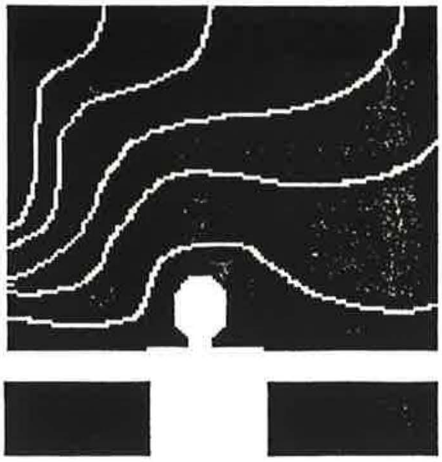
Building Systems: Room Air and Air Contaminant Distribution



December 5-8, 1988
Allerton House
University of Illinois
at Champaign-Urbana

Introduction

We have the responsibility and opportunity to define the state-of-the-art and research needs on room air and air contaminant distribution. That information will guide research efforts, regulatory activities, and the development of standards in many important federal agencies, professional societies, and industries. The most important federal agencies conducting and supporting ventilation and indoor air quality research and development are supporting our effort financially.

The planning committee has deliberately chosen engineers and other professionals from diverse disciplines and applications to participate in the symposium. We have selected people from all parts of the United States and numerous other countries. We want to learn from each other. Most importantly, we want to work together to prepare a well-written and supported definition and summary of the state-of-the-art and research needs. Ultimately, we all benefit from more healthful, comfortable, and productive indoor environments.

Leslie L. Christianson
Symposium Chair

Co-Sponsors

We gratefully recognize the **National Science Foundation** as the principal sponsor of this symposium. In addition, the following agencies and associations have provided financial and professional assistance in the preparation of the program:

<u>Government:</u>
National Institute for Occupational Safety and Health
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United States Environmental Protection Agency
University of Illinois at Champaign-Urbana

<u>Industry:</u>
National Association of Home Builders,
National Research Center
TSI, Incorporated
Honeywell, Inc.

Symposium Program

December 5, 1988 - Monday

2:00 p.m.	Participant interactions/demonstrations of software and products (Great Hall)
5:00 p.m.	Social Hour
6:00 p.m.	Dinner
7:30 p.m.	Welcome; Recognition of Sponsors; Keynote speech: "Perceptions and Projections" **Gifford Albright**, Architectural Engineering Dept., Pennsylvania State University (Library)

Mathematical Modeling Session
Building Systems: Room Air and Air Contaminant Distribution
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Introduction:

The subject of room air and air contaminant distribution has many facets and aspects. One of these aspects is the demonstrated understanding of the physical phenomena involved by mathematical modeling. These computerized mathematical models have been and can be developed for many purposes, ranging from theoretical computational fluid dynamics research to applied design. A quick examination of the field shows that the uses are as many as the different type users. Research scientists may develop and use these math models to guide entire lines of research. Manufactures will use models for design of components. Architects and engineers can use models to analyze affects on and to design for; the flow of air; comfort; indoor air quality; special requirements (e.g. clean rooms, equipment rooms, etc.); maintenance requirements; etc.. Organizations, from those writing voluntary standards to government agencies, from the local level to the federal, can use these models to develop codes, standards and regulations. These models can also be used to design field experiments. It can be further expected that these models will guide the expansion of knowledge and will form the basis for practical implementation of controlling indoor air pollution and achieving a satisfactory level of indoor air quality.

One of the underlying reasons for the spectacular advancements which have taken place in mathematical models for airodynamics and interactions is the advances in computer technology. Many of the design and analysis programs can be run on personal computers, while advances in mainframe computers have allowed complicated fluid dynamic models to address problems which just a short while ago were thought to be beyond computational capability. These advances have allowed the scientific principles, defined in physic and mathematical form, to be applied to the solution of real world problems. This advancement has been rapid and thus it is difficult for a person to be aware of the already developed tools available, their applicability and their limitations, there is a need for a survey of these tools to be made available to interested parties.

In this section the various type mathematical models will be discussed, as mentioned above this discussion may not cover all available models in detail, but is general enough to address the models in concept.

Macroscopic Modeling

Definition

Macroscopic models are used to predict the time and spatial variation of global measures of airflow, contaminant dispersal, and heat transfer in whole-building systems. They are based upon the application of mass, momentum, and energy balances, expressed in terms of ordinary differential equations, to one or more discrete control volumes chosen to represent the building system. Typically, the global measures include spatially discrete estimates of temperature, pressure, concentration, and air flowrate that are expected to approximate the state of the building system at some point or region in the system.

State of the Art

Presently macroscopic models are avalible for contaminant dispersal analysis, steady airflow analysis, and thermal analysis of whole building systems and moisture transfer and HVAC system analysis in subsystem or portions of building systems. For both contaminant dispersal and flow analysis building systems are, typically, modeled by single or multiple well-mixed zones linked by discrete air flow paths through which flow is assumed to be practically instantaneous. Element assembly approaches are available that allow additional mass transport phenomena, beyond that driven by instantaneous flow between zone, to be considered in contaminant dispersal analysis and that allow the consideration of a variety of pressure-flow "laws" for the discrete flow paths to be considered in flow analysis.

- Macroscopic modeling methods are theoretically simple, numerically straightforward, computationally non-demanding, and practically easy-to-use. They do not, however, provide within-the-room detail and are largely limited to modeling building systems that may be reasonably idealized by zones linked by discrete flow paths.

- The accuracy of macroscopic contaminant dispersal analysis is limited by a) the need to know all flows in the system accurately to complete the analysis and b) the completeness and accuracy of contaminant source or sink models used to drive the analysis. When these quantities are well-known comparisons between predicted and measured behavior have been excellent.

- The accuracy of macroscopic flow analysis is limited by a) the accuracy of the flow "laws" used to characterize the discrete flow paths, b) the accuracy of the temperature distribution that must be known apriori, at this time, that determines buoyant affects, and c) the accuracy in modeling the pressure distribution acting on the building due to wind. Individually, each of these sources of error can introduce significant inaccuracies and together inaccuracies are compounded. These methods can not, in general, be expected to provide accurate results.

- Element or component models are available for modeling bulk bi-directional and/or bulk net flow through large openings connecting individual rooms modeled as single zones for macroscopic flow analysis. The limitations and accuracy of these element or component models has yet to be established.
- Some attempts have been made to integrate macroscopic modeling techniques with microscopic modeling techniques to provide detailed information in parts of a building system while still considering whole-system interaction. While it appears that such a micro-macro modeling

approach may be possible for contaminant dispersal, mosture transfer, and thermal analysis, its application to the area of flow analysis is yet untried and may be expected to be of limited value.

- Some attempts have been made to also integrate macroscopic models of different classes. In particular, building (envelope) thermal models have been integrated with HVAC system models to account for HVAC system-building interaction. HVACSIM+ developed at NBS is one example.

- The International Energy Agency, through the Air Infiltration Center and Annex 20, is presently in the process of reviewing the state-of-art of both macroscopic and microscopic modeling methods with the expectation of developing guidelines for the selection and use of these modeling techniques.

Research Needs

- Macroscopic contaminant dispersal analysis models need to be extended to provide greater resolution of the details of dispersal within single rooms. This may be accomplished, for example, through the development of semi-empirical/semi-physical models of single rooms (e.g., multiple-zone-single-room idealization) using microscopic and/or experimental studies to determine correlations or through the use of the identification procedures presented by Berkmans in this symposium to relate local state variables to macroscopic state variable.

- Development of source models that may be incorporated in macroscopic contaminant dispersal analysis models that comprehensively account for the dependency of source emission (or sink removal) characteristics on the state parameters governing the dispersal in the building.

- Validation of both macroscopic contaminant dispersal and macroscopic flow analysis models through comparisons with field measured data (e.g., determined by tracer techniques), laboratory measured data, and data generated through microscopic simulation.

- Extend present capabilities to account for HVAC system interation and control in macroscopic flow analysis.

- Development of models for filtration devices that may be incorporated in macroscopic contaminant dispersal analysis models.

- Improve understanding and ability to predict wind driven pressure distributions on buildings through microscopic simulation, field and laboratory investigations.

- Determination of internal surface heat and mass transfer coefficients needed for macroscopic modeling.

- The integration of macroscopic flow and macroscopic thermal analysis models to deal with the coupled thermal-flow problem is needed.

- The integration of microscopic and macroscopic modeling techniques to provide detailed analysis within a portion of the building system yet account for whole system interaction warrants further consideration. The possiblity of integrating macroscopic and microscopic flow analysis in such a way so that the macroscopic model will determine pressure boundary conditions of the microscopic portion of the model may have some value.

MICRO MODELS

INTRODUCTION

These are computer programs which are capable of providing detail simulation of the flow, temperature and contaminant fields within an enclosure. They are based on the solution of the partial differential equations for continuity momentum, enthalpy and particle flow in discretized form. Differential equations for turbulence models are also required to describe the time-dependent variables.

Most available models use the finite volume solution technique with wall function expressions and the K-E turbulence model.

State-of-the-art

Most current micro models have been developed by small teams or individuals and they can only be used by themselves. Commercially available models are not "user friendly" and an expert is required to use them.

Current models with the K-E turbulence scheme can predict isothermal and low buoyancy flows reasonably accurately in most of the flow field with reduced accuracy close to boundaries and obstacles.

Research needs:

Flexible geometry is required to widen the scope of application of micro models in air flows and contaminant spread in buildings, e.g., transformation techniques, body-fitted co-ordinates etc.

Improved wall functions for momentum and heat flux are required for room boundaries. These can be obtained from high quality experimental measurements.

Improvement to turbulence closure models to deal with highly buoyant flows characterized by large Archimedes and Grashoff numbers.

Application of non-gird based CFD techniques to room flows such as Chorin's random vortex method.

Additional work on VAV systems particularly the investigation of 'short circuiting' of the supply air.

Application of existing models and future micro models to floor displacement ventilation and personal ventilation systems.

The inclusion of supply and extract air terminal device to the room flow and temperature fields.

The inclusion of radiant heat transfer in existing micro models.

MATHEMATICAL MODELING AT THE MICRO LEVEL

State-of-the-Art:

The analytical aspects of computational methods in fluid mechanics (dynamics) called "CFD" are highly developed, and a wide range of computer code implementations are available in the commercial sector.

The reliable application of CFD analysis to practical room air motion geometries is not mature for a number of reasons including theoretical inadequacies (accuracy, stability) in adequate mesh resolution capability, appropriate boundary conditions unknown, and inadequate non-isothermal turbulent closure models.

Present CFD codes are hard to use by the "non expert," and typically require "expert" adjustments to achieve a converged numerical solution. This prompts the new user to develop his own code, so as to be knowledgeable regarding the adjustable built-in parameters.

Even with these limitation, present CFD codes are being successfully applied to practical problem analyses by expert users in a research environment. Conversely, these codes are not generally useful in supporting alternative design assessments by HVAC engineer.

RESEARCH NEEDS

The mathematical analysis aspects of accuracy, convergence and stability of CFD algorithms, for the room air problem class, must be expanded to address and solve the principal fault of code unreliability.

The computer codes based on these improved CFD theories must be designed for efficient utilization of vector/parallel supercompter features, to admit adequate mesh resolution for prediction accuracy. The improved theories and codes must be highly flexible with respect to implementing improved turbuelnce models, as they become developed, especially with respect to boundary conditions and local mesh resolution and flow unsteadiness.

A cooperative project is required to bring the experimental and computational fluid mechnanics researcher into close contact to generate the detailed data base required for code/theory/turbulence model validation.

Use of the new mathematically robust CFD code that result must be improved by application of expert system concept to accomplish reiable use regarding online error estimation, mesh adaptation and overall user-friendlines including input/output work-station based graphics.

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Sources And Sinks:

When using the mathematical models, especially the macro or whole building models being used for pollutant concentration calculations, there often exists a need for source (generation) definition as well as sink (removal) and interaction (species change) terms. At the present time there is a paucity of adequate source, sink and interaction terms. Often the physics of the source is not well understood and the emission rate dependencies on the other factors is ill defined. For example, the diffusion of formaldehyde and other volatile organic compounds through composite materials has not been examined to the point where the physics and chemistry of this diffusion can be used to develop an applicable model. Even the single value of emission rates for a compound from a material are not well catalogued, available or understood. Often a person is forced to use a single value for the emission rate from a pollution source of interest. This value may be based on single set of measurements, taken under unspecified conditions, and may or may not be in the range that represent the real situation of interest.

While some work has been done on modeling the sorption of pollutants and the deposition of particles and radon progeny on surfaces, at the present time, the state of the knowledge is at best rudimentary and primarily indicates the need for a better understanding of the basic phenomena involved and upon which models can be developed. The interactions or attachments in air with other pollutants or particles is another area where only a very preliminary understanding of some of the phenomena exists.

Thus one finds that at the present time the contaminant distribution in buildings is severely hampered by lack of models and data for sources, sinks and interactions.

Present State of the Art:

There are a few emission rate source terms for some pollutants from sources of interest e.g. for cigarettes - particulates, CO, CO_2; kerosene heaters - particulates, CO, CO2, NO_x, VOC; unvented gas space heaters - particulates, CO, CO2, NO_x, VOC; Moth crystals - p-dichlorobenzene; dry cleaning - perchloroethylene; etc.. For formaldehyde emissions from pressed wood products there exists a physically based empirical model which allows for the consideration of temperature and relative humidity. Considerable work has also been done on radon and its progeny production modeling. For sinks there exists some simple models for NO_2, formaldehyde, perchloroethylene, formaldehyde, radon and radon progeny, and several others. A little work has been done on interaction of pollutant species in air, both as a first order reaction and for radon interactions.

Research Needs:

The research and data so far indicates that for some sources, sinks and interactions there may exist underlying phenomena which can be used to form emission models including their dependency on environmental factors and other controlling factors. The form and applicability and limitations of these models needs to be developed. In addition for some emission sources, e.g. combustion devices, it may be necessary to include the other chemical and physical dependencies.

Chemical Interactions

Particle and gaseous emissions may interact with one another after entering the air. Gaseous pollutants may react with other gaseous species. An example is the reaction of ozone produced by an electronic air cleaner with hydrocarbons. Particle size distributions can be modified by the coagulation. It is also suspected that hydrocarbons can be absorbed onto particles. In addition, many particles such as tobacco smoke are semivolitile and the particle size is modified by evaporation/condensation processes. Finally, particles may interact with water vapor changing the size of the particle and modify their physical behavior.

The particle size less than 10 micrometers defines the respirable fraction of aerosol. Therefore the particle size distribution is important in determining potential health effects of the pollutants. The chemical composition of the respirable fraction chemical properties defines dose.

Present State-of-the-art

Recently, efforts have been made to apply the research results from atmospheric science to the air in indoor spaces. The particle size distributions in indoor spaces are quite similar to atmospheric aerosol because the processes forming the size distribution are similar. Major field projects have been mounted to characterize indoor environments with respect to ventilation, hydrocarbons, radon and recently the respirable particle concentration. However considerable work will be required to develop theoretical concepts to generalize and model this information. At the present time the modeling has not kept pace with the data.

Research Needs

- the sorption and desorption isotherms of hydrocarbons with aerosol particles needs to be measured and generalized theoretically.
- the mathematical models developed to describe outdoor aerosols using mechanisms such as nucleation, coagulation, sedimentation need to be applied to problems in indoor air quality.

ON-LINE MODELING FOR CONTROL OF HVAC-SYSTEMS

INTRODUCTION

Because of the role of ventilation rate in the HVAC system's dynamic behavior, the applied control algorithm has an important influence on the resulting indoor climate and on energy use.Moreover, the internal gas-, heat, moisture production of occupants, whether it be people or livestock, as well as their desired environmental conditins are time varying. Under this condition, advanced on-line modeling based adaptive control algorithms, as they can be realized with today's technology, can offer new possibilities to improve indoor climate control in ventilated space.

State of the art.

- Once there is a model available that gives the dynamic response of the state variables to variations of the control inputs, there are a number of techniques available to develop an optimized (adaptive) control algorithm.

- It is possible by using on-line modelling techniques to predict the dynamic behaviour of inside temperature (energy), inside volumetric humidity concentration and volumetric gas concentration (mass) to non-linear variations of ventilation rate and heat sypply. This at condition that all those variables can be measured and that measured signals to contain enough "excitation" (dynamics).

- Once an SVD*-chip (Singular Value Decomposition) is available (development is going), this modeling technique can be implemented in the controller.

Research needs.

- If the principle works for energy and mass, it should be possible to make an extension to air velocity (includes moment).

- It is necessary to develop criteria for the on-line selection of these dataparts that permit reliable mathematical solution. This particularly for systems that are controlled already. The dynamic/noise ratio of the measured signal, the value of the sample period and the number of samples to be used for calculation are related problems.

- Today's on-line modeling gives problems with systems that have more input variables with different time delay's.

- Today's concept is based on a general system-part (to be simulated with model based on physical laws) and a particular system-part to be simulated with mathematical identification procedure. It has to be analysed for which variables the "control volume"(as defined in this concept, Berckmans 1986) is similar. For which variables is it different (f.e. gases with different specific weight), how many control volumes have to be taken into account ?

- To use physical scale models for developing on-line modeling techniques, the scaling problem has to be reviewed from the viewpoint of dynamic behaviour of the system.