

Modeling Indoor Contaminant Dispersion

Darrell W. Pepper¹ and Xiuling Wang²

Extended Abstract

The study of indoor air pollution requires understanding fundamental principles of fluid mechanics, species transport, heat transfer, and systems engineering. Buildings have become complex entities with considerable electronic control features embedded within the structures. Of particular concern are issues involving contaminants that routinely enter or lie dormant within building interiors, and their effects upon human health. Articles can be commonly found in newspapers printed throughout the world describing groups of people becoming sick while staying in a hotel, cruising on a ship, or travelling in planes or buses.

Efforts to define and describe pollutant transport within buildings and interiors has become complex. Modeling pollutant transport within indoor environments now requires computational methods and techniques that were utilized only in research laboratories a few years ago. Knowledge of fundamental principles of ventilation and building systems, including HVAC, must now be coupled with computational fluid dynamics techniques in order to accurately assess human health and predicting contaminant transport.

Toxic fumes and airborne diseases are known to produce undesirable odors, eye and nose irritations, sickness, and occasionally death. Other products such as tobacco smoke and carbon monoxide can also have serious health effects on people exposed to a poorly ventilated environment; studies indicate that indirect or passive smoking can also lead to lung cancer. Recommendations for outdoor airflow rates to dilute indoor polluted air vary considerably.

In recent years there has been extensive activity in the development and use of CFD tools and special programs for room air movement and contaminant transport applications. These investigations range from the prediction of air jet diffusion, air velocity and temperature distribution in rooms, spread of contamination in enclosures, to fire and smoke spread inside buildings. In most cases the predicted results have been promising when compared to available experimental data. However, numerical modeling of ventilation and associated interior contaminant transport is still at an early stage of development. A considerable amount of research and development work is still needed, particularly in the areas of efficient computational schemes, irregular and adaptive grids, turbulence modeling and wall functions.

One of the earliest attempts to numerically simulate airflow in rooms was conducted by Nielsen (1974) using the stream function-vorticity approach for the de-

¹Professor of Mechanical Engineering, Director of Nevada Center for Advanced Computational Methods (NCACM), University of Nevada Las Vegas (UNLV), Las Vegas, NV, 89154-4027

²Research Assistant Professor, NCACM, UNLV, Las Vegas, NV, 89154 -4027

pendent variables, along with a two-equation ($k-\epsilon$) model for turbulence based on the numerical procedure developed by Gosman et al (1969). The computations produced realistic room flows, but was limited to 2-D. Numerous papers have appeared over the years utilizing the stream function-vorticity approach for simulating 2-D flows within enclosures; however, the approach is *practically* limited to 2-D flows, and does not permit one to easily incorporate turbulence and 3-D effects inherent in actual ventilated enclosures. Efforts were later undertaken by Hjertager and Magnussen (1977) using the finite volume approach and the SIMPLE algorithm developed by Patankar and Spalding (1972) to solve the 3-D primitive equations of motion with the $k-\epsilon$ two-equation model for turbulence. They modeled the flow from an air jet exhausting into a rectangular room with two ceiling exits. While the point of jet separation from the ceiling was well predicted, the predicted velocity of the jet near the lower region of the room was higher than the measured value.

Gosman et al (1980) extended their two-dimensional finite volume model to solve isothermal flows within 3-D enclosures with small ventilation openings. They achieved good correlations of velocity profiles and jet velocity decay with measurements. Sakamoto and Matsuo (1980) similarly predicted 3-D isothermal flow in a room using the marker and cell (MAC) technique (Harlow and Welch, 1965) and two turbulence models: the $k-\epsilon$ approach and the large-eddy simulation (LES) technique (Deardorff, 1970). Results compared favorably with measured velocity profiles; they recommended that the $k-\epsilon$ approach for turbulence be used for room flow predictions over the LES model because it is simpler to use and requires less computing time for comparable accuracy. A computer program called CAFE, developed by Moulton and Dean (1980), was used to solve the 3-D velocity components, temperature, concentration, and $k-\epsilon$ turbulence parameters for flow in industrial enclosures and clean rooms. Results were in good agreement with measurements in regions where velocities were large.

Murakami et al (1987) investigated the three-dimensional airflow and contamination dispersion in six (rectangular) types of ceiling supply clean rooms both numerically and experimentally for isothermal flow. They used the MAC method coupled with a central difference approach for the velocity components, and a second-order upwind scheme for k , ϵ , and concentration, to solve the transient transport equations. Results showed good agreement between prediction and measurement, as well as some interesting flow phenomena regarding the spread of a jet exhaust as it reached the floor. Awbi (1989) numerically solved 2-D air flow and temperature distributions within rooms with diffusers and various vent locations in an effort to simulate 3-D effects; the 2-D non-isothermal predictions compared well to measured vertical velocity and temperature profiles in the room. An early historical discussion and descriptions of numerical methods for solving 2-D and 3-D ventila-

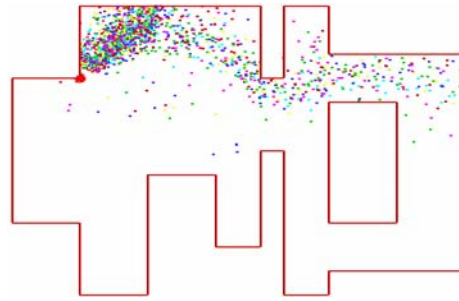
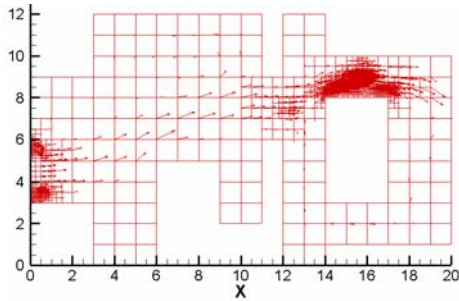


Figure 1: Flow of air within office complex Figure 2: Particle dispersion pattern case 1

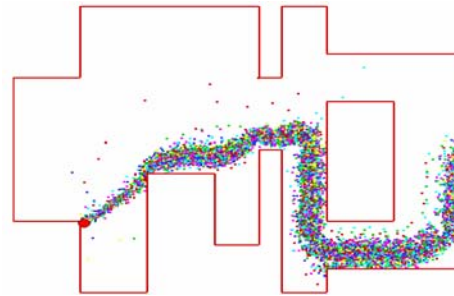
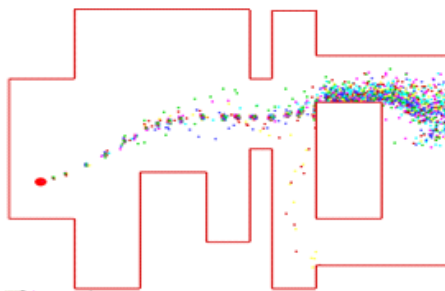


Figure 3: Particle dispersion pattern case 2 Figure 4: Particle dispersion pattern case 3

tion and contaminant transport is given by Awbi (1991). More recent descriptions of modeling efforts can be found in such journals as *Numerical Heat Transfer*, the *ASHRAE Transactions*, *Indoor Air*, and other related technical journals.

In this paper, a review of computational methods used to simulate indoor ventilation and species transport will be presented. In addition, recent methods employing hp-adaptive finite element techniques and use of stochastic schemes including Lagrangian particle transport will be discussed, including the use of meshless techniques (Atluri, 2005). The use of finite element schemes, as well as meshless methods (although limited in applicability at this time), permit irregular computational domains to be simulated; adaptive technologies provide highly accurate results, but require more computational storage than meshless methods. Current efforts have centered on the use of general probability distributions for the random component of motion due to turbulent diffusion (Runchal, 1980). Using a random walk model and Lagrangian particles to represent concentration, particle displacement in each coordinate direction can be calculated independently. Recent efforts utilizing these coupled computational techniques appear attractive for homeland security purposes.

Preliminary Results

Simulated air distribution patterns and pathways of a powder dispersing within

an office complex are shown in the following series of pictures. Both the door and the windows are open, and the contaminant powder spreads into the inner office. The flow of air and resulting velocity vectors are shown in Fig. 1 for a simple 1.5 m/s inflow into the office.

Particle dispersion patterns (where the red dot denotes contaminant source) are shown in Fig. 2, Fig. 3 and Fig. 4. The contaminant source has been placed on table 1 (case 1), center of the room (case 2), and table 2 (case 3), respectively.

The pollutant is transported and diffused by the ventilation pattern that affects the office complex. It is important that first responders be aware of the trajectory of the spreading contaminant. It is also critically important that inhabitants be aware of the contaminant pathway, and take evasive action. A fully automatic hp-adaptation strategy is used to adjust elements size and order according to the error distribution for solving the Navier-Stokes equations. A series of movies will be shown illustrating the transport of contaminant transport under varying indoor conditions.

References

1. American Society of Heating, Refrigerating and Air-Conditioning Engineers, *ASHRAE Handbook 1981 Fundamentals Volume*, Chpt. 22, Atlanta, GA, 1981, pp. 22.1-22.20
2. Atluri, S. N. , *Methods of Computer Modeling in Engineering and the Sciences*, Vol. 1, Tech. Sci. Press, Forsyth, GA, 2005, p. 560.
3. Awbi, H. B., "Application of Computational Fluid Dynamics in Room Ventilation," *Build. Environ.*, 24, 1989, pp. 73-84.
4. Awbi, H. B., *Ventilation of Buildings*, Chapman and Hall, London, 1991.
5. Deardorff, J. W., "A Numerical Study of Three-Dimensional Channel Flow at Large Reynolds Numbers," *J. Fluid Mech.*, 41, 1970, pp. 453-480.
6. Gosman, A. D., Pun, W. M., Runchal, A. K., Spalding, D. B., and Wolfshtein, M., *Heat and Mass Transfer in Recirculating Flows*, Academic Press, London, 1969.
7. Gosman, A. D., Nielsen, P. V., Restivo, A., and Whitelaw, J. H., "The Flow Properties of Rooms with Small Ventilation Openings," *Trans. ASME, J. Fluid Engr.*, 102, 1980, pp. 316-323.
8. Gresho, P. M., Chan, S. T., Lee, R. L., and Upson, C. D., "Modified Finite Element Method for Solving the Time-Dependent Incompressible Navier-Stokes Equations, Part 1, Theory," *Int. J. Num. Meth. Fluids*, 4, 1984, pp. 557-598.

9. Harlow, F. H. and Welch, J. E., "Numerical Calculation of Time-Dependent Viscous Incompressible Flow of Fluid with Free Surfaces," *Phys. Fluids*, 8, 1965, pp. 2182-2189.
10. Hjertager, B. H. and Magnussen, B. F., "Numerical Prediction of Three-Dimensional Turbulent Buoyant Flow in a Ventilated Room," *Heat Transfer and Turbulent Buoyant Convection*, D. B. Spalding and N. Afgan (Eds.), Vol. II, Hemisphere, Washington, DC, 1977, pp. 429-441.
11. Moulton, A. and Dean, R. B., "CAFE-A Computer Program to Calculate the Flow Environment," CAD 80, *4th Int. Conf. on Computers in Design Engineering*, Brighton, UK, 1980.
12. Murakami, S., Kato, S., and Suyama, Y., "Three-Dimensional Numerical Simulation of Turbulent Airflow in a Ventilated Room by Means of a Two-Equation Model," *ASHRAE Trans.*, 93(2), 1987, pp. 621-642.
13. Nielsen, P. V., "Flow in Air Conditioned Rooms," PhD Thesis, Tech. Univ. of Denmark, 1974.
14. Patankar, S. V. and Spalding, D. B., "A Calculation Procedure for Heat, Mass, and Momentum Transfer in Three-Dimensional Parabolic Flows," *Int. J. Heat Mass Transfer*, 15, 1972, pp. 147-163.
15. Runchal, A. K., "A Random Walk Atmospheric Dispersion Model for Complex Terrain and Meteorological Conditions," *2nd AMS Joint Conf. on Appl. of Air Pollution Meteor.*, March 24-27, 1980, New Orleans, LA.
16. Sakamoto, Y. and Matsuo, Y., "Numerical Predictions of Three-Dimensional Flow in a Ventilated Room using Turbulence Models," *Appl. Math. Modelling*, Vol. 4, 1980, pp. 67-71.

