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Numerical prediction for indoor air movement

Current status and future research needs in the development of room convection modeling

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THE RECENT RAPID progress in computer technology has made it possible to perform large-scale computations at much lower costs than just a few years ago. Excellent articles on this subject are found in a recent publication called "Super Computing."[1]

In addition, the increasing demand for developing a detailed design method for constructing extremely clean factories, in which LSI circuits are manufactured, has accelerated research concerning the micro modeling of local contaminant dispersion processes under uniform temperature conditions. Under these circumstances, an extensive effort has been made in Japan for the development of numerical prediction methods for room air motion in the last decade.

In the United States, room convection modeling is considered important for predicting thermal comfort, indoor air quality and smoke migration. ASHRAE Task Group on Indoor Environmental Calculation is currently evaluating several proposals to develop computer programs for predicting two- and three-dimensional room convection. Japanese experience on room air convection simulation developed in conjunction with clean room air flow analysis should be very valuable for ASHRAE task group efforts.

Turbulence models

The numerical calculation approach using the turbulence model with the finite difference technique is considered the most promising and recommendable method as far as practical applications are concerned, based on a number of experimental validations.[2,3,4] The turbulence models which have been tested by Japanese researchers in building physics are called the k-ε model[5] and the large eddy simulation (LES) method.[6,7]

The former is a model for Navier-Stokes equations for average velocities and pressures (Reynolds equations), and are given in Equation 1 in tensor notation omitting molecular viscous stress terms. This model relates the Reynolds stress terms appearing in the Reynolds equations to the local gradients of mean velocity using eddy-viscosity concept as in Equation 2.

$$\frac{DU_i}{Dt} = -\frac{1}{\varrho}\frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j}(-\overline{u_i u_j}) \qquad (1)$$

$$-\overline{u_i u_j} \sim \nu_t \cdot e_{ij} - \frac{2}{3}k\delta_{ij} \qquad (2)$$

In the k-ε model, two additional partial differential equations are employed for the turbulence kinetic energy (k) and its dissipation rate (ε) in order to estimate the spatial distribution of eddy viscosity (ν_t). The k-ε model for the high Reynolds number flow is given in tensorial forms in Equations 3-5.

$$\frac{Dk}{Dt} = \frac{\partial}{\partial x_j}\left[\frac{\nu_t}{\sigma_k}\left(\frac{\partial k}{\partial x_j}\right)\right] + \nu_t\frac{e_{ij}e_{ij}}{2} - \varepsilon \qquad (3)$$

$$\frac{D\varepsilon}{Dt} = \frac{\partial}{\partial x_j}\left[\frac{\nu_t}{\sigma_E}\left(\frac{\partial \varepsilon}{\partial x_j}\right)\right] + C_1\frac{\varepsilon}{k}\nu_t\frac{e_{ij}e_{ij}}{2} - C_2\frac{\varepsilon^2}{k} \qquad (4)$$

$$\nu_t = C_D\frac{k^2}{\varepsilon} \qquad (5)$$

On the other hand, the LES method employs the spatially filtered Navier-Stokes equations over the computational grid scale as the governing equations for large-scale fluid motion. The nonlinear interaction between large-scale and small-scale (subgrid scale) motion is approximated through the subgrid scale eddy viscosity model. The least complicated and commonly used version of the LES model is expressed in Equations 6 and 7 (again in a tensorial form).

$$\frac{\partial (U_i)}{\partial t} + \frac{\partial (U_i)(U_j)}{\partial x_j} = -\frac{1}{\varrho}\frac{\partial (P)}{\partial x_i} + \frac{\partial (\nu + \nu_s)(e_{ij})}{\partial x_j} \qquad (6)$$

$$\nu_s = (C\Delta)^2 \cdot \left[\frac{(e_{ij})^2}{2}\right]^{1/2} \qquad (7)$$

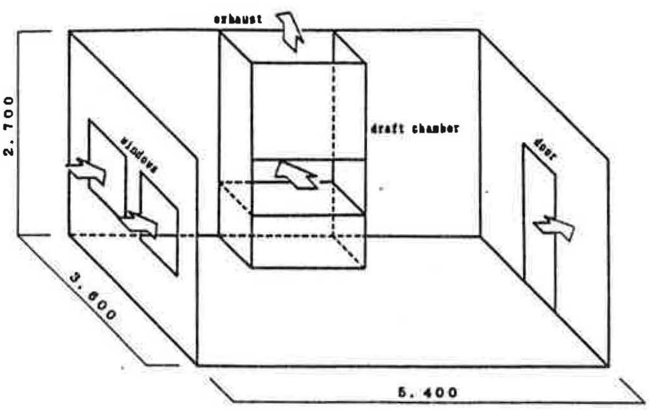

Figure 1—Room geometry (dimensions in mm)

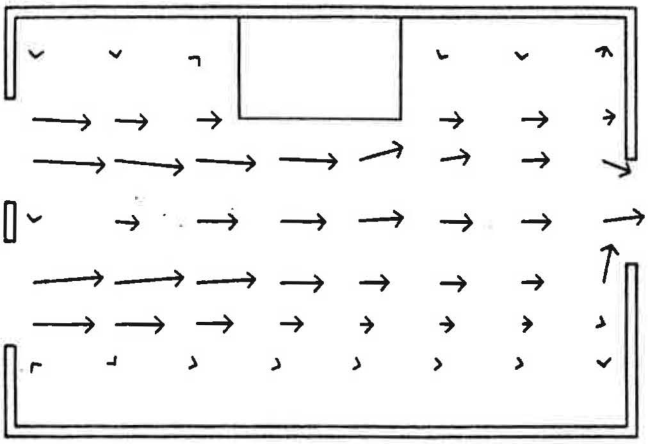

Figure 2—Measured velocity vectors in the representative plane at 1.260 mm above floor level

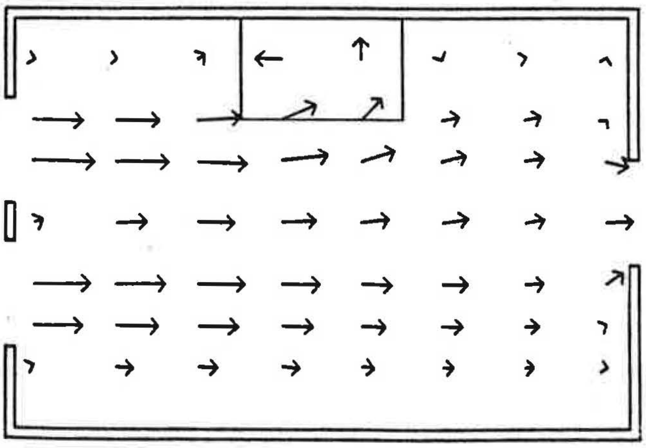

Figure 3—Predicted velocity vectors in the representative plane at 1.260 mm above floor level

The LES method

The LES method has several significant advantages. For example, the model consists of the filtered Navier-Stokes equations themselves and only one empirical constant, "C" in Equation 7, is sufficient to complete the subgrid scale model. Moreover, the general modeling for the subgrid scale stresses can be made more universal and acceptable than those required in the derivation of other transport type turbulence models, provided that the representative Reynolds number is large enough and the computational grid sizes lie in the inertial subrange, where energy cascade across each wave number is approximately conservative so that the energy flux takes the constant value of ε.

In spite of these superior characteristics, it appears that the LES method has not been widely used for predicting a variety of practical problems because of its computational difficulty.

As has been already mentioned, the LES method uses the filtered Navier-Stokes equations with respect to grid space but not time, the solution of these equations is never stationary (as the actual turbulent flow is not). If mean flow quantities have to be predicted, transient calculations must be conducted over time large enough to make the averaged values reliable. Unfortunately, these calculations still require too much computational time and computer memories even for the current super-computers. The LES method still will be applied, however, to limited problems requiring very fundamental understanding of flow phenomena or used for the verification of some more economical models.

The k-ε model

As a contrast, the k-ε turbulence model has a less stiff theoretical background, especially on the ε equation. Nevertheless, this model has been applied to many engineering problems partly because it requires moderate calculation efforts and has been proven to be capable of predicting practical turbulent flow problems with better accuracy than expected.

NOMENCLATURE

C	empirical constant in large eddy simulation method
C_1, C_2, C_D	empirical constants in k-ε turbulence model
e_{ij}	$\frac{\partial U_i}{\partial x_i} + \frac{\partial U_i}{\partial x_j}$
k	kinetic energy of turbulence
P	pressure
U_i	mean velocity component in x_i direction
u_i	fluctuating velocity component in x_i direction
x_i	coordinate
Greek Symbols	
ε	dissipation rate
ρ	density
ν	kinematic viscosity
ν_t	eddy viscosity
ν_s	subgrid scale eddy viscosity
δ_{ij}	kronecker delta
σ_k, σ_E	empirical constants in k-ε turbulence model
Special Symbols	
overbar	correlations of fluctuating quantities
D/Dt	substantial derivative
( )	spatially filtered value over the computational grid
Δ	mean local grid size = $(\Delta_x\Delta_y\Delta_z)^{1/3}$

Numerical prediction

In order to demonstrate the power and accuracy of the k-ε model, recent calculations of an indoor air pollutant dispersion problem using the k-ε model are described below.[8] Calculations were made by the senior author of this article at the University of Tokyo.

The room geometry used in the study represents a hypothetical chemical laboratory in which windows (fresh air intake) and a door opening (exhaust) were located on the opposite side of the room and a mechanical ventilation device (draft chamber) was installed as shown in *Figure 1*.* Comparative data were obtained using the 1/6 scale reduction model of the geometry with duct circulation systems.

In the experiment, concentration distribution was measured using C_2H_4 as tracer and the concentration analyzer which is composed of suction tube, pump and gaschromatography. Velocity distribution also was measured on a representable cross section using tandem special hot wire anemometer which is able to measure instantaneous velocity component as well as its direction.

In order to simulate the experimental condition, the room was subdivided into 30 × 20 × 15 rectangular "cells," and partial differential equations governing the mean velocity distributions were solved together with the k-ε turbulence model equations to account for the turbulence effect. The solution procedure used in the study was the finite difference technique based on the "MAC method,"[9] and the main feature of the solution technique is described briefly:

- Staggered grid system is used for discretion of dependent variables, which means that scalar quantities such a k, ε, P are defined in the center of the "cell" and velocity vector components on the "cell" surface perpendicular to it in each direction.
- Each partial differential equation is cast into finite difference form using upwind differencing for scalar quantity and central differencing for momentum equations.
- A pressure relaxation technique is used to handle the coupling between momentum and continuity equation.

Following the original "MAC" method, a time-marching technique is used to obtain the converged solution; that is, each partial differential equation is rewritten in a time-depending parabolic form. Thereafter, numerical time integration using explicit formulation (Adams-Bashforth scheme) is carried out over a sufficiently large amount of time until the solution becomes steady state.

Figures 2 and 3 show calculated velocity distribution in a representative cross section including all openings and the corresponding experimental results in case of the draft chamber under operation, where calculated velocity arrows are given only on the measured points for the convenience of comparison. The calculated velocity distributions are slightly smoother than those of the experiments, partly due to the overestimation of the eddy viscosity, though the general flow pattern is predicted fairly satisfactory.

Figures 4 through 7 present the predicted and measured concentration distribution in the same cross section when the neutral buoyancy contaminant is emitted from a point source just in front of the draft chamber inlet.

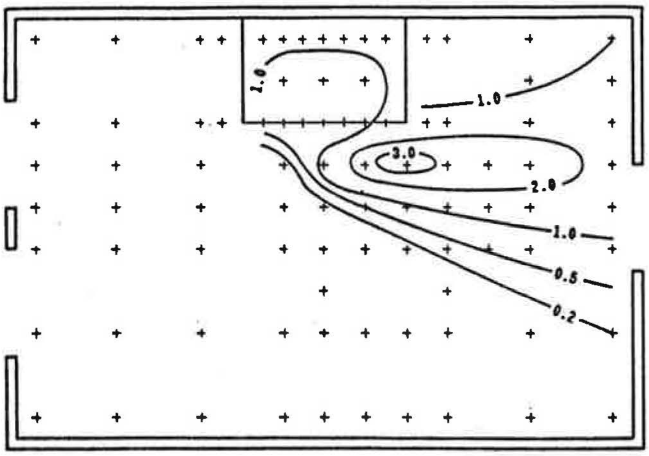

Figure 4—Measured non-dimensional concentration distribution in the representative plane at 1.260 mm above floor level—draft chamber: off (mark denotes measurement location)

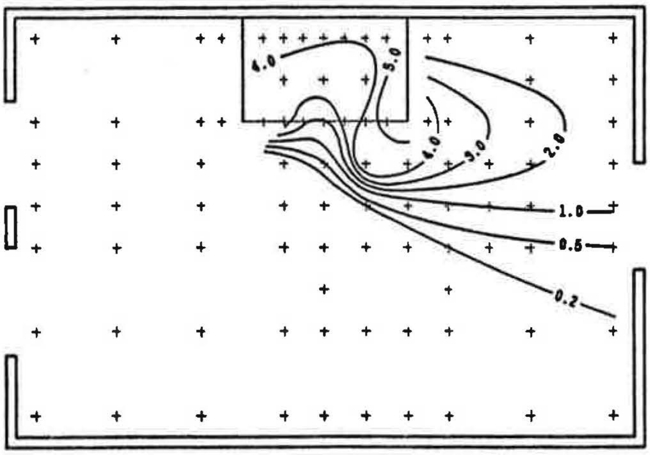

Figure 5—Measured non-dimensional concentration distribution in the representative plane at 1.260 mm above floor level—draft chamber: on (mark denotes measurement location)

Experimental iso-concentration lines show that, in the case where the draft chamber is out of operation, the peak concentration occurs just downstream of the point source and most of the contaminant disperses along the flow direction (from left to right in *Figure 4*) whereas a considerable amount of contaminant is dispersed toward the draft chamber and the peak concentration moves toward its edge of the right side wall under the condition of the draft chamber in action (as shown in *Figure 5*). *Figures 6 and 7* show that the numerical method can correctly simulate this dramatic change in the dispersion process due to the effect of the local ventilation system.

Current limitations

As briefly demonstrated in the above example, the numerical method is powerful and is able to predict room air motion and contaminant distribution fairly well. Nevertheless, it is important to recognize the following limitations inherent in the current calculation method:

1. The calculation domain including air inlet and outlet is a rectangle or a rectangular parallelpiped.

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*While this particular model may not be realistic, it is used nevertheless to demonstrate the capability of numerical model that can handle airflow through open boundary in combination with internal convection.

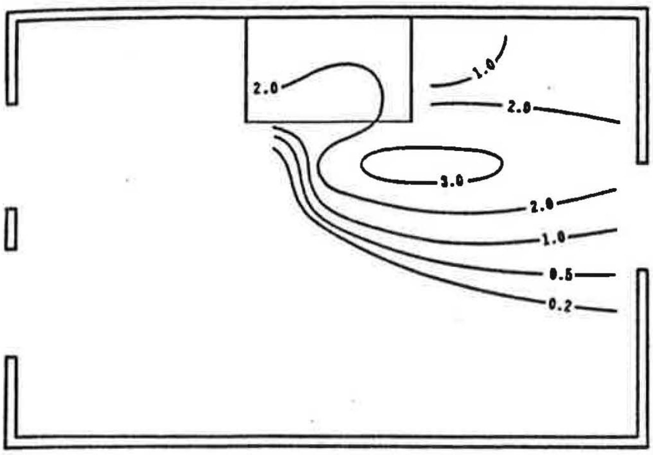

Figure 6—Predicted non-dimensional concentration distribution in the representative plane at 1.260 mm above floor level—draft chamber: off

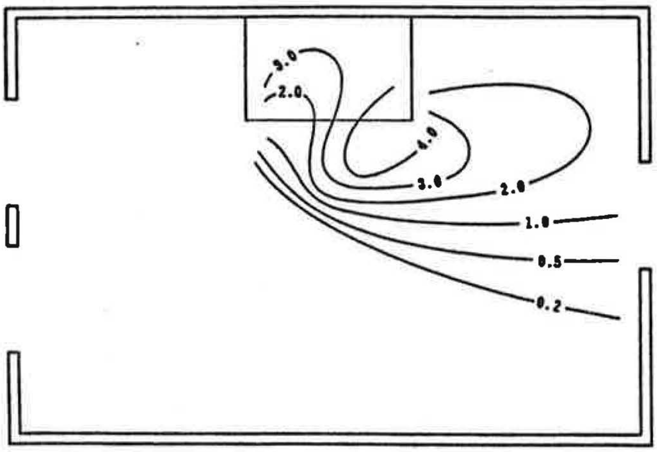

Figure 7—Predicted non-dimensional concentration distribution in the representative plane at 1.260 mm above floor level—draft chamber: on

2. The reference Reynolds number is sufficiently large so that the viscous effect can be perfectly negligible except near the wall region.

3. The temperature gradient in the flow regime is so small that buoyancy exerts little effect on the turbulence structure.

In these limitations, the first is caused by the use of standard finite-difference approximations based on the rectangular coordinate systems. This may be a serious limitation for the application of the numerical method to spaces enclosed by curved surfaces, such as air domes. This difficulty is expected to be removed, however, by using the recently developed approximation techniques such as finite-element method or grid generation method,[10] which have not yet been widely used in the field of building physics.

The other two limitations are much more serious than the first one because they originate from the inadequacies of the basic turbulence model itself.

The k-ε turbulence model consists of a set of equations governing the transport process of turbulent kinetic energy and its dissipation rate. These equations for k and ε together with the eddy viscosity formulation are not the exact forms derived from the Navier-Stokes equation, but they are model equations derived from several assumptions such as nearly equilibrium flow, isotropic dissipation of turbulence energy and gradient-type diffusion with constant Prandtl number, etc. Hence, there is a fair possibility that the numerical results become unrealistic when Reynolds number is not large enough so that eddy viscosity is as small as molecular viscosity, or when the buoyancy effect is so large that the gravitational force exerts a strong directional influence on turbulence.

Proposed modifications

So far, several authors have proposed modified versions of the k-ε turbulence model or different approaches, which can account for these additional effects.

An interesting attempt to extend the applicability of the k-ε turbulence model for high Reynolds number was carried out by Jones and Launder.[11] Their modification was mainly to make the empirical constants appearing in the conventional k-ε turbulence model to be the functions of the local turbulence Reynolds number by a semi-empirical approach so that the molecular viscosity effect in the very near wall region can be accounted for. Although their modified equations have been applied to the two-dimensional low Reynolds number wall flows with relative success, they are not likely to be applicable to the general recirculating low Reynolds number flows.

For strongly buoyant flows, several researchers proposed different schemes[12, 13, 14, 15] called second-order closure model which is much more complicated than the k-ε turbulence model. Recently, Rodi and associates[16, 17] attempted to simplify the model equations proposed by Launder and associates and clarified the applicability of their simplified version to various buoyancy influenced flows.

At the present, the study for buoyant flow prediction has not been conducted as extensively in Japan as for isothermal flow. This is partially due to the difficulty of experimental verification but mainly due to the uncertainty of the basic model equations. It should be an urgent task to determine the applicable range of the current method by providing careful comparative studies with experimental observations for fundamental buoyant flows to develop effective modifications. ■

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T. Kurabuchi is a research associate at the Department of Architecture, University of Tokyo. He has been working on room convection simulation problems since 1981 when he used three-dimensional room air convection as his graduate thesis for a Bachelor of Science degree at the University of Tokyo. Kurabuchi was a guest worker at the U.S. National Bureau of Standards, assisting the indoor air quality simulation modeling activities in the Building Environment Division at the Center for Building Technology.

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