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Numerical Modelling of Contaminant Dispersion Around Buildings

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As the computation of turbulent flow around a building has almost reached the point of routine calculation on a medium size computer, it is time to look at the next step of computation of contaminant dispersion around a building. The diffusion equation approach is a logical extension of the two equation model used for turbulent flow around a building. This approach still awaits a better model of turbulent diffusion of scalars. The alternative stochastic models, especially the large eddy simulation, have met with some success. Unfortunately, for the latter method, spectral information of the turbulence of the approach flow and a powerful computer are prerequisites.

INTRODUCTION

THE STUDY of air pollution in a high-rise crowded urban area is fundamentally different from a low-rise city or rural area. In most high-rise cities only office blocks in downtown are multistorey towers. Even when they are closely packed, the pollution problems are not serious, as offices generate little pollution. The intake air of ventilation systems may be contaminated by exhaust air which may cause corrosion or loss of efficiency of cooling systems. The effect of gas-heater exhaust is another minor problem. More serious is the street canyon effect on the dispersion of motor vehicle exhausts.

In Hong Kong, due to the lack of space, almost all residential blocks are high-rise towers. The towers are built sometimes so close to each other that the hot exhaust of a window air-conditioner can be blown into the living room of another apartment. Due to the nature of Chinese cooking, restaurant exhausts are major complaints of nearby residents. Worst of all, industrial establishments are also located in multistorey factory buildings. The factory buildings intermingle with residential blocks, especially in older industrial zones. Exhausts from steam generating boilers and other manufacturing processes are emitted into the air from low stacks or sometimes from street level vents. To formulate and enforce laws on air quality, the urban pollution workers need to have some knowledge of gas dispersion near buildings.

In a high-rise city, each building is usually inside the wakes of other buildings. The most practical approach for such a complex problem is to perform a scale model experiment inside an atmospheric boundary layer wind tunnel. This is expensive and time consuming. Just as in other areas of engineering, computer model is quicker and more cost-effective. The commonly used computer model of dispersion, such as the Industrial Source Complex Dispersion model of the United States Environmental Protection Agency (Bowers *et al.* [1]) depends on the Gaussian plume model. However, the effect of building wake is represented very crudely. Most unfortunately, the Pasquill–Gifford dispersion coefficients (σ_z) used are valid only for ranges beyond 100 metres, which is of little use inside crowded high-rise cities.

For very short range dispersion, such as the re-entry problems of exhaust air from vents on building roofs, Wilson's [2] semi-empirical formula derived from wind tunnel tests can be used. This formula has been validated by Lam *et al.* [3] during a field study on the roof-top of an urban high-rise building. The formula is good for design purposes but does not give a detailed concentration pattern of contaminant near the building for a polluting source in the building.

The dispersion of pollutant is a manifestation of the highly turbulent flow around the building. Recently, with the advance in turbulence modelling, numerical techniques and computer power, the calculation of the mean and turbulent flow around at least an isolated building has become successful. The details of the computations are presented in the other contributions to this special issue of *Building and Environment*. It is time to look critically at the next step of the incorporation of a turbulent dispersion model into the existing model of turbulent flow past buildings. To search for the right equations or models for numerical computation, an understanding of turbulent diffusion from sources in complex flows is required. An excellent review paper on this matter has been prepared by Hunt [4]. The computation of turbulent dispersion around buildings requires input from other actively researched fields such as turbulence modelling, simulation and numerical methods. A detailed review or survey of these areas will not be given in this paper. Instead, the different approaches will merely be outlined and interested readers directed to the many existing excellent reviews for further relevant information.

Two approaches will be discussed in this paper. The first approach is an extension of using zero, one or two equation models of turbulence for calculating flow around buildings. An extra equation for diffusion of

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scalar properties, e.g. temperature or concentration of contaminant, will be proposed. The diffusion of the scalar property has to be modelled consistently, such as the modelling of turbulent transport of momentum, for the set of equations to be closed and solvable. A second approach is the stochastic approach, where the turbulent diffusion is treated as a random phenomenon. Two different methods of simulating the turbulent flow, namely large eddy simulation and discrete vortex method, will be outlined.

DIFFUSION EQUATION APPROACH

According to Rodi [5], the distributions of mean velocity (u_i), mean pressure (p), density (ρ) and mean scalar quantities such as pollutant concentration (c) are govenered by the following equations.

Continuity:

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u_i)}{\partial x_i} = 0, \tag{1}$$

momentum equations:

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = -\frac{1}{\rho}\frac{\partial P}{\partial x_i} + \frac{1}{\rho}\frac{\partial}{\partial x_j}(-\rho\overline{u_i'u_j'}) + g_i \tag{2}$$

concentration equation:

$$\frac{\partial c}{\partial t} + u_j \frac{\partial c}{\partial x_j} + \frac{1}{\rho}\frac{\partial}{\partial x_l}(-\rho\overline{u_l'c'}) + S_c, \tag{3}$$

where the primed variables are fluctuations, overbars are averages in either ensemble or time sense, g_i is the buoyancy term and S_c is the source term of pollutant. For simplicity, only incompressible flow is considered. The pollutant is assumed to be passive, hence the equation of state can be neglected. The continuity and momentum equations are then decoupled from the concentration equation, i.e. turbulent flow past a building can be calculated first.

Historically, the solution of turbulent flow progresses in an evolutionary fashion in phase with the advancement of computer power. Starting with a crude approximation of Reynolds stress $\rho\overline{u_i'u_j'}$ in terms of a product of constant mixing coefficient and the gradient of the mean velocity, we progress to multi-equation models of Reynolds stress. Either finite difference or finite element methods can be used to solve the set of equations numerically. Other papers in this special issue address the computation of turbulent flow around buildings.

Once the flow around a building is obtained, the remaining concentration equation should be solved to the same degree of sophistication in the modelling of $\rho\overline{u_i'cu'}$. For the simplest case a prescribed eddy viscosity for $-\rho\overline{u_i'u_j'} = \nu_t(\partial u_i/\partial x_i)$ is used, then with direct analogy the turbulent mass transport can be related to the gradient of concentration by a mixing coefficient (Γ_t), namely $-\overline{u_i'c'} = \Gamma_t(\partial c/\partial x_i)$. In many calculations Γ_t is given by empirical measurements. A calculation along this line has been attempted by Chung and Kot [6] for the calculation of SO_2 dispersion around complex terrains. The program can readily be adapted to the prediction of dispersion around rectangular building blocks.

The next level of sophistication is the use of one or two equation models. The most popular is the k–ε two equation model, where k is the turbulent kinetic energy and ε is the dissipation rate. The success of this model in predicting turbulent flow past buildings can be seen from Paterson and Apelt [7]. To match the two equation modelling of Reynolds stress, two analogous equations for scalar flux, $\overline{u_i'c'}$ and $\overline{c'^2}$ have to be derived. The equation for $\overline{u_i'c'}$ is:

$$\underbrace{\frac{\partial \overline{u_i'c'}}{\partial t}}_{\text{rate of change}} + \underbrace{u_l\frac{\partial \overline{u_i'c'}}{\partial x_l}}_{\text{convective transport}} = \underbrace{-\frac{\partial}{\partial x_l}\left(\overline{u_i'u_l'c'} + \frac{1}{\rho}\delta_{il}\overline{p'c'}\right)}_{\text{diffusive transport}}$$

$$\underbrace{-\overline{u_i'u_j'}\frac{\partial c}{\partial x_j} - \overline{u_j'c'}\frac{\partial u_i}{\partial x_j}}_{\text{mean-field production}} \underbrace{-\beta g_i\overline{c'^2}}_{\text{buoyancy production}} + \underbrace{\frac{1}{\rho}\overline{p'\frac{\partial c'}{\partial x_i}}}_{\text{pressure scalar gradient correlation}}$$

$$\underbrace{-(\lambda+\nu)\frac{\partial \overline{u_i'}}{\partial x_l}\frac{\partial \overline{c'}}{\partial x_l}}_{\text{viscous destruction}}. \tag{4}$$

The viscous destruction term vanishes in local isotropy. If there is no buoyancy in the fluid, then the buoyancy production term vanishes and an extra equation for $\overline{c'^2}$ is not necessary. Model approximations have to be introduced for pressure–scalar gradient correlation and diffusion terms. The extra equation for the scalar fluctuation $\overline{c'^2}$ is:

$$\underbrace{\frac{\partial \overline{c'^2}}{\partial t}}_{\text{rate of change}} + \underbrace{u_j\frac{\partial \overline{c'^2}}{\partial x_j}}_{\text{convection}} = \underbrace{-\frac{\partial}{\partial x_j}(\overline{u_j'c'^2})}_{\text{diffusive transport}} \underbrace{-2\overline{u_j'c'}\frac{\partial c}{\partial x_j}}_{\text{production by mean field}}$$

$$\underbrace{-2\lambda\frac{\partial \overline{c'}}{\partial x_j}\frac{\partial \overline{c'}}{\partial x_j}}_{\text{dissipation } (\varepsilon_c)}. \tag{5}$$

This is the counter-part to the k-equation. Diffusion terms are usually modelled by gradient transfer type, and a model for the dissipation term has to be provided.

The pressure–scalar gradient correlation counteracts the production of scalar flux and is split into three parts for modelling:

$$\overline{\frac{p'}{\rho}\frac{\partial c'}{\partial x_i}} = \pi_1 + \pi_2 + \pi_3 \tag{6}$$

where:

$$\pi_1 = -C_1\frac{\varepsilon}{k}\overline{u_i'c'} \quad \text{turbulent part,}$$

$$\pi_2 = -C_2\overline{u_i'c'}\frac{\partial u_i}{\partial x_l} \quad \text{mean-strain part,}$$

$$\pi_3 = -C_3\beta g_i\overline{c'^2} \quad \text{buoyancy part.}$$

For the diffusive transport of $\overline{u_i'c'}$, the following gradient approximation is used:

$$\frac{\partial}{\partial x_l}\left[C_s\frac{k}{\varepsilon}\left(\overline{u_k'u_l'}\frac{\partial \overline{u_i'c'}}{\partial x_k} + \overline{u_k'u_l'}\frac{\partial \overline{u_i'c'}}{\partial x_k}\right)\right]. \tag{7}$$

The diffusive transport in the scalar fluctuation equation is modelled by:

$$-\overline{u_j' c'^2} = C_c \frac{k}{\varepsilon} \overline{u_j' u_l'} \frac{\partial \overline{c'^2}}{\partial x_l}, \tag{8}$$

which is again of a gradient transfer type. For the dissipation term denoted by ε_c a time-scale ratio R can be defined as:

$$R = \frac{\varepsilon}{k} \frac{\overline{c'^2}}{\varepsilon_c}. \tag{9}$$

If R is specified then $\varepsilon_c = Rk/\varepsilon \overline{c'^2}$. Unfortunately from experimental evidence R may range from 0.5 to 1.0 Zeman and Lumley [8] proposed another equation for modelling ε_c.

Values for various parameters can be found in Launder [9] and Rodi [5]. The modelling of the various terms in these two equations are still under intensive development. See Rodi [5] and Lumley *et al.* [10] for detailed discussions. The major difficulty in this type of modelling is due to the kind of averaging operation used in deriving the governing equations. No space averaging has been performed, i.e. motions of all length scales, from very large to microscales, are present in the averaged equations. It is difficult to model accurately by simple terms for motions of all scales. In addition, the empirical parameters used in various models for the diffusion of scalar properties have not been as thoroughly studied as in the k–ε equations.

For environmental flows, the basic boundary conditions are not known very accurately. The surface boundary condition for a pollutant can sometimes be a complete adsorption/absorption or reflection from the surfaces. More usually, it is somewhere in between needing a lot of experimental data for guidance. With a more complex model of turbulence, extra detailed initial and boundary conditions, say on $\overline{u'c'}$ and $\overline{c'^2}$, are needed for the increased number of variables and equations to be solved. The concentration flux and fluctuation of pollutant at the surface are difficult to prescribe. Few experiments have been performed to facilitate the understanding of these quantities, not only on the boundary but also within the flow field. Numerical experiments will have to be tried to obtain some indications of the sensitivity of various boundary conditions. Added to these, is the extra effort in computer programming and CPU time required for solving extra equations. All of these do not seem to justify the use of more sophisticated models other than the empirically determined simple mixing coefficient model used at this moment.

STOCHASTIC APPROACHES

Direct numerical simulation

To by-pass the difficulty of modelling turbulence, statistical or stochastic simulations of turbulence have been attempted. The most advanced, but conceptually the simplest, is the direct numerical simulation of turbulence. The original Navier–Stokes equations are integrated directly on the computer without any approximations. The initial velocities of tagged particles are chosen randomly, but their spectral properties have to be prescribed. Thousands of fluid particles are then tracked accurately to provide statistical information on the turbulence. If the tagged fluid particles are assumed to be passive scalar pollutants and if they are all released from the same source point, then the concentration of the tagged fluid particles at a small volume around some receptor point can be easily obtained by counting the number of tagged particles entering the finite volume for a given time. As a bonus, the dispersion study is inadvertently built into the main program used for the study of turbulence. The development of direct numerical simulation depends strongly on fast and accurate numerical methods, such as spectral methods, and powerful supercomputers. So far the problems studied were usually with periodic boundary conditions to suit spectral methods. Problems with physical boundaries are difficult to solve. So it is years away from using direct numerical simulation to calculate any meaningful engineering problems.

Other methods can be devised which retain some statistical details of turbulence, but use less, though still considerable, computer power. Large eddy simulation, sometimes also called sub-grid scale modelling, is one such method. Another method uses discrete vortices to calculate the flow around bluff bodies, in conjunction with the random flight method of tagged fluid particles, to obtain dispersion results.

Large eddy simulation

In terms of computer effort and also of conceptual complexity, the large eddy simulation is somewhere between direct numerical simulation and multi-equation models of turbulence. It was first used in meteorological computation by Smagorinsky [11]. Later it was shown by Deardoff [12] to be able to simulate the convective boundary layer.

At first glance, the governing equations obtained by filtering the continuity equation and Navier–Stokes equations are similar to Reynolds equations, but instead of the Reynolds stress term, a new stress term appeared. This term is called the Leonard stress. The modelling of the Leonard stress when compared to the modelling of the Reynolds stress is very much simpler. The filtering of equations is a kind of spatial averaging. The motion of a computational grid resolvable scale part is separated from the non-resolvable part, also called the sub-grid motion. The Leonard stress term is an interaction term between the resolvable large scale motions and sub-grid scale motions. Almost by definition, the modelling is more accurate when only a single length scale of motion is involved. By using very simple modelling, say, a gradient transfer type for the Leonard stress, reasonable results have been obtained in meteorological computations. A good review on this subject was written by Schumann *et al.* [13].

Murakami *et al.* [14] used large eddy simulation to calculate the flow around a cube. To show the fluid particle trajectory, tagged fluid particles were released from a single point in front of the cube. This, of course, simulated the emission of a passive pollutant from a point source and the subsequent dispersion around the cube.

The governing equations assuming incompressible flow for this problem after filtering were:

$$\frac{\partial u_i}{\partial x_i} = 0 \tag{10}$$

$$\frac{\partial u_i}{\partial t} + \frac{\partial u_i u_j}{\partial x_j} = -\frac{\partial p^*}{\partial x_i} + \frac{\partial}{\partial x_j} \nu_{SGS} e_{ij} + \nu \frac{\partial^2 u_i}{\partial x_j \partial x_j}, \tag{11}$$

where:

$$p^* = \frac{p}{\rho} + \frac{1}{3}\overline{u_i' u_i'},$$

$$e_{ij} = \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i},$$

$$\nu_{SGS} = (C_s \Delta)^2 \left(\frac{e_{ij}^2}{2}\right)^{1/2},$$

and: C_s = Smagorinsky constant; Δ = characteristic filter length.

The model for the Leonard stress was a simple eddy viscosity and graident transfer type. For boundary conditions, cyclic boundary conditions were used for downstream and spanwise direction. A free slip condition is used for the upper boundary and power laws were assumed for tangential velocities near the surfaces of walls and the ground. Two types of normal velocity boundary conditions were tried, namely zero and non-zero conditions. Initial velocity fluctuations were generated randomly by computer. The turbulence intensity was given by related wind-tunnel measurements.

According to the authors, this calculation demonstrated the feasibility of large eddy simulation in predicting flow around a building. The flow pattern was reasonably predicted. Even though the primary purpose of that calculation was for the flow around a cube, the concentration of tagged fluid particles arriving at a small volume around a receptor point for a given time can easily be accounted for.

To accurately track tagged fluid particles, once the Eulerian velocity field is obtained, requires a Lagrangian description of fluid particle motion. The equation of motion of a fluid particle in a vector form is:

$$\frac{\partial \underline{X}^L}{\partial t}(\underline{y}, t) = \underline{u}^L(\underline{y}, t), \tag{12}$$

where the superscript L refers to Lagrangian quantities. $\underline{X}^L(\underline{y}, t)$ and $\underline{u}^L(\underline{y}, t)$ denote the position and velocity at time t of the fluid particle that occupied the position $\underline{y}$ at $t = 0$, i.e.

$$\underline{x}^L(\underline{y}, 0) = \underline{y}. \tag{13}$$

The relationship between Lagrangian velocity $\underline{u}^L(\underline{y}, t)$ and Eulerian velocity $\underline{u}(\underline{x}, t)$ is given by:

$$\underline{u}^L(\underline{y}, t) = \underline{u}(\underline{x}^L(\underline{y}, t), t). \tag{14}$$

The accuracy of integration is important. Yeung and Pope [15] gave a discussion and a method dealing with this problem.

Discrete vortex—random flight method

Another method of simulating the gross features of separated flow is the discrete vortex method. There are several advantages of this method. Firstly, it is not a grid based method. Secondly, the main flow field is considered to be inviscid, so the governing equation is the Laplace equation for irrotational and incompressible flow. The viscous effects are limited only to the thin surface layers and the vortex cores for more sophisticated models. Thirdly, it is very successful in the computation of separated flow past 2-D bluff bodies. The gustiness of the wake flow can be reproduced.

Briefly, the method uses a vortex sheet to represent the thin viscous boundary layer near the bluff body and the ground. The distribution of vortex filaments that formed the vortex sheet is determined by the surface boundary conditions. Since the remaining flow field is a potential field, the Biot–Savart law is used to determine the induced velocity on various vortex filaments and at the point of interest in the flow field. The subsequent movement of the vortex filaments can also be traced. If the chaotic turbulent motions are to be simulated, randomness can be introduced into the motion of the vortex filaments. For a review of the discrete vortex method, the reader is directed to a detailed survey paper by Leonard [16]. This method does not require a fixed grid as is needed for finite difference or finite element methods, but book-keeping of the whereabouts of the various vortex filaments is necessary. In two dimensions, the book-keeping is manageable. Applications to flow past bluff cylinders in ocean-engineering and combustion in a channel with a back-step have been successful. For three dimensions, further research into the book-keeping programming is necessary.

Turfus [17] was successful in combining a random flight method of a tagged fluid particle to a discrete vortex solution of a 2-D wake flow. The problem solved was the dispersion of the emission from a vent in the downwind facing vertical wall of a 2-D building. This was used to model the exhaust of a gas heater and its effect on the contaminant concentration in the wake of the building. The random flight method is again a trajectory method similar to the fluid particle tracing in the large eddy simulation. The governing equation was:

$$\mathrm{d}\underline{x} = \underline{u}(\underline{x}, t)\,\mathrm{d}t + (2K_e)^{1/2}\,\mathrm{d}W_i, \tag{15}$$

where $\mathrm{d}W_i$ was a white noise process in two dimensions. K_e was an effective eddy diffusivity that could be chosen to be constant. For time stepping, a Runge–Kutta method was used. The intermediate step was:

$$\hat{\underline{x}} = \underline{x}(t) + \underline{u}(\underline{x}, t)\frac{\Delta t}{2} + (K_e \Delta t)^{1/2}(N_1, N_2). \tag{16}$$

and the final expression at $t = t + \Delta t$ was:

$$\underline{x}(t+\Delta t) = \underline{x}(t) + \tfrac{1}{2}[\underline{u}(\hat{\underline{x}}, t) + \underline{u}(\hat{x}, t+\Delta t)] + (K_e \Delta t)^{1/2}(N_1 + N_1', N_2 + N_2'), \tag{17}$$

where N_1, N_1', N_2, N_2' were independent unit normal random variables. The effect of the non-absorbing boundary was modelled by the usual reflection of a fluid particle off the surface.

According to the author, the comparison between the calculation and experiments of Castro and Snyder [18] was encouraging. The main discrepancies were in the representation of the mean flow conditions rather than in the inadequate representation of turbulent flow. If a 3-D computation by discrete vortex method for separation

flow past a building is available, the extension of the 2-D random flight method is straightforward.

CONCLUSIONS

The k–ε model is well established for computation of turbulent flow past bluff bodies. Engineers tend to be more comfortable in using such deterministic methods. Its advantages are: (i) the initial conditions are required on mean flow only; (ii) the computer power required is less. The disadvantages are: (i) the model of turbulent diffusion of scalar properties is still not standardized yet; (ii) a time dependent solution is difficult to obtain.

The stochastic models can handle inhomogeneous turbulence and unsteadiness which are the main features of separated flow past building. Simple modifications can also readily adapt the models to sources with buoyancy or particulate contaminant with settling velocity. The disadvantages are in the increase of computer power required and extra statistical information for initial conditions. For practical engineers, the statistical initial conditions are usually not available.

Both the above mentioned methods suffer from the requirements of assuming values for many parameters. The black art of fixing the values of various parameters can only be eliminated when the direct numerical integration of the Navier–Stokes equations becomes routine on accessible supercomputers. For the moment, the k–ε model of turbulence plus the hydrodynamic plume model have been used to calculate dispersion on a large scale such as accidental release of radioactive contaminant during a nuclear reactor accident in complex terrain, see Liu and Chieng [19]. For dispersion near a building, this type of computation should be able to provide a time-averaged concentration pattern. The stochastic model, namely the large eddy simulation, is more successful in presenting a fluctuating numerical solution to contamination near a building.

In conclusion, much research effort is required to bring the numerical models up to the practical usable level of scale wind tunnel modelling.

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