PARTICLE CONCENTRATION CALCULATIONS USING CFD

- A COMPARISON -

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Summary

Three approaches for the calculation of the particle contaminant distribution in a room using CFD are described. The approaches are tested for two types of flow problems. The results indicate that the Euler approach, in which only the particle settling velocity is incorporated, presents an attractive alternative for the more precise Lagrange approach. The Passive Scalar approach should not be used when calculating the particle distribution in a room.

Introduction

The use of CFD for the calculation of the exposure of persons to airborne particles (carcinogenic, biological; particle diameter (D_p) in the order of 0.3 – 20 μm) in a room gains interest as legislation on this subject becomes more strict. In this paper options to calculate particle concentrations in a room, using CFD, are discussed. A comparison is made between three approaches: the Passive Scalar (Gaseous), the Euler and the Lagrange approach. This comparison is made within the context of the development of a measurement protocol for bioaerosol measurements. The measurement location in the room is one of the items that are addressed in this protocol.

The three approaches are compared for two types of flow problem. The first comparison uses particle measurement results from literature for cleanroom ventilation conditions. The second one uses new measurement results obtained from bioaerosol measurements in an office room. The latter measurements have been performed within the context of the above described protocol development.

Methodology

The main difference between the three approaches to calculate the contaminant distribution in a room lies in the complexity with which individual particles are tracked in the flow. The Passive Scalar and the Euler approach deal with the particles as if it where a gas. In the Euler approach however the gravity force that acts upon a particle is included in the calculation of the particle contaminant distribution. The Lagrange approach not only includes the gravity force, but all other possible forces that may act upon a particle. It calculates individual particle trajectories instead of a bulk of particles. From the individual particle trajectories the contaminant distribution can be derived.

The most important difference between the Passive Scalar and the Euler approach and the Lagrange approach therefore is that inertial effects are only dealt with in the Lagrange approach. The other two approaches assume that a particle will follow the flow instantly. Inclusion of the gravity in the Euler approach is only possible through the fact that the gravity force is constant and in a constant direction. The resulting settling velocity nevertheless is imposed instantly on the particle.

As inertial effects are neglected the Passive Scalar approach and the Euler approach are not able to calculate the turbulent diffusion of the particles near the particle source, i.e. they ignore the correlation of the velocity fluctuations. Applying the analytical solution for a homogeneous turbulent velocity field with zero average velocity (Hinze 1975), one can derive that these approaches are only valid for time scales that are larger than the integral time scale (T_L) of the turbulent flow (Lemaire 2000). This time scale can be calculated from $T_L = C_L k/\varepsilon$, with $C_L = 3/2\ C_\mu/\sigma_s$. The Lagrange approach does not have this restriction, however the main disadvantage of the Lagrange approach is the calculation time. The Passive Scalar and the Euler approach obtain their result a factor 100 or more faster than the Lagrange approach.

The gravity force is normally the most important force that acts upon a particle in the indoor air flow. Use of the Euler approach therefore is attractive when many contaminant concentration calculations are required.

This study investigates the criteria for choosing a modelling approach when calculating the particle concentration. A distinction is made for rooms with a high air exchange rate and normal office room configurations, i.e. relative high and relative low average velocities.

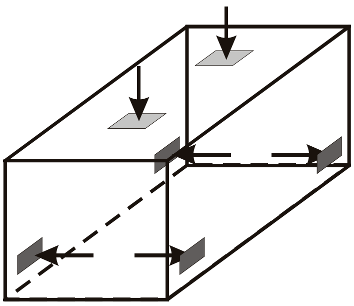

Figure 1. Sketch of the flow problem investigated by Murakami et al. (1992).

Implementation

The Passive Scalar approach uses the scalar conservation equation and numerical techniques found in most CFD-programmes.

The Euler approach also applies this method. In this case however the particle settling velocity is added to the stationary velocity field from which then the particle concentration is calculated (Murakami et a. 1992). The turbulent diffusion in both approaches is derived from the results of the applied standard k-ε turbulence model.

The Lagrange approach does not use the conservation equation. It uses the particle trajectory equation that can be found in e.g. Hinze (1975) and Auton et al. (1988). This equation balances the different forces that can act upon a particle under the assumption that the particles do not interact and are smaller than the smallest wavelength present in the turbulence. This applies to the investigated particles and the type of room air flow. In the here described results only the acceleration force, the resistance force and the gravity force are included. Electrostatic forces and Brownian movement are neglected ($D_p > 0.3$ μm). This also accounts for terms as the Basset-history integral, as the particle density is assumed to be a factor thousand larger that the fluid medium density. As $Re_D < 1$, Stokes' law can be applied to calculate the drag coefficient. For a turbulent flow field the particle trajectory is derived by applying Reynolds decomposition, i.e. a time-averaged part and a fluctuating part. The instantaneous particle position then is calculated by integrating the particle velocity over a time-step.

The Euler and Lagrange approach have been implemented in the in-house CFD-code WISH-3D (Lemaire 1996 and Lemaire 2000). In all cases it is assumed that the particles do not influence the flow field or the turbulence characteristics.

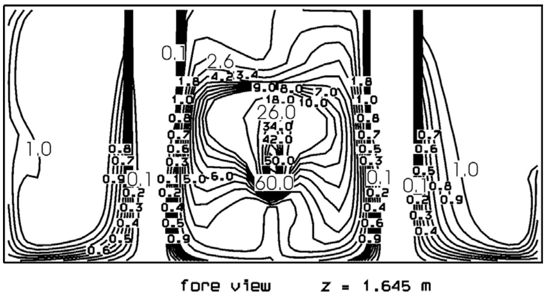

Figure 2. Particle distribution in the centre plane using the Euler approach (D_p = 10 μm).

Validation

The implemented approaches have been validated with measurement and simulation results from Murakami et al. (1992). Murakami et al. used a clean room configuration with two supplies in the ceiling and four exhausts in the wall (see Figure 1). The air exchange rate was set at 40 h^{-1}. The particle source was modelled as a 'source volume' in the centre of the room with its centre point at a height of 0.8 m. It was regarded transparent for the fluid flow.

The particle concentration in the room has been calculated for three different sizes of particle diameter (D_p = 0, 10 and 50 μm). An example of the result for the Euler approach is shown in Figure 2. In Table 1 the simulation results for the three approaches have been normalised in order to compare them with the measurement results as reported by Murakami et al. Normalisation was done to the particle concentration at the exhaust for D_p = 0 μm.

Table 1. Measured and calculated normalised average particle concentrations.

D_p [μm]	Murakami et al. (1992)	Passive Scalar	Euler	Lagrange
		in the exhaust		
0	1.0	1.0	1.0	1.0
10	0.91	1.0	0.93	0.96
50	0.11	1.0	0.11	0.14
		in the room		
0	1.70	1.59	1.59	1.72
10	1.59	1.59	1.51	1.62
50	0.52	1.59	0.58	0.66

The results in Figure 2 and Table 1 show that the different approaches are implemented correctly. The obtained results also show good resemblance with the measurement results.

Different values are found for the different approaches. Nevertheless, the Euler and Lagrange approach show similar results. This indicates that the more simple Euler approach is able to calculate the particle distribution in the room correctly. Though minor local differences

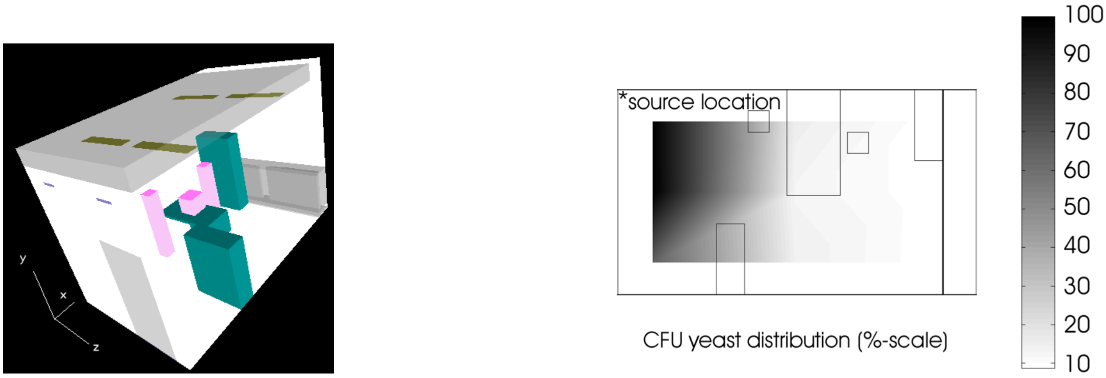

Figure 3. Sketch of the investigated flow problem and a result of the measured CFU-distribution in the room near floor level (source location at 1.50 m height at the indicated position).

can be found the Euler approach is applicable for this type of flow problem. The Passive Scalar approach is only valid for small particle sizes. For the investigated clean room configuration the particle size should be smaller than 10 µm.

Office room

The flow problem that was investigated by Murakami et al. (1992) was a clean room configuration. Also the particle concentration distribution in an office room is investigated. The flow field in an office room differs to that in a clean room, as for example the average velocity and the air exchange rate are an order of magnitude smaller. This obviously has its effect on the integral time scale (T_L).

In the context of developing a measurement protocol for bioaerosol measurement the particle distribution in an office room as a function of the source location and configuration has been investigated. Measurements as well as simulations have been performed applying the described modelling approaches.

The measurements have been performed using two types of micro-organisms; a bacteria ($D_p \approx 1.5$ µm) and a yeast ($D_p \approx 5$ µm). The deposition method was used to count the total Colony Forming Units (CFU) that deposited on different media that were distributed over a grid in the test room. The test room was equipped with an induction unit. Several heat sources were used to generate a realistic flow profile in the room. Figure 3 presents additional information. More information is found in Loomans et al. (2002).

As the results for the Passive Scalar approach can be derived from the Euler calculation, only the Euler and Lagrange approach have been used to calculate the contaminant distribution in the room. In Table 2 the results are compared similar to Table 1. For the Lagrange approach an extra result is given for which $T_L = 0$ s, implicating that the correlation of the velocity fluctuations is neglected and the results can be compared directly with the Euler approach.

Table 2. Calculated normalised average particle concentrations for the office room.

		in the exhaust	
D_p [µm]	Euler [T_L = 0 s]	Lagrange [$T_L(k,\varepsilon)$]	Lagrange [T_L = 0 s]
0	1.0	1.0	-
5	0.81	0.88	0.86*
10	0.39	0.48	-
		in the room	
0	17.4	22.8	-
5	15.3	25.7	26.1*
10	9.15	17.9	-

* Normalised to D_p = 0 µm, Lagrange [$T_L(k,\varepsilon)$].

The results in Table 2 indicate that the influence of the settling velocity is apparent at smaller particle diameters compared to the clean room example. The settling velocity in this case thus should not be neglected for particles > 5 µm. A comparison of measurement and simulation results indicates that the qualitative distribution is predicted correctly with both approaches. A high contaminant concentration is found at floor level near the source. An absolute comparison with the measurement results is not possible.

When the results of the two approaches are compared, it is obvious that the average contaminant concentration in the room derived from the Lagrange approach remains higher than from the Euler approach (also in absolute sense). The difference is caused by the fact that the (turbulent) particle dispersion over the room is significantly smaller for the Lagrange approach so that values are higher near the source. The result with the Lagrange approach using $T_L = 0$ s, indicates that this difference does not result from the difference in the treatment of the particle distribution close to the source. The results for $T_L = 0$ s and $T_L = f(k,\varepsilon)$ are similar. The difference therefore touches the calculation of the instantaneous particle position using the k- and ε-information. From the available measurement results it is not possible to indicate the accuracy quantitatively.

Discussion

Investigation of the particle distribution in a room gains interest as exposure to airborne pathogenic particles is regarded an important topic of the indoor air quality. As particle dispersion is closely related to the air flow pattern, CFD is a very suitable tool to calculate the particle distribution in a room.

The three approaches to calculate the distribution from a CFD-result, described in this paper, each have their specific advantages. When the accuracy of the result is regarded most important, in principle the Lagrange approach is the single approach to be used. In that case it is important to include all particle forces in the model that are expected to affect the investigated particle trajectories. The calculation of the instantaneous particle position in a turbulent flow as applied in the here described results remains a topic for further research. The main disadvantage of the use of the Lagrange approach is the simulation time.

The Euler approach presents a useful alternative to calculate the particle distribution in the room when the gravity force is regarded the single force that acts upon a particle. The results presented in this paper indicate that the calculated particle distribution agrees with that using the Lagrange approach. As inertial forces are neglected, analytical analysis indicates that close to the source the particle distribution is not calculated correctly. For normal office room configurations the Euler approach therefore should be applied carefully. Qualitatively the distribution normally will be predicted correctly.

As the extra calculation costs for the Euler approach are small, the Passive Scalar approach should not be used to calculate the particle distribution in a room. Then the effect of the particle settling velocity is not underrated and not dependent on the room air flow. Besides the described approaches, the particle cloud tracking technique must be mentioned. This technique uses a Gaussian probability density function to calculate the dispersion of particles on the basis of a limited number of particles (Valentine and Smith 1997). Particle cloud tracking combines the advantages of the accuracy of the Lagrange approach and the calculation time of the Euler approach.

The boundary conditions for the described results in this paper only assumed deposition on horizontal surfaces. On other surfaces elastic boundary conditions were prescribed. Deposition on vertical surfaces nevertheless also takes place. Abadie et al. (2000) even found a relation with the wall texture. These assumptions do not influence the here described comparison. Nevertheless a correct description of the boundary conditions may become important when researching environments with a high ‘fleecy’ factor.

Quantification of the source strength is an other important parameter that is difficult to derive from experiments or for in-situ flow problems. In that case the particle distribution is determined relative to the source strength.

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