On the boundary conditions of numerical particle simulation in indoor environment

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SUMMARY

Computational fluid dynamics can predict contaminant dispersion in enclosed environments, provide valuable information about indoor air quality, contaminant concentration and thermal comfort. It is widely known that the accuracy of numerical simulations strongly depends on the appropriate setting of boundary conditions and parameters.

The present study explores the role of boundary conditions on prediction of particle distribution, dispersion, and sedimentation in an enclosed environment. In addition, grid resolution and numerical approaches (that is, Eulerian or Lagrangian methods) were also discussed. Two C++ User-Defined Functions that calculate particle concentration distribution based on Eulerian or Lagrangian methods were also discussed.

1. INTRODUCTION

Particles suspended in the air can cause many health problems and are identified as a major enclosed environment pollutant (Roberts, 2006). Particles carrying aerobic bacteria can spread and initiate infectious diseases (Xie, Li, Sun, & Liu, 2009). Generally, particle distribution and deposition is assessed by conducting studies; however, possible danger and cost involved should be carefully considered. Though the computational fluid dynamics (CFD) technique has been widely used to predict particle transport and deposition in enclosed environments, challenges remain. Several factors in a numerical simulation can undermine accuracy, including boundary conditions (BCs), discretization scheme, turbulence modelling, grid type, and user knowledge. Depending on operator experience and abovementioned influential factors diverse results may be obtained for the same problem (Zhai, Zhang, Zhang, & Chen, 2007). However, proper physical and numerical treatment of BCs may become much more important when the simulation deals with particle prediction. In enclosed environments, the particle deposition and rebound behavior over the wall boundary are much more important and can highly influence the predicted concentration. In addition to the boundaries, the particle modelling approach is important and should be correctly applied.
Commonly, there are two modelling approaches for two-phase flow problems: Eulerian–Eulerian, and Eulerian–Lagrangian; however, selection between them is based on the research field, the computational cost, and numerical approach. This study highlighted the most accurate and applicable approach and settings for numerical particle prediction in indoor environments.

2. Modelling Approach

2.1. Eulerian–Eulerian model

This model is usually referred to as the Eulerian model and considers the particle phase as a continuum in a form similar to that of the fluid phase. Several Eulerian models have been developed for low-volume fraction of indoor particles (Lai & Chen, 2007; Zhao, Yang, Yang, & Liu, 2008). As the convective velocity of the air and particle phase is the same, the two-phase flow complexity is reduced. The governing equation for particle transport can be written as:

$$\frac{\partial C}{\partial t} + \nabla.\left[(u + v_s)C\right] = \nabla.\left[(D + \varepsilon_p)\nabla C\right] + S_C$$

(1)

where $u$ is the air phase velocity vector, $C$ is the particle mass concentration, $v_s$ is the particle settling velocity, $\varepsilon_p$ is the particle eddy diffusivity, and $S_C$ is the mass concentration source term. $D$ is the Brownian diffusion coefficient in a turbulent flow and particle size distribution of greater than 0.01 µm; the Brownian diffusivity is negligible compared to turbulent diffusivity.

When the Eulerian model estimates particle concentration within a computational domain, wall surface particle deposition remains a challenge part as most of commercial software, such as ANSYS Fluent, has no such built-in function. In this case, a C++ User-Defined Function (UDF) compiled by the operator can define a “sink” term in the cells near the wall surfaces. UDFs can be modified for specific applications and to adjust certain modeling parameters to meet simulation requirements. An example of such a particle deposition-modelling UDF is the following:
The idea is to define a sink term near the wall boundaries to remove the particle mass from the computational domain. There are different approaches proposed by others (Heiredal, 2010; Longmire, 2007).

2.2. Eulerian–Lagrangian model

This model is usually referred to as the Lagrangian model and computes the flow field based on the Eulerian framework, but treats the particle phases differently. In this method, the discrete behavior of each particle is considered to determine its trajectories based on Newton’s 2nd Law of Motion. Compared to the Eulerian model, the Lagrangian model may be rather memory intensive. The trajectory of a discrete phase particle is calculated by integrating the force balance over the single particle in terms of a Lagrangian reference frame. This force balance equates the particle inertia regarding the gravity, drag and Brownian forces, and can be written as follows:

\[
\frac{du_p}{dt} = F_D (\mathbf{u} - u_p) + \frac{g (\rho_p - \rho_p)}{\rho_p} + F_a
\]

(2)

Here, \(\frac{du_p}{dt}\) and \(F_D (u - u_p)\) represent the inertial and drag forces per unit particle mass, respectively. \(\mathbf{u}\) is the velocity vectors, \(\rho\) is the density, and \(g\) is the gravitational acceleration. In this equation, the subscript \(p\) refers to the particle, whereas the un-subscripted terms refer to the air. The term \(F_a\) is used to incorporate additional terms such as Brownian force, the thermophoretic and life terms. \(F_D\) is the inverse of relaxation time and is defined as follows:

\[
F_D = \frac{18 \mu C_D Re_p}{\rho_p d_p^2} \frac{C_D Re_p}{24}
\]

(3)
where $\mu$ is the molecular viscosity of the air, $d$ is the particle diameter, and $Re$ is the Reynolds number based on the particle diameter. $C_d$ is the drag coefficient for the sphere-shaped particles and can be computed from:

$$C_d = \frac{\xi_1}{Re} + \frac{\xi_2}{Re^2} + \xi_3$$  \hspace{1cm} (4)

where $\xi_1$, $\xi_2$ and $\xi_3$ are the constants given by Morsi and Alexander (Morsi & Alexander, 1972).

The stability of this method is highly important as stochastic particle tracking may introduce great uncertainty into predicting particle concentration. Therefore, some sort of statistical analysis should control and ensure the stability of the solution. The stability of the solution became statistically reliable as an adequate number of particles were explored (Zhang & Chen, 2006).

For the Lagrangian model the concentration can be calculated by the particle source in cell (PSI-C) method (Zhang & Chen, 2007):

$$C_j = \frac{M \sum_{i=1}^{m} dt_{(i,j)}}{V_i}$$ \hspace{1cm} (5)

where $C$ is the mean particle concentration in a cell, $V$ is the volume of a computational cell, $dt$ is the particle residence time, and subscript $(i,j)$ represents the $i^{th}$ trajectory and the $j^{th}$ cell, respectively. The stability of this method is highly dependent on the number of trajectories tracked (Zhang & Chen, 2006). The Lagrangian model does not directly calculate the particle concentration and thus to implement the PSI-C method in ANSYS Fluent, a UDF needs to be compiled. The following UDF is an example of this method:
In the Lagrangian model, different particle boundary conditions such as “tarp”, “escape” and “reflect” are usually available as built-in functions. The performance of the Eulerian and Lagrangian models in indoor environments has been the subject of many academic studies (Lai & Chen, 2007; Zhang & Chen, 2007; Zhao et al., 2008).

The calculation of these methods is different as they were developed using different frames of reference. In steady state conditions, the Eulerian model needs much iteration to obtain a converged concentration of particles. However, the Lagrangian model uses a time-marching manner and does not need iterations as long as particles are treated as one-way coupling.

2.3. Grid types

The CFD simulation grid type and quality is essential and can affect accuracy, computational robustness, and solution convergence. The importance is increased when the numerical simulation deals with two-phase flow. In CFD simulations, a higher grid refinement is normally used close to the walls to obtain very low dimensionless wall distance ($y^+$) and several cell layers within the boundary layer (Fig. 2-a). In two-phase flow simulation, a high grid resolution in the boundary layers prevents over-prediction (Béghein, Jiang, & Chen, 2005; Zhao, Zhang, Li, Yang, & Huang, 2004).

Fig. 1: Comparison of measured and predicted particle concentration at three different locations (Zhao et al., 2008)
Due to the high computational demand in indoor airflow simulations, interaction between the particles and airflow field is considered a one-way coupling; as a result, the effects of the discrete phase trajectories on the continuous phase were neglected (Sadrizadeh & Holmberg, 2014; Sadrizadeh, Tammelin, Ekolind, & Holmberg, 2014). This method is called post-processing simulation where particles are injected after the fully solved airflow field instead of by continuous injection (PSI-C method). In this case, a uniform grid over the full domain (Fig. 2-b) can provide a much more reliable solution. To predict particle concentration based on this method, the airflow field should be solved with a fine boundary layer grid; a converged solution further interpolates the uniform grid for post-processing particle simulation.

3. CONCLUSION

The importance of boundary conditions for precise prediction of particle concentration and deposition in indoor environments is well known among numerical simulation experts. The performance of Eulerian and Lagrangian models for prediction of particle concentrations in enclosed spaces was discussed. Two C++ user-defined functions for each method were provided and detailed. According to previous studies, the models, both of which have their pros and cons, were able to predict the particle concentration and distribution in indoor spaces, with their application being case-dependent.

The Eulerian model treats the particle phase as a continuum and develops its conservation equations on a control volume similarly to the fluid phase. As the convective velocity of the particle and air phase is the same, a one-way coupling with flow can reduce the complexity of the two-phase flow system. As a result, the Eulerian model used only particle concentration equations to couple with turbulence and momentum equations. A major weakness of this method is particle boundary condition unavailability. Particles are normally trapped on the solid walls and no recycling is considered in indoor simulations. However this boundary is not available with Eulerian model and this should be handled by a complimentary code.
When the Lagrangian model determines particle dispersion patterns, the interaction between the airflow field and the particles has normally been assumed to be a one-way coupling. This assumption can be made based on the effect of particles on the turbulent flow being negligible due to low solid loading, relatively small particle settling velocity, and particles not coagulating. If particles are treated as a one-way coupling, a post-processing particle simulation method can be employed to reduce the computational demand. A potential weakness of Lagrangian model is that particle concentration cannot directly calculated and some complimentary coding is required.

REFERENCES


