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Multi-zone IAQ model
Indoor air quality analysis

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

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During the past decade, indoor air pollution emerged as an international health issue, and as a result a new field of simulation, indoor air quality analysis, is emerging. James Axley of the Indoor Air Quality and Ventilation Group at NIST, formerly National Bureau of Standards at Gaithersburg, has developed an integrated set of computer-aided tools and this paper reviews the present capabilities of the IAQ model, presents examples of its application and briefly outlines its theoretical base.

Au cours de la dernière décennie, la pollution de l'air intérieur est apparue comme un problème majeur pour la santé, d'où la naissance d'un nouveau domaine de simulation, l'analyse de la qualité de l'air intérieur. James Axley du Groupe Qualité de l'air intérieur et Ventilation au NIST, ex- National Bureau of Standards, Gaithersburg, a développé des outils informatiques intégrés. Cet article passe en revue les possibilités actuelles du modèle d'IAQ (Qualité de l'air intérieur), donne des exemples de son application et souligne brièvement ses fondements théoriques

Indoor air quality analysis

International health issue

During the past decade, indoor air pollution emerged as an international health issue and, as a result, a new field of simulation, *indoor air quality analysis*, is emerging to provide the means to predict exposure to indoor air contaminants in existing and proposed buildings and, thereby, to assess the nature and severity of potential indoor air quality problems. It may be expected that this new field will come to play a key role in the development of strategies to mitigate indoor air quality problems and, eventually, become central to the design of high-quality indoor air environments.

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 air movement into, out of, and within the building system; the influence of the heating, ventilating, and air conditioning (HVAC) systems; the possibility of removal, by filtration, or contribution, by generation of contaminants; and the possibility of chemical reaction, radiochemical decay or sorption of contaminants. In indoor air quality analysis, we seek comprehensively to model all of these phenomena.

Three-dimensional fields

More precisely, in indoor air quality analysis we consider building air flow systems to be three-dimensional fields within which we seek completely to describe the state of infinitesimal air parcels. The state of such an air parcel is defined by its temperature, pressure, velocity, and contaminant concentration(s) – the *state variables* of indoor air quality analysis (Fig. 1).

The central problem of indoor air quality analysis is, then, the determination of the spatial (x,y,z) and temporal (t) variation of contaminant species concentrations or *contaminant dispersal analysis*. For a single non-reactive species, α, contaminant dispersal is driven by the air

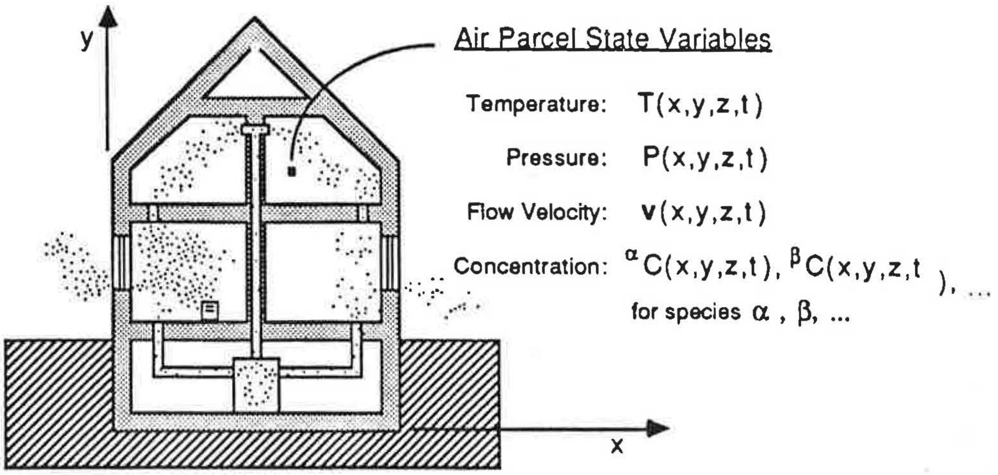


Fig. 1. Indoor air quality state variables

velocity field and its variation with time and thus the contaminant dispersal analysis problem, for this case, may be represented as:

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

Non-reactive Contaminant Dispersal Analysis

where the ellipses, ..., are used to indicate initial 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.

Analysis and measurement approaches

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. 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. Functionally, these related problems take the following forms:

Coupled flow/thermal analysis

$$\begin{array}{lcl|l} \boldsymbol{v}(x,y,z,t) & = & \boldsymbol{v}[P(x,y,z,t), \ldots] & \textit{flow analysis} \\ P(x,y,z,t) & = & P[T(x,y,z,t), \ldots] & \textit{buoyancy effects} \\ T(x,y,z,t) & = & T[\boldsymbol{v}(x,y,z,t), \ldots] & \textit{thermal analysis} \end{array}$$

Inverse contaminant dispersal analysis

$$\boldsymbol{v}(x,y,z,t) \overset{?}{=} \boldsymbol{v}[{}^{\alpha}C(x,y,z,t), \ldots]$$

(the basis of tracer gas techniques)

When contaminant reaction or sorption kinetics 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.

Reactive contaminant dispersal analysis

$$^{\alpha}C(x,y,z,t) = {}^{\alpha}C[\boldsymbol{v}(x,y,z,t), {}^{\alpha}C(x,y,z,t), {}^{\beta}C(x,y,z,t) \ldots]$$

Properly, then, a complete indoor air quality analysis package should provide the analyst with tools to consider this relatively complex set of analytical problems related to the central task of contaminant dispersal analysis. These analytical tasks and their relationships to the central task of contaminant dispersal analysis can be illustrated as in Fig. 2.

The NBS IAQ project

Tools to perform analytical tasks

The Indoor Air Quality Model Project, initiated in 1985 by the Indoor Air Quality and Ventilation Group at the National Bureau of Standards (ref. 1) with the support of the Department of Energy, the Environmental Protection Agency and the Consumer Products Safety Commission, has been organized to develop a set of computational tools to perform the analytical tasks indicated by Fig. 2. The primary product of this project is the CONTAM series of programs, their user's manuals, and the documentation of the underlying theory. The first member of this series, CONTAM86, and its supporting documentation (ref. 2) is available, the second member of the series, CONTAM87, was released in the Spring of 1988, and the third member of the series, CONTAM88, is under development. The capabilities of these programs may be summarized as follows:

- CONTAM86: non-reactive contaminant dispersal analysis for specified air flows; steady-state response and time constant analysis for steady flow conditions: dynamic response analysis for arbitrary flow and contaminant generation time histories
- CONTAM87: as above plus reactive contaminant dispersal analysis
- CONTAM88: as above plus non-reactive inverse contaminant dispersal analysis and air flow analysis for specified air temperatures

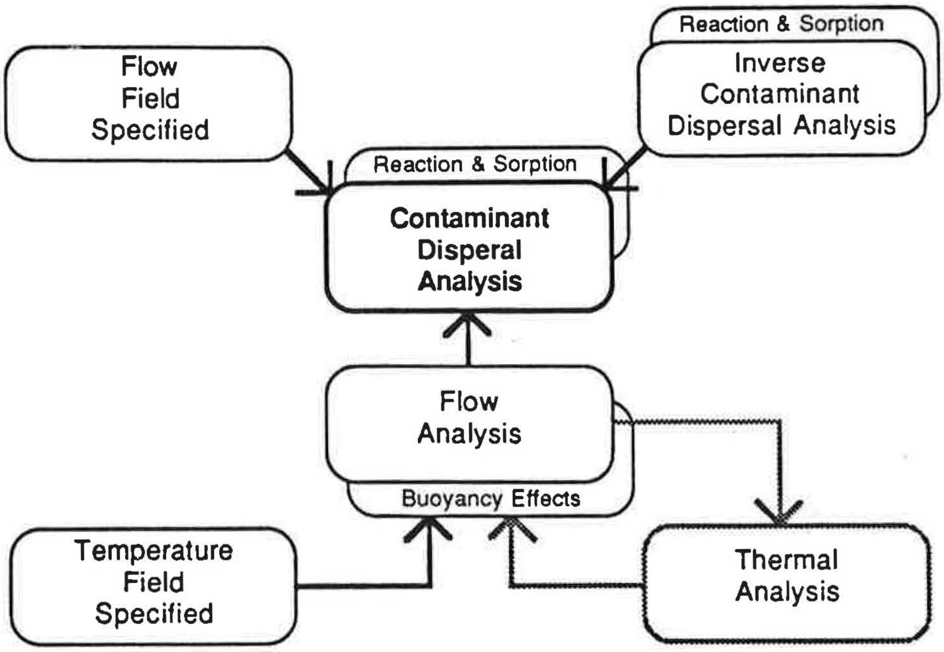


Fig. 2. The central and related problems of indoor air quality analysis

Command processors

These programs have been developed as command processors, providing a higher-level programming language for indoor air quality analysis, that accept commands interactively or from command/data files. The development of each successive member of the family involves, simply, the development and addition of new commands. Other researchers should be able easily to extend the capabilities of the series by developing additional commands; a set of specialized commands to aid in the development of new commands is available for this purpose.

The present scope of the project does not include consideration of the coupled thermal analysis problem and, therefore, we shall limit subsequent considerations to the problems of contaminant dispersal analysis, inverse contaminant dispersal analysis, and flow analysis for a specified temperature field. The modelling approach employed has, however, been designed to be compatible with a thermal analysis method introduced earlier by the author (ref. 3).

Modelling approach

Element assembly

The NBS IAQ model, like other existing IAQ models (refs 4, 5, 6), is based on a well-mixed zone simplification of the macroscopic equations of motion (i.e. mass, momentum and energy balances for flow systems) that, in essence, transforms the indicated field problems above into spatially discrete, but temporally continuous, ordinary differential equations. The NBS IAQ model differs from existing models in that an *element assembly* approach is taken to formulate the respective analytical problems. That is to say:

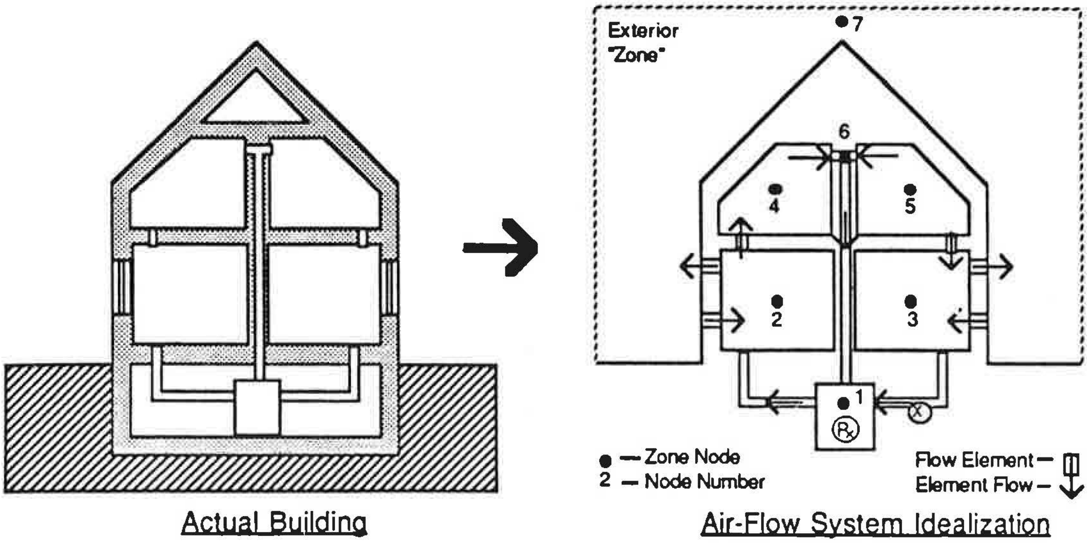
the building air flow system (field) is idealized as an assemblage of discrete air flow elements linking well-mixed building volumes or zones.

The equations governing the behaviour of the system are, then, *assembled* from individual *element equations* that describe specific instances of mass transport phenomena occurring in the building to form *system equations* governing the behaviour of the system as a whole.

From a practical point of view, the element assembly approach is intuitively satisfying and allows consideration of systems of arbitrary complexity. From a research and development point of view this approach separates the general problem of indoor air quality analysis into two primary sub-problems; element development and development of solution method. Research efforts can, thus, focus on the modelling of specific mass transport phenomena to develop improved or new elements or, alternatively, focus on developing improved methods of solving the resulting equations while accounting for the complex coupling that exists between the thermal, dispersal, and flow analysis problems. The approach has been formulated to be completely analogous and compatible with approaches based upon Generalized Finite Element method (ref. 7) 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 the Finite Element and associated methods.

This idealization of a building air flow system may be represented graphically in a rather direct and very intuitive way as illustrated in Fig. 3 for a hypothetical building system. With a knowledge of the air flow paths in the building system, the analyst selects from the library of available air flow elements to assemble graphically, and hence mathematically, the building idealization. At present, the library of flow elements contains those indicated in Fig. 4. It is worth noting that the convection–diffusion contaminant dispersal flow element is based on a finite-element solution of the one-dimensional convection–diffusion dispersal equations.

With each well-mixed zone we associate a set of discrete state variables with a distinct but arbitrary point in the



Actual Building

Air-Flow System Idealization

Fig. 3. Idealization of building air flow system

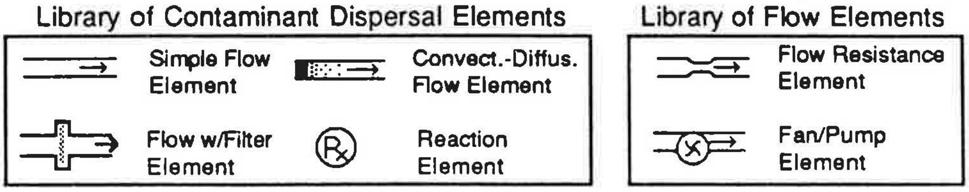


Fig. 4. Current library of indoor air quality analysis elements

zone, the zone *node*. These are meant to approximate the corresponding field variables in the zone at that point. For a system idealized as n well-mixed zones, then, the key discrete state variables would include:

$\{\boldsymbol{P}\} = \{P_1, P_2, \ldots P_n\}^T$

the vector of system pressure variables (1)

$\{\boldsymbol{T}\} = \{T_1, T_2, \ldots T_n\}^T$

the vector of system temperature variables (2)

$\{{}^{\alpha}\boldsymbol{C}\} = \{{}^{\alpha}C_1, {}^{\alpha}C_2, \ldots {}^{\alpha}C_n\}^T$

the vector of system α concentration variables (3a)

$\{{}^{\beta}\boldsymbol{C}\} = \{{}^{\beta}C_1, {}^{\beta}C_2, \ldots {}^{\beta}C_n\}^T$

the vector of system β concentration variables (3b)

. . . etc.

where the subscripts are zone/node indices. These variables will be referred to as the *system variables* to distinguish them from subsets of these variables which will be referred to as the *element variables*.

With each element e in the system assembly we associate two or more element state variables and note their association with the system variables. For 'two-node' flow elements, in particular, the element state variables are, for contaminant dispersal analysis:

$\{{}^{\alpha}\boldsymbol{C}^e\} = \{{}^{\alpha}C_i^e, {}^{\alpha}C_j^e\}^T$

the vector of element α concentration variables (4)

where i and j are node indices. The element air mass flow rate, w^e (for mass flow from i to j) is the key non-state variable for these elements.

With these element variables in hand, element equations are formulated that describe the specific mass transport phenomena that the element is meant to represent (e.g. mass transport from zone to zone by flow processes or mass transport from contaminant species to contaminant species by chemical processes). As an example, by assuming that flow through a two-node flow element is practically instantaneous and well mixed, the mass transport of species α from element node i to j due to an air mass flow rate w^e may be described by the following element equations (allowing for the possibility of a fraction η of the contaminant being removed by filtration):

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

or $\{{}^{\alpha}\boldsymbol{w}^e\} = [\boldsymbol{f}^e]\{{}^{\alpha}\boldsymbol{C}^e\}$ (5)

where ${}^{\alpha}w_j^e$ are the mass flow rates of species α into the element from the node at element nodes i and j respectively. Fig. 5 should help to clarify the meaning of these element variables. The matrix $[\boldsymbol{f}^e]$ is referred to as the element flow matrix. For mass transport due to reaction between contaminants or with the building fabric, there is a corresponding element reaction matrix that we will represent as $[\boldsymbol{r}^e]$ for our purposes here.

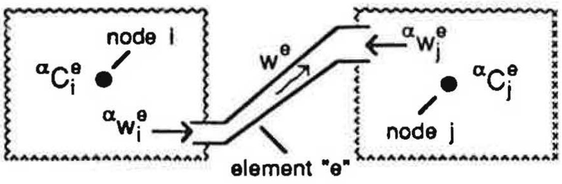


Fig. 5. Two-node contaminant dispersal flow element variables

Finally, these element equations are then assembled, for the given building idealization, to form the governing indoor air quality analysis equations:

$$[\boldsymbol{W}]\{^{\alpha}\boldsymbol{C}\} + [\boldsymbol{M}]\left\{\frac{\mathrm{d}^{\alpha}C}{\mathrm{d}t}\right\} = \{^{\alpha}\boldsymbol{G}\}$$

the contaminant dispersal equations (6)

$$[^{\alpha}\boldsymbol{C}]\{\boldsymbol{w}^{e}\} = \{^{\alpha}\boldsymbol{G}\} - [\boldsymbol{M}]\left\{\frac{\mathrm{d}^{\alpha}\boldsymbol{C}}{\mathrm{d}t}\right\}$$

the inverse contaminant dispersal equations (7)

$$[A(\{\boldsymbol{P}\})]\{\boldsymbol{P}\} = \{\boldsymbol{W}\}$$

the flow analysis equations (8)

where, here, consideration has been limited to the dispersal of a single species α. Although a discussion of the assembly process is beyond the scope of this paper, the nature of the assembly process is suggested by the following equation for the system mass transport matrix $[\boldsymbol{W}]$:

$$[\boldsymbol{W}] = \underset{e = a,b,\ldots}{\mathbf{A}} [\boldsymbol{f}^{e}] + \underset{f = q,p,\ldots}{\mathbf{A}} [\mathbf{r}^{f}] \tag{9}$$

The assembly operator **A** involves Boolean transformations of the element matrices followed by a summation process and is, therefore, a generalization of the summation operator Σ. We say, then, that the system mass transport matrix $[\boldsymbol{W}]$ is *assembled* from the element flow and reaction matrices. Similarly, the system pressure-flow matrix $[\boldsymbol{A}]$ is assembled from element pressure-flow matrices. The system volumetric mass matrix $[\boldsymbol{M}]$, nodal species generation vector $\{^{\alpha}\boldsymbol{G}\}$, and air mass flow vector $\{\boldsymbol{W}\}$ are assembled from both element contributions, in general, and discrete nodal contributions (e.g. the volumetric mass of each zone, discrete contaminant generation within each zone, and direct generation, as by fire, of air mass within each zone).

The inverse contaminant dispersal analysis equations are formed by collecting appropriate tracer gas test concentration data that are then used to assemble the concentration matrix $[^{\alpha}\boldsymbol{C}]$ and, possibly, the vector $\{\mathrm{d}^{\alpha}\boldsymbol{C}/\mathrm{d}t\}$ (tests are often designed, however, to ensure that this vector is zero and this term is then ignored). Alternatively, Equation 7 may be integrated over a discrete time interval to create an integral form of the inverse contaminant dispersal equations, and again test data would be used to form the corresponding integral equations.

The solution of these equations is beyond the scope of this paper. The inverse contaminant dispersal problem is inherently ill-conditioned and, therefore, especially stable numerical methods must be employed in its solution; single-value decomposition and constrained least-squares methods are presently being investigated. The flow analysis problem is highly non-linear and, therefore, a variety of non-linear solution strategies are presently being considered with modified forms of the Newton–Raphson method showing most promise at this time.

Examples of application

Test cases

At this time, the NBS IAQ model has been applied to a number of test cases to provide preliminary validation of the program. Comparisons between computed results and exact solutions for special cases of single and two-zone buildings and numerical solutions computed by one other contaminant dispersal program (ref. 8) have been proved to be practically identical. Comparisons between computed results and measured data have also been encouraging, although, here, good data sets are wanting. Two of these comparisons are considered. A programme of model validation was carried out in 1988.

Fifteen-storey office building

Infiltration studies of a fifteen-storey office building have been conducted by members of the Indoor Air Quality and Ventilation Group at NBS. Some of these studies involve hourly injections of a commonly used tracer gas, SF_6, into the fresh air supply ports of the building HVAC system. Flows in the supply ducts were measured, with significant uncertainty, by pitot traverse, SF_6 concentration time histories were recorded, and fresh air infiltration was estimated by tracer decay. Using the air flow measurements the upper two floors of this building were idealized as shown in Fig. 6.

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. 7 we compare measured SF_6 concentration time histories (measured centrally within the 'space' and at the 'exhaust' ports) to computed values of the 15th floor for two supply flow rates: 100% and 75% of the measured flow. In this case, the agreement between measured and computed time histories is within the uncertainty of the measured flows and validation is therefore indicated.

Two-storey townhouse with basement

Borrazzo and his colleagues at Carnegie Mellon University have conducted detailed field investigations of a two-storey townhouse measuring CO, NO, and NO_2 emission characteristics of the gas appliances within the townhouse, and the dispersal of these contaminants throughout the townhouse under a variety of different weather conditions (ref. 9). Illustrated in Fig. 8 is an idealization of the townhouse and the measured dynamic emission characteristics of the principal pollutant source, the gas range. The instantaneous emission rate, $G(t)$, is plotted relative to the steady-state value, G_{ss}. The NO_2 emission characteristics were more or less constant and are, therefore, not illustrated. NO_2 is a reactive contaminant and was modelled as such using the measured reactivity of $K = 2.4\,\mathrm{hr}^{-1}$.

In Fig. 9 we compare computed response with measured

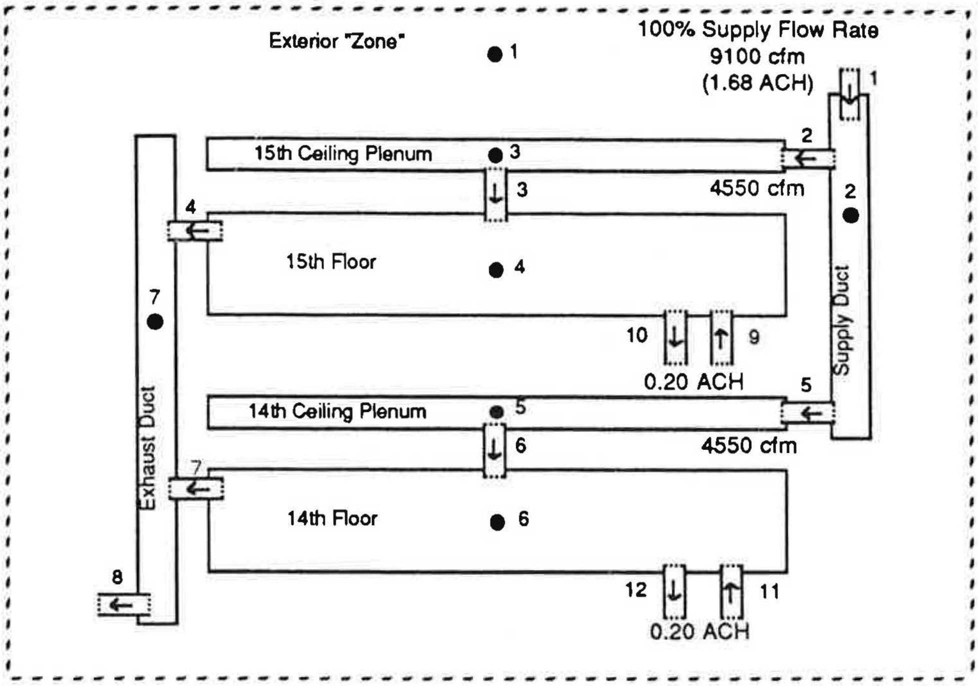


Fig. 6. Idealization of the 14th and 15th floors of an office building

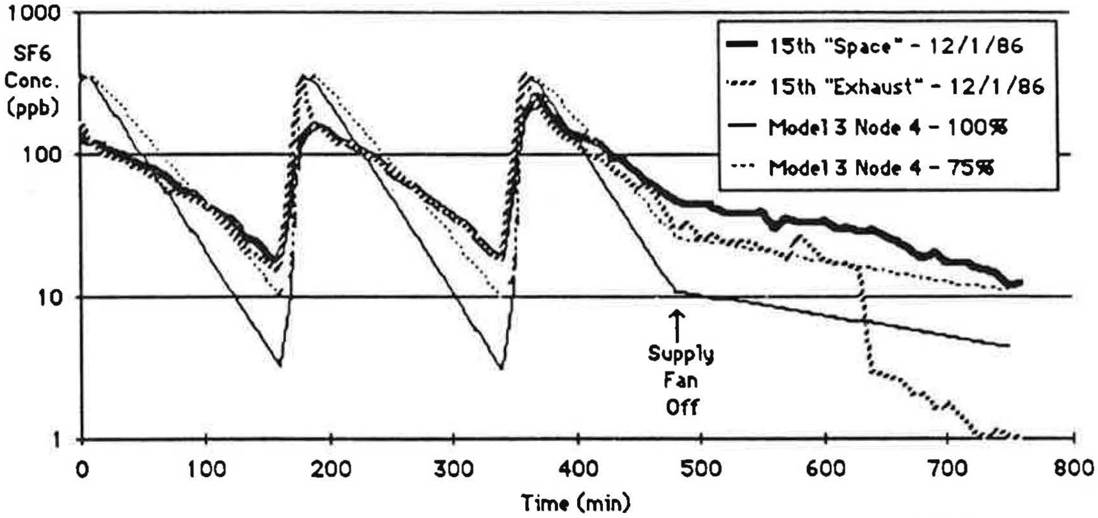
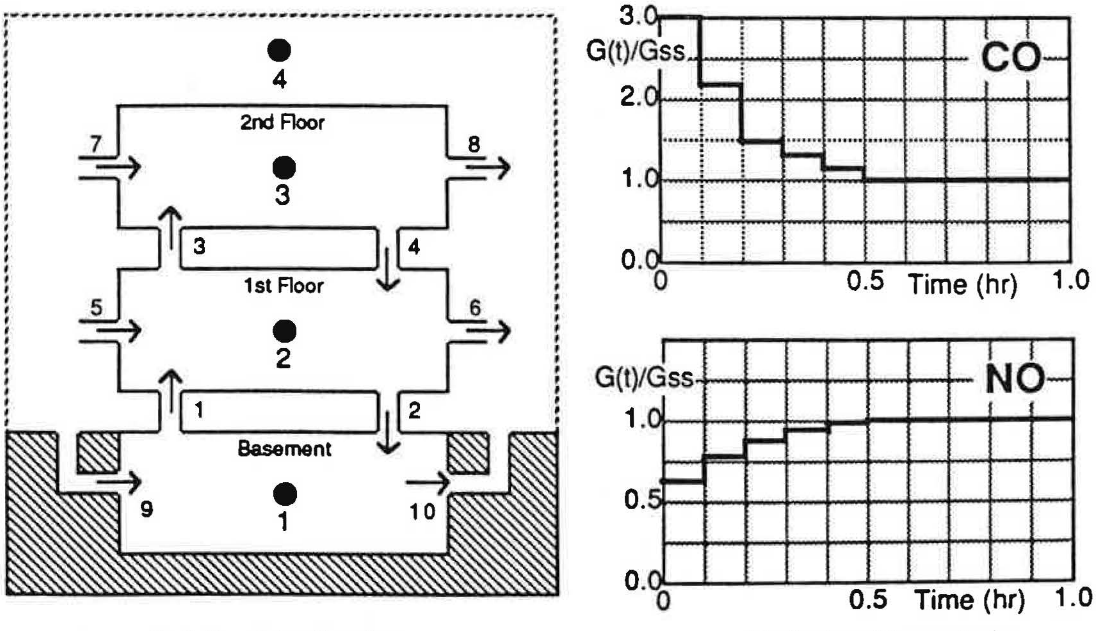


Fig. 7. Comparison of computed and measured response for an office building



Building Idealization

Emission Characterics

Fig. 8. Townhouse building idealization and range emission characteristics

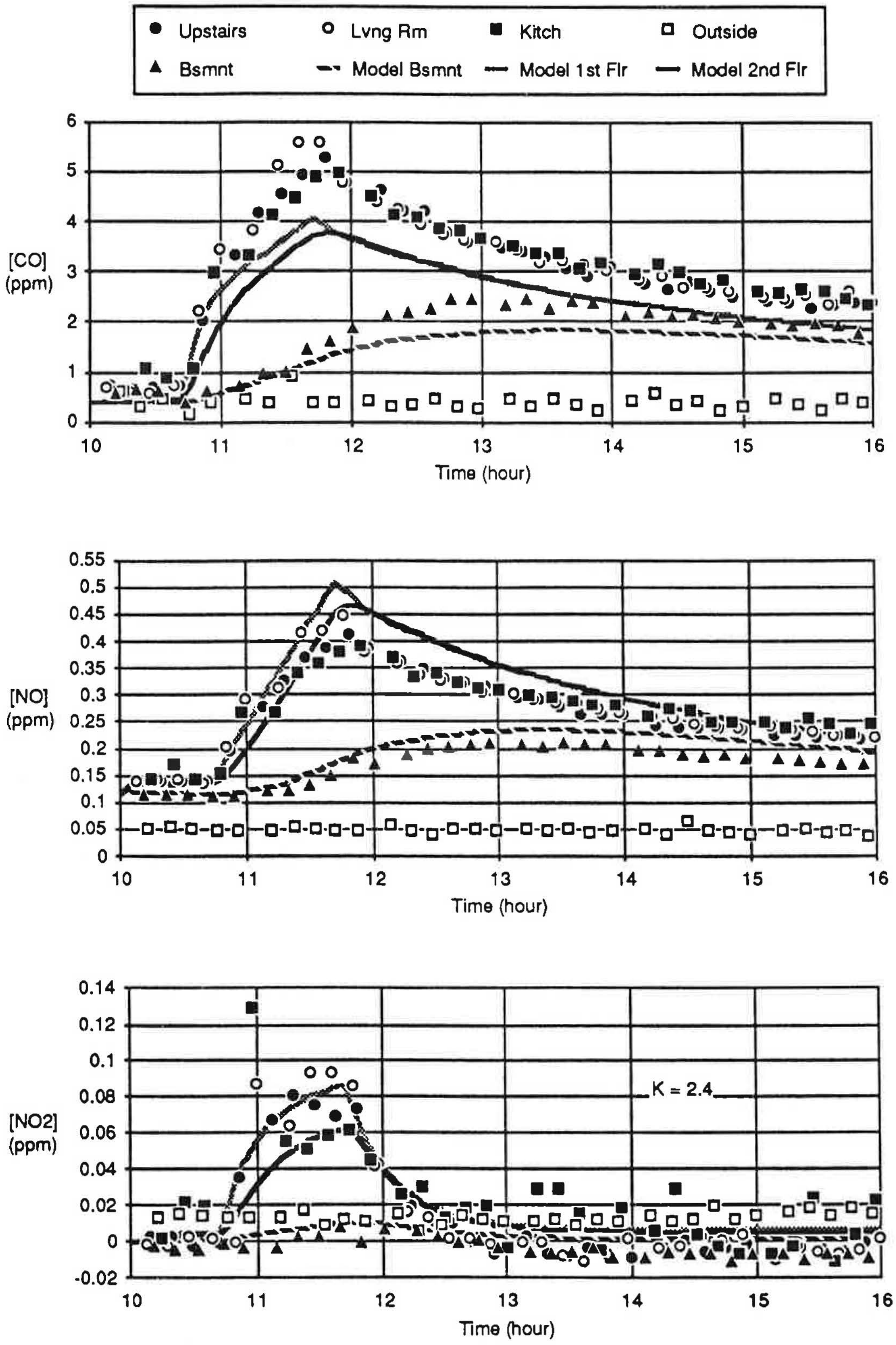


Fig. 9. ***Comparison of computed and measured response of a town house***

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% and NO: 6.5%). Regrettably, the NO_2 data set contained suspicious negative values and a great deal of scatter, but nevertheless the results are encouraging.

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