Use of COMSOL Multiphysics® for IAQ Monitoring in Cleanrooms

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Abstract: COMSOL Multiphysics was exploited for monitoring microclimate and Indoor Air Quality (IAQ) in a real Operating Theatre (OT). In the present paper we report some results carried-out during this activity, obtained by a multi-physical modelling, mainly based on the fluid dynamics solution, and the consequent determination of several transport-diffusion equations for passive scalar variables, such as temperature, relative humidity, carbon dioxide and particles concentration. A special procedure is proposed to simulate person movement and sliding door opening/closing. It is mainly based on the definition of specific source terms in the governing equations, assuming assigned values in the portions of computational domains where the solid objects are located at a chosen time. Exploiting an iterative cross-comparison of numerical results with experimental data carried out by a monitoring campaign in the studied OT, an innovative methodology is also presented to assess the number of particles, for a chosen class of diameter, released by the occupants to the environment. From our analyses some IAQ indexes were deduced, allowing monitoring the local and overall OT air quality level due to the ventilating system during real operational conditions.

Keywords: Operating Theatre; CFD; Moving Object; Air Quality, Particle Dispersion.

1. Introduction

The increasing development of computational fluids dynamics (CFD) in recent years have opened up the possibilities of a low-cost through real method for improving HVAC systems in the design phase, with fewer experiments required (1). High levels of IAQ in OT is an important issue to contribute in prevention of Surgical Site Infections (SSI). Despite of specific plant layouts are applied for OT ventilation (e.g. unidirectional flow), the effective use conditions can heavily modify the design microclimate and air quality levels. Medical staff presence and movements and sliding doors opening/closing can cause the compliance or not of some environmental parameters with national and international standards threshold values. Experimental measurements in the OT are usually expensive and invasive. In many countries they require complex procedures for legal authorization. CFD simulation can contribute in giving useful indications on proper indoor microclimate and IAQ conditions (2,3). Special efforts have been made by some authors to study different ventilation systems against resulting effectiveness in protecting the surgical site inside the OT (4,5,6). Some other studies investigate the air stream perturbations in OT induced by solid objects statically "plunged" in the forced flow. Other authors presented interesting results concerning the airflow and temperature distribution modifications connected to different surgical lamps shapes and locations (7). A comprehensive experimental and numerical analysis has been proposed by (8) concerning airflow and heat transfer inside an OT, taking into account all the medical staff standing up, operating bed, surgical lamps and equipment. Most of the above mentioned studies consider correct use on-design operational conditions for the outlined OTs. Few analyses have been proposed concerning the moving object effects on the airflow inside OTs (9,10). In the above papers the moving mesh approach is applied in order to manage the fluid-solid interface during transient simulations. An important investigation on the influence of movements on contaminant transport in OT has been proposed by (11). From a numerical point of view, an indirect approach, based on the consideration of distributed momentum sources, as well as a turbulent kinetic energy source, is applied for keeping into account the solid object movements by using fixed computational grids. In the present work we explain the fundamental numerical modeling methodology that was used in a recent research of the authors (12). Then, the airflow and climate in an existing OT, under "at rest" and actual use conditions, were investigated by numerical simulations. The "operational" conditions should be understood with faked

surgery, split into two use conditions respectively "correct operational" and "incorrect operational". Simulations were developed considering real events such as surgical staff movements through the door and walking inside the room, and sliding door opening/closing. We investigated the airflow and microclimatic parameter variations induced by the effective use conditions of the room. Then the impact of surgical staff on the indoor air quality was studied. An Euler-based approach was applied to solve the concentration fields of gaseous contaminant and small particles (up to 5 μm in diameter) in the indoor air. Existing databases generally refer to constant particle mass emission of a person as a function of his/her activity. At present, there are not many articles in the literature concerning numerical modelling in which the contaminant concentration for the IAQ analysis has been performed starting from sources of particle emission with a distribution dependent on particle diameter. There is also a lack of data concerning specific emission sources in terms of particles issued in time unit by people. Our investigation, widely explained in a recent work of the authors (13) was applied to estimate, by an iterative comparison between experimental data and numerical results, the emission rate of particles (differentiated by diameters) released by the occupants.

2. Use of COMSOL Multiphysics

COMSOL Multiphysics was applied to solve turbulent fluid-dynamical and thermal fields inside the OT. Air velocity distributions were then exploited as transport vector fields in solving some other passive-scalar equations, referring to the following microclimatic and IAQ variables, such as relative humidity, mean age of air, carbon dioxide concentration and particles concentration (for different particle diameter). The Reynolds Averaged Navier-Stokes and energy equations were considered as governing equations for fluid-dynamics and thermal analysis of the system. Under the assumptions of Newtonian fluid and uncompressible flow, applying a standard k-ε closure scheme, they read as follows:

$$\rho \frac{\partial \mathbf{U}}{\partial t} + \rho \left(\mathbf{U} \cdot \nabla \right) \mathbf{U} =$$
$$= \nabla \cdot \left[-p\mathbf{I} + \left(\mu + \mu_T \right) \left(\nabla \mathbf{U} + \left(\nabla \mathbf{U} \right)^{\mathrm{T}} \right) \right] + F \tag{1}$$

$$\nabla \cdot \mathbf{U} = 0 \tag{2}$$

$$\rho \frac{\partial k}{\partial t} + \rho \mathbf{U} \cdot \nabla k = \nabla \cdot \left[\left(\mu + \frac{\mu_T}{\sigma_k} \right) \nabla k \right] +$$
$$+ \frac{1}{2} \mu_T \left[\nabla \mathbf{U} + \left(\nabla \mathbf{U} \right)^{\mathrm{T}} \right]^2 - \rho \varepsilon \tag{3}$$

$$\rho \frac{\partial \varepsilon}{\partial t} + \rho \mathbf{U} \cdot \nabla \varepsilon = \nabla \cdot \left[\left(\mu + \frac{\mu_T}{\sigma_\varepsilon} \right) \nabla \varepsilon \right] +$$
$$+ \frac{1}{2} C_{\varepsilon 1} \frac{\varepsilon}{k} \mu_T \left[\nabla \mathbf{U} + \left(\nabla \mathbf{U} \right)^{\mathrm{T}} \right]^2 - \rho C_{\varepsilon 2} \frac{\varepsilon^2}{k} \tag{4}$$

$$\rho C_p \frac{\partial T}{\partial t} + \rho C_p \mathbf{U} \cdot \nabla T = \nabla \cdot \left(\lambda \nabla T \right) + Q \tag{5}$$

Further diffusion-convection equations were also considered in our model for computing the relative humidity, the mean age of air (it quantifies the average lifetime of air at a particular location), the CO_2 and particles concentration (depending on the diameter). Figure 1 shows the OT geometry. Some geometrical elements were used to simulate medical staff and the patient, lighting system and equipment. Two rectangular supply ceiling diffusers are located in the central zone of the ceiling: each of them provides a constant flow rate of fresh air. Two groups of 14 conical outgoing grilles are arranged over two smoothed corners of the room. For the "at rest" conditions, the values of the dependent variables at the ceiling diffusers, were assumed. Outflow conditions were considered at the recovery grids. At every solid/fluid interface, logarithmic wall functions were applied in the near wall flow, that was considered parallel to the wall and being in a wall offset equals one hundred viscous units. Turbulent production was assumed to equal dissipation at walls.

Movements of sliding door and one healthcare assistant were numerically simulated, to represent operational use conditions. In transient analyses, once the sliding door is opened, one assistant is expected to walk from the corridor

space inside the room, moving along the surgical table up to the patient's head, then turning around and leaving the room. The procedure adopted for simulating the "moving objects" inside the room was used in previous studies (14,15).
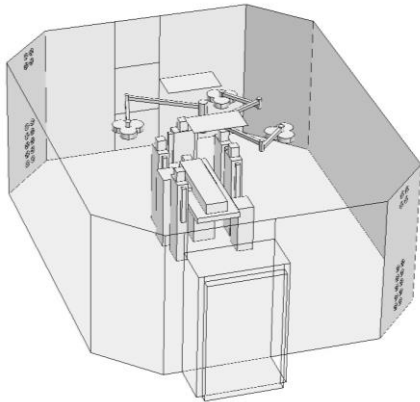

Figure 1. Geometry of the numerical model.

It is mainly based on the definition of specific source terms in the governing equations, assuming assigned values in the portions of the computational domains where the solid objects are located at a chosen time. Solid objects are not explicitly designed in the geometrical model because their movement is driven by assumed values 0 or 1 in specific logical functions during time. The binary value assumed by the logical functions depends on assigned geometrical coordinates for each object. In those regions fluid-dynamical properties and source terms assume specific values determining rest conditions for fluid. Time-dependent functions allow modification of the geometrical coordinates identifying the position of the "solid" objects during time, so that a prescribed motion law can be assigned to the moving objects. The procedure applied in order to characterize the portion of the domain wherein solid objects are located at a chosen time is presented below. Let us first consider the door. The following expressions were used to define its spatial coordinates:

```
x1_door=x10_door
x2_door=x20_door-dx(t)
y1_door=y10_door
y2_door=y20_door
z1_door=z10_door
z2_door=z20_door
```

A graphic representation is given in Figure 2 to better elucidate the meaning of the above reported expressions. In this figure the solid objects (door outlined in pink and person in blue) are geometrically represented only for clarity, these geometries not really being outlined in the numerical models used for computations. The above expressions assume constant or variable values in time. The time-function `dx(t)` denotes the motion law assigned to the door in the x direction. When `dx` assumes the value "0" the door is closed, otherwise, when the assumed value is "1.4" the door is completely open (the door width being 1.4 meter).
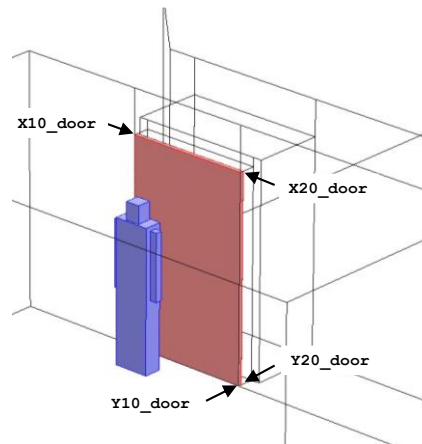
Figure 2. Graphic representation of expressions used to define positions of the "solid objects".

The following logical functions were defined in order to identify the coordinates' range, along each axis, identifying the door position:

```
x_door=if((x>x1_door)and(x<x2_door))then
1 else 0
y_door=if((y>y1_door)and(y<y2_door))then
1 else 0
z_door=if((z>z1_door)and(z<z2_door))then
1 else 0
```

Position of the solid object "door" analytically corresponds to value "1" assumed by the following expression:

```
door=x_door*y_door*z_door
```

The same procedure is applied for defining position of the other "solid objects" (head, harms and body for person) during time. In this case, a

second motion law (`dy(t)`) is defined to simulate the person movements along the y-direction throughout the free door-space once the door is open. Time evolution of the functions applied to define the "solid objects" movements are graphically reported in Figure 3.
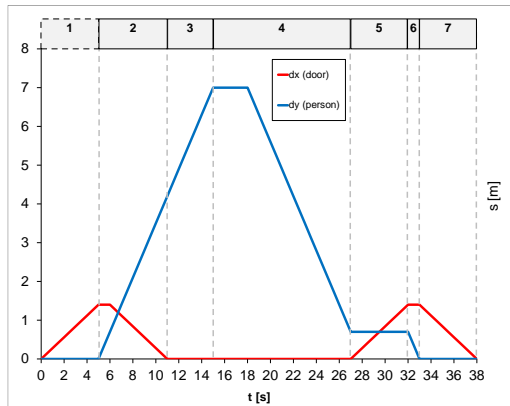
Figure 3. Graphic representation of expressions used to define positions of the "solid objects".

Due to its formulation, the present numerical procedure can be applied to prismatic solid objects only. Once the solid object position is defined during time, some further functions could be used for assigning physical properties to these portions of the numerical domain, as given below:

```
eta_dom=if((door>0)or(person>0)) then
eta_solid else eta_fluid

rho_dom=if((door>0)or(person>0)) then
rho_solid else rho_fluid

k_dom =if((door>0)or(person>0))then
k_solid else k_fluid

Cp_dom=if((door>0)or(person>0))then
Cp_solid else Cp_fluid
```

where expressions `person` relate to medical assistant entering and walking into the OT. In analogy with expression `door` used for the door, they identify the person position where their value is "1". It should be noticed that this procedure makes it possible to use average values of the physical properties for all the solid objects only. This does not represent an inconvenience for viscosity in the momentum equations, as its value is chosen arbitrarily high (1E+5) in order to contribute to motion enabling.

Therefore, some special source terms were implemented in the governing equations. In order to enable motion in the solid objects, we defined:

```
S_dom=if(P>0) then 0 else 1
Fx_dom=(C*(1-S_dom)^2)/(S_dom^3+ES)*u
Fy_dom=(C*(1-S_dom)^2)/(S_dom^3+ES)*v
Fz_dom=(C*(1-S_dom)^2)/(S_dom^3+ES)*w+(1-
person)*Fg
```

where C=1.6E+6 and ES=1E-4 are constant values. Note that `Fx_dom` and `Fy_dom` become null where `S_dom`=1 (volume of fluid), while `Fz_dom` corresponds to the buoyancy force. In order to enable thermal transport in solids, in the energy equation we defined the components of thermal transport vector as follows (door as example):

```
u_dom = if(door>0) then 0 else u
v_dom = if(door>0) then 0 else v
w_dom= if(door>0) then 0 else w
```

where u, v, w are the components of the velocity vector. Finally, we considered the following source term in the energy equation for considering the metabolic heat:

```
Q_dom = if(P>0) then Q else 0
```

Computational domain representing the corridor was kept into account only for simulations involving the opening/closing of the sliding door (incorrect use conditions). In this case, open boundary conditions were considered at the corridor transversal section. In thermal analysis, we applied a convective thermal flux at walls, considering a constant temperature for adjacent rooms. Insulation conditions were applied at solid/fluid interfaces for all other dependent variables that were solved. In the "at rest" conditions, we only considered the lamps as internal sources of sensible heat. Otherwise, in operational "correct use" conditions, internal heat sources were related to the medical staff and patient presence, their thermal load being both sensible and latent. Other boundary conditions did not change from operational "correct use" to "incorrect use" conditions. As pointed-out, interfaces between moving object and surrounding environment are in fact "fictitious", the moving objects not being bounded by additional geometrical boundaries. Internal heat and vapor sources were unchanged in values, except for the additional load due to the walking

healthcare assistant, whose location was variable in accordance with the moving object position during time.

The occupants contribution for particle emission rate was applied as a boundary flux at the occupants / surrounding air interfaces. The procedure adopted to assess the particulate flux depending on the particle dimension is explained in (13) can be summarized as follows: we evaluated particle emission due to each occupant, differentiated for diameter dimension, exploiting the experimental acquisitions of particle concentration in the real OT with and without patient and medical staff presence. Then, we combined the available experimental data with results coming out from numerical simulations to assess the emission rate of particles per person assessing distribution of emission rate by occupants as a function of particle dimensions.

4. Results

Some results obtained by simulations are presented in this section. Distribution of velocity magnitude in the operational zone is significantly modified from the "at rest" towards both the "operational conditions". The velocity profiles along x (y=8; z=1.5) direction is reported for the different room conditions in Figure 4. The "incorrect use conditions" refer to the time instant when the door is completely closed and the medical assistant walks through the room, until he reaches the top of the operating table. In these diagrams zero values represent the "imprint" of a fixed object/person or moving person standing in that location for the considered instant. Velocity profiles underline air flow patterns modifications due to the operational conditions. The air flow in the surgical zone is strongly modified by the medical staff presence: important differences are shown with the gap between green line and black/red lines in the figure. The effect due to the person movements on the airflow patterns in the surgical zone, appears less important. Velocity profiles show variable trends and high curve slopes in every cases, that is particularly important when the efficacy of "unidirectional" airflow is discussed for similar applications. The effect of sliding door opening/closing during the "incorrect operational conditions" is now discussed. Figure 5 provides the air velocity field

on a horizontal plane (z=1.5) for the simulated condition when the medical assistant is walking and the sliding door is shutting behind his back.
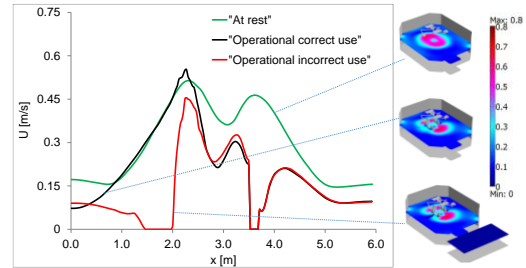
Figure 4. Velocity profiles along the x-direction for the different analyzed use conditions of the OT. In the right side, a slice of the velocity field is reported for each condition.

The picture shows the air velocity vector distribution for the zone close to the sliding door and velocity field variation. As a consequence, it was expected that an important rate of air outflows the room. In fact, a total amount of 16.3 m^3 of air outflows toward the corridor during the simulated condition of door opening/person crossing/door closing.
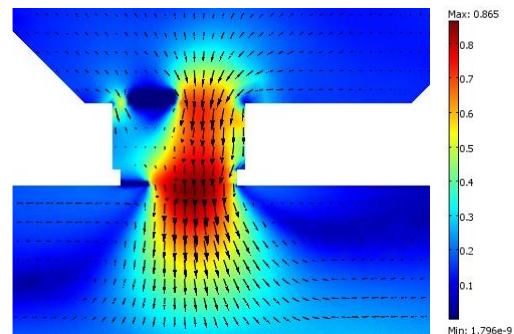
Figure 5. Velocity field and velocity vector in a horizontal slice in proximity of the sliding door, during sliding door closing and medical assistant walking inside the OT.

Figure 6 provides the airflow rate (blue line) outgoing the OT during the door opening. The door opening effect on the average pressure level inside the OT was also investigated. Figure 6 also shows the average pressure trend as a function of time (red line), during the phase of door opening: a significant pressure decrease can be gathered from plotted data. Therefore, the overpressure variation due to an "unforeseen

event" occurring during an "incorrect use condition" can determinate a temporary not compliance of the pressure scheme with the limits suggested by the present standards.
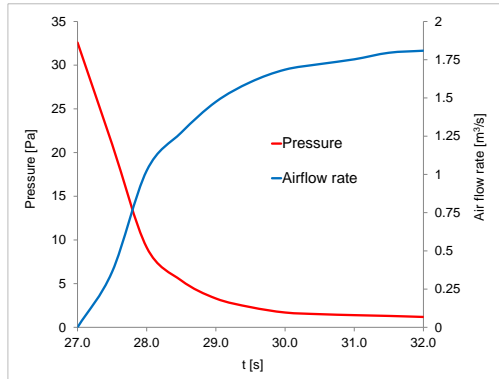

Figure 6. Time evolution of the OT pressure and the out coming airflow rate, during the sliding door opening.

The influence of OT use conditions on indoor thermal variations was analysed also. We observed an evident temperature variation in the "correct operational" condition compared with the empty room characterized by almost isotherm condition inside the OT. The additional thermal load due to the walking person, produces a further local temperature increase. Anyway, in the operating zone thermal levels remain very close to the design value despite of different use conditions. Analyzing the relative humidity results, it was detected that vapor production, due to the persons presence, produces an air moisture content that is not well balanced by the incoming air at the considered hygrometric conditions. The mean value computed all over the room is 67.8%, that exceeds any maximum threshold advised by all the standards. It can be noticed an increasing level of the moisture content at the back of the operating zone. This could be due to lacking ventilation all over the room that can determinate stagnation zones.

Concerning the IAQ, once the CO_2 concentration was solved and the particles emission rate per person were assessed for each diameter considered (Table 1), we had data for deriving some widely used local and global IAQ indexes. As an instance, Figure 7 shows the Ventilation Effectiveness (VE) computed for CO_2 in different OT zones. The VE index measures how quickly a contaminant is removed

from an air volume by quantifying the efficiency with which the internal pollutant is diluted or removed. It clearly depends on the airflow patterns.

	VE (CO2)
■ Breathing zone	88.80%
■ Occupied zone	92.16%
■ Total volume	98.85%
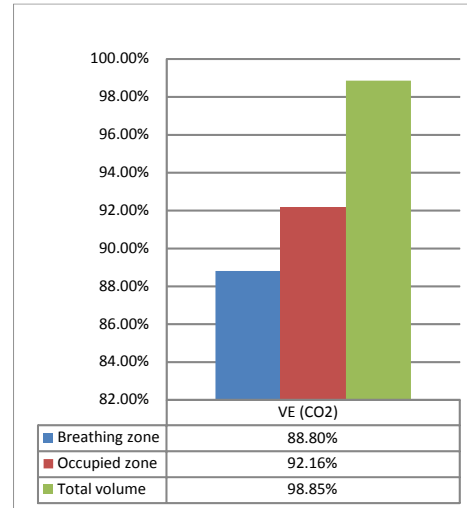
Figure 7. VE computed for CO_2 in different OT zones.

	Metabolic heat		
	Sensible	Latent	Total
	[W]	[W]	[W]
Medical staff	73.3	58.6	131.9
Patient	65.9	30.7	96.6
	Breathing		
	Airflow rate	CO2 emission rate	
	[m3/h]	[m3/h]	
Medical staff	2.0	0.080	
Patient	0.3	0.012	
	Particles emission rate		
	Particles diameter		
	0.4	0.75	3
	[μm]	[μm]	[μm]
Medical staff	1.01E+05	2.94E+04	1.36E+04

Table 1. Source terms adopted in numerical models for simulating the medical staff and patient presence inside the OT.

5. Conclusions

A numerical analysis on the airflows, heat transfer and contaminant diffusion in a real OT is presented in this paper. Our investigation provides, through quantitative parameters comparison, the influence of unforeseen movements of chirurgical/medical staff and the sliding door opening and closing phases on air temperature distribution, velocity field and air flow displacement but also on particles and CO_2 dispersion. Different scenarios were considered,

then measured and simulated, representative of the "at rest" and "operational/effective use" conditions. The COMSOL models provided the possibility for checking, during operational conditions of the studied OT, the ventilation efficiency and indoor air quality levels.

6. References

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7. Acknowledgements