A Cost-Effective Model for Indoor Contaminant Simulation

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ABSTRACT

A cost-effective numerical model has been developed which employs hp-adaptive finite elements to construct velocity fields and Lagrangian particles to predict contaminant dispersion patterns. The adaptive finite element method is based on both mesh enrichment (h-adaptation) and spectral order incensement (p-adaptation). The use of Lagrangian particles permits rapid visualization and assessment of contaminated areas within rooms and buildings. By coupling the model with AutoCAD/ProE drawings of a building, a domain model of offices on a floor including ventilation pathways can be readily implemented.

Simulation results for contaminant transport in an office complex consisting of three rooms and an adjacent hallway are presented. A sequence of movies and results for various ventilation scenarios are available at web site: www.unlv.edu/NCACM/IAQ.

INTRODUCTION

Numerous investigators have conducted considerable research over many years to address issues dealing with indoor air quality [1-5]. Fast and accurate predictions of health effects, mitigation, and regulation of emissions are especially important when dealing with indoor air quality. This has become extremely important as a result of the increase in terrorist activities over the past few years.

The finite element method (FEM), with its ability to easily deal with irregular geometries while employing the use of general-purpose algorithms, is especially attractive as a numerical method for simulating indoor contaminant transport. The use of adaptive FEM is even more attractive

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for it can produce accurate results with less computational effort than conventional, fine mesh approaches.

Generally, four main categories exist for adaptation: (1) h-adaptation, where the element sizes vary while the order of the shape functions are constant; (2) p-adaptation, where the element sizes are constant while the order of the shape functions increase to meet desired accuracy requirements; (3) r-adaptation, where spring analogy is used to redistribute the nodes in an existing mesh; (4) hp-adaptation, which is the combination of both h-and p-adaptation. Hp-adaptive schemes are among the best mesh-based schemes with the potential payoff of obtaining fast convergence rates. In this model, the hp-adaptive FEM is employed to construct indoor velocity fields.

In Lagrangian methods, a large number of particles are used to approximate advection and dispersion instead of solving the PDE for concentration directly. In this model, a random walk/stochastic Lagrangian particle approach is applied. This scheme uses a general probability distribution for the random component of motion due to turbulent diffusion and generates Lagrangian particles that define the contaminant dispersion trajectories.

Coupling the model with the ability to read AutoCAD/ProE drawings of a building, a domain model of offices on a floor including ventilation pathways can be quickly implemented. The Cad drawings permit the room and floor boundaries to be established while serving as a preload for the coarse mesh generation of the interior spaces. Coupling room sensors that would automatically trigger the model and set up appropriate response actions would allow immediate preventive measures to take affect.

Simulation results for contaminant transport in an office complex consisting of three rooms and an adjacent hallway are presented. A sequence of movies and results for various ventilation scenarios can be accessed at web site: www.unlv.edu/NCACM/IAQ.

MESH GENERATION

The establishment of a suitable coarse mesh is very important. The first step in creating a valid mesh is to establish the domain boundaries, which is easily done by reading a Cad file. Generally mesh generation can be quite time consuming, especially for the FEM. Even though numerous commercial meshing software exists, it is usually hard to integrate them with other codes. In this study, the initial coarse mesh is generated using Gambit – a well known and easily obtained commercial code. Coupling the model with the ability to read AutoCad/ProE drawings, a separate mesh module integrates the output from Gambit with the hybrid numerical model for discretizing interior domains for indoor contaminant transport simulation.

Meshing begins from the initial AutoCAD drawings for an office complex; in the following example, an interior domain consists of three rooms and an adjacent hallway. AutoCAD exports ACIS files, which are importable to Gambit. The configuration for the office complex is shown in Fig. 1.

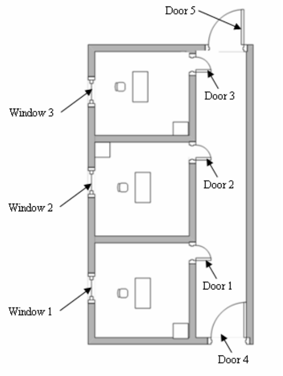

Figure 1 Office complex configuration

After importing the ACIS file from AutoCAD, Gambit creates an initial coarse mesh. The mesh in this expel simulation consisted of 389 quadrilateral elements and 500 nodes, as shown in Fig. 2.

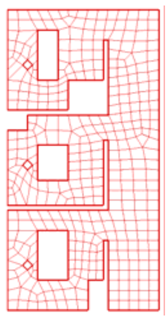

Figure 2 Initial coarse meshes

The meshing information from Gambit Neutral files is extracted after running the computer program "Mesh Converter" module. "Mesh Converter" is a bridge which connects the commercial meshing software to the hp-FEM codes. In order to minimize the bandwidth of the stiffness matrix in FEM, Quicksort Partitioning algorithms have been adopted [6].

NUMERICAL MODELS

The governing equations used to describe indoor air flow and contaminant transport are based on the conservation of momentum and species transport:

Conservation of Momentum

$$\rho\left(\frac{\partial V}{\partial t}+V\cdot\nabla V\right)=-\nabla P+\nabla\cdot\left(\mu\nabla V\right)+\rho B \tag{1}$$

Species Transport

$$\frac{\partial C_m}{\partial t}+\nabla\cdot\left(VC_m\right)=\nabla\cdot\left(k_h\nabla C_m\right)+S_{C_m} \tag{2}$$

Applying the Galerkin weighted residual method, and replacing the variables V and C_m with the trial functions:

$$V(\mathbf{x},t) = \sum N_i(\mathbf{x}) V_i(t) \tag{3}$$

$$C_m(\mathbf{x},t) = \sum N_i(\mathbf{x}) C_{mi}(t) \tag{4}$$

matrix equivalent forms for the integral expressions, Eq. 2 and Eq. 4, are obtained as:

$$[M]\{\dot{V}\} + ([K]+[A(V)])\{V\} + C\{p\} = \{F_V\} \tag{5}$$

$$[M]\{C_m\} + ([K]+[A(V)])\{C_m\} = \{F_{C_m}\} \tag{6}$$

A Petrov-Galerkin scheme is employed to weight the advection terms in the momentum and species concentration equations:

$$W_i = N_i + \frac{\alpha h_e}{2|V|}\left[V \cdot \nabla N_i\right] \tag{7}$$

$$\alpha = \coth\beta - \frac{1}{\beta}, \beta = \frac{|V|\, h_e}{2K_e} \tag{8}$$

where K_e is the streamline component of the diffusion tensor.

Mass lumping is used to obtain a fully explicit time scheme. The inverse of the mass matrix becomes:

$$[M]^{-1} = \frac{1}{m_i} \tag{9}$$

In the hp-adaptive FEM procedure, unstructured meshes, anisotropic and I-Irregular mesh adaptation rules are followed for the h-adaptation portion: an unstructured anisotropic mesh is allowed which is an efficient, directionally refined mesh where refinement in one directional is needed. The I-Irregular mesh refinement rule allows an element to be refined only if its neighbors are at the same or higher level (I-Irregular mesh). The minimum rule is followed in p-adaptation: the order for an edge common for two elements never exceeds orders of the neighboring middle nodes. The adaptation rules for h- and p- are combined together in hp-adaptation. In addition to these rules, it is important to maintain continuity of the global basis functions – this is achieved by employing constraints at the interfaces of elements supporting edge functions of different order.

The hp-adaptive FEM strategy employed in this model is based on an extension of the automatic hp-adaptation scheme originally described by Demkowicz et al. [7]. An optimal mesh is obtained by minimizing a local projection error for a reference solution to the incompressible equations of fluid motion. The technique is used to predict the movement of air within indoor environments.

A Random Walk Advective and Dispersive Model (RADM) is used to predict contaminant transport trajectories. This method, based on the early work of Runchal [8], solves the transport equation for species concentration through a large number of particles, each of which is advected according to the equation:

$$x_p^{n+1} = x_p^n + \Delta x + Z \tag{10}$$

where Z is the random displacement associated with dispersion.

FLOW SOLVER

A projection-step algorithm is used for the Navier-Stokes flow solver. This method is based on the Helmholtz-Hodge Decomposition Theorem (see Chorin et al [9] for details). The theorem states that a vector field, w, on domain, D, can be uniquely decomposed in the form

$$w = u + \nabla p \tag{11}$$

where u has zero divergence and is parallel to the boundary ∂D.

Applying this concept to the Navier-Stokes equations, a linear orthogonal projection operator L is applied to both sides of the equation, i.e. ,

$$L\left(\frac{\partial U}{\partial t} + \nabla P\right) = L\left(-(U \cdot \nabla)U + \frac{1}{\text{Re}}\nabla^2 U\right) \tag{12}$$

where $L(\nabla P) = 0$. Equation (12) becomes:

$$\frac{\partial U}{\partial t} = -(U \cdot \nabla)U + \frac{1}{\text{Re}}\nabla^2 U \tag{13}$$

Splitting the overall velocity into two components, V^* and V, the momentum equation under the linear orthogonal projection operator L becomes:

$$\frac{V^{*n+1} - V^n}{\Delta t} + V^n \cdot \nabla V^n = \frac{1}{\text{Re}}\nabla^2 V^n \tag{14}$$

The projection of V^* is a perturbed velocity onto the divergence free-space. Under the decomposition of the vector field $L(V^*)$, one can make the projection

$$V^* = V + \Delta t \nabla P \tag{15}$$

Taking the gradients of both sides of Eq.15, and since $\nabla \bullet V = 0$, a Poisson equation for P is obtained:

$$\nabla^2 P = -\nabla \cdot V^* / \Delta t \tag{16}$$

In a discretized finite element representation, this can be written as:

$$M(V - V^*) + \nabla P = 0 \tag{17}$$

where M is the mass matrix. Eq.17 can be rewritten as:

$$\frac{M}{\Delta t}(V - V^*) + CP = 0 \tag{18}$$

where C is the gradient operator. The equation is subject to the constraint of continuity

$$C^T V = 0 \tag{19}$$

Applying mass lumping,

$$C^T M^{-1} CP = C^T V^* \tag{20}$$

eventually permits the velocity to be solved using the relation

$$V = V^* - \Delta t M^{-1} CP \tag{21}$$

SIMULATION RESULTS

There are three test cases: (1) in the first case all the windows are closed; (2) in the second case only the first window is closed but all the other windows are open; (3) in the third case only the second window is open. The boundary conditions for these three cases are shown in Fig.3.

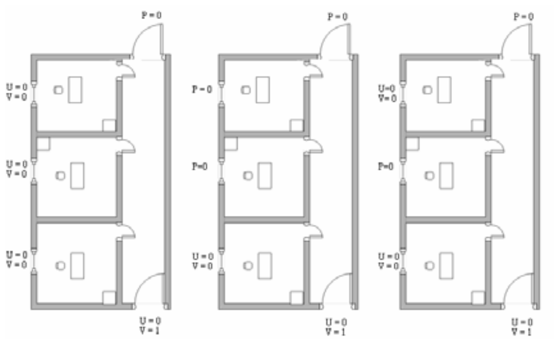

Figure 3 Boundary condition settings for the three test cases

The final hp-adaptive meshes are shown in Fig.4 for the three cases. The h-adaptation achieved 4 levels of refinement while the p-adaptation proceeded to 4th order. In the first case, the final element number is 530 and the total degrees of freedom (DOF) is 1374. In the second case, the final element number is 560 and the total DOF is 1517. For the third case, the final element number is 401 and the total DOF is 1216.

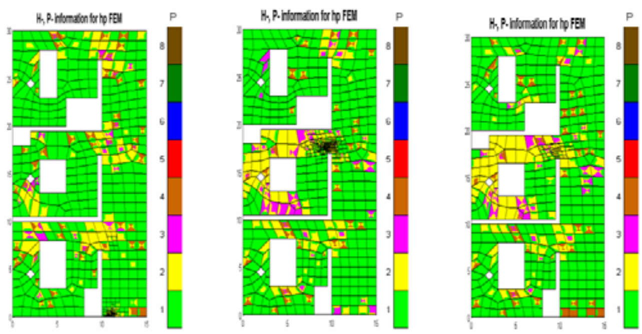

Figure 4 Final hp-adaptive FEM meshes for three cases

The equidistributed error shows the efficiency of the numerical algorithm, as displayed in Fig.5. Air distribution patterns and pathways of a powder dispersing within the office complex are shown in Figs. 6 and 7. Both the office doors and the windows are open, and the contaminant powder spreads into the inner office. A plan view of the flow of air and velocity vectors is shown in Fig.6 for all three cases.

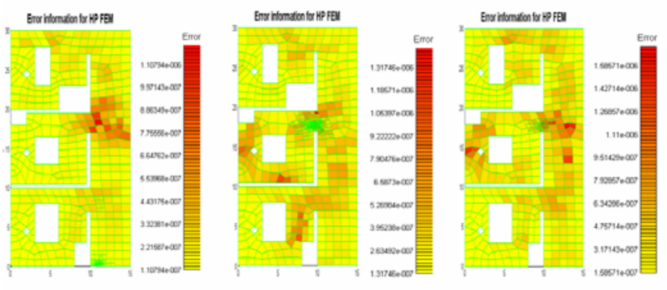

Figure 5 Computational error distributions for three cases

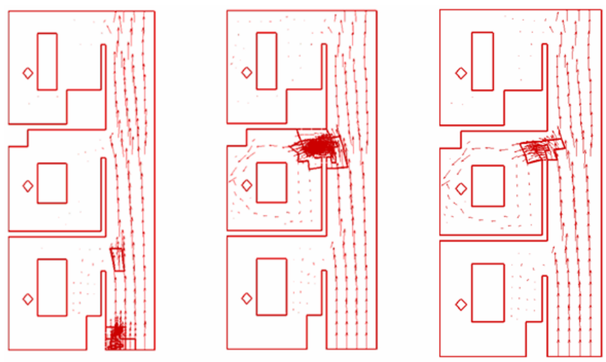

Figure 6 Velocity vectors

Particle dispersion patterns (large dot denotes contaminant source) are shown in Fig.7. The contaminant flows down the hall when all three windows are closed. However, contaminant can be seen entering various rooms when only the first window is closed and only the second window is open.

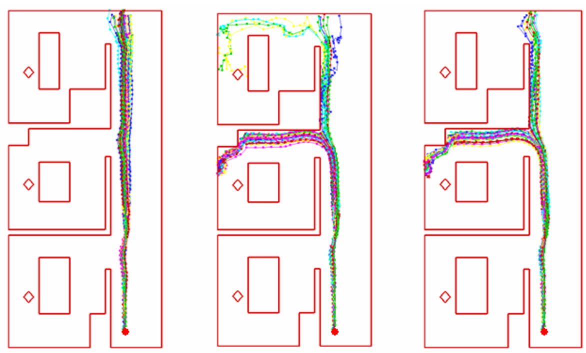

Figure 7 Particle dispersion patter for three cases

As shown in the particle dispersion patterns, the pollutant is transported and diffused by the ventilation pattern that affects the office complex. When all three windows are closed, it is relatively safe to stay inside the office. When only the first window is closed, contaminant will diffuse into the hallway and out the second and the third room windows. With only the second window open, the most dangerous place would be at the top part of the second room and the left part of the hallway. The location of the source is also a factor, and can produce significantly different dispersion patterns [10].

The performances of hp-adaptive algorithms are compared with non-adaptive algorithms with uniform h- and p- refined mesh. The compare is based on the first test case.The uniform refined and enriched solution is very time consuming, here we choose uniform refined mesh which goes up to 2 level h and uniform enriched mesh which goes up to second order, instead of using the uniform refined mesh which goes up to 4 level h and uniform enriched mesh which goes up to forth order.

Compare results are shown in Table 1. To reach the same error criteria 10E-5, it is easy to see that the hp-adaptive algorithms (with h- goes up to 4 level and p-goes up to 4^{th} order) is almost 3 times faster than non-adaptive algorithm (with 2 level h- uniform refine and second order uniform enrichment).

Table 1.Performances compare for different algorithms

Compare Cases	# of element Initial	# of element Final	# of DOF Initial	# of DOF Final	Total CPU Time (sec)	Per DOF CPU time (sec/DOF)	# of iteration
Uniform h (2 level) and P (2^{nd} order)	1556	1556	6683	6683	100561	15.55	16249
Hp adaptive algorithms(4 level both h, p)	389	530	500	1374	31080	22.62	16509

CONCLUSIONS

A cost effective numerical model is presented for indoor contaminant simulation. Accurate velocity fields are first constructed using an hp-adaptive FEM method. Contaminant transport is quickly simulated using a Lagrangian technique based on a random walk stochastic approach. Coupling model input capabilities with AutoCad/ProE drawings of a building, and employing an in-house “Mesh converter” with the use of the commercial mesh software Gambit, interior building domains can be easily integrated into the numerical model.

Examining preliminary simulation results for contaminant transport in an office complex, valuable information with regards to ventilation pathways and contaminant dispersion can be quickly established for risk assessment studies. The model seems particularly attractive for use in emergency response studies.

ACKNOWLEGMENTS

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NOMENCLATURE

D Domain

B	Body force
V	Velocity vector
V^*	Perturbed velocity vector
t	Time
k_h	Diffusion coefficient
k_e	Streamline component of the diffusion tensor
h	Characteristic of element length
M	Mass matrix
N_i	Shape function
p	Shape function order
P	Pressure
R_e	Reynolds number
S_c	Schmidt number
x_p^{n+1}	New time step particle location
x_p^n	Old time step particle locaiton
h_e	Element size
Z	Random displacement associated with dispersion
α	Petrov-Galerkin coefficient
β	Cell Peclet number
μ	First coefficient of viscosity or dynamic viscosity
ρ	Density
L	Linear orthogonal projection operator
∇	Divergence operator
$\nabla \bullet$	Dot product

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