Title

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PREDICTING INDOOR POLLUTANT CONCENTRATIONS, AND APPLICATIONS TO AIR QUALITY MANAGEMENT

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1. INTRODUCTION

Because most people spend more than 90% of their time indoors, predicting exposure to airborne pollutants requires models that incorporate the effect of buildings. Buildings affect the exposure of their occupants in a number of ways, both by design (for example, filters in ventilation systems remove particles) and incidentally (for example, sorption on walls can reduce peak concentrations, but prolong exposure to semivolatile organic compounds). Furthermore, building materials and occupant activities can generate pollutants.

Indoor air quality depends not only on outdoor air quality, but also on the design, maintenance, and use of the building. For example, "sick building" symptoms such as respiratory problems and headaches have been related to the presence of air-conditioning systems, to carpeting, to low ventilation rates, and to high occupant density (1). The physical processes of interest apply even in simple structures such as homes.

Indoor air quality models simulate the processes, such as ventilation and filtration, that control pollutant concentrations in a building. Section 2 describes the modeling approach, and the important transport processes in buildings. Because advection usually dominates among the transport processes, Sections 3 and 4 describe methods for predicting airflows. The concluding section summarizes the application of these models.

2. POLLUTANT TRANSPORT

The basic indoor pollutant transport model treats a building as a collection of locations that store pollutant mass, linked by flows that represent the transport processes of interest. For example, the physical processes of advection, filtration, and deposition correspond, respectively, to pollutant storage in air, on filters, and on walls and furniture. Other processes affect the pollutant identity, for example chemical reaction, phase change, and coagulation. Still other processes represent pollutant sources, for example the release of toxins by molds.

The overall transport model assembles these individual flows, to track pollutant mass through the building (2). The model comprises a system of coupled ordinary differential equations, which describe the time rate of change of pollutant mass at each storage location. While these equations require careful numerical treatment, in principle their solution is straightforward. Thus the discussion here focuses on the individual transport processes.

Airflow is the main process responsible for transporting gaseous contaminants and aerosolized particles through a building, and between the building and the outdoors. For particles, the transport depends on the type of flow path as well as the airflow rate, since doors, cracks, and ducts trap different fractions of the particles passing through them (3). The loss rates also vary with the particle size. For example, particles of about 0.3 micron in diameter penetrate cracks more effectively than do larger and smaller particles. Therefore the transport model may have to distinguish among the size ranges of interest in its handling of the flow paths and storage locations (4).

Other transport processes that affect the airborne concentration of particles include filtration, deposition, and resuspension. Resuspension due to occupant activity may account for the fact that measurements of particulate matter typically find higher personal exposure than would be predicted based on room concentrations (the "personal cloud"). In addition, tracking of particles (e.g. on shoes) can move contaminants between surfaces. Again these processes depend on the particle size.

Buildings have a higher ratio of surface area to volume than outdoors, so sorption is relatively more important. As noted above, sorption can moderate and prolong exposure. This effect may be especially pronounced in the face of temperature variations. For example, the daily cycling of temperatures in a ventilation system can cause particles trapped on the filters to sorb and release large quantities of pollutant.

While the important pollutant transport processes are known, many suffer from poor experimental characterization (3). Size-resolved penetration through cracks, and deposition in rooms and in ductwork, remain poorly understood at a theoretical level as well.

One important simplification of the modeling approach deserves special mention. Idealizing a building as a single, well-mixed zone, in which the room air serves as the only storage location of interest, produces a single transport equation with an analytical solution. This simple "box model" can provide good estimates of exposure in a residence, or in a single space of a commercial building where the flows are well known, for example because a mechanical ventilation system controls the entry of air into the space.

3. AIRFLOW BETWEEN ZONES

The airflows in a building depend on its leakage characteristics and operation, as well as on three driving forces: wind, buoyancy, and mechanical ventilation. For unventilated dwellings, a number of models predict infiltration as a function of wind speed and indoor-outdoor temperature difference (5). Thus they couple directly to the box model mentioned above. Since these models make assumptions about construction details of the residence, they do not apply to all housing types.

To predict airflows in complex structures, multizone models idealize a building as a network of well-mixed spaces or zones, connected by discrete flow elements such as doors, windows, cracks, fans, and ducts. The model finds the steady-state airflows that satisfy both the flow element relations and mass balance in the zones (6). A number of public and commercial codes implement this basic model. Most integrate a pollutant transport model as well.

To set up a multizone model, the practitioner divides the building into zones, then adds flow paths. Choosing model parameters, for example crack leakage areas, requires experimental techniques such as blower-door and tracer gas tests (5), or reference to lists of equivalent leakage areas for typical flow components (5, 7). Direct measurement of airflows in ventilation systems can quantify this major driver of pollutant transport, without the need to parameterize individual ducts, fans, dampers, and so on.

An extensive literature describes the validation of multizone models using whole-building tracer gas tests. However, this literature largely neglects important issues such as: (1) the number, type, and location of flow paths required to achieve a good fit to the data; (2) the sensitivity of the computed solutions to the model parameters; and (3) the model's performance with the ventilation system shut off, when uncertainties in the driving forces become relatively greater. Thus, multizone modeling remains an art, requiring a good understanding of the important flow paths, and an awareness that, although adding zones and paths to a model makes it easier to match the observed flows, it does not necessarily improve the model's predictive ability.

Multizone models have a number of limitations, which do not affect their utility in typical applications. For example, some codes cannot predict two-way vertical flows in stairwells and elevator shafts, potentially causing problems when simulating naturally-ventilated buildings. In the pollutant calculations, treating each zone as well-mixed ignores the flow complexity in large spaces. Furthermore multizone models usually represent pollutant transport as instantaneous, without accounting for either pollutant storage or transit time in the flow elements. Thus, problems dominated by the dynamics of pollutant transport in ducts may require more detailed transport models than multizone tools provide.

4. AIRFLOW WITHIN ROOMS

The well-mixed assumption fails in some rooms, due to: (1) local effects such as a pollutant source located near an airflow outlet; (2) buoyancy of dense or hot gases, including smoke and pollutants resulting from cooking; or (3) lack of mixing by the room airflow, for example due to short-circuiting between the ventilation system's supply and exhaust. Failure of the well-mixed assumption leads to under- or over-estimates of exposure. Unfortunately, the likelihood of failure may increase for large spaces, such as auditoria, which can contain many occupants.

Some models, known as zonal or subzonal, divide the poorly-mixed space into subzones connected by multizone-style flow elements. This approach does not capture the flow physics, since it neglects momentum in the airflow (8). The more appropriate technique, of computational fluid dynamics (CFD), discretizes the governing Navier-Stokes equations on a grid of points in the room (9). Building applications tend to use finite-volume discretizations and Reynolds-averaged turbulence models.

Typical uses of CFD in buildings focus on thermal comfort, ventilation efficacy, and detailed studies of phenomena such as mixing (10). These applications require tens of thousands of computational nodes, and hours of computer time, to find the flows in a single room (multizone models, by comparison, take a minute to find airflows for a whole building). Fortunately a relatively coarse CFD grid may prove sufficient to predict gross features of pollutant transport, at a significantly lower cost (8).

However, even with coarse grids whole-building CFD remains largely unattainable using current computers and solution algorithms. The obvious compromise, a combined multizone-CFD application, has appeared in the research literature, but has not gained widespread use. Probably the next few years will produce a number of validation studies for software tools that couple single-room CFD to multizone models.

5. DISCUSSION

Models for predicting airborne pollutant concentrations in buildings take a system-dynamic approach, assembling submodels that quantify the transport processes of interest. For ideal, nonreactive gases, most of the modeling uncertainty surrounds the choice of zones, zone volumes, and airflow rates. Reactive, volatile, and semivolatile gases introduce transport processes besides advection. Aerosols introduce issues of particle size as well as new transport processes. All these models contribute to uncertainty in the simulation, and the practitioner should perform some type of uncertainty analysis, such as Monte Carlo simulation, as part of any prediction effort.

A qualitative difference exists between uncertainty in the airflow and other transport processes. Airflow models are relatively well-understood, but require a large data collection effort in each building. By contrast, other transport processes are poorly understood, but once experimental work to develop models for specific pollutants is complete, they may apply across many buildings.

This paper does not list specific airflow and pollutant transport models. Many of the appropriate codes may be found in (4, 6, 7, 8, 9, 10).

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