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CFD SIMULATIONS OF POLLUTANT SPATIAL DISTRIBUTION IN A LARGE OFFICE

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Abstract: Computational Fluid Dynamics (CFD) is applied to analyse the flow and the concentration patterns of floor-emitted pollutants inside a mechanically ventilated office of simple geometry. The simulation results show complex airflow and high heterogeneity of concentration distribution. Alternative scenarios mainly of the vents' position and airflow strength are also examined and reliability issues are discussed. Studies like this contribute to the determination of the parameters that influence the modelling results and prepare the ground for improved and more reliable future simulations of indoor pollutant dispersion.

Key words: CFD, indoor air pollution, ventilation optimization, simulation reliability, ADREA

INTRODUCTION

Scientific interest on indoor air pollution increases, since modern people mainly live indoors and several equipment and construction materials provide additional pollution sources. While at external atmospheric flows common practices have more or less been developed and best practice advices are available, this is not the case with indoor flows. At buildings' interiors, basic CFD research is not that frequent and most studies attempt to solve a particular practical problem. Thus it is not clear enough which physical and numerical parameters affect the modelling results and this obstructs reliable simulations.

In this study the pollutant distribution in a large office of Athens is investigated using CFD and it is shown that concentrations can vary significantly among various working positions. This fact justifies the attempt to examine some influencing physical/modelling parameters like the geometry and the mass flow, but also the grid and the inlet conditions.

The specific office is chosen because it was examined in the past as the "GR22" case of the European collaborative project "OFFICAIR" (Sakellaris et al., 2016) and both experimental measurements and CFD results from a commercial code were available. No pollutant concentrations were measured, while for the CFD studies the whole floor was supposed to emit. The office dimensions are: 22.26 m (length – Y axis) x 7.80 m (width – X axis) x 2.54 m (height – Z axis). The office has nine windows facing outdoors and four doors (fig. 1a). On the ceiling there are seven air inlets and six air outlets related to the mechanical ventilation. The inflow/ outflow rates from the vents were measured explicitly (fig. 1b), while from the doors and windows they were modelled using the COMIS model and given as input to CFD.

METHODOLOGY

The current CFD investigations are performed using the ADREA-HF code. Mainly the RANS (Reynolds-Averaged Navier-Stokes) methodology is used for the simulations, but also a preliminary LES (Large Eddy Simulation) is tested. The geometry of walls and openings is reproduced using EDes (fig. 1c), the ADREA-HF geometrical pre-processor. The flow domain does not extend outdoors and furniture is initially ignored. The inflow/ outflow rates are chosen to be the same as in the actual "GR22" case. A 10 cm gap exists around each door and window in order to define the relevant outflows. Walls are treated as slightly rough (z_0 =0.001m), having the measured temperatures for the case the energy equation is solved. No-slip condition and rough wall functions are used for the solid surfaces. The standard *k*- ε model is used for the turbulence modelling. The pressure and velocity equations are decoupled with the use of the ADREA/SIMPLER algorithm. The upwind numerical scheme is used for the convection terms (central differences for LES) and the fully implicit first order for the time advancement (second order Crank-Nicolson for LES). The flow is treated as transient, with a time step restriction through the maximum CFL that is limited to the value of 0.5. Simulation is stopped at 14000 s, after the errors have dropped many orders of magnitude. The OpenMP-parallel version of the code is used, with the BiCGstab solver.

PC simulations' time is some hours for the normal grid (60060 cells) and few days for the fine one (493276 cells). Several other scenarios/ cases were examined, included in table 1. In all cases the passive pollutant is emitted uniformly from the floor and concentrations are presented non-dimensionalized with the same global average theoretical in-room concentration C_{av} that the office would have in case of full homogeneous commixture. Due to no uniform flow, actual $C_{av,act}$ differs depending on the case examined (slightly higher at cases 1, 2, 9, 10 and 11 and slightly lower at the rest of the cases). The air change rate is always 3.5 changes per hour. Twelve specific working positions are considered and 'sensors' (white spheres of fig. 4) are placed at the nose level at those positions in order to monitor the concentrations. Sensors are placed at 1.6 and 6.2 m of X axis, at 2.6, 6, 9.4, 12.8, 16.2, 19.6 m of Y axis, at Z=1.1 m.



Figure 1. Office plan (a), ventilation data (b) and geometrical representation at EDes (c)

RESULTS AND DISCUSSION

Base case

In general, the inlet flow from the roof vents, even weak, makes its way to the floor, where it impinges and spreads horizontally (fig. 2a). Depending on the position of the outlet vents and the neighbouring walls, full-height recirculations may be formed (fig. 2c). The flow is more complex between the areas of influence of the vents and close to the solid boundaries. Complicated three-dimensional flow patterns are formed in the whole office (fig. 2d). For example streamtrace 3 (fig. 2d) starts from inlet vent number 11, follows a complex route towards wall 2 at the back of the room, comes again to the front, tracks a full-height recirculation and exits from the last window's gap. The flow is believed to actually be unsteady, especially where flow fronts collide. As expected, the concentration distribution depends heavily on the flow field and varies throughout the office, presenting high non-uniformity. C/C_{av} has values from nearly zero at the inlets till four (4) at some places close to the junction of the floor with wall 2. One employee can have almost 3 times higher exposure than another (table 1, fig. 3). Generally the sensors close to the front wall (the one with the windows) have lower concentrations (fig. 3), especially sensor 7 that is almost bellow an inlet vent with strong flow. Different working positions' places (sensors) were also examined. While a small change at the height had insignificant influence to the concentration values, a displacement of 1 m towards the walls/ centre resulted in about 8% higher/ 15% lower average concentrations.

Influence of physical parameters – alternative scenarios

Alternative scenarios (additional cases 2 to 6, explained at table 1) were studied in order not only to examine how could the ventilation be improved, but also to see the influence of various physical

parameters to the modelling results. At table 1 the average, minimum, maximum and max/min values of C/C_{av} of the sensors is presented for each case. Keeping the same vent layout and just making the flow more uniform (case 2) gives the same average at the twelve positions, but the uniformity (ratio max/min) is improved. The fact that higher concentrations are close to wall 2, along with the fact that vents are far from that wall, makes us examine the scenario of vents being 60 cm closer to wall 2 (case 3), with same flows' strength as in the base case. That gives a 10% improvement in the average concentration. At case 4 the same geometry as in the base case is kept, but the vents from which the flow enters the room are changed: the inlet vents are all at the side of wall 2 (which is the 'problematic area' – see also fig. 4). In this case there is a 20% average improvement, but no improvement at uniformity.



Figure 2. Results for the base case. (a), (b): Velocity vectors at bottom and top planes. (c): Fluid flow and concentrations at 8 in-room surfaces. (d): 0.02 m/s velocity magnitude isosurface along with 3 streamtraces

Table 1. The cases examined and the ma	in results of the conce	intrations at the sensors	' positions
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Case	C/C _{av} at the 12 sensors:	Average	min	max	max/min
1 – BASE		1.18	0.69	1.97	2.85
2 – Uniform inflow rate at vents		1.18	0.76	1.78	2.34
3 – Wall 2 vents 60cm closer to wall 2		1.05	0.69	1.74	2.51
4 - Other inlets/outlets (uniform inlets/ at	wall 2 side)	0.95	0.53	1.53	2.89
5 - New vents design (inlet from the side	walls)	0.42	0.29	0.67	2.33
6 – New vents design (inlet from center)		1.14	0.94	1.28	1.36
7 – Base case with 12 desks		1.01	0.43	1.58	3.68
8 – Base case with 12 desks and 12 "people"		0.99	0.42	1.64	3.91
9 – Fine grid		1.16	0.65	1.88	2.88
10 – Given T at inlets – energy equation also		1.18	0.62	1.99	3.20
11 - Given k at inlets		1.14	0.70	1.57	2.25
12 – Preliminary LES		0.87	0.57	1.26	2.23



At case 5 the vent geometry is redesigned. Two rows of inlet vents are placed close to the side walls (see fig. 4), almost above of the working positions. Thus the employees receive fresh air directly and the average concentration at the sensors is 3 times lower (table 1). This is a serious improvement and explains why the concept of "personalized ventilation" has attracted so much interest. Case 6 has the same geometry as that of case 5, but the inlet/ outlet vents are interchanged: the flow enters from the centre. The employees' exposure in this case is much more uniform, but average C/C_{av} is almost the same as that of case 1. At fig. 4 though, it is noticed that at case 6 with a small shift of the working positions towards the blue oval areas, we can achieve an average concentration of about 0.75 (35% improvement). The uniformity of case 6 and the low concentrations of case 5 are also seen at fig. 3, which presents the persensor C/C_{av} for the 6 alternative scenarios. Sensors 1-6, which are close to wall 2, have lower values in case 5 than sensors 7-12, in contrast to case 1 (figs. 3, 4). From fig. 4, which contains much concise information, it can be noticed that cases 5 and 6 present less complex flow.



Figure 4. C/C_{av} contours plotted at the sensors' level (z=1.1m) along with the sensors (in white) for all the 12 cases examined. Blue areas have concentrations below the global in-room theoretical average C_{av} . Also the vents (orange: inflow, grey: outflow), the tangential velocity vectors and the W=0 iso-lines are presented.

Influence of simulation parameters – reliability issues

Concerning the velocity field, the specific problem examined has the characteristic of very low velocities. In such cases the accurate calculation of the flow is a tricky task, since very small absolute deviations can result in big relative differences, locally dissimilar flow patterns and even higher divergence at concentration values. In order to see the sensitivity of the results to some additional parameters that might affect the flow field, six more cases are examined (table 1, cases 7-12). Cases 7 and 8 consider the influence of the detail of the in-room geometry representation, by adding desks and employees. The rest four cases are: Finer grid case 9 (almost 10 times more cells), non-isothermal case 10, case 11 with given (uniform) turbulent kinetic energy at inlets and an LES instead of RANS case.

Cases 7 and 8, reveal that the heterogeneity of concentrations is highly increased as we add in-room geometrical objects (table 1, fig. 4). The local flow and concentration patterns can change substantially around various solid items. For example, the desk that corresponds to sensor 7 is just below the vent number 11. As a result the fresh air spreads above the desk and keeps the values of sensor 7 very low.

About cases 9 to 12, the closer their results are to the base case, the better it is for the modeller, since the simulation would me more insensitive to the modelling parameters and more robust. Present results (fig. 4) show that while the general flow and concentration patterns are maintained, the differences at the sensors are not always small. Table 1 shows that the average concentrations at the sensors are preserved at cases 9, 10, they start dropping at case 11 and drop a lot at the preliminary LES case. It is noted though that at the LES case the whole-room average concentration drops. Concerning the values at the sensors' positions, concentrations up to 50% higher or lower can be observed at specific sensors, compared to case 1. The differences are higher especially at sensors 2 and 3 for all the four additional simulations (while at

most of the other sensors differences are comparatively low). A better look at fig. 4 reveals that sensors 2 and 3 are close to vortex-centres, which are not at exactly the same place across the simulations. Analysis of the time-series of velocity U at the specific points from the LES simulation reveals slightly bimodal probability density function distribution at sensor 2 and slightly skewed at sensor 3 (while it is Gaussian at the other sensors). This means that there is no unique solution of the flow field, as RANS assumes: the flow is unsteady. This could explain the different behaviour of RANS simulations for (even slightly) different simulation parameters. It should be noted that unsteadiness at one point could theoretically result in unsteadiness at most of the flow field in RANS simulations in a confined space. This could explain why some sensors' values oscillate at various RANS cases examined.

An additional issue is that at a specific place the flow field may be the same at two particular simulations, but the concentrations may differ due to transfer of pollutant from other places (where the velocity field might be slightly different). In case of sensor 2, this is probably the main reason concentrations between runs are different: in some cases clean-air flow towards wall 2 that passes from sensor 2 is stronger/ cleaner and thus concentrations there drop. Further examination is not an easy task: the flow is too complicated to try to find the causes for a specific behaviour and differences between the cases. Simpler cases should be examined in order to facilitate such tasks.

Concerning the turbulent kinetic energy k, even if a high value is given at the inlets (constant throughout each inlet), the physical production of turbulence at the corners of the inlet vents is deteriorated and the k field is more unphysical. The problem is more critical at LES. An improvement to this might be the extension of the flow field by including part of the duct geometry of the ventilation system.

CONCLUSIONS

Personal exposure at large offices can present high heterogeneity. In the specific case examined max/min concentration at the working positions can be up to 4, if in-room geometry is taken into account. CFD can help in determining the best working positions for a specific ventilation layout and, even better, in designing improved ventilation systems. For example, in this case, vents almost above the working positions with exits at the centre, decrease the average concentrations by a factor of three. Concerning the parametric studies, apart from the obvious parameters of source strength and position and air refresh rate (that are kept the same throughout this study) the most influencing physical/ simulation parameters from those examined that should be taken into account when performing indoor modelling are: geometry/ layout/ strength distribution of vents, in-room geometry, choice of RANS vs. LES (LES is tricky at the boundary conditions and needs orders of magnitude more simulation time), boundary conditions, selection of isothermal/ non-isothermal (needs more input data) case, selection of grid.

The unsteadiness of the flow seems to be a serious problem concerning the reliability of indoor CFD runs. Actually, as seen from this study, indoor CFD results can occasionally be questionable, especially at tricky points of the flow field. For the future it is suggested to build some kind of validation database for indoor simulations: Some basic, very simple cases should be defined (of ventilation, cross-ventilation etc) and thoroughly examined both experimentally and numerically (with RANS and especially with LES). Thus basic flow features and influencing parameters will be made clear for some typical indoor problems. Those cases could be validation cases for future studies. Then, best practice advices could be formulated for indoor simulations and even if CFD (especially RANS) is proven not being able to reproduce all physical flow/ dispersion details, we will know to some extend its limitations and the cases it might fail.

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