Title
Modeling transient contaminant transport in HVAC systems and buildings.

Authors
Federspiel, C C
Li, H
Auslander, D M
et al.

Publication Date
2002-06-01

Peer reviewed

MODELING TRANSIENT CONTAMINANT TRANSPORT IN HVAC SYSTEMS AND BUILDINGS

CC Federspiel[1], H Li[1], DM Auslander[2], D Lorenzetti[3], AJ Gadgil[3]

[1]Center for the Built Environment, University of California, Berkeley, CA, USA
[2]Dept. Of Mechanical Engineering, University of California, Berkeley, CA, USA
[3]Indoor Environment Dept., Lawrence Berkeley National Laboratory, Berkeley, CA, USA

ABSTRACT
A mathematical model of the contaminant transport in HVAC systems and buildings is described. The model accounts for transients introduced by control elements such as fans and control dampers. The contaminant transport equations are coupled to momentum equations and mass continuity equations of the air. To avoid modeling variable transport delays directly, ducts are divided into a large number of small sections. Perfect mixing is assumed in each section. Contaminant transport equations are integrated with momentum equations in a way that guarantees mass continuity by using two non-negative velocities for computing the mass transport between elements. Computer simulations illustrate how the model may be used to analyze and design control systems that respond to a sudden release of a toxic contaminant near a building. By coupling transient flow prediction with transient contaminant prediction, the model overcomes a number of problems with existing contaminant transport codes.

INDEX TERMS
Air transport, HVAC, Modeling pollutant concentrations

INTRODUCTION

Contaminant transport indoors is influenced by the motion of indoor air (advection) and by diffusion. In buildings with mechanical ventilation, the movement of air by mechanical equipment plays a significant role in the transport of contaminants. Mechanical equipment such as fans and dampers continually adjust the flow rates of air in buildings, sometimes slowly, but other times abruptly.

Two kinds of computer codes exist for modeling contaminant transport indoors. One kind, called computational fluid dynamics (CFD), solves the partial differential equations governing mass, momentum, and energy transport on a fine grid. CFD codes are complex, expensive, and difficult to use, so simpler models have been proposed that use lumped or zonal models to predict contaminant transport. Examples of such zonal models are CONTAM (Walton, 1997) and COMIS (Fuestel, 1999).

Existing zonal models assume steady-state air motion. Airflows are determined by solving a set of nonlinear algebraic equations for air mass conservation at a set of zones. After the flows have been determined, mass transport of the contaminant is predicted by equations governing zone-to-zone mixing.

The model described in this paper is motivated by the need for a zonal model that can predict contaminant transport under conditions where the air motion is highly transient. The intended application is the prediction of controlled response following the release of a toxic contaminant in or near a building. If the release could be detected, then the building controls could be used to rapidly redistribute air to minimize injury. Existing zonal models are not suited to predicting rapid response.

The approach is to couple equations governing zone-to-zone mixing with equations of motion for the air. Transient behavior due to both mixing and unsteady air motion are solved simultaneously. Flow rates from the equations of motion are used in the advection terms of the mixing equations. Mass conservation of the contaminant is ensured by using two non-negative velocity terms in the mixing equations derived from the equations of motion.

METHODS

The equations of motion for airflow in ducts has been described elsewhere (Federspiel et al., 2001). A summary is provided here. Equations of motion are derived from momentum equations in HVAC system ducts. The change of momentum in a duct is equal to the sum of forces acting on the boundaries of a control volume draw at the surfaces and ends of the duct. Forces include pressure at duct end points, which are often junctions with other ducts, fluid friction, pressure drops across minor loss components such as elbows, and pressures developed by fans. The momentum equations for a network of ducts can be expressed by the following set of differential equations:

$$M\dot{V} = -F\langle V|V|\rangle - K\langle V|V|\rangle + A_f P_f + A_e P_e + A_j P_j \tag{1}$$

where M is a mass matrix, V is a velocity vector, F is a matrix of friction terms, K is a matrix of loss coefficient terms, P_f is a vector of fan static pressures, P_e is a vector of external pressures, and P_j is a vector of junction pressures.

Conservation of mass at each junction in the network is described by the following set of linear equations:

$$A_j^T V = 0 \tag{2}$$

Together, Equations 1 and 2 form a set of differential algebraic equations (DAE) with index 1. They can be reduced to a set of ordinary differential equations by differentiating the conservation constraint (Equation 2), substituting Equation 1, solving for the junction pressures, then substituting the junction pressures into Equation 1.

Contaminant transport in ducts and in rooms is modeled using mixing equations with advection from one zone to another. Figure 1 shows a schematic of a three-zone mixing system. To ensure conservation of mass of the contaminant two non-negative flow terms connect the zones.

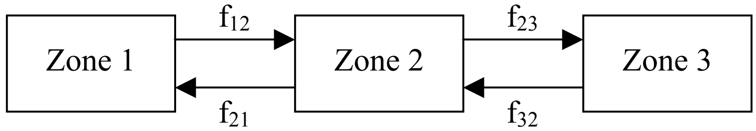

Figure 1: Schematic diagram of a three-zone mixing system.

The mixing equation for zone 2 is as follows:

$$\frac{d}{dt}\left(M_2\omega_2\right) = f_{12}\omega_1 - f_{21}\omega_2 - f_{23}\omega_2 + f_{32}\omega_3 \tag{3}$$

where M_2 is the mass of air in zone 2, ω denotes mass concentration, and f denotes mass flow rate. When a sequence of zones is used to model a duct, all of the flow terms in one direction equal the flow computed from the momentum equation, and all of the flow terms in the opposite direction are zero. Using the non-negative flow terms simplifies the switching in the mixing equations that results from flow reversals in the equations of motion, and adds very little overhead to the simulation code.

The transport delay resulting from contaminant transport in ducts is modeled by breaking the duct into a large number of adjacent sections in a so-called “tanks-in-series” model. As the number of sections approaches infinity, the behavior of the multi-zone mixing model approaches that of a plug-flow model. Figure 2 shows how well mixing models with increasing numbers of sections approximate a plug flow system.

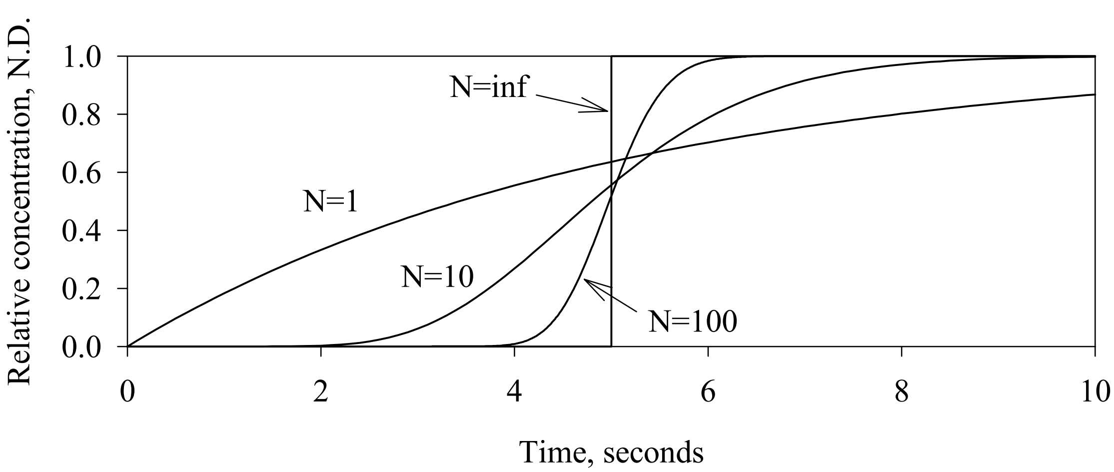

Figure 2: Approximation of plug flow by mixing systems.

RESULTS

In this section we show examples of simulations of a simplified system configured to model an air-handling system serving a single zone. The system has five ducts (outdoor, recirculation, supply, return, and exhaust), with the following diameters: 1.2, 0.7, 0.6, 0.5, and 0.4 meters, respectively. The duct lengths are 3, 5, 100, 80, and 3 duct diameters, respectively. The room is 11.5 by 23 meters in area, and is 3 meters high. The system has a supply and return fan, and control dampers in the outdoor, recirculation, and exhaust ducts.

We modeled a scenario where a contaminant suddenly enters the outdoor air intake at a fixed concentration of 345 μg/kg. We assumed that the contaminant would enter the exhaust duct at that concentration if the flow there reversed, and that the contaminant would enter the room by infiltration at that concentration if the room pressure became negative. When the contaminant first enters the system a control action is taken. We modeled two control actions. The first is the standard shutdown action for an air-handling unit. The fans shut down together, the outdoor and exhaust dampers close, and the return damper opens. We also considered an alternative action in which the return damper closes in order to reduce air motion as quickly as possible. The damper actuators move at a fixed speed of one degree per second. The fans slow down exponentially with a time constant of 90 seconds.

Figure 3 shows the room concentration as a function of time for both actions. The standard shutdown procedure is more effective at controlling the concentration of the contaminant. While closing the return damper clearly reduces the supply flow rate as shown in Figure 4, it also increases the outdoor airflow rate (Figure 5), increasing the concentration in the supply duct (Figure 6).

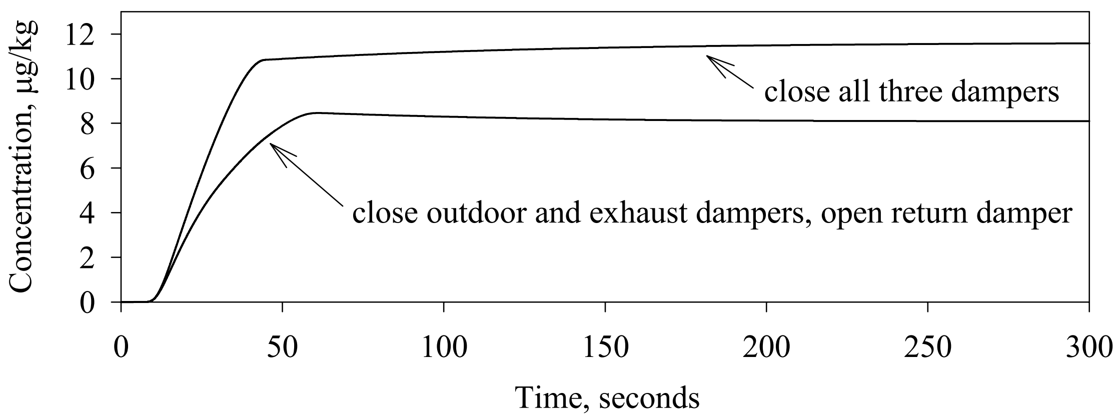

Figure 3: Room concentrations for both actions.

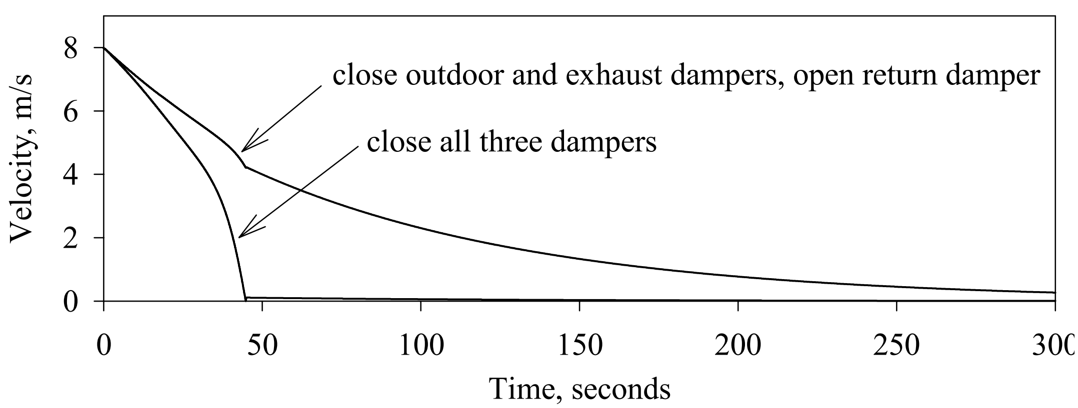

Figure 4: Velocity in supply duct for both actions.

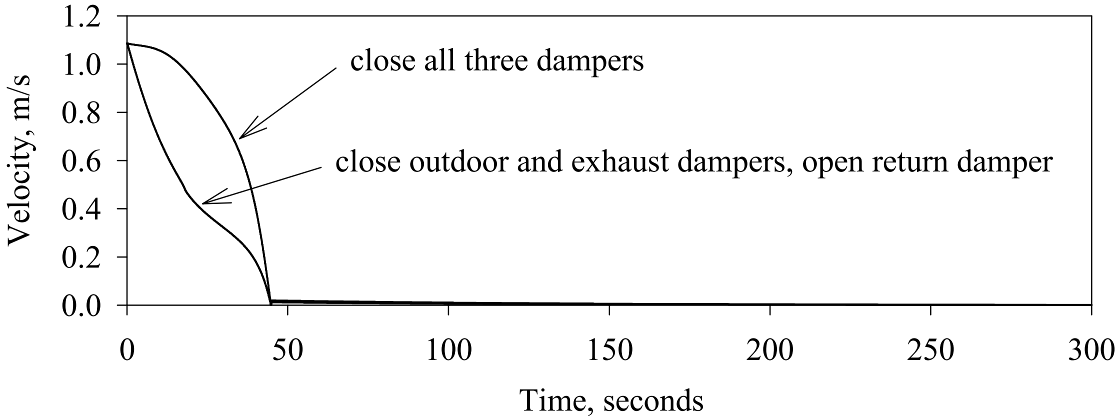

Figure 5: Velocities in outdoor air duct for both actions.

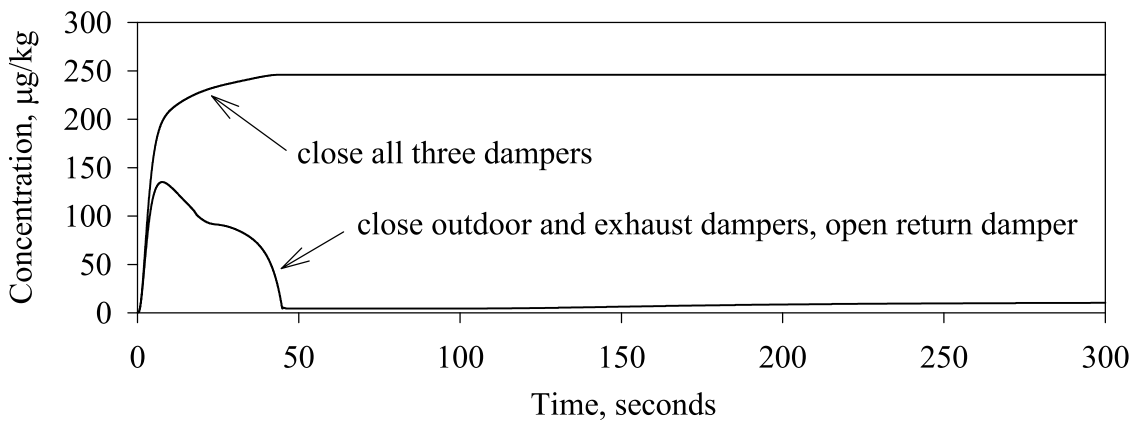

Figure 6: Concentration at the inlet of the supply duct for both actions.

DISCUSSION

The model proposed in this paper was developed specifically to analyze and design control systems that respond to accidental or intentional releases of toxic contaminants. The simulations in the previous section illustrate how it can be used for that purpose. However, it could also be used to study how the normal transient behavior of HVAC controls impacts indoor air quality. For example, the model could be used to assess how start-stop operations of small, packaged equipment impact the indoor concentration of normally occurring volatile organic compounds indoors.

The model described in this paper may require a solver that can handle stiff systems, which are systems that have a wide range of eigenvalues. The momentum equations will be stiff if some ducts are very short relative to others or if the loss coefficients in some ducts are very high. In practice both of these conditions are common. Furthermore, the contaminant transport equations will be stiff if zones of widely varying sizes are used. This is likely since some zones will represent duct sections while others will represent rooms. To get acceptable behavior from the simulations in the previous section it was necessary to use a solver designed to handle stiff systems, to tighten the tolerances, and to force it to use no more than second-order integration, which is absolutely stable.

The model proposed in this paper could help overcome some of the significant problems associated with zonal models such as CONTAM and COMIS, which rely on fairly limited types of steady-state flow models. Using transient models provides one way to escape the modelling restrictions in these programs. Furthermore, for airflow applications it is trivial to provide consistent initial conditions for the simulation simply by setting all velocities and fan speeds to zero. Therefore it is always possible to arrive at a solution to the airflow system using transient models, even if the modeller is only interested in steady-state behavior.

Another problem associated with zonal models that rely on steady-state flow is that the models assume that contaminants move instantaneously between rooms. They don't normally treat duct sections as zones, so they don't account for the fact that the HVAC system itself can store contaminants. This means that they may over-predict concentrations after events such as the kind show in the simulations in this paper.

The momentum of fan wheels and air mass in ducts causes air to continue to move even after fans have been de-energized or fan speeds changed. If existing zonal models are used to predict transient behavior, then errors may be made in predicting flows because fan speed lags fan commands and air velocity lags fan speed. The model in this paper overcomes this problem.

CONCLUSION AND IMPLICATIONS

We have developed a model that predicts the concentrations of contaminants in HVAC systems and buildings during sudden transient conditions. It differs from existing zonal models by simultaneously predicting unsteady airflow and unsteady contaminant transport. The model can be used to analyze and design control actions taken in response to an accidental or intentional release of a toxic contaminant in or near a building.

ACKNOWLEDGEMENTS

This work was supported by the Office of Non-proliferation and National Security, Chemical and Biological Non-proliferation Program of the US Department of Energy under Contract No. DE-AC03-76SF00098.

REFERENCES

Federspiel, C. C., S. D. Lanning, H. Li, and D. M. Auslander, 2001, "Coordinated Control of HVAC Systems," *Proceedings of the International Conference for Advanced Building Operations*, Austin, TX.

Feustel, H. E., 1999, "COMIS--an international multizone air-flow and contaminant transport model," *Energy and Buildings*, 30(1), 3-18.

Lorenzetti, D. M., 2001, "Computational Aspects of Nodal Multizone Airflow Systems," LBNL Report #46949.

Walton, G. N., 1997, "CONTAM96 User Manual," U.S. Department of Commerce, National Institute of Standards and Technology, report no. NISTIR 6056.