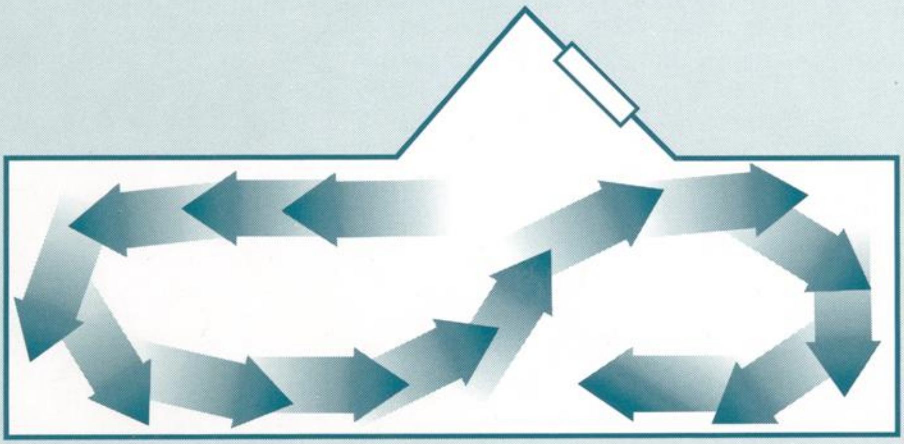
MODELING OF INDOOR AIR QUALITY AND EXPOSURE



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Foreword

This publication, *Modeling of Indoor Air Quality and Exposure*, contains papers presented at the symposium of the same name held in Pittsburgh, PA on 27–28 April 1992. The symposium was sponsored by ASTM Committee D-22 on Sampling and Analysis of Atmospheres and Subcommittee D22.05 on Indoor Air. Dr. Niren L. Nagda of ICF Incorporated in Fairfax, VA presided as symposium chairman and is the editor of the resulting publication.

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Overview

Concern for the quality of air in buildings and exposures to toxic substances has been rising in recent years. Mathematical modeling of indoor air quality is commonly used to improve the understanding of chemical and physical processes that affect indoor pollutant concentrations and to predict indoor concentrations and human exposures under different situations.

Most indoor air quality models are based on the principle of conservation of mass: the accumulation of a contaminant is equal to the difference between the mass generated within or entering a particular air space and the mass leaving that air space. In this conceptual framework, pollutant concentrations are increased by emissions within a defined volume and by transport from other air spaces, including the outdoors. Similarly, concentrations are decreased by transport exiting the air space, by removal to chemical and physical sinks within the air space, or by conversion of the contaminant to other forms. Relationships are in the form of one or more differential equations representing the rate of accumulation and the contaminant gain and loss.

Models to quantify human inhalation exposure to contaminants need to consider air quality in various microenvironments such as residences, workplaces, and outdoors. Because many people spend a large fraction of their time indoors, inclusion of an indoor air quality model is an important component of total or 24-h exposure modeling. Another important component of exposure modeling is consideration of human activity patterns, that is, where and how people spend their time during the conduct of their daily activities.

In the past, simplifying assumptions have been made in modeling, such as a constant source rate over time, a negligible sink rate, steady-state conditions, or an isothermal air mass. In addition, activity patterns have not been considered or have been treated with simplistic assumptions. These may be appropriate assumptions under some limited circumstances but, to obtain greater generalizability and to better understand the behavior of indoor contaminants or the factors that affect exposures, it is important to examine situations in a more realistic manner.

This Special Technical Publication (STP) has been published as a result of the 1992 symposium entitled, "Modeling of Indoor Air Quality and Exposure" held in Pittsburgh, PA in an effort to present recent advances in various aspects of indoor air and exposure modeling. The papers presented at this symposium are grouped in three areas:

(1) Modeling and measuring sources and sinks,
(2) Model validation and application, and
(3) Modeling of exposures.

Research over the last several years has shown that emissions from indoor sources dominate indoor air concentrations and exposures much more so than factors such as ventilation. Understanding of complexities such as re-emitting sinks is just beginning. As sources and sinks are basic components of indoor air quality modeling, and considerations of sources and sinks are often linked, the papers on that subject form the first major section of the STP.

The second section of this STP contains papers that address a variety of indoor air quality modeling issues: validation of models, modeling of air flows, including consideration of computational fluid dynamics, and application of models to predict indoor air concentrations of contaminants. The third section extends considerations of indoor air quality modeling to exposure modeling. Activity patterns are treated as assumed scenarios, as measured profiles for specific individuals, and as general mobility patterns for subgroups defined by factors such as age and occupation.

Individuals who are involved in indoor air quality and exposure research can use this STP to assess the state-of-the-art, and as a foundation to further on-going research. The STP will assist environmental and public health officials with responsibilities in the areas of indoor air quality and public health in understanding the impact of various factors on indoor concentrations and exposure. With the diversity of topics covered in this STP, all focused towards modeling, it should be a valuable resource for undergraduate and graduate students and faculty.

The remainder of this overview provides some highlights of the papers included in the STP.

Modeling and Measuring Sources and Sinks

Clausen et al. determined time-varying profiles for emissions of cyclohexanone and phenol from a vinyl floor covering using two 234-L chambers and a much smaller, 0.035-L chamber. The emission rates of both compounds decreased rapidly during the first 24 h followed by a much slower decrease over the next several days. The experimental data for the initial period indicated evaporation-controlled emissions; the authors have suggested diffusion-controlled emissions for the period after the first 24 h. However, parameters for the diffusion-controlled model could not be reproduced with the data collected from this study.

Keating and McKone measured and modeled the water-to-air transfer efficiency for trichloroethylene (TCE) during showering using a specially constructed chamber and different nozzles. As expected, the nozzle producing smallest drop diameters had the highest transfer efficiency. Significant differences were observed between measured air concentrations and those predicted using transfer efficiencies and air exchange rates. The authors examined possible impacts of various factors such as measurement precision, aerosol concentrations, scavenging, deposition, and incomplete mixing. In a different study, Borrozzo et al. measured partition coefficients for TCE and ethanol to nylon, wool, polypropylene, jute, styrene-butadiene rubber (SBR), glass, cotton and polyester surfaces, as well as partition coefficients for chloroform, tetrachloroethylene, and p-dichlorobenzene to nylon, cotton, wool, and glass surfaces. For nonpolar species, sorption to polypropylene and SBR was greater than sorption to nylon or wool. For polar species, the opposite was true. The authors suggested that "*ad*sorption" can explain the majority of the experimental results but "*ab*sorption" may be a dominant mechanism in some cases. Since various components of a composite material may display different affinities for a single compound and different mechanisms of interaction, first-order kinetics may not adequately describe sorption of indoor volatile organic compounds.

Complexities of source and sink terms are further magnified when mixtures of compounds, such as environmental tobacco smoke, are considered. In such cases, it is not practical to measure or even model all constituents of the mixture as one considers their transport and removal in an indoor environment, thereby making the selection of suitable tracers an important issue in modeling. Eatough examined various components of environmental tobacco smoke (ETS) with respect to uniqueness to ETS, ease of determination at concentrations present in indoor air, and relationship to other components of ETS. The author contends that gas-phase 3-ethenylpyridine and isoprene, and particulate-phase solanesol could be better ETS tracers than nicotine and respirable particles, that have been used as tracers in the past.

The existence of re-emitting sinks for VOCs is well recognized, but the mechanisms by which VOC sinks operate are not well understood. Diffusion mechanisms have been considered to play a role in interactions of VOCs with indoor sinks. Dunn and Chen proposed and tested three unified, diffusion-limited mathematical models to account for such interactions. The phrase "unified" relates to the ability of the model to predict both in the sink accumulation and decay phases. A linear isotherm model adequately described data when a pillow functioning as a sink was exposed to ethylbenzene and a single-parameter diffusion model described pillow-sink/perchloroethylene data well, but neither could adequately describe data for carpet when exposed to ethylbenzene. A hybrid, sorption/desorption model was required to describe carpet-sink/ethylbenzene data, consistent with the complex nature of that sink.

The concept of ''deposition velocity,'' as used in describing the interaction between an airborne contaminant and indoor surfaces, is defined as the net flux of a species to a surface divided by the concentration of that species in air. Deposition velocities have been used in modeling the amount of a given substance removed by indoor surfaces. Nazaroff et al. discussed, measured, and modeled deposition velocities for four different species: fine particles, radon progeny, ozone, and nitrogen dioxide. The authors showed that the factors that may limit useful application of the concept include lack of uniform mixing in the indoor space, limited data on air motion near surfaces within buildings, spatial variability of deposition, and the inflexibility of the concept to deal with subsequent release or re-emission of contaminants into indoor air.

Sorption of contaminants on suitable filtration media is one means of improving the quality of air in buildings, yet models that fully accommodate filtration processes are not availble. Axley and Lorenzetti proposed models formulated as mass transport modules that can be combined with existing indoor air quality models. Four generic families of models proposed by the authors include: equilibrium adsorption, boundary layer diffusion, porous adsorbent diffusion transport, and convection-diffusion transport. The authors present applications of these models and propose criteria for selection of models that are based on the boundary layer/conduction heat transfer problem.

Model Validation and Application

Model validation is perhaps the weakest aspect of indoor air quality model development. Recognizing a critical need, ASTM has published a *Standard Guide for Statistical Evaluation of Indoor Air Quality Models* (ASTM D 5157) that provides quantitative tools for evaluation of indoor air quality models. These tools include statistical formulas for assessing the general agreement between predicted and measured values as well as for evaluating bias. The guide also proposes specific ranges of values for various statistical indicators that can be used in judging model performance.

As in the case of indoor air quality models in general, Guo observed that few source and sink models have been validated. The author outlined five major problems areas: (1) elusive model parameters, that result from attempts to model complex reality with a simple model, so that some adjustable parameters are necessary; (2) confusion in parameter estimation methods, specifically uncertainty in selecting appropriate regression models to accurately fit various portions of emissions decay; (3) uncertainty in scale-up and misleading scaling factors, for example, the commonly used ratio of air exchange rate to the chamber loading factor is incorrect unless the source is constant at steady state; (4) unspecified valid range, particularly the limited time over which a model is valid and the limited degree of air turbulence for which a model is valid; and (5) weakness in quantitative comparisons between models and observations, that is caused by an almost exclusive dependence upon graphic comparisons and a failure to use statistical methods.

Solutions suggested by Guo included the need to check the agreement between the model and multiple sets of observations as well as performing scale-up verification. This should be coupled with the use of statistical comparisons to complement graphic comparisons. Finally, he proposed that the key to developing relatively simple mass transfer models lies in selecting proper expressions for mass transfer coefficients, and he suggested criteria for choosing an expression. It was also noted that the degree of accuracy of model predictions necessary is an important consideration; in some cases, a simple model may do a reasonable job.

Girman expanded in some detail upon one of the concerns described by Guo: chamber air velocity and its effect on the scale-up of model results. Through simple modeling of air with chambers of different dimensions, Girman suggested that air velocities in small test chambers as currently operated may be essentially stagnant, possibly resulting in inaccurate emission factors. He proposed that boundary-layer effects be examined for a range of representative materials, especially wet sources, to determine the importance of controlling air velocities in small chambers. If chamber air velocities are currently too low to obtain representative emission factors, guidance for selecting appropriate operating conditions was suggested: operating chambers with high loading and high air exchange rates to produce representative chamber concentrations and representative air velocities. Other suggestions include varying the design of chamber air inlets and outlets.

Yamamoto et al. present a model that can be used as an analytical tool for engineers to evaluate potential ventilation performance and indoor-air-quality implications of a proposed indoor space design. The ventilation model is capable of determining distributions of time-averaged, steady-state flow fields, assuming isothermal conditions. Klobut demonstrated, through a modeling simulation, that unevenly distributed thermal load tends to increase the spread of contaminants in the building. His numerical simulations consider non-isothermal, two-way flow through large openings and illustrate differences among different scenarios, including an isothermal case with examples. Although his work represents an important step, the potential sources of uncertainties, especially those introduced by flow relations for each path, still need to be examined. The author urges a comprehensive verification of the simulation through measurements.

Jones and Waters dealt with the application of airflow and smoke modeling for building environmental design using three-dimensional computational fluid dynamics (CFD). CFD modeling can assist in design of a building in three main areas: (1) comfort, by predicting variation in thermal comfort due to air temperature and velocity and permitting optimization of space heating or cooling efficiencies; (2) health, by predicting ventilation effectiveness of the spatial distribution of fresh air; and (3) safety, by predicting the movement of smoke during a fire for a given smoke management strategy. The authors presented examples of applications of CFD modeling including design and assessment of natural ventilation strategies and prediction of smoke movement arising from accidental fires for the development of a smoke ventilation strategy.

As a number of buildings, especially in Europe, rely exclusively on natural means for ventilation, natural ventilation systems are important for indoor air quality. Panzhauser et al. pointed out that few generally accepted design rules and codes are available to assist in the design of natural ventilation systems. An effective design of natural ventilation systems could be achieved through properly designed and constructed window and shaft systems that consider regional climate, occupancy requirements, and geometric configuration of the building. Based on long-term studies of residual buildings in Austria, and mathematical modeling, the authors have developed a single-cell model to support the design and evaluation of natural ventilation systems. The model has undergone limited testing and enhancements are planned.

Applications of indoor air quality modeling to specific pollutants are presented in three papers: Panzhauser and Mahdavi predict formaldehyde concentrations and Wray et al. and Persily address radon. Panzhauser and Mahdavi extend the work on formaldehyde conducted almost 20 years ago to distinguish two types of formaldehyde sources, those that depend on indoor air conditions and those that do not. Their model calculates formaldehyde concentrations under steady-state and dynamic conditions for different sources, spaces and boundary conditions. Wray et al. used a model to make a comparative assessment of the effectiveness of subslab radon mitigation systems in residential structures. They found that, consistent with the measured data, a subslab depressurization system was more successful than a subslab pressurization system in reducing indoor radon concentrations. Persily presents results of a limited number of computer simulations of multizone airflow and radon transport for a simplified representation of a multi-family, high-rise building. His simulation considers the influence of two different radon source terms, indoor-outdoor temperature difference, and exterior wall leakage. Although the analysis is limited by the lack of measurement data, one conclusion of the study is that vertical shafts are critical pathways for air and radon transport in these tall buildings.

Modeling of Exposures

Sparks et al. have developed an indoor-air-quality based exposure model that enables analysis of individual exposures for a wide variety sources and sinks. Assuming certain activity scenarios, the model allows for calculating exposures in a multiroom residential environment. The authors provided examples to explain the impact of source emissions on exposures and modifications to those exposures due to behavior of sinks.

Rosenbaum and Anderson summarized a demonstration study of the use of dispersion modeling to estimate carcinogenic risk to residents of southern California from benzene emitted into the atmosphere. The model addresses exposures and risks due to inhalation of contaminants considering different geographic subregions, age-occupation groups, daily activities, and respiration rates. The impact of building ventilation rates on indoor air quality is considered, but indoor sources and sinks are not included in this model. With the exclusion of indoor sources and sinks in their model, the opportunity to test the correspondence between predicted and observed concentration is limited: the results of the model are in the same range as the measured outdoor benzene concentrations.

Koontz et al. described a model that is under development for estimating the distribution of Californians' indoor exposures to various pollutants. The model will address various contaminants such as VOCs, inorganic gases, and particulate matter. The model can either use existing indoor concentration and exposure information to generate exposure distributions across microenvironments or it can estimate indoor air concentration distributions for different microenvironments based on principles of indoor air quality modeling. The model utilizes recently collected data on individual activity profiles of California residents and will use Monte Carlo techniques to combine data on activity patterns, microenvironmental concentration distribution, and mass-balance parameters.

Behar et al. simulate exposures of a sample of residents in an urban area during the conduct of their daily lives and combine the exposure levels with pharmacokinetic models. The estimates of exposure are based on human activity patterns, indoor concentration distributions, and outdoor concentration distributions and are simulated using Monte Carlo techniques. The results indicate: (1) that contributions to exhaled air and arterial blood concentrations from indoor air exposures are large compared to those solely resulting from outdoor exposures, and (2) that changes in exposure rapidly translate into similar changes in blood and exhaled breath concentrations.

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