\} + [M]\frac{d\{C\}}{dt} = \{G\}. \quad (31)$$

To complete the definition of a contaminant dispersal analysis problem these equations will have to be augmented with specifications of initial and boundary conditions. Some elements assemblages will lead to system equations that are either difficult to solve or have no (unique) solution at all, therefore, before considering solution options and methods it will be necessary to identify the conditions that will have to be met to produce system equations that will not only yield solutions, but those that will yield accurate solutions in a numerically efficient and stable manner.

To simplify subsequent discussion we shall limit consideration to assemblages resulting in diagonal system mass matrices (i.e. we shall limit the convection-diffusion element equations to the lumped mass approximation, Equation (20e)). The extension to the nondiagonal case is straightforward.

Boundary conditions

The variation of species concentration or generation rate, but not both, may be specified at system nodes. Concentration or generation conditions in the discrete model are equivalent to boundary conditions in the corresponding field problem and will, therefore, be referred to as such.

Formally then, we may distinguish between those

nodes for which species concentration will be specified, $\{C_c\}$, (e.g. nodes associated with outdoors) and those for which the generation rate will be specified, $\{G_g\}$, and partition the system equations accordingly:

$$\begin{bmatrix} [W_{cc}][W_{cg}] \\ [W_{gc}][W_{gg}] \end{bmatrix} \begin{Bmatrix} \{C_c\} \\ \{C_g\} \end{Bmatrix} + \begin{bmatrix} [M_{cc}] & [0] \\ [0] & [M_{gg}] \end{bmatrix} \times \begin{Bmatrix} \frac{d\{C_c\}}{dt} \\ \frac{d\{C_g\}}{dt} \end{Bmatrix} = \begin{Bmatrix} \{G_c\} \\ \{G_g\} \end{Bmatrix}. \quad (32)$$

Using the second equation and simplifying we obtain:

$$[\tilde{W}]\{\tilde{C}\} + [\tilde{M}]\frac{d\{\tilde{C}\}}{dt} = \{\tilde{E}\} \quad (33a)$$

where we have introduced the new terms:

$$[\tilde{W}] \equiv [W_{gg}];$$

the generation-driven transport matrix; (33b)

$$\{\tilde{C}\} \equiv \{C_g\};$$

the generation-driven concentration vector; (33c)

$$[\tilde{M}] \equiv [M_{gg}];$$

the generation-driven mass matrix; (33d)

$$\{\tilde{E}\} \equiv \{G_g\} - [W_{gc}]\{C_c\};$$

the system *excitation*. (33e)

The system is seen to be driven by the system *excitation*, $\{\tilde{E}\}$, that includes both specified contaminant mass generation rates and contaminant concentrations which may, in general, vary with time.

The *response* of the system is defined by the solution of Equation (33) for the generation-driven concentration variables, $\{C_g\}$. The generation rates, $\{G_c\}$, required to maintain the specified concentrations, $\{C_c\}$, may be determined from the computed response of the system to the specified excitation using the first equation of Equation (32) as:

$$\{G_c\} \equiv [W_{cc}]\{C_c\} + [W_{cg}]\{C_g\} + [M_{cc}]\frac{d\{C_c\}}{dt}. \quad (34)$$

While Equation (33) is theoretically important, it may not represent a computationally efficient scheme for imposing required concentration constraints. It is possible to impose the concentration specified conditions without actually rearranging the system equations by either directly scaling the concentration-specified diagonal elements of Equation (31) by a large number and setting the corresponding generation rate equal to the product of the specified concentration and the scaled diagonal term or by including "processing jumps" within the numerical solution algorithms employed [15, 16]. These strategies are not only computationally convenient but would be especially useful for systems with limiting controls placed upon some nodal concentrations.

System transport matrix $[W]$

The character of the system transport matrix $[W]$, being a direct assembly sum of the element transport

matrices $[x^*]$, is intimately related to the character of these element arrays. The simple flow element, simple flow element with filtration, and convection-diffusion flow element transport matrices, equations (16b), (17b), (20b) and (20c), are, respectively:

$$w^e \begin{bmatrix} 1 & 0 \\ -1 & 0 \end{bmatrix}; \quad w^e \begin{bmatrix} 1 & 0 \\ (\eta-1) & 0 \end{bmatrix};$$

$$\frac{w^e}{2} \begin{bmatrix} 1 & 1 \\ -1 & -1 \end{bmatrix} + \left(\phi + \frac{2}{P^e e} \right) \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix},$$

where:

$$P^e e = \frac{w^e L^e}{\rho A D}, \quad (35)$$

is the so-called *element Peclet number* and, here, we have limited consideration to the dispersal of a single species.

For convection-diffusion element, Huebner and Thornton show [12] that numerical instability may be avoided if the upwind parameter, ϕ , is selected so that:

$$(\phi + 2/P^e e) \geq 1; \quad 0 \leq \phi \leq 1. \quad (36)$$

Thus, assuming this stability condition will be satisfied, we may rewrite the convection-diffusion element transport matrix as:

$$w^e \begin{bmatrix} 1 & 0 \\ -1 & 0 \end{bmatrix} + \frac{\theta w^e}{2} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix};$$

$$\theta = (\phi + 2/P^e e) - 1 \geq 0. \quad (37)$$

If, now, we consider the details of the assembly process we can conclude that the assembly of simple flow elements, flow elements with filtration, and the first term of the convection-diffusion element equations above, all being nonsymmetric, will result in a nonsymmetric contribution to the system transport matrix, which we shall designate as $[W_{\text{non-sym}}]$, while the assembly of the second term of the convection-diffusion element equations will result in a symmetric contribution to the system transport matrix, which we shall designate as $[W_{\text{sym}}]$:

$$[W_{\text{non-sym}}] = \sum_{\text{simple}} w^e \begin{bmatrix} 1 & 0 \\ -1 & 0 \end{bmatrix} + \sum_{\text{filter}} w^e \begin{bmatrix} 1 & 0 \\ (\eta-1) & 0 \end{bmatrix}$$

$$+ \sum_{\text{con-diff}} w^e \begin{bmatrix} 1 & 0 \\ -1 & 0 \end{bmatrix}, \quad (38)$$

$$[W_{\text{sym}}] = \sum_{\text{con-diff}} \frac{\theta w^e}{2} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}, \quad (39)$$

and we note that in both cases the diagonal elements will be positive and the off-diagonal elements nonpositive (i.e. negative or zero).

Furthermore, for a given system node i : (a) the diagonal elements of the nonsymmetric contribution will equal the total mass flow out of a node; (b) the row sum of the off-diagonals will equal the sum of total mass flow into the node weighted by the filter efficiency factors, $(\eta-1)$, for flow elements with filtration; (c) the column sum of the off-diagonals will equal the sum of total mass flow out of the node weighted by the filter efficiency factors, $(\eta-1)$, for flow elements with filtration.

Thus, if the total mass flow into a system node is equal

to the total mass flow out of a system node (i.e. if total flow is conserved), then we may conclude:

$$W_{\text{non-sym},ii} \geq \sum_{j=1}^n |W_{\text{non-sym},ij}| \equiv \text{row sum of row } i, \quad (40a)$$

$$W_{\text{non-sym},ii} \geq \sum_{j=1}^n |W_{\text{non-sym},ji}| \equiv \text{column sum of col. } i. \quad (40b)$$

By inspection, the diagonal terms of the symmetric contribution simply equal their respective column and row sums. We may thus conclude that the sum of the nonsymmetric and symmetric contributions satisfy the following inequalities:

$$W_{ii} \geq \sum_{j=1}^n |W_{ij}|, \quad (41a)$$

$$W_{ii} \geq \sum_{j=1}^n |W_{ji}|, \quad (41b)$$

for assemblies of flow elements only. If all filter efficiencies are zero or, equivalently, no flow elements with filtration are contained in the assemblage, then the equalities will be strict in Equations (40a)–(41b). (This last conclusion follows directly from a consideration of the dispersal of the "species" air which by definition has a concentration of 1.0 at all nodes, $\{C\} = \{1\}$, which is unchanging in time, $d\{C\}/dt = \{0\}$, and which, for our considerations, is not being generated, $\{G\} = \{0\}$; thus, by Equation (31) we obtain the equivalent result that $\{W\}\{1\} = \{0\}$.)

Using these results we may show that the important submatrix of the system transport matrix identified above as the generation-driven submatrix, Equation (33b), is nonsingular (i.e. will lead to unique solutions of the contaminant dispersal problem), but to do so we must introduce some relatively esoteric theorems relating to the general class of matrices known as M -matrices.

An M -matrix may be defined in a number of alternative, but equivalent ways. Using the alternative employed by Funderlic and Plemmons [17] an M -matrix is a square non-zero real matrix with all off-diagonal elements non-positive that has eigenvalues with non-negative real parts. It may be shown [18] that a real square matrix $[A]$, with positive diagonal elements and non-positive off-diagonal elements: (a) is an M -matrix (possibly singular) if and only if it can be shown that $[[A] + \xi[I]]$ is a non-singular M -matrix for all scalars $\xi > 0$; (b) is a nonsingular M -matrix if $[A]$ is strictly diagonally dominant.

In the case at hand, clearly $[[W] + \xi[I]]$ is strictly diagonally dominant, and therefore a non-singular M -matrix, for all scalars $\xi > 0$ (if, of course, total mass flow is conserved at all nodes). Thus we can conclude that $[W]$ is an M -matrix, although it will be singular for the limiting case when all filter efficiencies are zero.

It has also been shown that each principal submatrix of an irreducible M -matrix (other than the M -matrix itself) is a non-singular M -matrix [18]. The system transport matrix would be said to be *reducible* if it is possible, using an appropriate numbering of the system nodes, to assemble the transport matrix in the form:

$$[W] = \begin{bmatrix} [W_{11}] & [W_{12}] \\ [0] & [W_{22}] \end{bmatrix}, \quad (42)$$

where $[W_{11}]$ and $[W_{22}]$ are square matrices, otherwise $[W]$ would be said to be irreducible. Recalling that super-diagonal terms of flow element assemblages, W_{ij} ; $j > i$, correspond to flow(s) from node j to node i and sub-diagonal terms, W_{ji} ; $j < i$, correspond to flow(s) from node i to node j , a flow matrix of the form of Equation (42) would correspond to a flow system idealization having a total mass flow from subassembly 2 to subassembly 1, without a return flow from 1 to 2, and, therefore, conservation of total mass flow would be violated.

We may conclude, then, that for assemblies of flow elements: (a) the system transport matrix, $[W]$, will be an irreducible M -matrix and, therefore; (b) the generation-driven transport matrix, $[\tilde{W}]$, a principal submatrix of the system transport matrix will be a non-singular M -matrix, if they are formed based upon a flow idealization that satisfies conservation of total mass flow (assuming the stability condition, Equation (36), for convection-diffusion elements has been satisfied).

Non-singular M -matrices have the important additional property that they may be factored into the product of lower, $[L]$, and upper, $[U]$, triangular matrices by procedures relating to Gauss elimination *without the need of pivoting* in an efficient and numerically stable manner (i.e. resulting in no more accumulation of error than that which would result if pivoting were employed) [19]. Therefore, not only may we be certain that a properly formed flow transport matrix will lead to the possibility of solution but it will also allow the use of very efficient methods of solution associated with LU decomposition *without pivoting*:

$$[\tilde{W}] = [L][U]; \text{ for assemblies of only flow elements.} \quad (43)$$

Unfortunately extending the consideration of singularity to the addition of kinetics elements to the assemblage is problematic. The analyst who chooses to employ the linear kinetics element will, most often, face the challenging task of forming an appropriate linearization (or a series of linearizations) of non-linear empirical rate expressions. If the analyst forms linear rate coefficient matrices having one of several suitable forms (e.g. positive diagonal matrices, diagonally dominant matrices with positive diagonals and non-positive off-diagonals, or M -matrices) then the resulting transport matrix may be shown to be non-singular, but other cases may also prove to be non-singular. At this point, then, we are not in a position to provide guidance and leave the responsibility in the hands of the analyst.

System mass matrix $[M]$

The system mass matrix $[M]$ is assembled from diagonal element mass matrices composed of non-negative real numbers. It, therefore, follows directly that the system mass matrix will also be a diagonal matrix of non-negative real numbers. In those cases where all element contributions are positive the inversion of the system mass matrix is trivial:

$$[M]^{-1} = \text{diag}(1/M_{11}, 1/M_{22}, \dots, 1/M_{nn}); \quad M_{ii} > 0. \quad (44)$$

In some cases, however, an analyst may consider an element mass contribution to be negligibly small or, at the other extreme, practically infinite and, therefore, may wish to model these contributions with either zero or infinite values. Both cases will tend to complicate numerical solution of the system equations and are best considered as special cases.

Zero mass terms. For cases where some elements of the system mass matrix are zero we partition Equation (33) into those equations associated with zero mass nodes (subscript z) and those associated with non-zero mass nodes (subscript n):

$$\begin{bmatrix} [\tilde{W}_{zz}][\tilde{W}_{zn}] \\ [\tilde{W}_{nz}][\tilde{W}_{nn}] \end{bmatrix} \begin{Bmatrix} \{\tilde{C}_z\} \\ \{\tilde{C}_n\} \end{Bmatrix} + \begin{bmatrix} [0] & [0] \\ [0] & [\tilde{M}_{nn}] \end{bmatrix} \begin{Bmatrix} \{\tilde{E}_z\} \\ \{\tilde{E}_n\} \end{Bmatrix} = \begin{Bmatrix} \{\tilde{E}_z\} \\ \{\tilde{E}_n\} \end{Bmatrix} \quad (45)$$

The equations associated with the zero mass nodes may then be *eliminated* from consideration by first solving the upper equation:

$$\{\tilde{C}_z\} = [\tilde{W}_{zz}]^{-1} \{ \{\tilde{E}_z\} - [\tilde{W}_{zn}]\{\tilde{C}_n\} \}, \quad (46)$$

and substituting this result into the lower equation to obtain a reduced system of equations:

$$[\tilde{W}]\{\tilde{C}\} + [\tilde{M}]\frac{d\{\tilde{C}\}}{dt} = \{\tilde{E}\}, \quad (47a)$$

where we have introduced the new terms:

$$[\tilde{W}] \equiv [\tilde{W}_{nn}] - [\tilde{W}_{nz}][\tilde{W}_{zz}]^{-1}[\tilde{W}_{zn}], \quad (47b)$$

$$\{\tilde{C}\} \equiv \{\tilde{C}_n\}, \quad (47c)$$

$$[\tilde{M}] \equiv [\tilde{M}_{nn}], \quad (47d)$$

$$\{\tilde{E}\} \equiv \{\tilde{E}_n\} - [\tilde{W}_{nz}][\tilde{W}_{zz}]^{-1}\{\tilde{E}_z\}. \quad (47e)$$

The elimination of these equations may be conveniently and efficiently realized by partial LU decomposition. Equation (47) is important from a theoretical point of view; the operations indicated in this equation are not numerically efficient and should be avoided.

Infinite mass terms. For cases where some elements of the system mass matrix are infinite we partition Equation (33) into those equations associated with infinite mass nodes (subscript ∞) and those associated with nonzero mass nodes (subscript n):

$$\begin{bmatrix} [\tilde{W}_{\infty\infty}][\tilde{W}_{\infty n}] \\ [\tilde{W}_{n\infty}][\tilde{W}_{nn}] \end{bmatrix} \begin{Bmatrix} \{\tilde{C}_\infty\} \\ \{\tilde{C}_n\} \end{Bmatrix} + \begin{bmatrix} [\tilde{M}_{\infty\infty}] & [0] \\ [0] & [\tilde{M}_{nn}] \end{bmatrix} \begin{Bmatrix} \{\tilde{E}_\infty\} \\ \{\tilde{E}_n\} \end{Bmatrix} = \begin{Bmatrix} \{\tilde{E}_\infty\} \\ \{\tilde{E}_n\} \end{Bmatrix} \quad (48)$$

From the first of these equations we obtain:

$$\frac{d\{\tilde{C}_\infty\}}{dt} = [\tilde{M}_{\infty\infty}]^{-1} \{ \{\tilde{E}_\infty\} - [\tilde{W}_{\infty n}]\{\tilde{C}_n\} - [\tilde{W}_{n\infty}]\{\tilde{C}_\infty\} \}, \quad (49)$$

but $[\tilde{M}_{\infty}]^{-1} = [0]$ thus we may conclude (for finite excitation) that:

$$\frac{d\{\tilde{C}_\infty\}}{dt} = \{0\} \therefore \{\tilde{C}_\infty\} = \{\text{constant}\}, \quad (50)$$

and hence the second equation may be simplified to give:

$$[\tilde{W}_{nn}]\{\tilde{C}_n\} + [\tilde{M}_{nn}]\frac{d\{\tilde{C}_n\}}{dt} = \{\tilde{E}_n\} - [\tilde{W}_{n\infty}]\{\tilde{C}_\infty\}. \quad (51)$$

This equation has the same form as Equation (33) and, thus, it is seen that the imposition of an infinite mass term is entirely equivalent to constraining the corresponding concentration variable to a specified constant value. The analyst may, then, avoid difficulties with infinite mass nodes by constraining these nodes with specified constant concentrations.

State matrix $[\tilde{M}]^{-1}[\tilde{W}]$

Equation (33) may be rewritten as:

$$[\tilde{M}]^{-1}[\tilde{W}]\{\tilde{C}\} + \frac{d\{\tilde{C}\}}{dt} = [\tilde{M}]^{-1}\{\tilde{E}\} \quad (52)$$

where it is assumed that zero mass terms have been eliminated and the effect of infinite mass has been accounted for through the specification of constant nodal concentrations.

The product matrix $[\tilde{M}]^{-1}[\tilde{W}]$, sometimes referred to as the *state matrix*, contains the essential dynamic character of the system being studied. For properly formed idealizations (being the product of a positive diagonal matrix and a non-singular M -matrix) it will be a non-singular M -matrix [20] and, therefore: (a) solutions to Equation (52) will exist; (b) the state matrix may be factored by LU decomposition without the need of pivoting in an efficient and numerically stable manner.

We may gain some insight into the general character of solutions to Equation (52) by limiting consideration to systems with constant transport and mass matrices. The response of such a steady flow system, with steady/constant kinetics, and without excitation (i.e. the homogeneous case) is defined by:

$$[\tilde{M}]^{-1}[\tilde{W}]\{\tilde{C}\} + \frac{d\{\tilde{C}\}}{dt} = \{0\}. \quad (53)$$

The governing equation for the familiar contaminant decay problem. The solution to this equation may be found by anticipating the solution:

$$\{\tilde{C}\} = \{\tilde{\Phi}\}e^{-t/\tau} \quad (54)$$

where: τ = decay time constant; $\{\tilde{\Phi}\}$ = vector of unknown magnitudes. When substituted into Equation (53), this leads to the standard eigenvalue problem:

$$[[\tilde{M}]^{-1}[\tilde{W}] - (1/\tau)[I]]\{\tilde{\Phi}\} = \{0\}. \quad (55)$$

The solution of this standard eigenvalue problem and its relation to the first order system of differential equations being considered is discussed elsewhere [21, 22] and is well beyond the present scope. Suffice it to say, for a properly formed system idealization of n unconstrained nodes there will be n solutions to this eigenvalue problem

consisting of n pairs of time constants, τ_i , (or equivalently their inverses, $1/\tau_i$ —the system eigenvalues) and their associated eigenvectors, $\{\tilde{\Phi}_i\}$, $i = 1, 2, \dots, n$.

Non-degenerate case. In some cases, the so-called *non-degenerate* cases, it will be possible to transform the state matrix, by similarity transformations, to diagonal form leaving the eigenvalues on the diagonal as:

$$[S]^{-1}[\tilde{M}]^{-1}[\tilde{W}][S] = \text{diag}((1/\tau_1), (1/\tau_2), \dots, (1/\tau_n)) \quad (56)$$

where $[S]$ = the similarity transformation.

Inasmuch as the state matrix is a non-singular M -matrix these eigenvalues will have positive real parts but may, in some situations, have imaginary components, see [2] for example.

For these cases it will be possible to express the general solution to the homogeneous problem, Equation (53), as a linear combination of simple exponential decay terms:

$$\{\tilde{C}(t)\} = a_1\{\tilde{\Phi}_1\}e^{-t/\tau_1} + a_2\{\tilde{\Phi}_2\}e^{-t/\tau_2} + \dots + a_n\{\tilde{\Phi}_n\}e^{-t/\tau_n}, \quad (57)$$

where the scalar coefficients, a_1, a_2, \dots, a_n , are determined from the initial conditions using the similarity transformation employed as:

$$\{a_1, a_2, \dots, a_n\}^T = [S]^{-1}\{\tilde{C}(t=0)\}^T. \quad (58)$$

For those (unusual) systems having eigenvalues with imaginary components, by Equation (57), we should expect to see harmonic oscillations in concentration time histories that decay in time, see [2, 23] for detailed examples and [24] for actual measured data.

The n pairs of time constants and associated eigenvectors are often referred to as the system *modes* and the response of the system is often described in terms of the degree to which each mode participates. From the form of the free response, Equation (57), it is clear that as time passes the contribution of those modes with larger time constants will dominate the character of the response—if they have been excited—until, eventually, the response, at all nodes, will be dominated by the mode with the largest time constant and therefore will appear to be a simple exponential decay.

The similarity transformation $[S]$ may be chosen as a matrix whose columns equal the eigenvectors, in this case, and, therefore, by Equation (58) we can see that we may trigger a decay response in any single mode if we simply set the initial conditions equal to the corresponding eigenvector (or a scalar multiple of it), although, for some modes the eigenvectors will have negative components that, for contaminant dispersal problems, would not be physically admissible.

From the Gerschgorin Theorem [21] we know that these system eigenvalues lie in at least one of the n circles on the complex plane with centers along the real axis at values equal to the diagonal terms of the state matrix and radii equal to the off-diagonal absolute row sums:

$$\left| (1/\tau) - \left(\frac{\tilde{W}_{ii}}{\tilde{M}_{ii}} \right) \right| \leq \left(\frac{1}{\tilde{M}_{ii}} \right) \sum_{j \neq i} |\tilde{W}_{ij}|. \quad (59)$$

For the special case of n independent zones (i.e. having no flow between zones), without kinetic transport, coupled to an $(n+1)$ th zone of specified concentration

(e.g. having infiltration and exfiltration flows to the exterior, constant concentration environment) the off-diagonal row sums of $[\tilde{W}]$ will be zero, the diagonal values of $[\tilde{W}]$ will equal the total mass flow out of each node (i.e. equal to the total infiltration or exfiltration to the $n+1$ zone, in this case) and, therefore, the n system time constants will be given by:

$$\tau_i = \left(\frac{\tilde{M}_{ii}}{\tilde{W}_{ii}} \right); \text{ for } n \text{ uncoupled zones.} \quad (60)$$

That is, the system time constants are simply equal to the familiar single-zone time constants for each of the n uncoupled zones. The ratios defined by Equation (60) are sometimes referred to as the *nominal time constants* of the system. It follows from the Gerschgorin Theorem that the nominal time constants will provide, in general, a poorly bounded, but computationally inexpensive, estimate of the (real part of the) system time constants.

Degenerate case. In some cases, the so-called *degenerate* cases, it will not be possible to diagonalize the state matrix, but in these cases it will always be possible to transform the state matrix to a form known as the Jordan canonical form, an upper block-triangular matrix with the eigenvalues (inverse time constants) on the diagonal. It will, however, still be possible to express the general solution to the homogeneous problem as a combination of exponential decay terms, but now some of these decay terms will have factors equal to powers of time (i.e. in addition to terms like $e^{-t/\tau}$ we will have to include terms like $t e^{-t/\tau}$, $t^2 e^{-t/\tau}$, $t^3 e^{-t/\tau}$, etc.).

Stability. In all cases the system time constants will have positive real parts, as the state matrix is a non-singular M -matrix, and therefore all components making up the general solution will approach zero with time. That is to say, the homogeneous contaminant dispersal equations are *stable*; the concentration at all nodes will approach zero. Furthermore, following the argument similar to that presented earlier, we may show that the sum of the state matrix and its transpose is also a non-singular M -matrix with positive (real parts of) eigenvalues and, therefore, the sum of the squares of the system concentrations (i.e. the *Euclidean* norm of the concentration vector) will decay at every instant of time [22]:

$$\frac{d\|\{\tilde{C}(t)\}\|^2}{dt} < 0; \quad t \geq 0, \quad (61a)$$

where:

$$\|\{\tilde{C}(t)\}\|^2 = |\tilde{C}_1(t)|^2 + |\tilde{C}_2(t)|^2 + \dots + |\tilde{C}_n(t)|^2. \quad (61b)$$

These results are consistent with experience (and intuitive expectation) that while some nodal concentrations may at first increase with time (e.g. due to zone-to-zone mixing) in the long run all concentrations will diminish toward the zero level and at all times (some reasonable measure of) the mean concentration will also be diminishing.

Solution options

The governing system of equations (i.e. Equation (33) or Equation (47)) have the form of a system of first order linear differential equation with constant coefficients. In many practical situations, however, element mass flow

rates and/or element kinetics may not be constant in time, and thus, in general, the system transport matrix should be considered to be non-constant. Here we shall consider the solution of these equations for steady state behavior, free response behavior, and general dynamic behavior.

Steady-state behavior

For systems with steady element mass flows and steady kinetics driven by steady contaminant generation rates and/or specified concentrations the response of the system will, eventually, come to a steady state given by the solution of:

$$[\tilde{W}]\{\tilde{C}\} = \{\tilde{E}\}. \quad (62)$$

This equation may be solved by LU decomposition without pivoting in an efficient and numerically stable manner.

Free response behavior

The free response behavior of steady flow/kinetics systems has been discussed above and shown to be closely related to the solution of the eigenproblem given by Equation (55) that yields system time constants and associated eigenvectors.

For steady flow/kinetics systems, knowledge of the system time constants provides invaluable insight into the dynamic character of the system yet eigenanalysis is computationally demanding. As noted above, Equation (60) provides a poorly bounded, but computationally inexpensive, estimate of the (real part of the) system time constants. A variety of techniques exist that will provide better estimates of the system time constants (and eigenvectors if desired) [25, 26].

Dynamic behavior

The governing systems of equations, Equation (33), may be solved numerically for cases of steady flow/kinetics with general unsteady contaminant generation using any number of different finite difference solution schemes. Here we shall describe a scheme based upon the so-called *generalized trapezoid rule*.

We begin by dividing time domain into discrete steps:

$$t_{(n+1)} = t_{(n)} + \delta t \quad n = 0, 1, 2, \dots, \quad (63)$$

where: $t_{(0)}$ = initial time; δt = integration time step (often constant but may be variable). At the $(n+1)$ th step the instantaneous mass balance defined by Equation (33) may be written as:

$$[\tilde{W}]\{\tilde{C}\}_{(n+1)} + [\tilde{M}]\left\{\frac{d\tilde{C}}{dt}\right\}_{(n+1)} = \{\tilde{E}\}_{(n+1)}, \quad (64a)$$

where:

$$\{\tilde{C}\}_{(n+1)} \equiv \{\tilde{C}(t_{(n+1)})\}, \quad (64b)$$

$$\left\{\frac{d\tilde{C}}{dt}\right\}_{(n+1)} \equiv \frac{d\{\tilde{C}(t_{(n+1)})\}}{dt}, \quad (64c)$$

$$\{\tilde{E}\}_{(n+1)} \equiv \{\tilde{E}(t_{(n+1)})\}. \quad (64d)$$

Substituting into this equation the difference approximation based upon a generalization of the trapezoid rule:

$$\{\hat{C}\}_{(n+1)} \approx \{\hat{C}\}_{(n)} + (1-\theta)\delta t \left\{ \frac{d\hat{C}}{dt} \right\}_{(n)} + \theta\delta t \left\{ \frac{d\hat{C}}{dt} \right\}_{(n+1)}, \quad (65)$$

where: $0 \leq \theta \leq 1$; $\theta = 0$ corresponds to the *Forward Difference* scheme; $\theta = 1/2$ corresponds to the *Crank-Nicholson* scheme; $\theta = 2/3$ corresponds to the *Galerkin* scheme; $\theta = 1$ corresponds to the *Backward Difference* scheme.

A general implicit finite difference scheme is obtained that may be conveniently organized into a three step algorithm:

Step 1.

$$\{\tilde{C}\}_{(n+1)} \equiv \{\hat{C}\}_{(n)} + (1-\theta)\delta t \left\{ \frac{d\hat{C}}{dt} \right\}_{(n)}. \quad (66a)$$

Step 2.

$$[\theta\delta t[\tilde{W}] + [\tilde{M}]] \left\{ \frac{d\hat{C}}{dt} \right\}_{(n+1)} \approx \{\tilde{E}\}_{(n+1)} - [\tilde{W}]\{\tilde{C}\}_{(n+1)}. \quad (66b)$$

Step 3.

$$\{\hat{C}\}_{(n+1)} = \{\tilde{C}\}_{(n+1)} + \theta\delta t \left\{ \frac{d\hat{C}}{dt} \right\}_{(n+1)}. \quad (66c)$$

It should be noted that: (a) this algorithm is self-starting; given initial conditions, $\{\hat{C}\}_{(0)}$, Equation (64) may be solved to obtain an estimate of the initial rate of change of nodal temperatures, $\{d\hat{C}/dt\}_{(0)}$, and the first step, Equation (66a), may then be computed; (b) Equation (66b) may also be solved by LU decomposition, without the need of pivoting; importantly then, the matrix $[\theta\delta t[\tilde{W}] + [\tilde{M}]]$ may initially be factored into the $[L]$ and $[U]$ product matrices and need not be refactored again (until there is a change in the system transport matrix, as discussed below).

This scheme has been analysed by Huebner [12] and a more general predictor-multicorrector scheme that includes this *implicit* scheme has been analysed by Hughes [27] for systems with constant coefficient matrices. For $\theta \geq 1/2$ this scheme leads to an unconditionally stable solution and for $\theta \geq 3/4$ (approximately) leads to an unconditionally stable non-oscillatory solution.

For cases of unsteady flow/kinetics one may approximate the solution by updating the system transport during the numerical solution process to capture the change in the system equations. That is, we would replace Equation (66b) with:

$$[\theta\delta t[\tilde{W}]_{(m)} + [\tilde{M}]] \left\{ \frac{d\hat{C}}{dt} \right\}_{(n+1)} \approx \{\tilde{E}\}_{(n+1)} - [\tilde{W}]\{\tilde{C}\}_{(n+1)}, \quad (67)$$

where:

$$[\tilde{W}]_{(m)} \equiv [\tilde{W}(t_{(m)})]; \quad t_{(m)} \in \langle t_{(i)}, t_{(j)}, t_{(k)}, \dots \rangle,$$

and the system transport matrix would be updated (i.e. reformed or reasssembled) at the discrete times belonging to the set of times $t_{(m)}$ selected so that the changes of the transport matrix are well represented. Going one step farther, for non-linear kinetics, Equation (67) would

become a non-linear equation and could, conceivably, be solved using one of several non-linear solution algorithms.

IMPLEMENTATION AND APPLICATION

A program, CONTAM87, has been developed at the National Bureau of Standards to provide a first example of a computational implementation of the contaminant dispersal analysis theory presented above. CONTAM87 is the second member of the CONTAM series of programs [6, 7, 8] 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 the 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 air flows in building systems, and, eventually, building thermal analysis commands, based upon earlier work [8] 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 air flows in building systems. Here we shall present the results of two 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 storey office building are presently being conducted by the Indoor Air Quality and Ventilation Group at NBS. Some of these studies involve periodic injections of a commonly used tracer gas, SF₆, into the supply air ducts of the building HVAC system. Flows in the supply ducts were measured (with significant uncertainty) by hot-wire traverse. SF₆ concentration time histories were recorded, and fresh air infiltration was estimated by tracer decay. Using the air flow measurements the upper two floors of this building were idealized as shown in Fig. 7.

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 Fig. 8 we compare measured SF₆ 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. The first injection of tracer occurred ten minutes before the zero time indicated in Fig. 8, and was modeled as such. The actual response was not recorded, however, during this first ten minute interval. Presumably the system responded to this first injection in a manner similar to that seen for the next injection (i.e. at

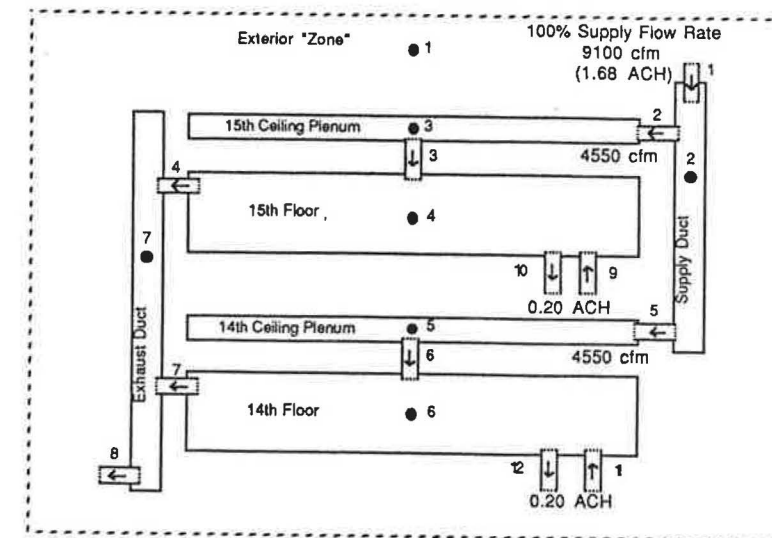


Fig. 7. Idealization of the 14th and 15th floors of an office building.

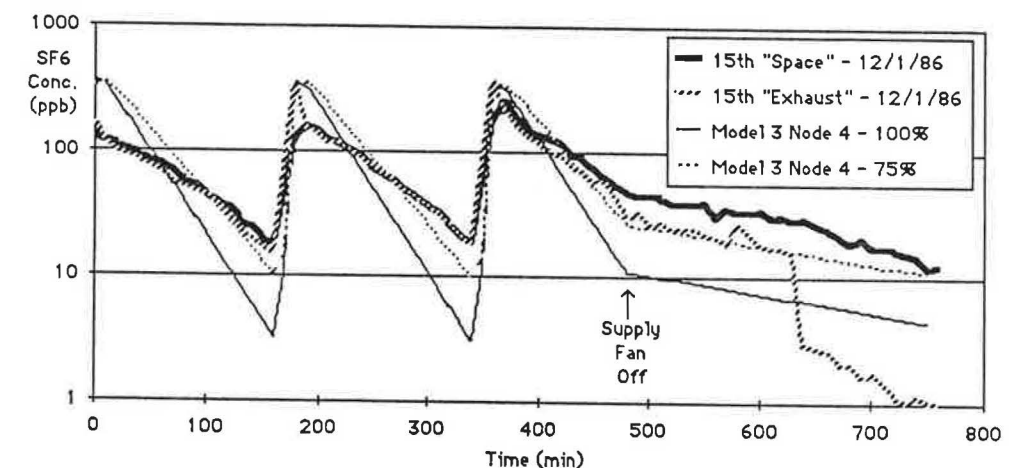


Fig. 8. Comparison of computed and measured response for an office building.

time ≈ 200 min in Fig. 8) and thus the apparent discrepancy between modeled and measured response at time zero is believed not to be significant. In this case, the agreement between measured and computed time histories is within the uncertainty of the measured flows and validation is therefore indicated.

Carnegie-Mellon townhouse study

Borrazzo and his colleagues at Carnegie-Mellon University have conducted detailed field investigations of a two-storey townhouse measuring CO, NO, and NO₂ 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 [28]. Illustrated in Fig. 9 is an idealization of the townhouse and in Fig. 10 the dynamic emission characteristics of the principal pollutant source; the gas range. The instantaneous emission rate, $G(t)$, is

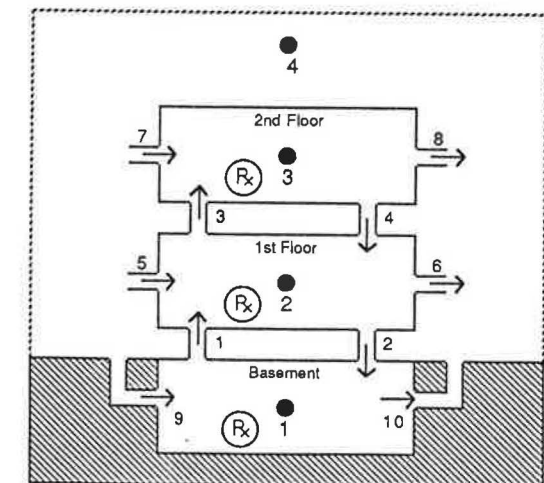


Fig. 9. Townhouse building idealization.

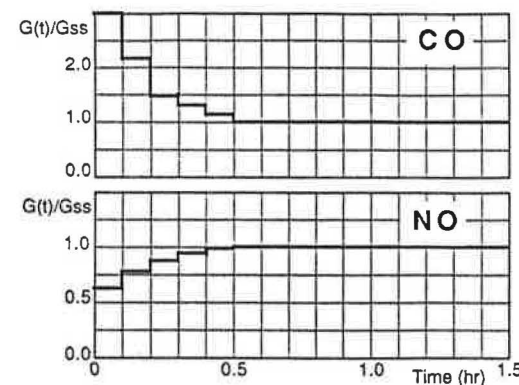


Fig. 10. Range emission characteristics.

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 $\kappa = 2.4 \text{ h}^{-1}$.

In Figs 11–13 we compare computed response with measured data. The details of air flow 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%). The computed response results were relatively insensitive to variations in the assumed first-to-second air exchange rate, more sensitive to variations in the distribution of infiltration and first-to-basement air exchange rates, and most sensitive to the dynamic details of the range emission characteristics. These range characteristics were reported to be very sensitive to the flow rate of fuel gas to the range. A relatively small reduction in the fuel gas flow rate could have corrected the under and over-predictions noted above.

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 the measured data was used to determine the reactivity constant the agreement here may be an artifice. The basis of determination of the reactivity and the basis of the computed response are more or less

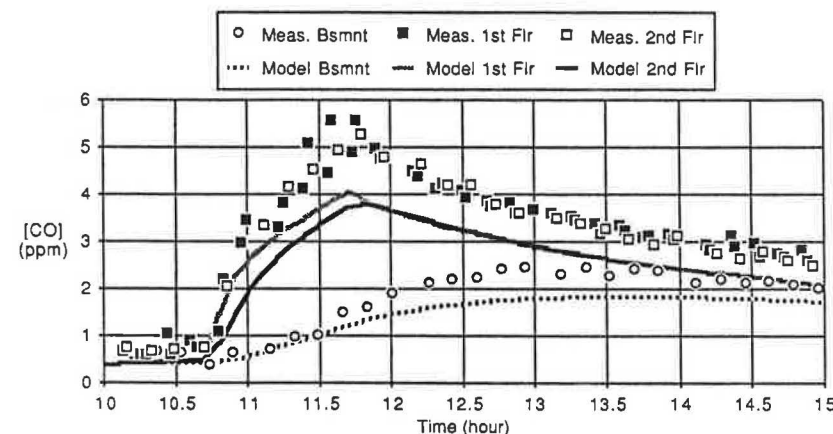


Fig. 11. Comparison of computed and measured CO response.

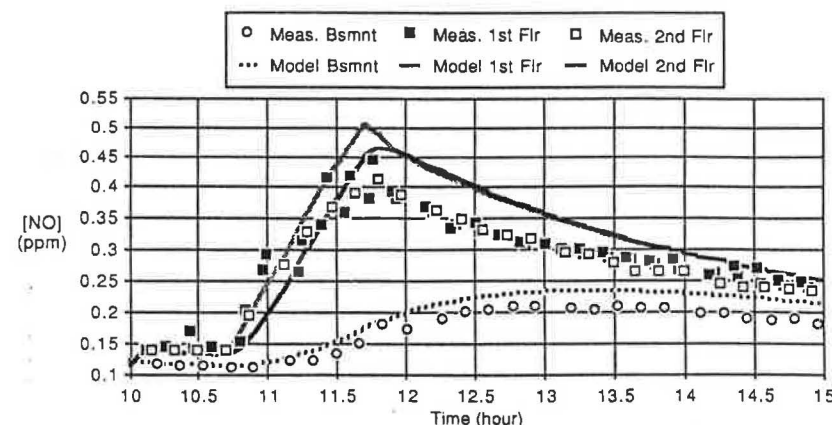
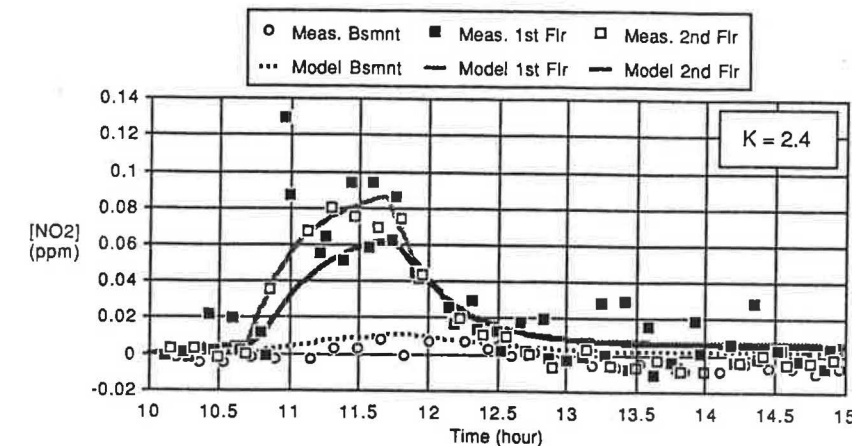


Fig. 12. Comparison of computed and measured NO response.

Fig. 13. Comparison of computed and measured NO_2 response (NO_2 reactivity = 2.4 h^{-1}).

the same as the system behaves, practically, as a single-zone system. Therefore the agreement may reflect no more than this.

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 account-

ing 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 [29] 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 air flow systems wherein a portion of the building air flow system would be modeled in detail using microscopic elements while the rest of the air flow 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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Analysis of Errors Associated with Passive Ventilation Measurement Techniques

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In small buildings where ventilation is the primary mechanism for removing indoor air pollutants, interest in converting the resulting energy load on the heating or cooling system of the building is significant. The desire of making field measurements of this time-varying quantity has led to the development of many approaches. The simplest one is called the passive ventilation measurement technique which typically measures the average concentration of a constantly emitted tracer gas from which the average ventilation rate can be estimated. This study relied on mathematical models combined with typical weather data to calculate how an ideal passive ventilation measurement would perform; simulations were then conducted based on two house types in four seasons and six climates. It was found that the passive technique significantly underpredicted the average ventilation and that the use of multiple tracers accomplished marginal improvement. Inadequate mixing was found to be a major impediment to the interpretation of the results and could completely invalidate the measurement. Not covered in this report are the additional errors associated with measurement uncertainty, instrumentation limitations and non-ideal experimental conditions.

NOMENCLATURE

A	air change (ventilation) rate (ach) (h^{-1})
\mathbf{A}	air change rate (matrix) (h^{-1})
C	instantaneous tracer volume concentration
\mathbf{C}	multizone tracer volume concentration (matrix)
ϵ	instantaneous ventilation efficiency
$\mathbf{\epsilon}$	multizone ventilation efficiency (matrix)
ϵ_m	mean ventilation efficiency (for a period of time)
$\mathbf{\epsilon}_m$	mean ventilation efficiency (matrix)
ϵ_o	overall multizone ventilation efficiency
η	distribution efficiency (matrix)
η_o	overall distribution efficiency
S	instantaneous (tracer) source strength (h^{-1})
\mathbf{S}	multizone (matrix) source strength (h^{-1})
σ_e	scatter in the multizone efficiency
t	time (h)
τ_e	instantaneous turn over time (h)
$\mathbf{\tau}_e$	multizone (matrix) turn over time (h)
Δt	discrete time step (h)
V_o	total volume of the building (m^3)
\mathbf{V}	(diagonal) room volume (matrix) (m^3)
\bar{X}	overbar: the time average of the instantaneous quantity X

INTRODUCTION

IN THE last few years the need for a simple and accurate way of measuring the average ventilation rates of large numbers of dwellings has increased. This growing demand has spurred the development of low-cost, long-term monitors that use an emitter, to provide a constant source of a tracer gas throughout the period of measure-

ment and a sampler to provide a time-averaged measurement of the tracer concentration. Any system that incorporates constant emission of tracer gas with a time-averaged concentration measurement, regardless of its physical details, falls into the category of a *passive ventilation measurement technique*.

Several different variations of this technique exist, but the most popular and generalizable system appears to be AIMS—the Average Infiltration Monitoring System. This system, which uses a tube filled with Per-Fluorocarbon Tracer (PFT) as an emitter and a diffusion-limited charcoal-like adsorber as a sampler, is the one to which most of the scientific [1], professional [2] and trade [3] refers. Although most studies reflect a fairly good understanding of the technique in highly controlled environments, large studies such as the Residential Standards Demonstration Program (RSDP) of the Bonneville Power Administration (BPA) are getting systematic differences, between the PFT and calculations based on leakage measurements, on the order of 50% [4]—a phenomenon that researchers do not understand.

It is the intent of this report to discuss some of the measurement errors associated with the generic technique—specifically, to quantify the errors caused by variations occurring in ventilation during the measurement period. We believe that much of the systematic under-prediction seen in the measurements obtained by these passive techniques, may be caused by this type of error.

BACKGROUND

In most small commercial buildings and virtually all residential buildings, unintentional air infiltration, or natural ventilation is the dominant mechanism for supplying fresh (i.e. outdoor) air. The rate of infiltration is

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