CFD Modelling of an Aerosol Exposure Chamber for Medical Studies

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An exposure chamber is an effective device that allows determining with precision the whole-body contact with an air contaminant. In this work the design of a vertical laminar exposure chamber (of about 18 m^3) for aerosol contaminants is described. In order to determine the velocity and concentration fields, a computational fluid dynamics approach (CFD) has been adopted. The proposed CFD model gives an effective method for sizing rooms constituted by a distribution device which works in turbulent conditions, and an exposure room volume with complex furnishings working in laminar conditions. Two types of aerosol have been taken into account: 1 μm spherical particles, acting as gaseous species, and 10 μm spherical particles, acting as solid. The transitory for reaching a steady-state concentration field, that is the minimum time required to reach a uniform particles distribution, have been evaluated for both the aerosols.

1. Introduction

In working environments people are often exposed to gaseous and/or condensed pollutants that can be potential causes of allergies, diseases and in general health damages. In the framework of the occupational and environmental health and medicine, it is essential to evaluate the hazardous level of an air contaminant with regard to the assimilated dose (Chung et al., 1999; Rogers et al., 2005). Such an evaluation can be carried out by determining, for the sake of examples, a time-weighted amount of contaminants assimilated by workers through lunges and skin, that is by measuring the whole-body exposure (Liden et al, 1998). The exposition is accurately determined if the working environment is well-mixed, as the contaminant concentration results uniformly distributed. On the contrary, when this condition is not met, as it is usually observed in real environments, which are characterized by local releases of contaminants and by an inhomogeneous fluid-mechanics field, the determination of the exposure is difficult and characterized by a poor accuracy.

An exposure chamber is an effective device that allows determining with precision the whole-body contact with an air contaminant. Brief descriptions of such rooms can be found in literature (Pauluhn, 2003), with reference to gaseous and condensed pollutants exposition, respectively (Søstrand et al., 1997; Liden et al, 1998). In these rooms, the contaminant concentration field is kept at high degree of uniformity by means of a strong mixing (turbulent exposure rooms) or by means of a top-to-bottom distribution device (laminar exposure rooms). When the pollutant is gaseous or, due to small dimensions, comparable to a gas, the design of exposure rooms is not critical; on the other hand, when inertial forces acting on contaminant solid particles are not negligible, the chamber design becomes complex and computationally expensive. In this work the design of a vertical exposure chamber for aerosol contaminants is described by means of a CFD approach. In particular, main process parameters are reported in Table 1.

Table 1: Main process parameters.

Parameter	
Operating temperature	25°C
Operating pressure	1.024 atm
Chamber air flow rate	36 $m^3 h^{-1}$ (at 25°C)
Aerosol concentration	$500 \cdot 10^{-6}$ g m^{-3}
Aerosol density	2800 kg m^{-3}
Range of aerosol dimensions	1÷10 μm

2. Design of a whole-body exposure chamber

In this study a whole-body laminar exposure chamber (of about 18 m^3) has been designed by a modelling approach, in particular by means of a computational fluid-dynamics (CFD) model, which represents today a competitive and reliable technique with regards to pilot scale tests. With such an approach, velocity, scalars and particles concentration fields can be obtained both in laminar and turbulent regime, both in stationary and transient conditions, allowing evaluating the operating performance of the exposure chamber. The design is targeted to reach a uniform aerosol concentration condition in the whole volume, that is a maximum spatial unbalance of 10% (Yakhot and Orszag,1986), in 2 hours.

Main dimensions of the exposure chamber are a 2.5 m width, 3.0 m length and 2.4 m height, and they have been defined in order to ensure the possibility to host the necessary medical equipment and instruments within the room. The total net volume, that is with internals, is about 15.7 m^3. At nominal operating conditions, the total flow rate is 36 m^3 h^{-1}, that gives an ideal, total replacement rate of 0.45 h.

Modelling exposure chambers is a challenging task as typically, to reach rapidly uniform conditions, fluid-dynamic turbulent regime is required. That involves two main problems, that are (i) the velocity and concentration fields depend strongly on the layout of internals, (ii) the CFD model is computationally expensive. For such reasons, in this study an exposure chamber arrangement that minimizes both the internal layout to fluid-dynamics dependence and the computational resources has been adopted. A sketch of the equipment is shown in Figure 1. In particular, the chamber is split into two zones, a *plenum*, the higher one, and the effective exposure chamber, also named the *chamber* in the following.

The upper part of the *plenum* is provided with four circular inlets of 0.1 m in diameter, located at 0.75 m and 0.625 m from vertical walls, whereas the floor of the *chamber* works as outlet. Conical deflector have been positioned immediately downward each circular inlet to improve the particles spreading. The intermediate plane, partitioning the *plenum* and the *chamber*, is a perforated plate with holes of 0.001 m in diameter equally spaced, located at 0.2 m from the plenum roof, and the total open area of the intermediate plane is the 0.13% of the total cross-section area of the chamber, introducing a pressure drop between the two zones.

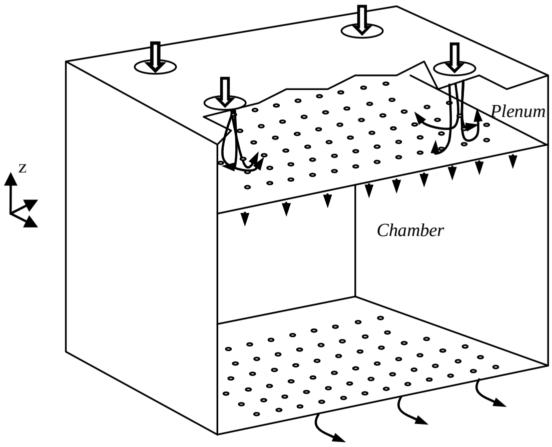

Figure 1: Sketch of the proposed exposure chamber.

With such an arrangement, the *plenum* works in turbulent regime as an equalizing chamber, ensuring a uniform aerosol concentration at the inlet of the *chamber* that, on the contrary, works in laminar regime. More in general, fluid-mechanics is independent with regard to the internal layout, which leads to an effective and reliable design.

3. CFD modelling

According to the chamber arrangement, the CFD model has been split into two independent cases, one for the *plenum* and the intermediate perforated plate, and the other one for the *chamber*. Computed velocity and concentration fields at the outlet of the perforated plate are applied as inlet boundary conditions for the *chamber* model. In Figure 2 the modelled geometrical domains for the whole chamber and for the internals are shown.

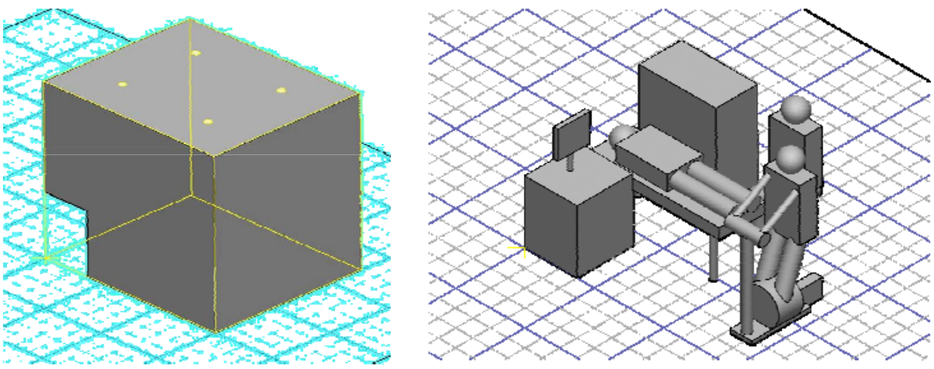

Figure 2: Geometrical domains for the whole chamber (left) and for internals (right).

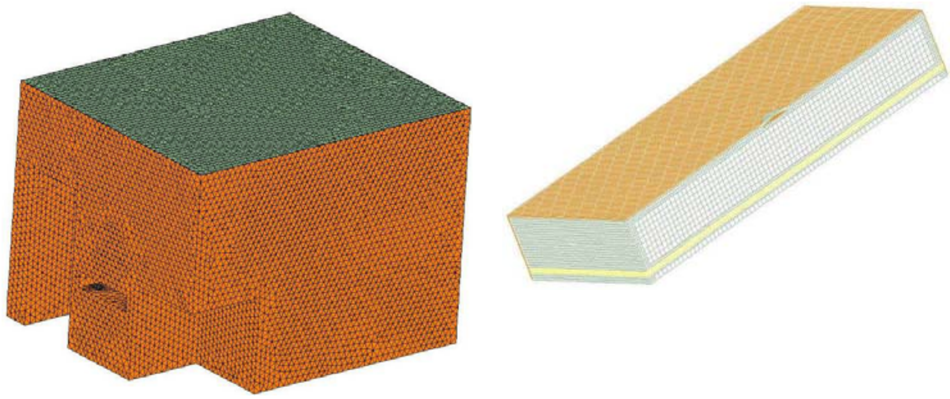

Figure 3: Computational domain for the chamber (left, unstructured mesh) and for the plenum (right, structured mesh).

The numerical technique adopted for the fluid-mechanics simulation is based on the finite volume method, consequently the geometrical domain has been converted into a computational domain by a meshing operation. Concerning the *plenum*, for which only a quarter has been considered due to symmetry, a structured mesh has been used, giving a model with 251k cells. On the contrary, an unstructured mesh has been adopted for the *chamber*, made by 700k tetrahedral cells. Two details of the mesh are shown, for the sake of example, in Figure 3.
In this study the air fed to the chamber has been considered incompressible and with constant physical properties; further, since the aerosol concentration is small the gas-to-particle coupling is of one-way type. CFD simulations have been carried out for two different cases, that is with 1 μm and 10 μm aerosol particles. In the first case, due to the small Stokes number, the particles are assumed as gaseous species; on the contrary, for heaviest particles a discrete trajectory approach has been accounted for. Governing equations for the case of small particles are mass continuity, Navier-Stokes and scalar concentration equations in transient form:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \tag{1}$$

$$\frac{\partial (\rho \mathbf{u})}{\partial t} + \rho \mathbf{u} \cdot \nabla \mathbf{u} + \nabla P = \rho \mathbf{g} + \nabla \cdot \left[\mu \left(\nabla \mathbf{u} + \nabla \mathbf{u}^{T} \right) - \frac{2}{3} \mu \mathbf{I} \nabla \cdot \mathbf{u} \right] \tag{2}$$

$$\frac{\partial (\rho Y_i)}{\partial t} + \rho \mathbf{u} \cdot \nabla Y_i = -\nabla \cdot (\rho D_i \nabla Y_i) \tag{3}$$

where **u** and **g** represent the velocity and gravity vectors, P, μ and ρ are the pressure, viscosity and density of the air, while Y_i and D_i are the mass fraction and mass diffusion coefficient of the aerosol, respectively. Subscript “T” and **I** identify the transposed matrix and the unit matrix. In order to simulate the behaviour of the heaviest aerosol, particles are considered of spherical shape, with constant physical properties, uniformly distributed on the inlet surfaces. The governing equations is the momentum balance on the particle:

$$m\frac{\partial \mathbf{u}}{\partial t} = \mathbf{F}_D + \mathbf{F}_T \tag{4}$$

where m is the particle mass and $\mathbf{F}_D$ and $\mathbf{F}_T$ represent the drag force and the turbulent dispersion force respectively. The last term is applied for the *plenum* only, where turbulent flow occurs. In order to properly size the transitory, particles colliding on the walls has been considered lost.
Then, turbulence is modelled by the RNG-k-ε model, which represents a good compromise between accuracy and computational resources for complex flow fields. Accordingly, conserving equations for turbulence kinetic energy and turbulence dissipation rate must be coupled to the above equations. The maximum computed velocity was 0.75 m/s, located at the inlets. The whole fluid-dynamics model was implemented by means of a commercial CFD code.

4. Results and discussion

On the basis of the proposed design, initial simulations have been performed for tuning the optimal arrangement of the *plenum*, that is the minimum necessary height and the best number and location of aerosol inlets. Once the more effecting geometry has been defined, a full simulation, starting from a clean chamber up to steady-state conditions, has been performed. Figure 4 summarizes the particles trajectories into the *plenum* for the two investigated cases. As expected, smaller particles are more entrained by the air flow rate; on the contrary, a larger amount of heavier particles are lost on the walls. The 1 μm particles that reach the *chambers* are about 44% of the total particles, whereas the same fraction drops to 33% for the 10 μm particles. In the worst case (heavy particles), uniform conditions within the *plenum* are reached in 540 s.

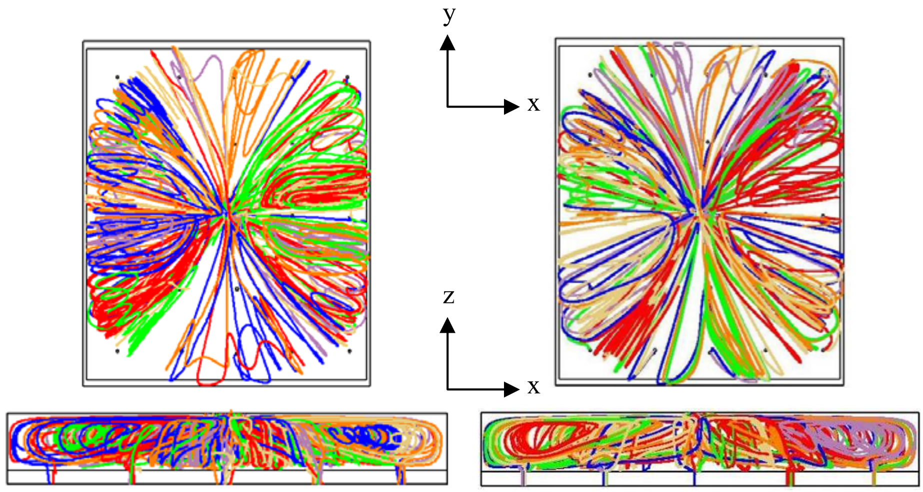

Figure 4: Particle trajectories into the plenum: 1 μm (left) and 10 μm (right) particles.

The velocity and concentration fields obtained at the *plenum* outlet in uniform conditions have been imposed on the upper horizontal plane of the *chamber* as inlet boundary conditions. It was found that, as worst case (light particles), the necessary transitory that allows for obtaining a uniform aerosol concentration within the *chamber* is about 2040 s. In Figure 5 concentration fields for two representative times, estimated at three locations, are reported. Clearly, the fluid-mechanics regime is laminar; however, the molecular transport is negligible with regards to the convective transport as obstacles are not promptly surrounded by the aerosol. The total transitory, for reaching sufficient uniform distribution in the *chamber*, was estimated to be 2580 s, which is considered satisfactory from a process point of view.
In order to check the quality of the numerical procedure, simulations have been performed also with a larger cells number, that is 1.5 times the described model. Grid convergence was checked by Richardson's technique (Roache, 1997); a minimum convergence of 10^{-3} was obtained for each degree of freedom.

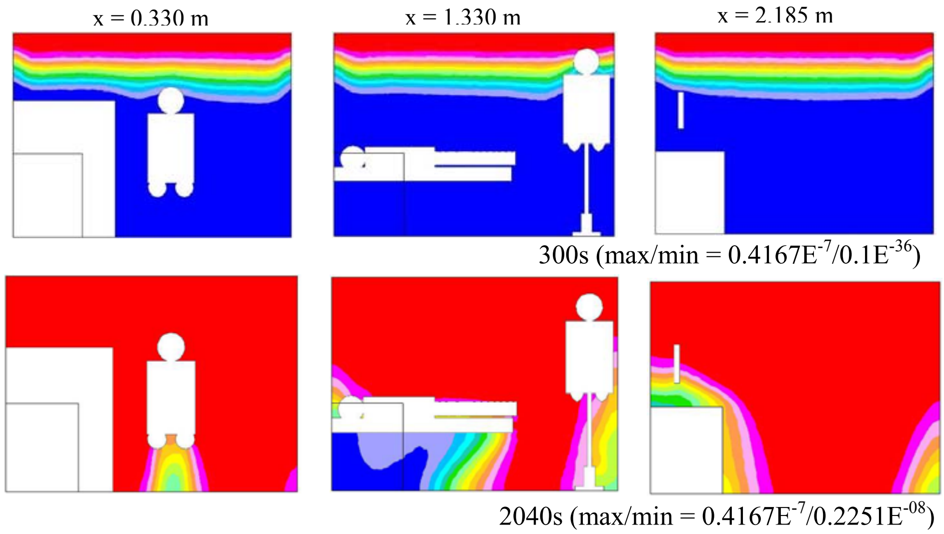

Figure 5: Aerosol concentration fields at three different locations within the chamber.

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