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A validation process for CFD use in building physics – study of contaminant dispersion.

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Abstract

Growing interests in environmental concerns oblige building engineers to develop new approaches and to get used to new skills. Among them, Computational Fluid Dynamics (CFD) holds more and more importance. This technique can help to improve the comfort of the occupants but also to predict very early building energy performance. Moreover, it is possible to study the quality of the air. This last point will greatly help building engineers to improve sanitary conditions in various cases such as hospitals, clean rooms or even in classical buildings. However, this approach is still new and need to be validated. Indeed, CFD is still new in the frame of building physics. This paper aims to prove the ability of CFD to predict accurately contaminant dispersion and to demonstrate the breakthroughs that CFD can bring in the near future.

1 Introduction

As a large part of energy consumptions is due to buildings (heating, ventilation, etc.), scientists are urged to develop new tools for architects and building engineers. Among them, Computational Fluid Dynamics (CFD) applied to building physics is in gestation for decades (Chen and Jiang [1]). This approach, first developed for aerospace applications, is now getting mature and will improve dramatically airflow description in buildings. This implies major breakthroughs in Internal Air Quality (IAQ) prediction, building energy efficiency and occupants' comfort.

Unfortunately, CFD is still new and needs to be validated. In the frame of a validation process already constituted of 7 different cases, this paper intends to address the contaminant dispersion problematic. Indeed, this topic constitutes one of the most interesting openings for CFD in building physics. It could modify deeply the design process concerning hospitals, museum, clean rooms or industrial premises.

2 Context

CFD have already been validated on several cases by different authors. Until now, in most of the cases, these papers focused on one case without tackling this problematic with a global point of view. For this reason, Barbason et al. [2] and Barbason and Reiter [3] have created a validation process based on a holistic approach. It aimed to select a narrow number of cases which cover most of the typical applications in building physics and which can be found easily in the scientific literature and reproduced by new operators. The validation process is decomposed in two main themes: the encountered physical phenomena and the different geometry scales implied in building physics.

The first axis is made up of four cases: a free float case, a mechanical ventilation case, a natural ventilation case and a radiation case. The second axis is also composed of four cases: a single room, a partitioned building, an open-floor building and a glazed atrium.

Every case of this validation process is based on experimental data available in the scientific literature. Thus, the operator can compare its numerical results to in-situ measurements and judge the quality of its simulations. Moreover, as this validation process covers various applications, it could be used also as a tool for new user to get use to the different approaches to adopt in function of the configuration.

However, a contaminant dispersion case was not included in the first version of this validation process. Indeed, this parameter is secondary in comparison with the description of the airflow and the air temperature field for residential and office buildings. So, it was logical to focus first on these aspects and to assess the ability of CFD to describe the different physical phenomena involved in building physics.

The contaminant dispersion topic has already been covered in numerous papers. For example, several papers tackled the problematic of the quality of the air in hospitals: Chow and Yang [4] have described the airflow inside an operating room while Méndez et al. [5] and Mazumdar et al. [6] have studied the patient's comfort inside their rooms. An other problematic concerns the sanitary conditions in clean rooms which could also be improved drastically thanks to CFD (Rouaud and Havet [7]).

Unfortunately, every case quoted above was only studied with a CFD approach. There was no comparison with experimental data. Thus, it is not possible to conclude anything related to the validity of the CFD.

This paper intends to introduce two new cases in the frame of the validation process to assess the quality of the results obtained with a CFD approach. It will also permit to the operator to know more precisely the incertitude range of such approach.

3 Method

Two cases will be described in details according to a procedure described by Chen and Srebric [8]. These authors have imagined a procedure to report CFD results in building physics. It should be done in three steps. The first one is called the verification and is mainly intended for code developers. Indeed, it aims to ensure the ability of CFD to produce results in this context. For this reason, this step will be skipped. The second one is called the validation and intends to describe every parameters used to help every new operator to reproduce the simulation. Eventually, the last step is the results report. It should be approached first qualitatively. Indeed, lots of information can be obtained directly by studying the airflow and the air temperature field. Then, a quantitative approach is required to assess the quality of the results and to know the incertitude range of the results. Eventually, the secondary variables, such as the contaminant dispersion, the age of the air of the turbulent kinetic energy can be studied in details.

For this paper, the first studied case comes from the work of Yuan et al. [9]. It has the same configuration than the free float case of the complete validation process. If the operator has already computed the airflow and the air temperature field, the contaminant dispersion is an easy parameter to describe. For this reason, this case was chosen as the first case. The second one is based on the study of Yang et al. [10]. The type of configuration is the same (a displacement ventilation in a single room) but it includes a detailed manikin. So, this case makes also the operator aware of the human description and the interaction between a body and its surroundings.

Eventually, it should be noted that these numerical studies were realized with Fluent (Ansys Inc. [12]) which is the world leading CFD software.

4 Case 1

4.1 Geometrical description

The experimental room dimensions are 5.16 x 3.65 x 2.43 m (length x width x height). It is composed of two computers, two basic manikins, six fluorescent lamps, a displacement ventilation and classical office furniture. The experimental room is linked to a control room by a 3.45 x 1.27 m window. The other walls, the floor and the ceiling have a same composition.

Figure 1 illustrates the geometrical configuration while every dimension is given in Chen and Srebric [8].

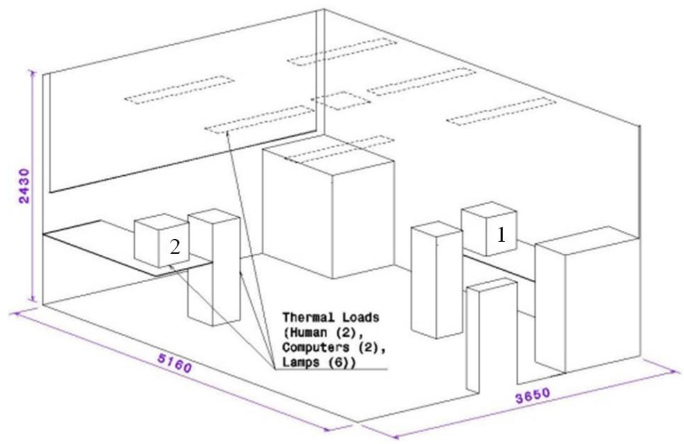


Figure 1. Free Float Case – Geometrical configuration (Yuan et al. [9])

4.2 Experimental description

The airflow rate was 4 ACH (Air Changes per Hour) which corresponds to an incoming air velocity of 0.09 m/s. The supply air temperature was 17°C while the measured exhaust air temperature was 26.7°C.

The heat released by the fluorescent lamp is 34 W per item. Every occupant releases 75 W while the computers 1 and 2 (cfr Figure 1) emit respectively 108.5 W and 173.4 W.

Concerning the wall properties, the thermal conductivity of every wall was 0.189 W/(m².K) except for the window which was 3.704 W/(m².K). Wall temperatures are also given. Unfortunately, it is known inside a range. The range and the chosen temperature for the CFD simulation are given in Table 1.

	Wall temperature range	**CFD temperature**
Floor	23.3°C – 26°C	23.3°C near the DV / 23.85°C faraway
Window	27.3°C – 28.1°C	27.7°C
Wall below the window	24.2°C – 26.6°C	25.4°C
Other Wall	23.3°C – 26°C	24.35°C
Ceiling	23.3°C – 26°C	25.85°C

Table 1: Wall temperature ranges

Air temperature and the mean velocity were measured during the experiment. However, it should be noted that the error on the air temperature is ±0.04°C. The repeatability on the air velocity measurements is 0.01m/s or 2% of the measurement. Moreover, when the magnitude is lower than 0.10m/s, the value cannot be considered as reliable.

Concerning the contaminant dispersion, a tracer gas (sulfur hexafluoride - SF_6) was used to simulate the CO_2 emitted by the two occupants. The rate of release was 40ml/h for each manikin-boxes. This value is very small but sufficient because the natural concentration of SF_6 in the air is very low. It should be noted that the incertitude range of the sensors is more or less 10% of the measured value.

4.3 Turbulence model

The Shear-Stress Transport k-ω approach was used to model the turbulence (Menter [11]). This approach gives satisfactory results in building physics (Barbason and Reiter [3]). It belongs to the Reynolds Averaged Navier-Stokes approach. However, it is important to understand that the choice of the turbulence model is always a matter of compromise. Indeed, some approaches could be more precise but requires much more computing time and resources. It should be noted that this turbulence model includes a low-Reynolds correction to take into account the interaction between the flow and the walls.

4.4 Boundary conditions

A uniform profile for the inlet conditions was imposed. This approach introduces errors but their importance decreases with the distance to the diffuser (Chen and Srebric [8]).

Concerning the heat emission, only the total amount of heat (radiative and convective part) is known. The ratio between these two transfer modes could be estimated but it would bring supplementary errors. Consequently, all the heat transfer was supposed to be done by convection. It was supposed to be uniformly distributed on the two manikins and the two computers. Again, it brings errors but one can assume that the sum of all these errors remains small in comparison with the expected precision.

Eventually, concerning the exhaust, a zero pressure boundary condition was used.

4.5 Numerical methods

CFD codes discretize the differential equations of Navier-Stokes by a finite volume method. The discretization of the pressure-velocity coupling was made with an algorithm called SIMPLEC. Gradients were discretized in accordance with a Green-Gauss cell-based method and every parameter respected a QUICK algorithm for their own discretization. These parameters were chosen to have a good compromise between accuracy and resources needs.

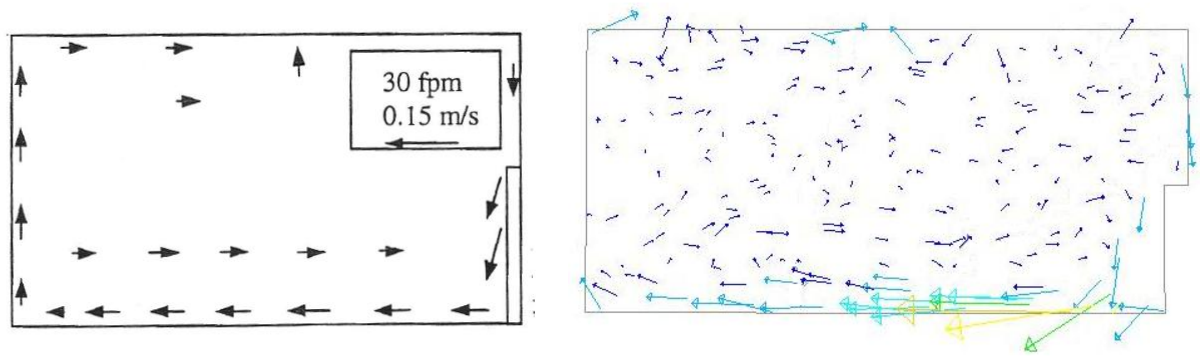
Concerning the convergence criterion, default criteria of Fluent (ANSYS Inc. [12]) are used. For every variable of the air flow, the sum of the imbalance in every cell should be inferior to 0.1% of a value representative of the flux of this variable. In this case, it is easy to evaluate the representative value. Indeed, it depends directly on the boundary condition at the inlet.

Concerning the time discretization, a false time-step of 0.5s was adopted. Indeed, Cook and Lomas [13] have proven that a false time-stepping approach permits to have better results in a smaller computing time.

At last, a tetrahedral mesh was used for convenient reason. Its size was 422 544 cells. A grid dependence study was performed to ensure that results would not evolve if the mesh was coarser. The difference in terms of quality was not significant.

4.6 Results

According to Chen and Srebric [8], it is important to have both a qualitative and a quantitative point of view to assess the quality of the results.



(a) (b)

Figure 2. Comparison of the airflow pattern observed by using smoke visualization and CFD - a) Experimental results (Yuan et al. [9]) - b) Numerical results

The Figure 2.a represents the results of an airflow visualization obtained experimentally with smoke in the central plane (Yuan et al. [9]). It permits to have access to the description of the airflow patterns inside the room. Results show that the airflow coming from the displacement ventilation goes straight away to the floor until it reaches the opposite wall. Then, the airflow, heated by the wall and the loads, goes upward. When it reaches around 50cm, the airflow splits in two components. The first part continues to go upward until the ceiling where it finally reaches the exhaust. The second part is redirected horizontally toward the displacement ventilation where it closes an other air loop.

These phenomena can also be observed at Figure 2.b. One of the main advantages of CFD is the detailed description of the airflow. Indeed, it is possible to describe precisely the different recirculation loop inside the room. As it can been seen, they are numerous in the upper part of the room where the heat loads create a strong natural convection.

The second step of the qualitative analysis concerns the air temperature field in the central plane. Displacement ventilation generally creates a strongly stratified configuration. This phenomenon can be evaluated precisely thanks to CFD. The Figure 3 proves that, in the current configuration, there is a 5°C difference between the floor and the ceiling level. These results seem correct and can now be compared to the experimental data.

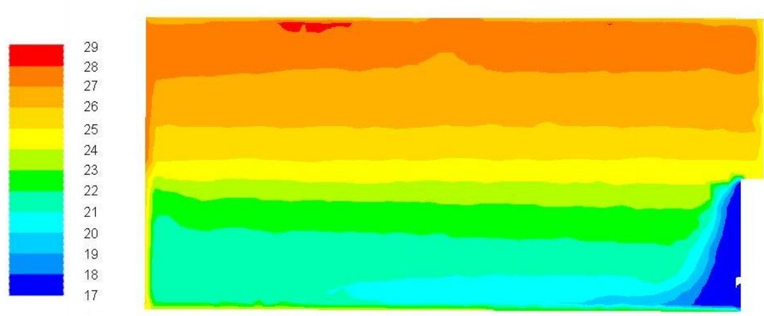


Figure 3. Air temperature repartition obtained thanks to CFD.

The experimental data were collected thanks to 9 columns composed of 9 temperature sensors, 6 anemometers and 6 SF_6 sensors. In sake of clarity, only the results of three columns (2 to 4) will be presented. These columns correspond to the central part of the room between the two manikins. The quality of the results of the other columns is similar (Barbason et al. [2]).

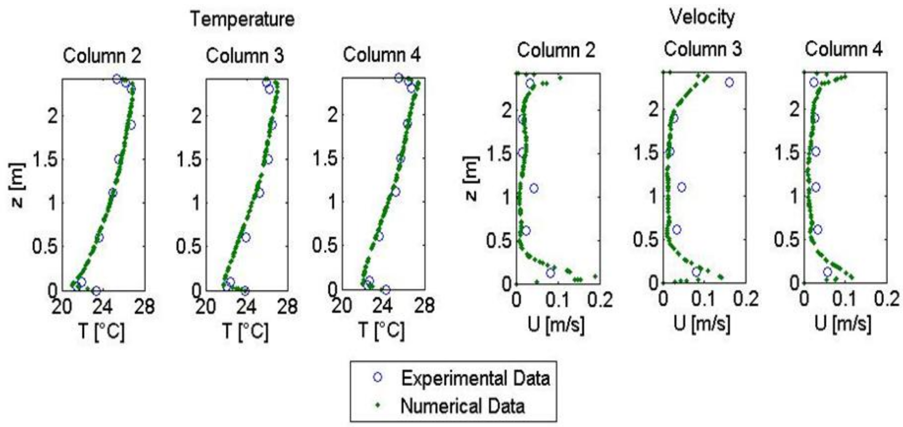


Figure 4. Air temperature and air velocity measured and computed results.

The Figure 4 shows that the results obtained for the air temperature and velocity by the numerical approach fit the experimental data. The agreement is very good. The mean error between numerical and experimental data concerning the air temperature is less than 0.4°C. It proves the ability of CFD to describe precisely this case. It is also interesting to see that the thermal gradient is well described.

Concerning the air velocity, first, it should be noticed that the air velocity is generally inferior to the 0.10m/s and so the experimental results could be erroneous. Nevertheless, it can be seen that there is a close agreement between numerical and experimental results. These results are very encouraging.

Eventually, Figure 5 illustrates the results obtained for the contaminant concentration. It can be seen that, once again, results are good. However, the mean error is about 20% of the contaminant concentration in the outlet (c_0). Results for secondary variables will generally be less accurate. Indeed, these variables are obtained on the basis of the primary variables and so are not directly computed. Moreover, given the range of incertitude on the measurements for contaminant concentration (10% of the value), a part of the incertitude comes from the experimental data. Then, it is clear that CFD can tackle this problematic.

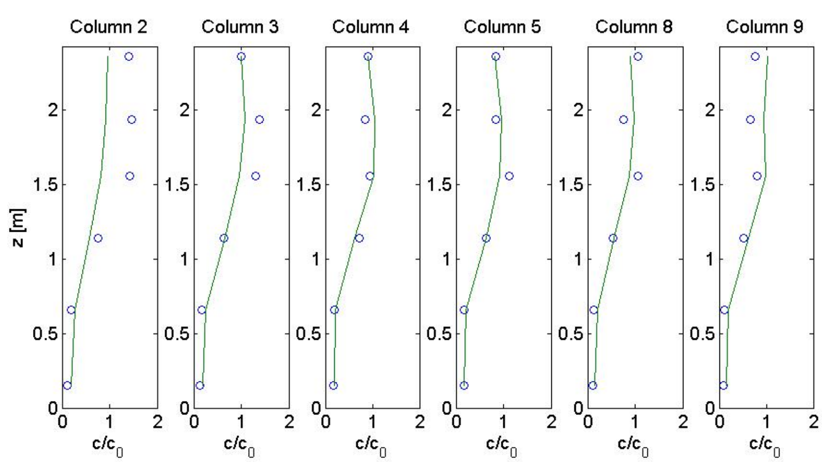


Figure 5: Results of the Free Float Case.

4.7 Conclusions

The ability of CFD to predict the airflow and the air temperature field is proven. The quality of the results for these primary variables assesses the interest to use CFD in building physics. Moreover, secondary variables have also been described precisely. So, CFD has proven on this case that it could be use to predict a contaminant dispersion case. However, the operator interested by such applications should know that the accuracy is not as good as for primary variables but CFD gives a very interesting description of the behaviour of the dispersion and these results are inside an incertitude range of about 20% of the range of concentration inside the room.

5 Case 2

5.1 Geometrical description

This case is also a single room equipped with a displacement ventilation and with a human simulator sitting in front of a computer. This case is very close to a real situation. The dimensions of the supply diffuser are 0.4m (length) x 0.15m (width) and the air supply rate is 43m³/h (0.79 Air Changes per Hour). The dimensions of the outlet diffuser are 0.34m x 0.14m. The air is injected with a temperature of 19°C. It should be noted that there is no other obstacles inside the room and that the outlet is in the ceiling. The complete plan of the case is given in Yang et al. [10].

5.2 Experimental description

This paper focuses on the distribution of air temperature and air velocity inside the room. Experimental data were obtained by five poles placed in the median plane and around the body. The position of the poles is described in Figure 6.

24 probes were placed on the poles at different height (0.4, 0.75, 1, 1.4 and 1.8m). The probes sampled data every 30 seconds in 30 minutes

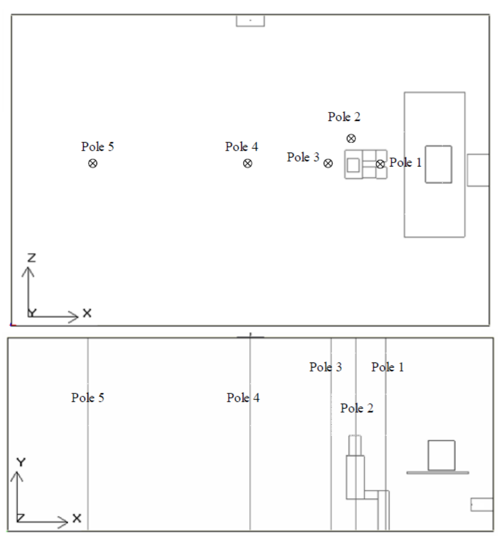


Figure 6: Experimental Poles Positions (Yang et al. [10]).

Concerning the body, the simulator is 1.6m height and the surface area is 1.68m² (mean value for a human body). A description of the human simulator is given at figure 7. Heating panels are placed inside the body and deliver 76W (typical value for a sat person). Eventually, the computer power is simulated by a lamp placed inside a box. The heat generated by this device is fixed to 40W.

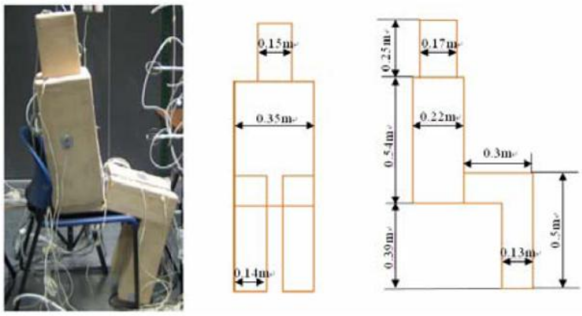


Figure 7: Human simulator description (Yang et al. [10]).

The contaminant is once again SF_6 and is emitted in the back of the manikin with a rate of 482ml/h. This contaminant is often used in experiments because it is non-reactive, non-toxic, odourless, colorless and detectable in small concentrations (Yang et al. [10])

5.3 Turbulence model

For the same reasons than for the first case, a SST k-ω model was used with a low-Reynolds correction.

5.4 Boundary conditions

Walls temperatures are supposed uniform and precise values for each wall are given in Yang et al. [10]. The temperature of the human body is not imposed but a constant heat flux is imposed (76W) equally distributed on the body surface. This hypothesis is not ideal because in the experimental case, the main part of the flux is emitted in the chest part (where the heating device is) and not in the legs. The error made by this approximation is supposed to be small. Concerning the computer, a constant flux of 40W is imposed on the whole surface.

The air velocity through the inlet is supposed to be uniform and the outlet is model by a uniform pressure distribution.

5.5 Numerical methods

Concerning the discretization, convergence criterion and the time discretization, the free float case parameters were used.

Eventually, a 400 000 tetrahedral cells was used. Once again, a convergence study was made on the mesh such that results do not change significantly if the mesh is finer.

5.6 Results

Figure 8 shows the air temperature repartition. It can be deduced from this image that there is two phenomena occurring: the natural convection due to the thermal loads and the forced convection due to the displacement ventilation. At first sight, the upper part of the room is dominated by the natural convection cell and the bottom part is driven by the forced convection. This repartition is logical.

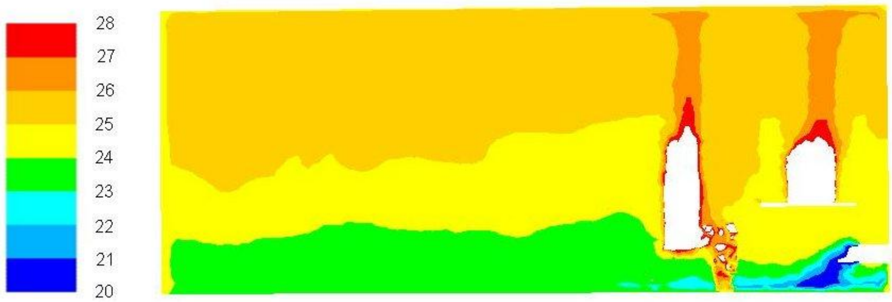


Figure 8: Air Temperature in the Median Plane.

It is interesting to focus on the zone between the legs of the simulated body. This zone is very hot due to the proximity of the two heated surface. Phenomena are probably strongly unstable and gradients important. It is not surprising to see that CFD software has some difficulty to converge to a smooth solution. This phenomenon is also visible at Figure 9 (Pole P1) for the first column: results for air temperature and velocity are varying strongly.

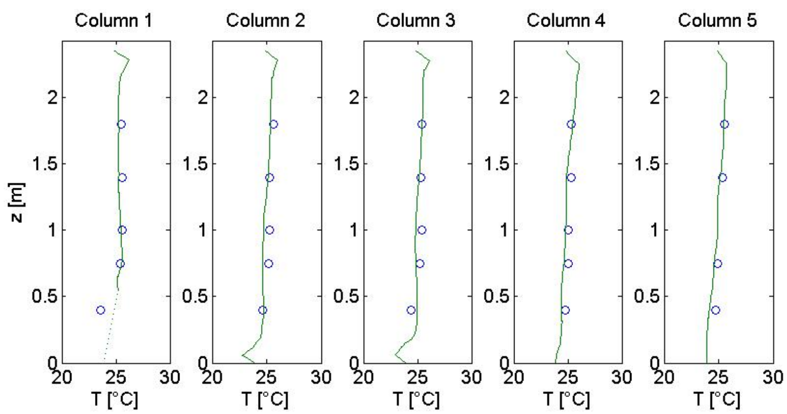


Figure 9: Results of the Mixed Convection Case.

Figure 9 illustrates the numerical results obtained for the air temperature. The agreement between experimental and numerical data is very good. The mean air temperature error is 0.25°C which is excellent given the range of temperature inside the room (8°C – 3% of error). This result do not include the first point of the first pole given the fact that results in this zone are varying extremely quickly and do not permit to have a precise idea of the thermal conditions.

Concerning the air velocity, it could be seen at Figure 10 that results are also very good. Nevertheless, due to very small measurements, the incertitude on the experimental results is quite important and do not permit to draw a strong conclusion. However, it can be seen that the magnitude of the velocity is well predicted: the mean error is about 0.02m/s.

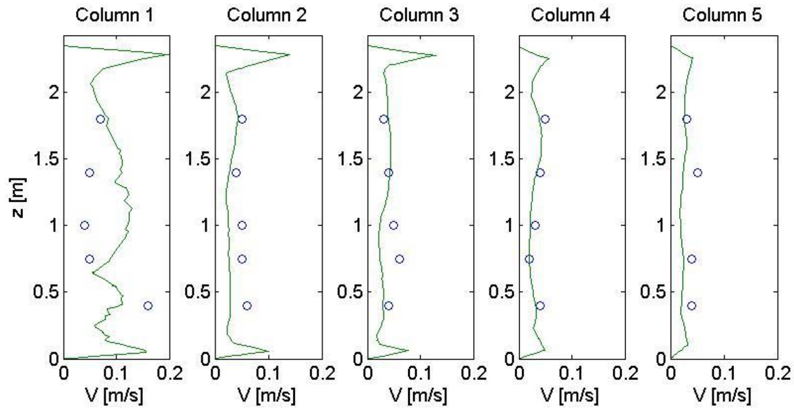


Figure 10: Results of the Mixed Convection Case.

Results for the contaminant concentration can be seen on Figure 11. It can be seen that results are very good. Unlike the free float case, the order of accuracy for this secondary variable is the same than for the primary ones. The mean error on the contaminant concentration is less than 5% of the concentration in the exhaust. Moreover, contaminant concentration gradients seem to be well predicted. This aspect is very important because it influences greatly the distribution of the contaminant inside a room.

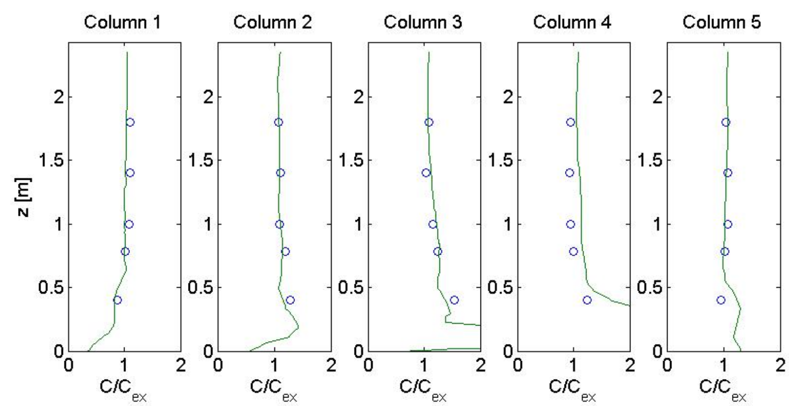


Figure 11: Results of the Mixed Convection Case.

5.7 Conclusions

This example proves the ability of CFD software to model correctly mixed convection. As the air temperature field and the airflow are well described, it is easy to predict the occupant's comfort.

Moreover, the good knowledge of the contaminant concentration inside the room permits to describe precisely the air quality. This validates the use the CFD in such cases. The expected accuracy can be very good (less than 5% of the range) and so CFD could serve as an optimization tool in the near future.

6 Conclusion

CFD will undoubtedly help building engineers and architects in the near future. Thanks to this new tool, industrials can make important breakthroughs especially in the prediction of the occupant's thermal comfort and the air quality description.

Comparisons between CFD simulations and experimental data prove the ability of CFD to predict the airflow, the air temperature field and the contaminant dispersion in a room.

Nevertheless, the results obtained with the two cases described in this paper should not be overstated. The validity of the CFD has been proven for single rooms equipped with a displacement ventilation. It appears now that for such cases (which could be an operating room or a patient's room in a hospital), CFD is able to produce very interesting results with a great accuracy. However, these results cannot be extended to other type of applications, such as big clean rooms.

Eventually, one should not forget that numerical simulations can greatly improve building energy performance, one of the main challenges of this century.

7 Acknowledgement

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