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PARTICLE DISPERSION IN ENCLOSED SPACES USING A LAGRANGIAN MODEL

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Abstract: *In this paper, an analysis of particulate matter dispersion in indoor spaces was made using a CFD (Computational Fluid Dynamics) model in steady state~~,~~ on a commercial software, ANSYS FLUENT. An Eulerian method was used to solve the fluid flow, applying the renormalization group (RNG) $k - \varepsilon$ turbulence model and a DRW (Discrete Random Walk) Lagrangian approach was used to predict the particle trajectories accounting for the turbulent dispersion. The numerical results obtained were compared with experimental data reported in the literature. The simulated velocity fluid flow agrees well with the reported experimental measurement. The Lagrangian model presents some discrepancies in the particle phase concentration on the bottom side, the predicted concentration is lower than expected, over-predicting the particle transport and the deposition rate, probably due to large turbulent kinetic energy estimation and the near wall region treatment.*

Keywords: *CFD, Lagrangian model, DRW, indoor particle dispersion.*

1. INTRODUCTION

Diverse mathematical models can be used to describe the governing processes of transport, diffusion and deposition of pollutants in open and indoor spaces. Following the spatial and temporal evolution of the pollutants realized by a specific source, these models allow to analyze the air quality, identifying distribution patterns and to evaluate the risk of areas with higher concentration exposure. The movement of pollutants in the air comprises transport, dispersion and deposition. Transportation is caused by wind flow, while the dispersion results from local turbulence. The deposition including precipitation and sedimentation causes the downward movement of particles in the atmosphere.

Among the models used to study particle dispersion the most common ones are the analytical models, which use a phenomenological basis, including a realistic solution description of the transport-diffusion equation applied to idealized conditions. Other treatments include statistical models, based on empirical relationships that can relate flow parameters with the concentration of solids from data analysis of experimental measurements. Finally, the numerical models, which may include particle deposition and settling phenomena, and are also used in the study of indoor particle flow. In terms of numerical models, the Computational Fluid Dynamic (CFD) models can be mentioned, those are based on numerical solution of basic conservation equations and transport phenomena principles, such as mass, momentum and energy conservation.

For the solution of a multiphase flow, two approaches can be adopted: Eulerian and Lagrangian methods. The first one considers the particle phase as a continuum medium, including an equation for the mass conservation of the species. In the latter, the trajectory of each particle is obtained by solving a balance equation (SEINFELD; PANDIS, 2006). In the present work, the commercial software ANSYS FLUENT was selected to analyze the particle dispersion in enclosed spaces applying a Lagrangian model in steady state regime.

2. METODOLOGY

In this paper the particulate matter dispersion in indoor spaces is analyzed. For the fluid flow an Eulerian model is applied and for the particle dispersion, a Lagrangian approach is selected. The computational domain adopted for the studies was based on the experimental setup proposed by Chen *et al* (2006), a rectangular cabin with the following description: $0{,}8m \; x \; 0{,}4m \; x \; 0{,}4m$ of length x width x height, single inlet and outlet, with centers located at

$(0m, 0{,}2m, 0{,}36m)$ and $(0{,}8m, 0{,}2m, 0{,}04m)$, respectively, with symmetry plane at $y = 0{,}2m$. The air velocity and the particle concentration were measured with a Phase Doppler Anemometer (PDA). Glass silver coated spheres were injected with a constant mass flow. The gas phase velocities were taken through lines located at $x = 0{,}2, 0{,}4, 0{,}6m$ positions, while the concentrations were evaluated at the symmetry plane. The cabin geometry is specified in Fig. 1.

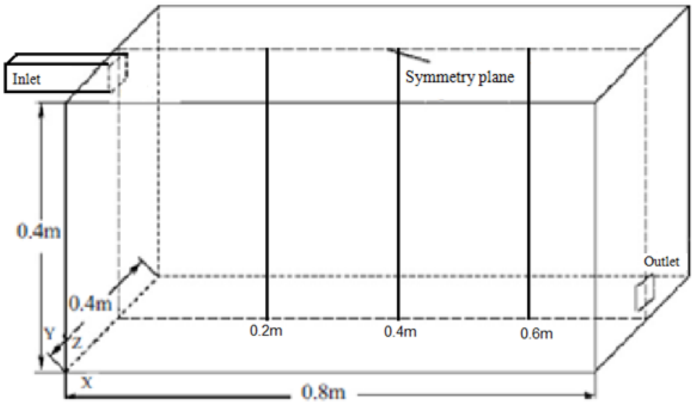

Figure 1. Cabien layout [Modified from:ZHOU (2008)]

2.1 Fluid flow modeling

According to Etheridge and Sandberg (1996), airflow in rooms is considered turbulent and particles are transported and dispersed by turbulence effect. In this work, the flow field is solved with the renormalization group (RNG) $k - \varepsilon$ turbulence model. This is an alternative to traditional models, and was proposed by Yakhot and Orzag (1986) for recirculating flows, detachment of the boundary layer among others. It is based on the theory of renormalization groups in the Navier-Stokes equations. The transport equations for turbulent kinetic energy and its dissipation are maintained, while the model constants differ from those of the standard model.

For the near wall region, a scalable wall function is used to avoid inconsistencies within the mesh refinement process.

2.2 Particle phase modeling

In Lagrangian models the displacement of each particle is followed through a complete track. The trajectories of the particles are calculated from integration of balance of forces acting over the particles, described next:

$$\frac{dx_p}{dt} = \boldsymbol{u_p} \tag{1}$$

$$m_p \frac{d\boldsymbol{u_p}}{dt} = \sum F_i \tag{2}$$

In which, x_p, is the particle position vector, u_p and m_p, are the particle velocity and mass, respectively. The term F_i represents the sum of all relevant forces:

$$\sum F_i = F_b + F_s + F_c \tag{3}$$

Where F_b, F_s represent the body, surface and collision forces, respectively. Among the body forces, the gravitational effect is considered, $F_{b,g}$. Among the surface forces, in this case the drag force($F_{s,D}$), buoyancy ($F_{s,b}$) and Saffman lift force ($F_{s,lf}$), are considered, according to the previous studies of Zhao et al. (2008). The Brownian dispersion is not relevant for the present study due to the large particle size considered.

$$m_p \frac{d\boldsymbol{u}_p}{dt} = m_p \frac{3}{4}\frac{\rho}{\rho_p d_p} C_D\left(\boldsymbol{u} - \boldsymbol{u}_p\right)\left|\boldsymbol{u} - \boldsymbol{u}_p\right| + m_p\left(\frac{\rho_p - \rho}{\rho}\right)\boldsymbol{g} + \frac{2K\nu^{1/2}\rho d_{ij}}{\rho_p d_p (d_{lk} d_{kl})^{1/4}}\left(\boldsymbol{u} - \boldsymbol{u}_p\right) \tag{4}$$

The first term on the right side represents the drag force, the second includes the buoyance and gravity, and the latter is the generalization of the Saffman expression, where $K = 2.594$ and d_{ij} is the deformation tensor (Saffman, 1965), this force accounts for the particle rotation induced by shear flow where velocity gradients generate that motion, this term can be relevant in the near-wall region treatment.

2.2.1 Stochastic tracking

The turbulent particle dispersion model is based on a stochastic approach. In ANSYS FLUENT, those tracks are calculated by the integration of a linearized form of Eq 2, with the mean fluid velocity, $\bar{\boldsymbol{u}}$, calculated from the RANS equations, and the instant velocity $\boldsymbol{u}^{'}(\boldsymbol{t})$ from the particle path for the integration. In this way, the random turbulent effects over the particle dispersion can be included by computation of the trajectories of a representative number of particles (*number of tries*).

The instantaneous velocity, $\boldsymbol{u}^{'}$, is described by the Discrete Random Walk model or Eddy life time model. This model describes particle interaction with the stylized simulated eddies, in which each eddy has a characteristic time scale. Assuming a Gaussian distribution for the fluctuation velocity, the $\boldsymbol{u}^{'}$, components adopt the form:

$$\boldsymbol{u}' = \zeta\sqrt{\boldsymbol{u}'^{2}} \qquad (5)$$

In which ζ is a random distributed number and the remaining part represents the Root Mean Square (RMS) values for the fluctuating velocities.

2.2.2 Particles concentration

To evaluate the distribution of particle concentration from the Lagrangian trajectories, the Particle Source in Cell method (PSI-Cell) is used, since it has been validated by Zhang and Chen (2006). This method estimates the number of particles in a control volume being represented in terms of the concentration C_j, explicitly by:

$$C_j = \frac{\dot{m}\sum_{i=1}^{m} dt_{i,j}}{V_j} \qquad (6)$$

Where $\dot{m}$ is the particle mass flow, dt the residence time and i, j are the subscripts that represent the ith and jth cell.

2.3 Numerical solution and Boundary Coditions

ANSYS FLUENT uses the finite volume method to discretize the integral form of the governing equations of the flow. Once the computational domain is defined and subdivided, the principles of conservation of the properties are applied discreetly in each volume element, integrating the equations in a conservative way on the volume (VERSTEGG; MALALASEKERA, 2007).

For the pressure-velocity coupling, the SIMPLE solver is used in the simulation, which follows a pressure-based, segregated algorithm, solving sequentially the pressure and momentum equations.

In ANSYS FLUENT, the variables are stored in the center of the control volumes, however to solve the transport equations presented in the previous item, it is necessary to know the value of these in the faces, this is done using interpolation schemes. The details of the model configuration are given on Tab. 1.

Table 1. Numerical methods and discretization schemes for the fluid flow

Numerical method	
Solver	*Pressure-based*
Pressure-velocity coupling	*SIMPLE*
Relaxation factors	0.3 –Pressure 0.7 - Momentum 0.7 –Turbulence
Regime	Steady state
Spatial discretization	
Pressure	*Standard*
Convective terms	U*pwind* schemes second order
Gradients	*Green-Gauss node-based*
Convergence criteria RSM residual	10^{-4}

For the solution of the continuous phase (fluid) a constant velocity is imposed at the inlet, and a no-slip condition is selected for the walls. The outlet is considered as pressure-outlet. For treatment of the dispersed phase (particles), the solid boundaries were defined as trap, thus every particle that reaches the surfaces is aborted from the subsequent cell calculations, no particle rebounds in consider on any surface. In Tab. 2, the initial and boundary conditions for each phase are listed.

Table 2. Initial and boundary conditions for continous and dispersed phase

Continuous phase	
Inlet	$\bar{u} = 0.225$
Outlet	$P = 0\ Pa$
Wall	$\bar{u} = (0\ 0\ 0)m/s$
Dispersed phase	
Particle diameter	$d_p = 10\mu m$
Particle density	$\rho_p = 1.4x10^3 kg/m^3$
Particle mass flow	$m_p = 5.04x10^{-7} kg/s$
Injection velocity	$u_p = 0.225$

A mesh independence study was conducted for the flow field in three structured meshes, with 96780, 176364 and 294808 equally spaced elements, generated with ANSYS MESHING software. The results were considered grid independent as the velocity profiles of the continuous phase remained unchanged with the mesh variations. Thus, in all other calculations just the coarse mesh is considered.

The particles were injected after the convergence of the fluid flow is achieved. A total of 36000 particles were used to achieve a representative number of particles per unit volume. The number of particles was increased until a statistically stable result for the particle concentration was reached, with a variation of less than 2%.

Since the solid fraction is very low ($\alpha_p = 3.73x10^{-6}$), the effect of particles on the turbulent flow can be neglected, by considering that the flow affects the particles but not in the opposite, therefore it can be treated as one way coupling (Elghobashi, 1994).

3. RESULTS

The velocity profiles of each phase are presented in Fig. 2. The particle axial velocities exceed the fluid velocity due to the sudden expansion at the inlet region, while at the bottom the opposite case is observed, probably due to cross stream transport. However, the experimental measurements in the near wall region normally may contain a high degree of uncertainty.

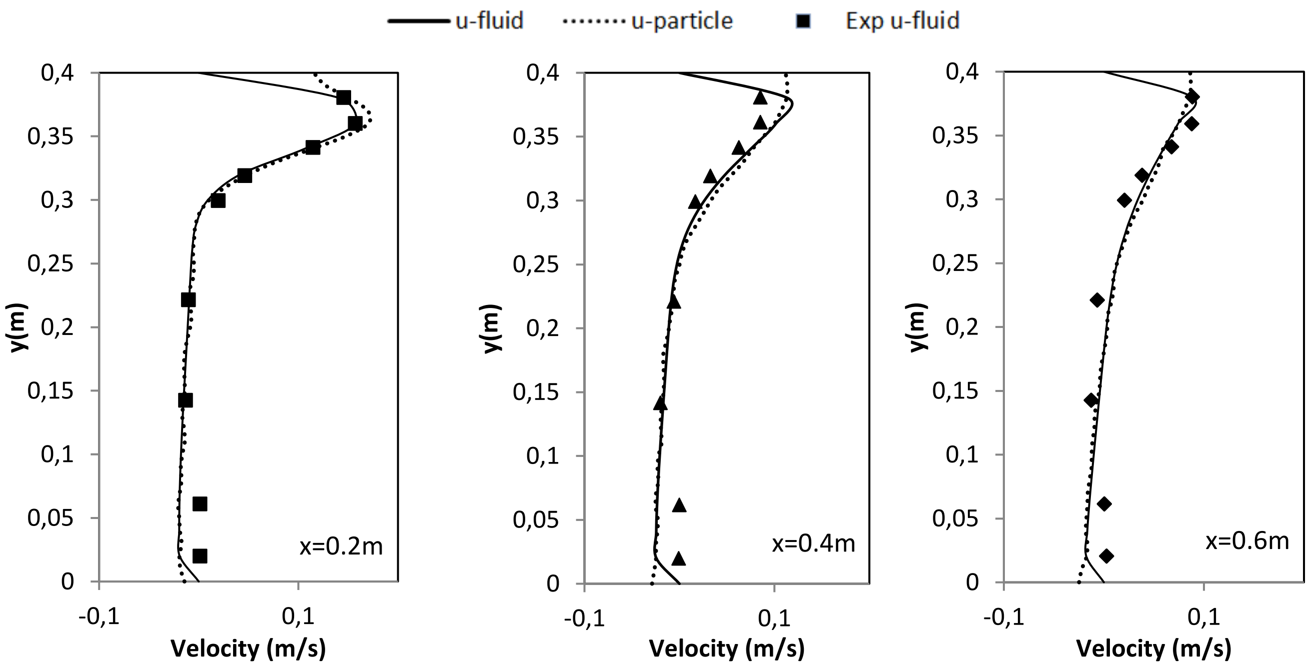

Figure 2. Fluid and particle velocity profiles (computed and experimental)

In Fig. 3, a comparison of experimental and simulated concentration profiles along the axis of symmetry is shown. The values are normalized, based on the input value. The concentration is higher at the inlet, then decreases along the x-axis due to particle deposition. The simulation could represent the distribution in the first plane, at x = 0.2m, but the discrepancy between measured and simulated values increases as the particles go forward (larger x values). The concentrations obtained with the model, in the last two positions, were lower than expected. The relative error to the mesasured data was defined as the difererence between calculated and measured data divided by the measured data. Its value is relatively high, especially in the wall region near the floor. The largest relative error (above 70%) is found at point (0.2, 0.02, 0.2), perhaps due to the overestimation of particle deposition, which may be due to the trap condition imposed to the walls and a larger turbulent kinetic energy estimation.

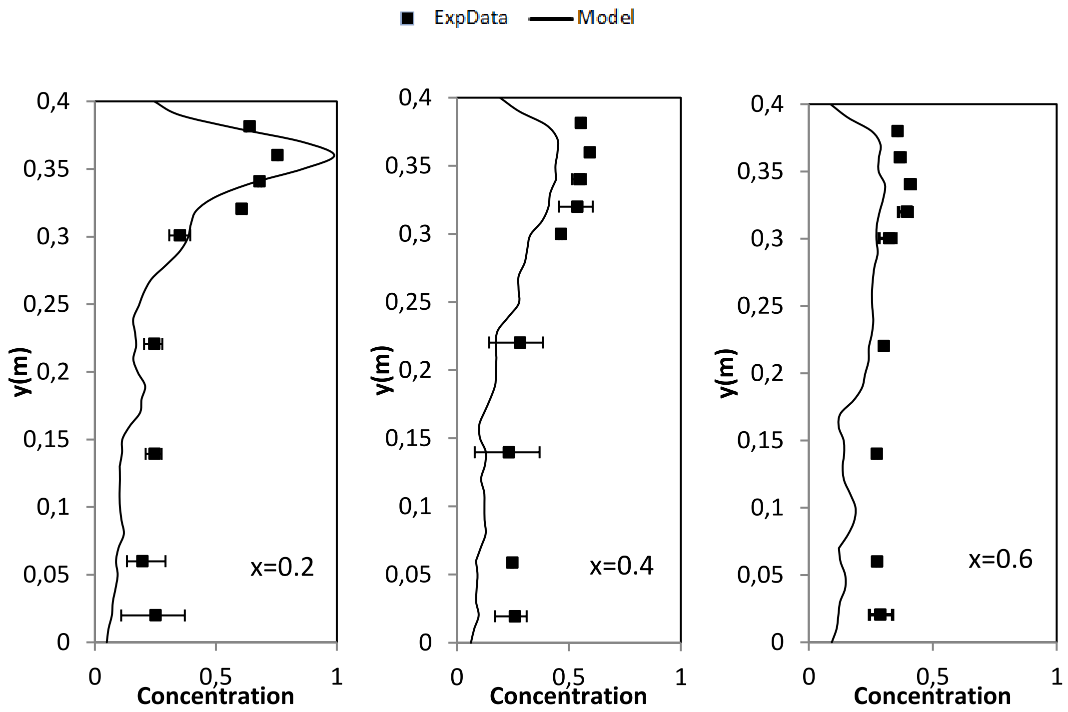

Figure 3. Particle concentration profiles (computed and experimental)

4. CONCLUSIONS

A CFD model was used to describe particulate matter dispersion in indoor spaces and was validated with the experimental data from Chen *et al* (2006). An Eulerian approach was selected for the continuous phase while a DRW (Discrete Random Walk) Lagrangian approximation was adopted for the disperse phase to predict the particle trajectories, accounting for the turbulent dispersion. A steady state case with one way coupling for the particulate phase was considered. After the mesh independence study, it was concluded that the numerical results are grid independent.

The numerically modeled velocity profiles of the fluid phase agree with the experimental data reported. The Lagrangian approach represented well the particle concentration distribution. Some discrepancies are observed in the near wall region probably due to a larger turbulent kinetic energy estimation and a trap condition imposed on the walls, generating a larger deposition rate than expected, or to the larger experimental errors in this region.

The DRW Lagrangian model successfully reproduced the particulate matter dispersion in indoor spaces, but a more suitable wall treatment must be included to account for particle resuspension and the lower deposition rate experimentally observed.

5. ACKNOWLEDGEMENTS

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6. REFERENCES

Chen, F., Yu, S.C.M., Lai, A.C.K.., 2006. “Modeling particle distribution and deposition in indoor environments with a new drift-flux model”, *Atmospheric environment*, Vol. 40, p. 357–367.

Elghobashi, S., 1994. “On predicting particle-laden turbulent flows”, *Applied Scientific Research*, Vol. 52, n. 4, pp. 309-329,

Etheridge, DW., Sandberg M., 1996. *Building ventilation: theory and measurement*. Chichester, New york: John wiley & Sons.

Saffman, P.G., 1965. “The lift on a Small Sphere in a Slow Shear Flow”. *J. Fluid Mech*., Vol. 22, p 385-400,

Seinfeld, J.H., Pandis, S.N., 2006. *Atmospheric Chemistry and Physics of Air Pollution*. New York: John Wiley & Sons.

Versteeg, H. K.; Malalasekera, W., 2007. *An Introduction to Computational Fluid Dynamics: The finite volume method.* Pearson.

Yakhot, V., Orszag, S.A., 1986. “Renormalization group analysis of turbulence. I. Basic theory”, *Journal of Scientific Computing*, Vol. 1, p. 3-51.

Zhao, B., Yang, C., Yang, X. and Liu, S., 2008. “Particle dispersion and deposition in ventilated rooms: testing and evaluation of different Eulerian and Lagrangian models”, *Building and Environment*, Vol *43*, n. 4, p. 388-397.

Zhang, Z., Chen, Q. 2006. “Experimental measurements and numerical simulations of particle transport and distribution in ventilated rooms”, *Atmospheric Environment*, Vol. 40, n. 18, p. 3396-3408.

7. RESPONSIBILITY NOTICE

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