A review of modelling particle deposition

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ABSTRACT

Particle deposition indoors has received increasing attention recently as a result of increasing concern about the effects of particle exposure on human health.

Recently, a review paper has been published on particle deposition indoors, focusing on the experimental side (Lai, *Indoor Air*, **12**:211–214;2002). In this paper, modelling efforts addressing indoor particle deposition were reviewed. The emphasis was put on the particle eddy diffusivity term of Eulerian approach. Both the conventional and unconventional methods modelling the particle eddy diffusivity were reviewed and their assumptions and limitations were discussed. The appropriateness of the methods for practical indoor measurement was also addressed.

INDEX TERMS

Deposition; Modelling

INTRODUCTION

From the mathematical point of view, there are two approaches to analyse the particle transport process. The first approach is the Eulerian method, which considers the particulate phase as continuous and applies the species conservation condition to deduce the equation of particle concentration as a function of position and time. The second one is the Lagrangian approach, which treats the dynamics of one single particle by a trajectory method and extends to a multiple particle system by statistical analysis.

EULERIAN APPROACH

The key challenge of most Eulerian modelling of particle deposition is to determine the particle eddy diffusivity ε_p. Corner and Pendlebury (1951) developed the first analytical solution for the deposition of particles onto surfaces of various orientations in a rectangular chamber under homogeneously turbulent flow.

They expressed the particle eddy diffusivity coefficient in the form of

$$\varepsilon_p = K_e y^2 \tag{1}$$

K_e being the turbulent intensity parameter and expressed as

$$K_e = \kappa^2 \frac{\mathrm{d}u}{\mathrm{d}y} \tag{2}$$

where κ is the von Kármán constant (usually assumed to be 0.4). u is the longitudinal mean flow velocity and du/dy is the mean flow velocity gradient. It should be noted that both Eqns (1) and (2) can be derived using Prandtl's mixing length hypothesis.

The next significant improvement in the Eulerian approach was the model developed by Crump and Seinfeld (1981). They derived an expression for the particle rate loss coefficient

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for an enclosure of arbitrary shape. They also generalized the expression for the turbulent diffusivity coefficient

$$\varepsilon_p = K_e y^n \tag{3}$$

instead of fixing $n = 2$ as in the model of Corner and Pendlebury (1951), n can be any real number.

As shown in Eqns (1)–(3), the conventional methods require two parameters, K_e and n, to estimate particle eddy diffusivity. There are three such approaches, all of which require the evaluation of the velocity gradient (cf. Eqn (2)). The applicability of the first method, which was adopted by Corner and Pendlebury (1951), is doubtful. Using boundary layer flow to approximate the flow along each surface is too idealistic and can be only used for rough estimation purposes. For a real enclosure, in which the flow pattern is so complex, this ideal hypothesis is unlikely to be true. In the literature, there are no data available to verify the appropriateness of the expression, e.g. detail CFD modelling comparison.

The other two approaches are analogous to each other in the sense that they both employ the statistical theory of turbulence advanced by Taylor (1935) to evaluate the velocity gradient term. The first approach employs the theory of local similarity, usually referred to as *universal equilibrium* (Kolmogoroff, 1941a). This theory states that if the Reynolds number of a system is sufficiently large, the small scale eddies will exhibit a common universal structure which applies to all types of turbulent flow. The rate of energy flow per unit mass in the system is determined by the motion of the larger eddies. The small-scale eddies must then adjust themselves to achieve the required rate of energy dissipation, through an *energy cascade* (Kolmogoroff, 1941b). Based on the above argument, the energy dissipation rate can be evaluated by estimating the net energy input of the system and the following expression resulted:

$$\varepsilon = \frac{\mathrm{d}q}{\mathrm{d}t} \tag{4}$$

where ε is the energy dissipation rate per unit mass of fluid. q is the turbulent kinetic energy per unit mass of the fluid

$$q = \frac{1}{2}(\overline{u_1^{'2}} + \overline{u_2^{'2}} + \overline{u_3^{'2}}) = \frac{3}{2}(\overline{u^{'2}}) \tag{5}$$

where $\overline{u_i^{'2}}$ is the rms component of the fluctuation velocity i. Further, assuming the turbulence is isotropic the last equality sign resulted. Etheridge and Sandberg (1996) assumed that the time taken to dissipate the energy, τ, is proportional to the time scale of the large eddies, they expressed τ as

$$\tau \approx \frac{L_t}{(\overline{u^{'2}})^{1/2}} \tag{6}$$

where L_t represents the size of the largest eddies or the width of the flow. They adopted the natural choice for L_t to be $V^{1/3}$, where V is the volume of the room. Combining Eqns (5) and (6), ε can be approximated as

$$\varepsilon \approx \frac{q}{V^{1/3}/(\overline{u'^2})^{1/2}} \tag{7}$$

By measuring the decay of the velocity and turbulence fluctuation $\overline{u'^2}$, ε in Eqn (7) can be estimated.

On the other hand, Hanzawa *et al*. (1987) calculated ε by another expression

$$\varepsilon = \frac{q^{3/2}}{\lambda} \tag{8}$$

where λ is the Taylor micro-scale eddy and is estimated by the following expression (Hinze, 1975):

$$\lambda = \sqrt{\frac{\overline{u^2} \cdot \overline{u'^2}}{2\pi^2 \int_0^\infty n^2 E(n) \mathrm{d}n}} \tag{9}$$

where u is the mean velocity, n is the frequency of the eddy and $E(n)$ is the energy spectrum.

The other approach is also based on the statistical theory of turbulence proposed by Taylor (1935). If the flow is isotropic, i.e. the mean properties are independent of the direction of the reference axes (although not strictly held in any confined-boundary conditions such as a room), ε can be expressed as

$$\varepsilon = \frac{15}{2} \upsilon \overline{\left(\frac{\partial u'}{\partial y} \right)^2} \tag{10}$$

where $\partial u' / \partial y$ is the velocity gradient of the fluctuation velocity in orthogonal directions. Rearranging the terms in Eqn (10), Okuyama, Shimada and their colleagues (e.g. 1977, 1986) evaluated the velocity gradient term by estimating stirrer power energy. They assumed that in the case of a stirred tank, the average value of the energy dissipation rate was approximately equal to the power input rate of the stirrer. They used a parameter called the *power number* (P_N) to calculate the input power experimentally. It is defined as

$$P_N = \frac{P}{N^3 L^5 \rho_a} \tag{11}$$

where P is the input power, N is number of stirrer revolutions per unit time and L is the length of the stirrer blade. Apparently, if we know the P_N of the stirrer, the evaluation of ε becomes straightforward. How to determine the power number, however, is not as simple as thought. Obviously, the power number depends on the type of the stirrer, i.e. propeller or turbine, and the detailed design of the stirrer, i.e. number of blades, blade diameter and blade areas, etc. It is also a function of the stirrer speed (Bates *et al*., 1966). For different types of stirrers, the magnitude of the power number can vary up to one order of magnitude (Okuyama *et al*., 1986). It is suggested that the power number method proposed by Okuyama and Shimada is only suitable for some specific stirrers or mixers and may not be appropriated for forced ventilation systems in which no power number can be defined. One point to note is that although Okuyama, Shimada and their colleagues used Eqn (2) to evaluate K_e, the exponent raised to the von Kármán constant was one and not two as used by Corner and Pendlebury.

After obtaining ε, one more parameter that needs to be determined is the exponent n in Eqn (3). In the literature, various values of n between 2 and ~3 have been reported. The dimensional inconsistency associated with the non-integer values of n makes the expression lack a strong physical foundation. Chen *et al*. (1992), Cheng (1997) and Lai and Nazaroff (2000) discussed the discrepancies among different studies. In some studies, the values of n were obtained by fitting the data (Okuyama *et al*., 1986). A new model has recently been developed with a different perspective by incorporating recent information on the structure of turbulent diffusivity in the vicinity of the surface. Only one parameter, the friction velocity, u_*, was used to describe the turbulence enhanced deposition feature (Lai and Nazaroff, 2000).

The application of u_* is very common in particle deposition on pipe/duct surfaces (Wood, 1981; Guha, 1997). Basically, it is a measure of the wall shearing stress exerted on the surfaces by the moving fluid, and can be determined by estimating the velocity gradient at the wall. For the flow over a smooth surface with a prevailing direction, the physical significance of u_* can be interpreted as being equal to the fluctuation velocity in the transverse direction (Davies, 1972). However, in the literature, very few results have been reported to justify the use of this parameter to describe indoor turbulent condition and further experimental validation is necessary (Schneider *et al*., 1994; Byrne *et al*., 1995).

LAGRANGIAN APPROACH

The Lagrangian approach splits the particle phase into a representative set of individual particles and tracks these particles separately through the flow domain by solving the equations of particle motion.

To the author's knowledge, there is no published work particularly for particle deposition in an enclosure or room in the literature. Several investigators studied particle transport in indoor environments numerically; however, the particle deposition parts of their work are very crude.

Lu and Howarth (1996) presented a Lagrangian model predicting aerosol particle deposition and migration in two interconnected ventilated zones. The turbulent airflow field was modelled by the standard k–ε model. Only the drag force and gravity were considered and the effect of turbulence was ignored. Chung (1999) performed similar Lagrangian simulation for particle transport in a multizone enclosure. However, only the trajectories of several sample particles were shown and his experiment did not consider particle motion. All of these investigations focus on the influence of the bulk air movement exclusively. The grids used were very coarse. The important turbulent dispersion and diffusion effects were not taken into consideration.

The main disadvantage of Lagrangian simulations is its cost. It is prohibitive to obtain a 'statistically significant' quantitative result for three-dimensional simulations. Flow dependent variables are the most difficult part for particle deposition modelling. For Lagrangian simulations in an enclosure, the mean velocity, turbulent intensity level returned by CFD solvers and stochastic instantaneous turbulent field returned by random walk schemes are of crucial importance. Most of the existing turbulence models are calibrated based on flows parallel to the wall and employ empirical wall functions. Airflows in indoor environments or enclosures always involve flow impingement, separation, small secondary vortexes in corners. The validity of conventional turbulence models has not been well addressed, or some recent improvement is not available in popular commercial CFD packages.

Currently, the authors are investigating particle deposition indoors by improving an Euler–Lagrange model. Figure 1 shows the distribution of particles depositing inside a chamber between 5s–10s. Only one-fourth of the test chamber is simulated (chamber size 0.4 × 0.4 ×

0.4 m^3). An ensemble of 16 000 10-μm particles initially uniformly distributed is released. The deposition points are recorded. It is observable from the figure that advection effect plays a dominant role in corners due to the non-negligible normal mean flow velocity component. Near the stagnation point, particles depart from fluid streamlines and strike on the floor due to impaction.

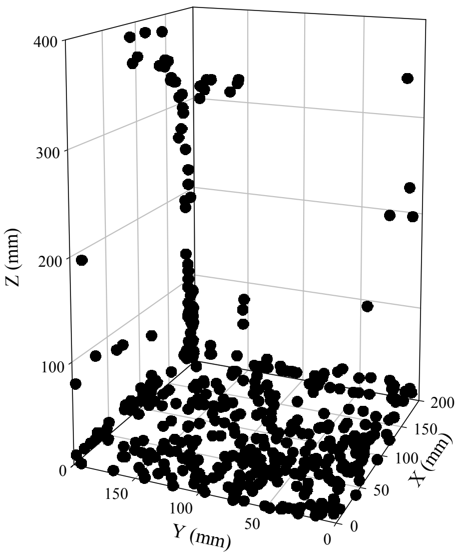

Figure 1 Distribution of particles depositing inside a chamber between 5s and 10s.

CONCLUSION

The knowledge of particle deposition has many practical implications. It is evident that the Eulerian and Lagrangian approaches are actually two extremes of particle deposition modelling. The current review highlights the particle diffusivity mandatory required by the Eulerian model and the limitations of the CFD model.

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