THE DEVELOPMENT OF MODELS FOR THE PREDICTION OF INDOOR AIR QUALITY IN BUILDINGS.

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ABSTRACT

The National Bureau of Standards has undertaken a research effort to develop a general indoor air quality simulation program for buildings. At present there exists three computer programs which can be used to analyze interzonal air movements in multizoned buildings and predict the level of contaminants due to a wide variety of contaminants. This paper will introduce the reader to the scientific and mathematical basis of the models, the preparation of building input data for these programs, and the use of the models for both residential and commercial buildings. Greater detail may be found in reference [1].

1. GENERAL CONSIDERATIONS

Airborne contaminants introduced into a building disperse throughout the building in a complex manner that depends on the nature of air movement in-to (infiltration), out-of (exfiltration), and within the building system, the influence of the heating, ventilating, and air conditioning (HVAC) systems on air movement, the possibility of removal, by filtration, or contribution, by generation, of contaminants, and the possibility of chemical reaction or physical-chemical reaction (e.g., adsorption or absorption) of contaminants with each other or the materials of the buildings construction and furnishings.

![Contaminant Dispersal in a Residence](image)

Fig. 1.1 Contaminant Dispersal in a Residence

Our immediate objective, here, is to develop a model of this dispersal process for building systems that comprehensively accounts for all phenomena that affect the actual contaminant dispersal process. We shall, however, attempt, to develop this modeling capability within a more general context so that techniques developed here may be extended to more complex problems of indoor air quality analysis. To this end, in this section, the problem is given a general definition and the basic modeling strategy used to address this problem is outlined.

1.1 Definition of Problem

The building air flow system may be considered to be a three dimensional field within which we seek to completely describe the state of infinitesimal air parcels. The state of an air parcel will be
defined by its temperature, pressure, velocity, and contaminant concentration (for each species of interest) - the state variables of the indoor air quality modeling problem.

Our immediate task is, then, to determine the spacial and temporal variation of the species concentrations within a building due to thermal, flow, and contaminant excitation driven by environmental conditions and the HVAC system and its control, given building characteristics and their control.

That is to say, we seek to determine;

\[ \alpha C(x,y,z,t) \] ; Contaminant "\( \alpha \)" Concentration

\[ \beta C(x,y,z,t) \] ; Contaminant "\( \beta \)" Concentration

... where;

- \( C \) = species mass concentration or mass fraction
- \( \alpha, \beta \) = species type indices
- \( x, y, z \) = spacial coordinates
- \( t \) = time

and shall refer to the process of determining the spacial and temporal variation of these species concentrations as contaminant dispersal analysis.

Contaminant dispersal analysis, for a single nonreactive species "\( \alpha \)", depends on the air velocity field and its variation with time;

\[ \alpha C(x,y,z,t) = \alpha C(\mathbf{v}(x,y,z,t)) \] & B.C. : Contam. Dispersal Anal. \hspace{1cm} (1.1)

But, the air velocity field depends on the pressure field which is affected by the temperature field thru buoyancy and, completing the circle, the temperature field is dependent on the velocity field;
Thus, in general, contaminant dispersal analysis, for a single nonreactive species, is complicated by a coupled nonlinear flow-thermal analysis problem. Therefore, a comprehensive indoor air quality model will eventually have to address the related flow and thermal problems.

For cases of reactive contaminants, contaminant dispersal analysis, itself, will become a coupled (and, generally, nonlinear) analysis problem as individual species' concentrations will depend on other species' concentrations in addition to the air velocity field:

\[ \alpha C(x,y,z,t) = \alpha C(v, \alpha C, \beta C, ...) \quad : \text{Species } \alpha \text{ Dispersal Analysis} \]  \quad (1.5a)

\[ \beta C(x,y,z,t) = \beta C(v, \alpha C, \beta C, ...) \quad : \text{Species } \beta \text{ Dispersal Analysis} \]  \quad (1.5b)

In this paper we shall focus on single, nonreactive species dispersal analysis and the associated problem of flow analysis, for a completely defined thermal field and its variation. The approach taken, however, has been formulated to be compatible with thermal analysis modeling techniques developed earlier [2]. Presently, we are addressing the reactive, multiple species dispersal analysis problem and see no difficulty with extending the approach to this more complex situation.

1.2 Modeling Approaches

We shall attempt to solve the general field problems posed above by attempting to determine the state of air at discrete points in the building air flow system. It will be shown that this spatial discretization allows the formulation of systems of ordinary differential equations that describe the temporal variation of the state fields. Two basic approaches may be considered, one based upon the microscopic equations of motion (i.e., continuity, motion, and energy equations for fluids) and the other based upon a "well-mixed" zone simplification of macroscopic mass, momentum, and energy balances for flow systems.

In the microscopic modeling approach one of several techniques of the generalized finite element method, which includes the finite difference method, could be used to transform the systems of governing partial differential equations into systems of ordinary differential equations that then can be solved using a variety of numerical methods. The macroscopic modeling approach leads directly to similar systems of ordinary differential equations.
In both approaches the building air flow system is modeled as an assemblage of discrete flow elements connected at discrete system nodes. Systems of ordinary differential equations governing the behavior of elements are then formed and assembled to generate systems of ordinary differential equations that describe the behavior of the system as a whole. These systems of equations may then be solved, given system excitation and boundary conditions, to complete the analysis.

Fig. 1.3 Basic Spacial Discretization Approaches

Virtually all computational procedures, except those used to form the element equations, would be practically identical for both approaches. From a practical point of view, however, microscopic modeling will involve on the order of 1000 nodes per room while the macroscopic model will involve on the order of only 10 nodes/room to realize acceptably accurate results. Consequently, the microscopic modeling approach can lead to extremely large systems of equations that therefore limit its use, at this time, to research inquiry. The macroscopic approach, resulting in systems of equations that are on the order of two magnitudes smaller than the microscopic approach, is a reasonable candidate for practical analysis, although it can not provide the detail of the microscopic approach.

Within this report we shall limit consideration to the macroscopic approach, although the specific techniques employed to implement this approach have been formulated to be compatible with the microscopic approach and it is expected that one may, in the future, be able to use both approaches in analysis to gain the benefits of detail in specific areas of the building system and yet account for full-system interaction.

1.3 The Well-Mixed Macroscopic Model

Here, the building air flow system shall be modeled as an assemblage of flow elements connected to discrete system nodes corresponding to well-mixed air zones.
 Limiting our attention to the contaminant dispersal and flow analysis problems we associate with each system node the discrete variables or degrees of freedom (DOFs) of pressure, air mass generation (typically zero), species concentration, species mass generation, and temperature;

\[
\begin{align*}
\{P\} & = \{P_1, P_2, P_3, \ldots \} : \text{Pressure DOFs} \\
\{W\} & = \{W_1, W_2, W_3, \ldots \} : \text{Air Mass Generation DOFs} \\
\{^{\alpha}C\} & = \{^{\alpha}C_1, ^{\alpha}C_2, ^{\alpha}C_3, \ldots \} : \text{Species Conc. DOFs} \\
\{^{\alpha}G\} & = \{^{\alpha}G_1, ^{\alpha}G_2, ^{\alpha}G_3, \ldots \} : \text{Species Gen. DOFs} \\
\{T\} & = \{T_1, T_2, T_3, \ldots \} : \text{Temp. DOFs}
\end{align*}
\]

as well as the key system characteristic of nodal volumetric mass, \(V_1, V_2, V_3, \ldots\). The pressure, concentration, and temperature DOFs will approximate the corresponding values of the state field variables at the spacial locations of the system nodes.

With each element "e" in the system assemblage we note the element connectivity - the system nodes that the element connects - and identify an element air mass flow rate, \(w^e\). The element mass flow rates will be related to the nodal state variables through specific properties associated with each particular element to form element equations.

In the formulation of both the contaminant dispersal model, presented in Section 2, and the flow model, presented in Section 3, we will assemble the governing element equations to form equations governing the behavior of the building system as a whole - the system equations - by demanding conservation of mass flow at each system node.

2. Contaminant Dispersal Analysis

In this section contaminant dispersal element equations are formulated. Demanding continuity of mass flow at each system node these element equations are then assembled to form contaminant
dispersal equations governing the behavior of the full building system. Finally, methods for solution of the system equations are outlined.

2.1 Element Equations

Two nodes and a total mass flow rate, \( w^e \), will be associated with each flow element, where flow from node \( i \) to \( j \) is defined to be positive. An element species concentration, \( C^e_k \), and an element species mass flow rate, \( W^e_k \), will be associated with each element node, \( k=i, j \). The element species mass flow rate is defined so that flow from each node into the element is positive.

\[ \{aW^e\} = W^e \begin{bmatrix} 1 & 0 \\ -1 & 0 \end{bmatrix} \{aC^e\} \quad ; \text{for} \; w^e \geq 0 \]  \hspace{1cm} (2.1a)

\[ \{aW^e\} = W^e \begin{bmatrix} 0 & -1 \\ 0 & 1 \end{bmatrix} \{aC^e\} \quad ; \text{for} \; w^e \leq 0 \]  \hspace{1cm} (2.1b)

or

\[ \{aW^e\} = [f^e] \{aC^e\} \]  \hspace{1cm} (2.1c)

where;
\[ \{aW^e\} = \{aW_i^e, aW_j^e\}^T \]  \hspace{1cm} ; \text{element species mass flow rate vector}
\[ \{aC^e\} = \{aC_i^e, aC_j^e\}^T \]  \hspace{1cm} ; \text{element species concentration vector}

\[ [f^e] = \text{element total mass flow rate matrix} \]

\[ = W^e \begin{bmatrix} 1 & 0 \\ -1 & 0 \end{bmatrix} \quad ; \text{for} \; w^e \geq 0 \]  \hspace{1cm} (2.1d)

\[ = W^e \begin{bmatrix} 0 & -1 \\ 0 & 1 \end{bmatrix} \quad ; \text{for} \; w^e \leq 0 \]  \hspace{1cm} (2.1e)
If the element acts as a filter and removes a fraction, $\eta$, of the contaminant passing thru the filter then the element flow rate matrix becomes:

\[
[f^e] = \text{element total mass flow rate matrix}
\]

\[
= w^e \begin{bmatrix} 1 & 0 \\ (\eta-1) & 0 \end{bmatrix} ; \text{ for } w^e \geq 0 \tag{2.1f}
\]

\[
= w^e \begin{bmatrix} 0 & (\eta-1) \\ 0 & 1 \end{bmatrix} ; \text{ for } w^e \leq 0 \tag{2.1g}
\]

The fraction, $\eta$, is commonly known as the "filter efficiency" and may have values in the range of 0.0 to 1.0.

### 2.2 System Equations

System equations that relate the system concentration DOFs, \{â©c\}, to the system generation DOFs, \{â©g\}, may be assembled from the element equations by first transforming the element equations to the system DOFs and then demanding conservation of species mass flow at each system node.

There exists a one-to-one correspondence between each element's concentration DOFs, \{â©c\}, and the system concentration DOFs, \{â©c\}, that may be defined by a simple Boolean transformation;

\[
\{â©c\} = [â©B]^e \{â©C\}
\]

where;

\[
[â©B]^e \text{ is an } m \times n \text{ Boolean transformation matrix consisting of zeros and ones; } m = \text{the number of element nodes (here, } m=2); n = \text{the number of system nodes}
\]

For example, an element with nodes 1 & 2 connected to system nodes 5 & 9, respectively, of a 12-node system would have ones in the 1st row, 5th column and the 2nd row, 9th column and all other elements of the 2 x 12 Boolean transformation matrix would be set equal to zero.

In a similar manner, we may define a "system-sized vector" to represent the net species mass flow rate from the system node into an element "e", \{â©w\}, and relate it to the corresponding element species mass flow rate using the same transformation matrix, as;

\[
\{â©w\} = [â©B]^e \{â©w\}
\]

For an arbitrary system node n, with connected elements "a", "b", ... as indicated below in Fig. 2.2, we then demand conservation of species mass as;

\[
\left( \sum \text{connected elements} \text{ (elem. species mass flow)} \right) + \left( \text{rate of change of species mass} \right) = \left( \text{generation of species mass} \right)_{\text{system node } n}
\]

\[
\left( \begin{array}{l}
\text{rate of change of species mass} \\
\text{generation of species mass}
\end{array} \right)_{\text{system node } n}
\]

\[
\text{connected elements}
\]

\[
\text{elem. species mass flow}
\]

\[
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\]
or, for the system as a whole;

\[ \sum_{e = a, b, ...} \{ \alpha^{a} \} + \{ V \} \left( \frac{d^{a} C}{dt} \right) = \{ \alpha G \} \]  

(2.6)

where:

\[ [V] = \text{diag}(V_1, V_2, ...) \quad ; \text{the system volumetric mass matrix} \]

\[ V_i = \text{the volumetric mass of node } i \]

Fig. 2.2 Conservation of Species \( \alpha \) Mass Flow at System Node \( n \)

Substituting relations (2.2) and (2.3) we obtain the final result;

\[ [F] \{ \alpha C \} + [V] \left( \frac{d^{a} C}{dt} \right) = \{ \alpha G \} \]  

(2.7a)

where:

\[ [F] = \sum_{e = a, b, ...} \left( [\alpha B^e]^T [f^e] [\alpha B^e] \right) \]  

(2.7b)

= the system mass flow matrix

= \( A[f^e] \) ; the direct assembly sum of element flow matrices

Equation (2.7a) defines the contaminant dispersal behavior of the system as a whole and is said to
be assembled from the element equations through the relation given by equation (2.7b). The assembly process, as formally represented in equation (2.7b), has found widespread application in the simulation of systems governed by conservation principles and is, therefore, often represented by the so-called assembly operator A as indicated above. It should be noted that while the formal representation of the assembly process is important from a theoretical point of view, it is generally far more efficient, computationally, to assemble the element equations directly, without explicitly transforming them (see, for example, the "LM Algorithm" in [3]).

2.3 Boundary Conditions and Solution of System Equations

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 continuum model and will, therefore, be referred to as such. Formally then, we may distinguish between those DOFs for which concentration will be specified, \( \{\alpha C_c\} \), and those for which generation rate will be specified, \( \{\alpha C_g\} \), and partition the system of equations accordingly;

\[
\begin{bmatrix}
F_{cc} & F_{cg} \\
F_{gc} & F_{gg}
\end{bmatrix}
\begin{bmatrix}
\alpha C_c \\
\alpha C_g
\end{bmatrix}
+ 
\begin{bmatrix}
V_{cc} & 0 \\
0 & V_{gg}
\end{bmatrix}
\begin{bmatrix}
d\alpha C_c \\ dt \\
d\alpha C_g \\ dt
\end{bmatrix}
= 
\begin{bmatrix}
\alpha G_c \\
\alpha G_g
\end{bmatrix}
\]

(2.8)

Using the second equation and simplifying we obtain;

\[
[F_{gg}]\{\alpha C_g\} + [V_{gg}]\{\frac{d\alpha C_g}{dt}\} = \{\alpha G_g\} - [F_{gc}]\{\alpha C_c\} 
\]

(2.9a)

or

\[
[\hat{F}]\{\alpha \hat{C}\} + [\hat{V}]\{\frac{d\alpha C}{dt}\} = \{\alpha \hat{E}\} 
\]

(2.9b)

where;

\[
[\hat{F}] = [F_{gg}] ; \text{ the generation driven mass flow matrix}
\]

\[
\{\alpha \hat{C}\} = \{\alpha C_g\} ; \text{ the generation driven nodal concentration vector}
\]

\[
\{\alpha \hat{E}\} = \{\alpha G_g\} - [F_{gc}]\{\alpha C_c\} ; \text{ the system excitation}
\]

(2.9c)

It should be noted that the response of the system is driven by the system excitation involving both specified contaminant mass generation rates and contaminant concentrations which may, in general, vary with time.

Equation (2.9b) most directly defines the contaminant dispersal behavior of the system. The formation and solution of equation (2.9b) will be considered the central task of contaminant dispersal analysis. Three classes of solution are important;

a) steady state solution for conditions of steady flow and excitation,
b) dynamic solution for arbitrary system excitation and flow variation, and
c) the associated eigen solution, defined only for conditions of steady flow, that provides the steady-flow system time constants.

It may be shown that the generation driven mass flow matrix is a nonsingular matrix of a special form, a nonsingular “M-matrix” [1], and as a result computationally efficient numerical methods based on LU decomposition of the generation driven mass flow matrix may be used to solve both the steady state and dynamic problems. The eigen solution is computationally more difficult.

3. Air Flow Analysis

In this section air flow element equations are formulated that relate mass flow rate through flow elements to pressure differences across the elements, the assembly of these element equations to form equations governing the flow behavior of the building air flow system is discussed, and methods of solving these equations are outlined. The formulation of the air flow equations presented herein is based, in large part, on the work of Walton [4], an example presented by Camahan et. al. [5], and Chapter 33 of the ASHRAE Handbook 1985 Fundamentals [6].

3.1 Pressure Variation within Zones

For the well-mixed macroscopic model, fluid density within any zone i, \( \rho_i \), will be assumed constant and thus the variation of static pressure within a zone, \( p_i(z) \), will be given by:

\[
p_i(z) = p_i + \frac{q}{g_c} \rho_i (z_i - z)
\]

where;

- \( z_i \) = the elevation of node i relative to an arbitrary datum
- \( z \) = elevation relative to an arbitrary datum
- \( g \) = the acceleration due to gravity
- \( g_c \) = dimensional constant (1.0 \( \text{kg m/} \text{N s}^2 \))

Static pressures (i.e., under still conditions) acting on exterior surfaces may be approximated as:

\[
p(z) = p_a - \frac{q}{g_c} \rho_a z
\]

where \( p_a \) and \( \rho_a \) are the atmospheric pressure and air density at the level of the outdoor datum.

To account for pressures due to wind effects the pressure on any exterior surface may be approximated using published wind pressure coefficients [6] as:

\[
p(z) = p_a + C_p \frac{\rho_a U^2}{2}
\]

where \( p_a \) and \( \rho_a \) are the atmospheric pressure and air density at the level of the outdoor datum.
where $C_p$ is a dimensionless pressure coefficient associated with the position on the exterior surface and the characteristics of the wind and $U_H$ is the wind speed at the roof level of the building.

![Diagram](image.png)

**Fig. 3.1 Elevations Defined Relative to a Datum**

### 3.2 Element Equations

Two classes of flow elements have been developed; *flow resistance elements* and *fan/pump elements*. The theoretical basis of the flow resistance element will be outlined here; the reader is referred to [1] for the development of the fan/pump element.

The flow resistance element is a very general element that may be used to model a large variety of flow paths that provide passive resistance to flow (e.g., conduits, ducts, ductwork assemblies, small orifices such as cracks, etc.); the fan/pump element may be used to model HVAC fans given the performance characteristics of a specific fan. These two classes of elements should allow modeling of a large variety of complex and complete building airflow systems.

Resistance to flow will be modeled by flow elements having a single entry and exit (e.g., simple ducts, openings between zones, orifices, etc.). Flow components with multiple entries, exits, or both may be modeled by assemblages of these simpler elements.

Flow resistance elements shall be two-node elements. With each node we associate element pressure, $P^e$, temperature, $T^e$, and flow rate, $W^e$, DOFs (i.e., for flow from the node into the element).

Fluid flow within each flow resistance element is assumed to be incompressible, isothermal, and governed by the Bernoulli equation as applied to duct design [6];

$$
(P_1 + \frac{\rho v_1^2}{2g_c}) - (P_2 + \frac{\rho v_2^2}{2g_c}) + \frac{\rho}{g_c} (Z_1^e - Z_2^e) = \sum \Delta P_e
$$

(3.4)
Where, for the purposes of developing the general element equations, the more conventional flow variables, indicated below, have been used:

- \( P_1, P_2 \) = entry and exit pressures, respectively
- \( V_1, V_2 \) = entry and exit mean velocities, respectively
- \( g_c \) = dimensional constant, \( 1.0 \text{ (kg-m)/(N-sec}^2) \)
- \( g \) = the acceleration of gravity (e.g., \( 0.980665 \text{ m/sec}^2 \))
- \( \rho \) = density of fluid flowing through the element
- \( z_1, z_2 \) = elevations of entry and exits, respectively
- \( \dot{w} \) = mass flow rate through the element
- \( \Sigma \Delta P_0 \) = the sum of all frictional and dynamic losses in the elements

The losses, \( \Sigma \Delta P_0 \), are commonly related to the velocity pressure, \( \rho V_o^2 / 2g_c \), of the fluid flow at reference cross sections, as:

\[
\Delta P_o = C_o \frac{\rho V_o^2}{2g_c}
\]

where; \( C_o \) = loss coefficient

Thus the loss sum takes the form:
Recognizing the mass flow rate, \( \dot{w}^e \), at each of these sections must be equal;

\[
\sum \Delta \rho = \left( \frac{1}{2g_c} \right) \left( C_o^2 \rho v_o^2 + C_p^2 \rho v_p^2 + C_q^2 \rho v_q^2 + \ldots \right) \tag{3.6}
\]

Equation (3.6) may be rewritten in terms of mass flow rate as;

\[
\sum \Delta \rho = \frac{d}{g_c} \rho v = \ldots = \rho V A_1 = \ldots = \rho V A_0 = \rho V A_p = \rho V A_q = \ldots = \rho V A_2 \tag{3.7}
\]

and equation (3.4) then simplifies to;

\[
(P_1 - P_2) + \frac{d}{g_c} \rho (z_1 - z_2) = C^e (\dot{w}^e)^2 \tag{3.9}
\]

where;

\[
C^e = \frac{1}{2g_c} \left( \rho - \ldots - \rho + \rho + \rho \right) \tag{3.10}
\]

Equation (3.9) may now be rewritten in terms of the element pressure DOFs, using equation (3.1), as;

\[
(P_m^e - P_n^e) + \frac{d}{g_c} \rho (z_m - z_1^e) + \rho (z_1^e - z_2^e) + \rho (z_2^e - z_n^e) = C^e (\dot{w}^e)^2 \tag{3.11}
\]

Introducing a new variable, \( B^e \), for the bouyancy induced pressure component;

\[
B^e = \frac{d}{g_c} \rho (z_m - z_1^e) + \rho (z_1^e - z_2^e) + \rho (z_2^e - z_n^e) \tag{3.12}
\]

Equation (3.11) may be rewritten as;

\[
|\dot{w}^e| = (C^e)^{-1/2} \left( |P_m^e - P_n^e + B^e| \right)^{1/2} \tag{3.13a}
\]

or
where

\[ w^e = a^e (P_m^e - P_n^e) + a^e B^e \]  
(3.13b)

where:

\[ a^e = (C^e | P_m^e - P_n^e + B^e | )^{-1/2} \]  
(3.13c)

where the second form, equations (3.13b) and (3.13c), will provide the correct sign for \( w^e \).

**Variation of Flow With Zone Pressure**

It is useful, at this point, to develop analytical expressions for the variation of mass flow with zone pressure. This expressions will be seen to be useful for solving the nonlinear flow system equations using schemes based upon the classical Newton-Raphson iteration method. Therefore, from equations (3.13b) and (3.13c) we obtain;

\[
\frac{\partial w^e}{\partial P_m^e} = -\frac{1}{2} (C^e)^{-3/2} \frac{\partial C^e}{\partial P_m^e} ( | P_m^e - P_n^e + B^e | )^{1/2} + \frac{1}{2} (C^e)^{-1/2} ( | P_m^e - P_n^e + B^e | )^{-1/2} \]  
(3.14a)

and from equation (3.10) we obtain;

\[
\frac{\partial C^e}{\partial P_m^e} = \frac{1}{2} q_c \rho (A_o^{-2} \frac{\partial C_o}{\partial P_m^e} + A_p^{-2} \frac{\partial C_p}{\partial P_m^e} + A_q^{-2} \frac{\partial C_q}{\partial P_m^e} + \ldots) \]  
(3.15a)

\[
\frac{\partial C^e}{\partial P_n^e} = \frac{1}{2} q_c \rho (A_o^{-2} \frac{\partial C_o}{\partial P_n^e} + A_p^{-2} \frac{\partial C_p}{\partial P_n^e} + A_q^{-2} \frac{\partial C_q}{\partial P_n^e} + \ldots) \]  
(3.15b)

that is, the variation of \( C^e \) with pressure is simply a weighted sum of the variation of individual pressure loss coefficients contributing to the total pressure loss along the element. Analytical expressions for these partial derivatives of the pressure loss coefficients are not easily formulated, but by considering limiting cases of flow we can gain some insight.

In general, the loss coefficients depend, in a rather complex and poorly understood way, upon the nature of flow, as indicated by the Reynolds number, \( Re \), and detailed characteristics of the flow geometry (e.g., roughness, constrictions, etc.). For many situations, however, the loss coefficients are practically constant for the limiting case of fully turbulent flow (i.e., \( Re > 10^6 \)), at one extreme, and proportional to \( 1/Re \) for laminar flow (i.e., \( Re < 2 \times 10^5 \)) at the other;

\[
C_o = \text{constant for fully developed turbulent flow} \]  
(3.16)

\[
C_o = C_o' Re = C_o' \mu / D_o V_o \text{ for fully developed laminar flow} \]  
(3.17)
where; \( C_{o} \) = constant

In fully developed turbulent flow, with each of the pressure loss coefficients constant, the partial derivatives of equations (3.15) become zero and consequently the first term of equations (3.14) becomes zero and, using equations (3.13), may be simplified to;

\[
\frac{\partial w}{\partial \rho_{m}} = \frac{1}{2} \frac{\partial a}{\partial \rho_{m}} \quad ; \text{for fully turbulent flow} \\
\frac{\partial w}{\partial \rho_{n}} = -\frac{1}{2} \frac{\partial a}{\partial \rho_{n}} \quad ; \text{for fully turbulent flow}
\]

Limiting consideration to flow resistance elements of constant cross-section, we may formulate a modified expression for laminar flow in an element, in a manner similar to that used to formulate equations (3.13). We obtain;

\[
w \approx a_{L} \left( \frac{\rho_{m} - \rho_{n}}{\rho_{m}} \right) + a_{L} b_{e}
\]

where:

\[
a_{L} = (2g_{o}p/\mu)(\frac{C_{o}^{*}}{D_{o}A_{o}} + \frac{C_{p}^{*}}{D_{p}A_{p}} + \frac{C_{q}^{*}}{D_{q}A_{q}} + ... )
\]

for which the evaluation of the variation of flow with pressure is straightforward;

\[
\frac{\partial w}{\partial \rho_{m}} = a_{L} \quad ; \text{laminar flow, constant cross section} \\
\frac{\partial w}{\partial \rho_{n}} = -a_{L} \quad ; \text{laminar flow, constant cross section}
\]

It is instructive to compare the fully turbulent flow equation, equation (3.13) with \( C_{o} \) constant, with this particular case (i.e., constant cross section) fully laminar flow equation as shown in figure 3.4 below.

It is seen that \( a_{o} \), the tangent slope of the fully turbulent curve, becomes unbounded as flow approaches zero-flow conditions while \( a_{L} \) does not.

If the variations of the pressure loss coefficients, \( C_{o} \), \( C_{p} \), \( C_{q} \), ... , with flow are well defined (i.e., for conduits: if the friction factor relations are reliable) then the flow defined by equations (3.13) should asymptotically approach these two curves at the upper and lower limits of flow. (Note: this is not to say that these two curves provide an upper or lower bound to flow magnitude, in fact, they do not.

Our purpose, here, is not to use these limiting-case flow relations in place of the more general relation of equations (3.13), but rather to use these limiting cases to provide an estimate of the variation of element flow with zone pressure to be used in nonlinear solution algorithms.
Specifically, we shall only employ equations (3.19) and (3.20) for very low flow conditions, when the more general expression for flow, equation (3.13b), and the approximation for the variation of flow with pressure, equations (3.18), will tend to become unbounded.

\[ w^e = a^e \left( \frac{P^e - P^e_0}{m^n} + B^e \right) \]

**Fig. 3.4 Limiting Case Flow Relations - Elements of Constant Cross-Section**

**Matrix Formulation of the Element Flow Equations**

The element equations may be recast into matrix form, using the element DOFs defined above, by first noting:

\[ w^e = w^e_m = -w^e_n \]

thus;

\[ \{w^e_{\text{net}}\} = \{a^e\} \{P^e\} + \{w^e_B\} \]  \hspace{1cm} (3.22a)

where;

\[ \{w^e_{\text{net}}\} = (w^e_m, w^e_n)^T \]  \hspace{1cm} (3.22b)

= the element net mass flow rate vector

\[ \{P^e\} = (P^e_m, P^e_n)^T \]  \hspace{1cm} (3.22c)

= the element pressure vector
\[
\begin{align*}
[a^e] &= a^e \begin{bmatrix} -1 & -1 \\ -1 & 1 \end{bmatrix} & \text{for all but very low flow conditions} \\
\ &= a^e \begin{bmatrix} -1 & -1 \\ -1 & 1 \end{bmatrix} & \text{for very low flow conditions} \\
\ &= \text{matrix of pressure-flow coefficients}
\end{align*}
\]

\[
\{w_B^e\} = a^e B^e \begin{bmatrix} 1 & -1 \end{bmatrix}^T & \text{for all but very low flow conditions} \\
\ &= a^e L^e B^e \begin{bmatrix} 1 & -1 \end{bmatrix}^T & \text{for very low flow conditions} \\
\ &= \text{bouyancy-induced mass flow rate vector}
\]

and;

\[
\frac{\partial \{w_{\text{net}}^e\}}{\partial \{P^e\}} = \frac{a^e}{2} \begin{bmatrix} -1 & -1 \\ -1 & 1 \end{bmatrix} & \text{for all but very low flow conditions} \\
\ &= a^e L^e \begin{bmatrix} -1 & -1 \\ -1 & 1 \end{bmatrix} & \text{for very low flow conditions}
\]

The element pressure-flow coefficients \(a^e\) and \(a_L^e\) are defined in such a way that they are always positive, therefore, the matrix of pressure-flow coefficients will be positive semi-definite.

Some complicating details deserve special note;

a) the direction of flow will be determined by the sign of \((P_m^e - P_n^e + B^e)\); if positive, the flow will be from \(m\) to \(n\),

b) the density \(\rho\), of the fluid flowing through the element, will depend on the direction of flow;

\[
\rho = \rho_m & \text{ for flow from } m \text{ to } n \\
\rho = \rho_n & \text{ for flow from } n \text{ to } m
\]

c) the flow coefficient, \(C^e\), will also depend on the direction of flow due to the dependency of \(\rho\) on direction and the dependency of the pressure loss coefficients \(C_0\) that also, in general, depend on the direction of flow,

d) the pressure-flow coefficient matrix \([a^e]\) will also be flow-direction dependent due to the flow-direction dependency of \(C^e\) and \(B^e\),

e) equation (3.22a) is highly nonlinear due to the flow-direction dependencies, noted above, the dependency of the pressure-flow coefficient matrix \([a^e]\) and the bouyancy-induced mass flow.
rate vector \( \{w_B^e\} \) on the pressure, and the dependency of density on fluid temperatures which are, in turn, dependent on the rate of flow.

### 3.3 System Equations and Their Solution

Element equations similar to those presented above may be developed for a fan/pump element [1]. Flow resistance and fan/pump element equations, for a given flow system idealization, may then be assembled by demanding the conservation of mass at each system node to form system flow equations:

\[
\{W\} = [A]\{P\} + \{W_B\} + \{W_O\}
\]

where:

\[
[A] = A[a^e] ; \text{the assembly of element matrices} \quad (3.24b)
\]

\[
\{W_B\} = A\{w_B^e\} ; \text{the assembly of element bouyancy vectors} \quad (3.24c)
\]

\[
\{W_O\} = A\{w_O^e\} ; \text{the assembly of fan free-delivery flow vectors} \quad (3.24d)
\]

The derivation of equation (3.24a) is similar to that used in the derivation of the contaminant dispersal equations (2.7a) and, again, solution will require the specification of at least one pressure boundary condition - a single zone's pressure will suffice.

Equation (3.24a) defines the flow analysis problem. It is assembled from nonlinear element equations and, therefore, is nonlinear. Two classic nonlinear solution strategies and their variations;

a) Method of Successive Substitutions or Fixed-Point Iteration
   - Direct
   - Jacobi Iteration
   - Zeid's Modified Jacobi Iteration
   - Gauss-Seidel Iteration
   - Successive Overrelaxation Method
b) Newton-Raphson Method
   - Classic Newton-Raphson Method
   - Modified Newton-Raphson Method

as well as incremental formulations of these methods, provide reasonable candidates for solving this system of nonlinear flow equations.

### 4. CONTAM86

CONTAM86 is the first program in a series of programs being developed to implement the NBS indoor air quality model; it is an implementation of the nonreactive contaminant dispersal theory presented above and is written in ANSI Standard FORTRAN77 with IBM PC™ and Apple Macintosh™ version available. Other programs currently under development include AIRMOV, a
partial implementation of the flow analysis theory presented above, CONTAM87 a FORTRAN 77 extension of CONTAM86 that allows consideration of reactive contaminant dispersal, and CONTAMEZ a C language adaptation of the CONTAM family designed to be particularly user friendly.

With CONTAM86 the analyst may consider steady state analysis, system time constant analysis for conditions of steady flow, and dynamic analyses for arbitrary conditions of unsteady flow and unsteady system excitation. Nonreactive contaminant dispersal systems of arbitrary complexity may be modeled with system size limited only by available memory.

CONTAM86 is a command processor; it responds to commands in the order that they are presented and processes data associated with each command. Commands may be presented to the program interactively, using keyboard and monitor, or through the use of command/data input files; that is to say, it offers two modes of operation - interactive and batch modes.

For most practical problems of contaminant dispersal analysis the batch mode of operation will be preferred. For these problems, analysis involves three basic steps;

**Step 1: Idealization of the Building System and Excitation**

![Diagram showing actual building and airflow system idealization](image)

**Actual Building**  
**Air-Flow System Idealization**

Fig. 4.1 Idealization of the Building System and Excitation

Idealization of the building flow system involves;

a) discretization of the system as an assemblage of appropriate flow elements connected at system nodes,
b) identification of boundary conditions, and
c) numbering of system nodes optimally (i.e., to minimize the bandwidth - node number difference - of system equations).

The excitation (i.e., specified contaminant concentrations and generation rates) may be modeled to be steady or defined in terms of arbitrary time histories. For the latter case initial conditions of nodal contaminant concentration will have to also be specified.
**Step 2: Preparation of Command/Data Input File**

![Diagram showing the process of preparing input file](image)

In the batch mode, the program reads ASCII text files of commands and associated data, collected together in distinct data groups, that define the building flow idealization and excitation. The command/data input file may be prepared with any available ASCII text editing program and given a file name, `<filename>`, specified by the user. The `<filename>` must, however, consist of 8 or less alphanumeric characters and cannot include an extension (i.e., characters separated from the filename by a period, ".").

**Step 3: Execution of CONTAM86**

![Diagram showing the execution of CONTAM86](image)

CONTAM86 is then executed. Initially CONTAM86 will be in the interactive mode. To enter the batch mode the command "SUBMIT F=<filename>" may be used to "submit" the command/data input file to the program. The program will then proceed to form element and system arrays and compute the solution to the posed problem. CONTAM86 reads the ASCII command/data input file and creates an ASCII (i.e., printable) output file `<filename>.OUT`. The results of an analysis, `<filename>.OUT`, may be conveniently reviewed using an ASCII editor and, from the editor, portions or all of the results may be printed out. Key response results are also written to the ASCII file `<filename>.PLT` in a format that may easily be transferred to some spreadsheet and plotting programs (i.e., data values within each line are separated by the tab character) for plotting or subsequent processing.

**Introductory Example**

Consider the two-story residence with basement shown, in section, below. In this residence interior air is circulated by a forced-air furnace and exterior air infiltrates the house through leaks around the two first floor windows. The flow system may be idealized using flow elements to model the
ductwork, room-to-room, and infiltration flow paths as shown below.

For this example, CO₂ generated in one room of a two story four room residence is dispersed throughout the building by the hot-air system and diluted by outside air infiltration at the rate of 0.5 ACH in the two lower rooms. The CO₂ is generated by a portable kerosene heater operated for 133 minutes and then turned off. The results of the analysis are plotted below illustrating the detailed dynamic variation of pollutant concentration in the building air flow system.

The CONTAM command/data input file used for this study is listed below.
5. **AIRMOV**

The solution of the simultaneous mass balance equations is presently accomplished by the computer program AIRMOV. This program was originally a series of subroutines in the Thermal Analysis Research Program (TARP) developed by George Walton of the National Bureau of Standards [4]. There are two versions of the program which are presently distributed: AIRMOV4 and AIRMOV10. AIRMOV4 is a Fortran-77 version which can be compiled and run on an IBM-PC compatible computer using the IBM Professional Fortran compiler. AIRMOV10 is a Pascal version which has been compiled using TURBO-Pascal on the IBM-PC. AIRMOV4 can handle up to 1000 openings and up to 50 zones. AIRMOV10 uses the dynamic memory allocation procedures available in Pascal and has no practical limitation as to the number of zones or openings. AIRMOV10 has also
taken advantage of the more sophisticated data structure possible in a structured language such as Pascal to implement a series of linked lists for storing the zone and opening data. A laminar flow model is also used for pressure differences across an opening of less than 0.1 Pa. This not only more closely approximates the physical flow through an opening, but also greatly improves the convergence of the numerical solution of the nonlinear equations for the conditions of small induced pressures (low wind or small temperature differences) or large openings (such as open doorways or open windows).

**Input Data**

The input file for AIRMOV must be called AIRMOV.DTA. A sample for a model of a two story office building is included. This office building is modeled as 6 zones. Each floor has two zones: an occupied zone and the ceiling plenum. The other two zones are the two stairwells which are treated as one zone and the elevator shaft.

![OVERHEAD VIEW OF TYPICAL FLOOR](image)

**Fig. 5.1 Schematic of Pittsfield Building**

The first line of the input file contains the building title. The second line contains program control parameters (the maximum number of iterations, a list parameter which controls output (usually set to 1) and the number of contaminants).

The next group of lines provide information on each zone. Each line corresponds to a zone and includes the following:

- Zone reference height in meters
- Zone temperature in Celsius
- Zone volume in m$^3$
- Initial concentrations of the contaminants in kg/kg of air

When you are finished describing all zone data, include a terminator line with a negative value for the reference height.

The next group of lines provide information on each flow opening. These make use of a zone numbering scheme based on the order of the zone data lines, i.e. zone 1 is the first zone listed and so on. Zone 0 corresponds to the outside. Each line in this group corresponds to an opening and contains the following:

- Near side zone number
- Far side zone number (may be 0 for outside)
- Opening Area in m$^2$
This group of input is terminated by a line with a near side zone number of zero or less.

The next group of lines proved zone information for the run. There must be one line for each zone. Each line contains the zone temperature in Celsius, a forced airflow rate in the zone in kg/s (negative flow rates indicate an exhaust) and contaminant generation and absorption rates in kg/s for each contaminant.

The last group of lines are the ambient conditions and there can be as many as desired. Each line contains a time in seconds for which the conditions are valid, the ambient temperature in Celsius, the barometric pressure in Pa, the wind speed in m/s, the wind direction and the ambient contaminant concentrations. If one is not calculating contaminant concentrations, the time step value may be set to 1. This will give only the air flows for each weather condition. The last line of the input file should have a time step of zero or less.

Included is a sample output for the first weather conditions for this description of the office building.

**Sample Input File (AIRMOV.DTA)**

PITTSFIELD: 2 ISOLATED ZONES, 3 EQUAL OPENINGS PER FACE

```
20 1 0
7.9 22. 2923. 0. 0. 0. 0.
7.9 22. 2894. 0. 0. 0. 0.
7.9 22. 335. 0. 0. 0. 0.
7.9 22. 30. 0. 0. 0. 0.
7.9 22. 974. 0. 0. 0. 0.
7.9 22. 965. 0. 0. 0. 0.
1 0 20. 60. 0. 0. 0. 0.
1 0 0.0167 .65 1.0 0. 0.0 7.9
1 0 0.0100 .65 1.0 0. 1.95 7.9
5 0 0.0100 .65 1.0 0. 3.5 7.9
1 0 0.0167 .65 1.0 90. 0.0 7.9
1 0 0.0167 .65 1.0 90. 1.95 7.9
5 0 0.0100 .65 1.0 90. 3.5 7.9
1 0 0.0167 .65 1.0 180. 0.0 7.9
1 0 0.0167 .65 1.0 180. 1.95 7.9
5 0 0.0100 .65 1.0 180. 3.5 7.9
1 0 0.0167 .65 1.0 270. 0.0 7.9
1 0 0.0167 .65 1.0 270. 1.95 7.9
5 0 0.0100 .65 1.0 270. 3.5 7.9
2 0 0.0167 .65 1.0 0. 4.0 7.9
2 0 0.0167 .65 1.0 0. 5.95 7.9
6 0 0.0100 .65 1.0 0. 7.5 7.9
2 0 0.0167 .65 1.0 90. 4.0 7.9
2 0 0.0167 .65 1.0 90. 5.95 7.9
6 0 0.0100 .65 1.0 90. 7.5 7.9
```

1 AIRMOV contaminant dispersal analysis is an early implementation; the CONTAM series of programs offer more advanced modeling capabilities.
Sample Output for AIRMOV (first weather conditions)

NBS INTERZONAL AIR MOVEMENT & CONTAMINANT DISPERSAL PROGRAM
Project Title: FITTSFIELD: 2 ISOLATED ZONES, 3 EQUAL OPENINGS PER FACE

Maximum Number of Iterations: 20
Print Output Control: 1
Number of Contaminants: 0

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<th>ZZ</th>
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<th>VOL</th>
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<td>2923.00</td>
</tr>
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<td>22.00</td>
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<tr>
<td>6</td>
<td>7.90</td>
<td>22.00</td>
<td>965.00</td>
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</table>

Number of Zones = 6
Building Volume = 8121 M^3
Begin next time step

<table>
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<th>Flows</th>
<th>Pressure Differences</th>
</tr>
</thead>
<tbody>
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<td>0.0171 kg/sec</td>
</tr>
<tr>
<td>Flow:</td>
<td>2 1  0</td>
<td>0.0068 kg/sec</td>
</tr>
<tr>
<td>Flow:</td>
<td>3 5  0</td>
<td>-0.0050 kg/sec</td>
</tr>
<tr>
<td>Flow:</td>
<td>4 1  0</td>
<td>0.0171 kg/sec</td>
</tr>
<tr>
<td>Flow:</td>
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<tr>
<td>Flow:</td>
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</tr>
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<tr>
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<tr>
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<tr>
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<tr>
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<tr>
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<tr>
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Opening Flows & Pressure Differences

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<th>Opening</th>
<th>Flows</th>
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<td>Flow:</td>
<td>36 4 6</td>
<td>-0.0020 kg/sec</td>
</tr>
<tr>
<td>Flow:</td>
<td>37 5 1</td>
<td>0.0485 kg/sec</td>
</tr>
<tr>
<td>Flow:</td>
<td>38 6 2</td>
<td>0.0423 kg/sec</td>
</tr>
<tr>
<td>Flow:</td>
<td>39 5 2</td>
<td>-0.0258 kg/sec</td>
</tr>
</tbody>
</table>

Infiltration Rate: 0.04 /hr  Exfiltration Rate: 0.04 /hr
No more time step data

REFERENCES

[1] Axley, J.W., Indoor Air Quality Modeling: Phase II Report, (presently under review for publication by the National Bureau of Standards, Building Environment Division, Center for Building


