The objective of this study is to develop an approach concerning the integration of volatile organic compounds (VOCs) emissions due to office equipment in computational fluid dynamics (CFD) simulations, in order to assess the indoor air quality (IAQ) in offices. The transport and diffusion phenomena of VOCs are taken into account in the CFD model by means of conservation equations of the mass fraction, written for each VOC that is intended to be considered in the simulation. These equations are added to the basic equations describing turbulent confined non-isothermal flows (conservation of mass, momentum, energy, and turbulent quantities) in CFD modelling. On the other hand, these equations should include source terms of mass for each VOC that is planned to be taken into account in the model. The values of these source terms are specified in the model according to experimental data available in the literature. The numerical model is applied in this study for a small office, taking into account two ventilation systems: conventional mixing ventilation system and displacement ventilation system. The simulations are carried out for low air flow rates with different air supply temperatures. Concerning the sources of VOCs in terms of electronic devices, the office is supposed to be equipped with 4 computers, 4 monitors, and 4 laser printers. The assessment of IAQ in the office is accomplished by taking into account in the CFD model the indoor levels of the following five VOCs: benzaldehyde, ethylbenzene, o-xylene, styrene, and toluene. The CFD model proposed in this study allows achieving values of VOCs concentrations throughout the entire indoor environment in a particularly comprehensive manner. Consequently, results are presented in terms of benzaldehyde, ethylbenzene, o-xylene, styrene, and toluene concentration contours in the office. The results show that the estimated VOCs concentration levels due to office equipment are far below the set threshold limit values, both in the case of mixing ventilation and displacement ventilation, despite low ventilation rates taken into account. However, it should be remembered that the results are based only on VOCs emissions due to electronic devices, VOCs generated from other indoor sources have not been taken into consideration during the simulations. On the other hand, the numerical description of VOCs sources for CFD modelling developed in this work may be easily extended for other indoor VOCs sources. Finally, the numerical approach proposed in this study can lead to relevant IAQ analyses, being an appropriate alternative to experimental investigations, challenging to carry out in situ.

KEYWORDS

IAQ - indoor air quality; VOCs – volatile organic compounds; ventilation efficiency; CFD – Computational Fluid Dynamics modelling
spend approximately 90% of the time indoors, 5% in different means of transportation (cars, trains, airplanes, etc.), and only 5% outdoors (Hancock, 2002); building ventilation rates reach often values below nominal ventilation rate conditions established according to standards for healthy indoor environments (Mendell et al., 2013); there are more and more sources of indoor air pollution due to our modern style of life (Zhang and Smith, 2003).

The best example related to the last point mentioned above is the dramatic growth of volatile organic compounds (VOCs) in classic indoor air samples because of new sources each year: from hundreds species in 1990s to thousands individual VOCs nowadays (Manivanan, 2006). In this context, office devices are becoming major sources of indoor pollution due to their widespread and increasing use in modern, well-equipped, office buildings. Studies have shown that the emissions from these devices (computers, monitors, printers, copiers, etc.) generate about 35 substances and most of these are VOCs (Maddalena et al., 2011).

Unfortunately, numerous recent studies (McGee, 2015) have been undoubtedly revealed that human exposure to VOCs can lead to acute effects (e.g. inflammation of mucous membranes, irritation, headache, asthma exacerbation) and even chronic effects (e.g. respiratory system, circulatory system, and central nervous system diseases, organs dysfunction, cancer). Consequently, the number of studies dealing with IAQ associated to VOCs emissions and indoor concentrations is continuously increasing, particularly for office work environment, as many people in developed countries spend large part of the day in office buildings, frequently improperly ventilated. Most of these investigations are based on experimental methodologies (Wang et al., 2011; Kowalska et al., 2015). However, experimental studies in this field are challenging to fulfil in situ. As a result, there are also a number of numerical approaches used to evaluate the IAQ, including the Computational Fluid Dynamics (CFD) technique. Indeed, thanks to amazing hardware development, the CFD approach can be employed nowadays as a pertinent simulation tool to assess the IAQ for different applications (Helmis et al., 2007; Stathopoulou and Assimakopulos, 2008; Corgnati and Perino, 2013; Zhuang et al., 2014; Yang et al., 2014).

Consequently, the objective of this work is to numerically predict the IAQ within small ventilated rooms in office buildings (based on CFD technique), taking into account VOCs emissions from office equipment. Results are presented in terms of VOCs concentrations contours in the office, for different air supply temperatures in the case of mixing ventilation and displacement ventilation. This allows to compare the performance (efficiency) of different ventilation strategies for the enclosure taken into consideration.

2 MODELLING OF VOLATILE ORGANIC COMPOUND CONCENTRATIONS

The development of the numerical model is based on VOCs transport and diffusion in the indoor air in order to assess the efficiency of the ventilation systems. As a result, the main hypotheses of the CFD model are the following:
- fluid, air-VOCs mixture;
- mixture air-VOCs, ideal gas of perfect gases (air and VOCs);
- mixture air-VOCs, incompressible Newtonian fluid;
- no chemical reaction between the species of the mixture;
- insignificant heat and mass transfer interactions within the mixture;
- density of mixture air-VOCs, ideal gas law formulation (based on the mixture temperature and the mass fraction of each species (air and VOCs));
- specific heat capacity of mixture air-VOCs, mixing law formulation (depending on the mass fraction average of the species, air and VOCs, heat capacities);
- thermal conductivity and viscosity of mixture air-VOCs, expressed through kinetic theory;
- diffusion coefficient of VOCs in air, constant values, based on data extracted from the literature.

Based on the above assumptions, the transport and diffusion phenomena of VOCs are taking into account in the CFD model by means of conservation equations of the mass fraction, written for each VOC that is intended to be considered in the simulation. These equations can be written as classic convection-diffusion equations. In addition, these equations are added to the equations describing turbulent confined non-isothermal flows (conservation of mass, momentum, energy, and turbulent quantities) in CFD modelling. As a result, VOCs conservation equations and the other equations, governing in the CFD model the conservation of variables in the computational domain, have similar expression:

$$0 = -\nabla \cdot (\rho \Phi v) + \nabla \cdot (\Gamma \nabla \phi) + S$$  \hspace{1cm} (1)

where $\rho$ – mixture density; $\Phi$ - variable of interest (it can be: mass fraction for each VOC considered, $1$ for the continuity, velocity components, temperature, or turbulent parameters); $v$ – mixture velocity; $\Gamma$ - diffusion coefficient; $S$ – source term.

The first term on the right-hand side of the Eq. (1) stands for the convection mechanisms and, in the case of VOCs, it is representing the change of the VOC concentration due to the flow. On the other hand, the second term on the right-hand side of the Eq. (1) signifies the diffusion term. It is worthwhile to mention that this term integrates in the numerical model both aspects of diffusion, molecular and turbulent. The molecular diffusion is based on Fick’s first law: diffusion flux is proportional to the concentration gradient, using constant diffusion coefficient in the case of each VOC, as mentioned above. On the other hand, the turbulent diffusion for each VOC is taking into account in a similar way to that of the Reynolds analogy. Consequently, mixture mass turbulent diffusivity is related to the eddy viscosity through the CFD turbulence model used to describe the flow in the computational domain. Finally, the third term on the right-hand side of the Eq. (1) refers to source terms. The values of these source terms for each VOC are based on VOC generation rates of different sources which are intended to be considered in the numerical model. Consequently, these source terms for each VOC will be specified in the model according to experimental data available in the literature (see the next section).

3 CASE STUDY

The numerical model briefly presented above is applied in this study for a small office (6.2 x 3.1 x 2.5 m$^3$), taking into account two ventilation systems:

- classic mixing ventilation system, air supply occurs at the upper part of the room, while air exhaust is located at the lower part of the room (Figure 1);
- displacement ventilation system, in this case the air supply is located in the occupied zone, while air exhaust is placed at the upper part of the room (Figure 2).

The simulations are carried out for low air flow rates with different air supply temperatures, both in the case of mixing ventilation and displacement ventilation, see Table 1.

<table>
<thead>
<tr>
<th>Test</th>
<th>Air flow rate (m$^3$/h)</th>
<th>Air changes per hour (h$^{-1}$)</th>
<th>Temperature (°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mixing ventilation</td>
<td>96.1</td>
<td>2.0</td>
<td>15.0</td>
</tr>
<tr>
<td>Mixing ventilation</td>
<td>96.1</td>
<td>2.0</td>
<td>30.0</td>
</tr>
<tr>
<td>Displacement ventilation</td>
<td>96.1</td>
<td>2.0</td>
<td>15.0</td>
</tr>
<tr>
<td>Displacement ventilation</td>
<td>96.1</td>
<td>2.0</td>
<td>30.0</td>
</tr>
</tbody>
</table>
Concerning the sources of VOCs in terms of electronic devices, the office is supposed to be equipped with 4 computers, 4 monitors, and 4 laser printers (see Figure 3).

The assessment of IAQ in the office is accomplished by taking into account in the CFD model the indoor levels of the following five VOCs: benzaldehyde, ethylbenzene, o-xylene, styrene, and toluene. The choice of these VOCs is justified by the fact that these VOCs are characterised by significant emissions from office equipment, according to data available in the literature (Maddalena et al., 2011; Kowalska et al., 2015). In addition, it is worthwhile to mention that these five VOCs are classified as possibly carcinogenic to humans. Consequently, the implementation of the CFD model requires in this case five supplementary equations expressing the conservation of mass fraction for each VOC taken into consideration (benzaldehyde, ethylbenzene, o-xylene, styrene, and toluene). As indicated before, these
equations have the classic formulation of advection-diffusion equations, see Eq. (1), and they are added to the basic equations expressing turbulent confined non-isothermal flows in CFD modelling. The values of the diffusion coefficient of each VOC, required in these conservation equations for each VOC, are specified in Table 2 (New Jersey, 2015).

<table>
<thead>
<tr>
<th>VOC</th>
<th>benzaldehyde</th>
<th>ethylbenzene</th>
<th>o-xylene</th>
<th>styrene</th>
<th>toluene</th>
</tr>
</thead>
<tbody>
<tr>
<td>diffusion coefficient x 10^{-6} (m^2/s)</td>
<td>7.3</td>
<td>7.5</td>
<td>7.5</td>
<td>7.1</td>
<td>8.7</td>
</tr>
</tbody>
</table>

On the other hand, the emissions of VOCs from office equipment are taken into account by mass source terms added in each of these five equations describing the conservation of mass fraction, for each VOC considered (benzaldehyde, ethylbenzene, o-xylene, styrene, and toluene). The values of these source terms for each of the five VOCs considered are specified in the model according to experimental data existing in the literature (Maddalena et al., 2011), see Table 3.

<table>
<thead>
<tr>
<th>VOC</th>
<th>benzaldehyde</th>
<th>ethylbenzene</th>
<th>o-xylene</th>
<th>styrene</th>
<th>toluene</th>
</tr>
</thead>
<tbody>
<tr>
<td>computer + monitor source term x 10^{-11} (kg/s)</td>
<td>0.209</td>
<td>1.414</td>
<td>0.930</td>
<td>0.921</td>
<td>2.056</td>
</tr>
<tr>
<td>laser printer source term x 10^{-11} (kg/s)</td>
<td>2.367</td>
<td>1.956</td>
<td>1.625</td>
<td>2.220</td>
<td>1.550</td>
</tr>
</tbody>
</table>

The numerical model developed as specified above was assembled using a finite-volume, Navier-Stokes solver (Fluent, version 15.0.0). The main elements of this model are shown in Table 4.

<table>
<thead>
<tr>
<th>Feature</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fluid</td>
<td>air-VOCs mixture</td>
</tr>
<tr>
<td>Flow</td>
<td>three-dimensional, steady, non-isothermal, turbulent</td>
</tr>
<tr>
<td>Computational domain</td>
<td>finite volumes, unstructured mesh (tetrahedral elements):</td>
</tr>
<tr>
<td>discretisation</td>
<td>5,744,884 cells for mixing ventilation; 6,007,026 cells for displacement</td>
</tr>
<tr>
<td>Turbulence model</td>
<td>Shear Stress Transport (SST) turbulent kinetic energy-specific</td>
</tr>
<tr>
<td></td>
<td>turbulent dissipation rate (k-ω), with low-Reynolds corrections</td>
</tr>
<tr>
<td>Numerical resolution</td>
<td>second-order upwind scheme</td>
</tr>
<tr>
<td></td>
<td>velocity-pressure coupling: SIMPLE algorithm</td>
</tr>
<tr>
<td></td>
<td>convergence acceleration: algebraic multigrid</td>
</tr>
</tbody>
</table>

4 RESULTS

The numerical model allows achieving VOCs concentration field all over the computational domain. Consequently, results are presented below in terms of benzaldehyde, ethylbenzene, o-xylene, styrene, and toluene concentration contours in the office, for each configuration taken into account (see Table 1). These results are reported in a vertical plane passing nearby the occupants. Figures 4 and 5 show the results for the cold air supply test and hot air supply test in the case of mixing ventilation system. The same results are presented in Figures 6 and 7 for the displacement ventilation system.

It should be first emphasized that, despite the numerous indoor VOCs sources taken into account, limited dilution volume and low ventilation rates, for all configurations taken into consideration, VOCs concentration levels in the office are well below the occupational
Figure 4: VOCs concentrations (mixing ventilation system, cold air supply, 2 h⁻¹ air changes per hour)

Figure 5: VOCs concentrations (mixing ventilation system, hot air supply, 2 h⁻¹ air changes per hour)
Figure 6: VOCs concentrations (displacement ventilation system, cold air supply, 2 h\(^{-1}\) air changes per hour)

Figure 7: VOCs concentrations (displacement ventilation system, hot air supply, 2 h\(^{-1}\) air changes per hour)
exposure limits established by different organisms: Permissible Exposure Limits – PELs, set by Occupational Safety and Health Administration – OSHA (California, 2015) or Threshold Limit Values – TLVs set by American Conference of Government Industrial Hygienists – ACGIH (Abdul-Wahab, 2011). These results confirm the experimental data summarised in (Levin and Hodgson, 2006).

On the other hand, there are differences in effectiveness between the two ventilation systems, as expected. Accordingly, the numerical results highlight the well-known behaviour of mixing ventilation systems and displacement ventilation systems. In the case of mixing ventilation, efficiency is different depending on the temperature of the air supply and room area: the efficiency can be decent in the case of cold air supply in the region where the fresh air jet falls in the occupied zone, while the VOCs concentrations can reach values twice as high in other regions of the occupied zone (Figure 4). In addition, the mixing ventilation efficiency is affected in the entire occupied zone in the case of hot air supply due to buoyant forces and Coanda effect even if the indoor levels of VOCs remain low (Figure 5).

Concerning the displacement ventilation, the overall effectiveness is constant in the occupied zone, regardless of the supply air temperature. Basically, in this case, the diffusion of the pollutants follows the air flow established in the enclosure.

5 CONCLUSIONS

The implementation of the CFD model proposed in this study allows achieving values of VOCs concentrations throughout the entire indoor environment. As a result, this methodology can lead to pertinent IAQ investigations, being an appropriate option to experimental analyses, difficult to perform in situ. In addition, the numerical model allows forecasting indoor VOCs values in a particularly comprehensive way. This makes possible to assess the levels of VOCs near the occupants, allowing more accurate estimations regarding the IAQ, contrary to analyses based on average values or on a small number of measuring points in the occupied zone.

On the other hand, the numerical description of VOCs sources for CFD modelling developed in this work may be extended for other indoor VOCs sources (e.g. carpets, furniture, paints, building materials, etc.).

The results of the case study taken into account show that the estimated VOCs concentration levels due to office equipment are far below the established threshold limit values, despite low ventilation rates taken into account. On the other hand, it should be remembered that the results are based only on VOCs emissions due to electronic devices, VOCs generated from other indoor sources have not been taken into consideration during the simulations. Furthermore, in spite of low concentrations of indoor VOCs from electronic devices numerically assessed in this study, long term exposure could be more harmful to the health than short term exposure to higher concentrations. Besides, cumulative chemical effects of multiple VOCs may lead to more detrimental impact on occupants’ health.

Consequently, investigations based on numerical model presented in this work should be continued to make available new data concerning IAQ related to VOCs emissions from indoor sources.

6 ACKNOWLEDGEMENTS

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7 REFERENCES


