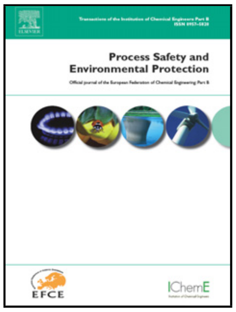


Title: Modelling of Volatile Organic Compounds
Concentrations in Rooms due to Electronic Devices

Author: C. Teodosiu V. Ilie R. Teodosiu

PII: S0957-5820(16)30099-4
DOI: http://dx.doi.org/doi:10.1016/j.psep.2016.06.013
Reference: PSEP 801

To appear in: *Process Safety and Environment Protection*

Received date: 18-12-2015
Revised date: 9-5-2016
Accepted date: 7-6-2016

Please cite this article as: <doi>http://dx.doi.org/10.1016/j.psep.2016.06.013</doi>

Study highlights:

- integration of VOCs emissions due to office equipment in CFD simulations
- transport and diffusion of VOCs by means of conservation equations for each VOC
- source terms of mass for VOCs using experimental data available in the literature
- model applied for a small office with conventional mixing ventilation system
- estimated VOCs concentration levels are far below the threshold limit values

Modelling of Volatile Organic Compounds Concentrations in Rooms due to Electronic Devices

C. Teodosiu[a], V. Ilie[a], R. Teodosiu[a]
[a]Faculty of Building Services and Equipment, Technical University of Civil Engineering,
Bucharest 020396, Romania
Corresponding author. Tel.: +40 21 252 46 20; Fax: +40 21 252 68 80
Email: cteodosiu@yahoo.com

Modelling of Volatile Organic Compounds Concentrations in Rooms due to Electronic Devices

ABSTRACT

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). 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 include source terms of mass for each VOC, based on VOC generation rates of different sources considered in the numerical model (computers, monitors, and laser printers). On the other hand, 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. The numerical model is applied in this study for a small office, taking into account a conventional mixing ventilation system (low air flow rates with different air supply temperatures). Health hazard assessments are 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. Consequently, results are presented in terms of benzaldehyde, ethylbenzene, o-xylene, styrene, and toluene concentration contours in the office, as well as mean and peak values of these VOCs in the occupied zone of the room. The results show that the estimated VOCs concentration levels due to office equipment are far below the set threshold limit values. However, the reported maximum concentrations of VOCs taken into account in the occupied zone tend to approach in some measure levels of concern with respect to odour or sensory irritation. Finally, the numerical description of VOCs sources for CFD modelling developed in this work may be extended for other indoor VOCs sources. As a result, the numerical approach proposed in this study can lead to relevant health hazard analyses, being an appropriate alternative to experimental investigations, challenging to perform in situ.

Keywords: CFD - Computational Fluid Dynamics modelling; IAQ – indoor air quality; VOCs – volatile organic compounds; indoor exposure

1. Introduction

Nowadays people are becoming increasingly aware of threats due to atmospheric pollution but people do not equally realize health consequences due to inadequate indoor air quality (IAQ). Indeed, according to recent studies carried out by the USA Environmental Protection Agency (EPA) of human exposure to air pollutants, indoor concentrations of different pollutants can reach values that are 2-5 times, and occasionally, more than 100 times higher than outdoor concentrations (Alves et al., 2013). This is particularly worrying as people spend more than 90% of their time in closed spaces (home, office, commercial buildings, schools, hospitals, vehicles, trains, airplanes, etc.) in the case of industrialized countries (de Blas et al., 2012). Indoor environment can contain different kinds of pollutants: inorganic pollutants (e.g. carbon dioxide, carbon monoxide, nitrogen dioxide, sulphur dioxide, ozone), organic pollutants (e.g. volatile organic compounds, formaldehyde, pesticides, polynuclear aromatic hydrocarbons, polychlorinated biphenyls), physical pollutants (e.g. asbestos, man-made mineral fibers, radon), radioactive pollutants, biological agents (e.g. fungi, bacteria), etc. (Maroni et al., 1995). Concerning the volatile organic compounds (VOCs), the number of species experienced a spectacular evolution in typical indoor air samples due to new sources each year: from hundreds in 1980s (Maroni et al., 1995) to thousands individual VOCs today (Anderson and Albert, 1998; Manivanan, 2006). Unfortunately, the negative effects of VOCs on the health of occupants have been clearly emphasized by numerous studies (McGee, 2015). Consequently, VOCs are currently considered as important pollutants in the indoor environment since they 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).

In addition, concerns about the exposure to VOCs in indoor air have increased lately because of lack of fresh air. This is due to the reduction of building ventilation rates in order to save energy with heating, ventilation, and air conditioning (HVAC) systems (Yang et al., 2009). Consequently, concentrations of VOCs in indoor air can be generally 5 to 10 times higher than outdoors, with even higher indoor air concentrations where extreme cold weather conditions exist leading to very low ventilation rates (Dales et al., 2008).

As a result, 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, therefore 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 Assimakopoulos, 2008; Corgnati and Perino, 2013; Zhuang et al., 2014; Yang et al., 2014).

Accordingly, the aim of this study is to predict the IAQ for small ventilated rooms in office buildings, based on CFD methodology. Studies focused on IAQ in offices are particularly important today because, in order to achieve more energy efficient buildings, many indoor office environments will have reduced ventilation while there are numerous sources of VOCs in these buildings (e.g. construction materials, furniture, office equipment, and contaminated outdoor air). In this context, it is worth mentioning that office equipment (computers, monitors, printers, copiers, etc.) are becoming significant sources of “pollution” due to their widespread and growing use in modern office buildings. Studies have shown that the emissions from these devices contain about 30-35 substances and most of these are VOCs (Maddalena et al., 2011). These are the reasons why the CFD model developed in this study focused on VOCs emissions from office equipment and prediction of VOCs concentration in small offices with low ventilation rates.

2. Modelling of Volatile Organic Compound Concentrations

The development of the numerical model is based on VOCs transport and diffusion in the indoor air. 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, written in a tensor notation as:

$$\rho \frac{\partial}{\partial x_i}\left(u_i m_{i'}\right) + \frac{\partial}{\partial x_i} J_{i',i} = S_{i'} \qquad (1)$$

In Eq. (1), the left-hand side terms stand for the convection mechanisms (in the case of VOCs, it is representing the change of the VOC concentration due to the airflow, with ρ – mixture density;

x_i - spatial coordinate; u_i – velocity component in i direction; $m_{i'}$ – mass fraction for each VOC taken into account) and diffusion phenomena respectively (with $J_{i,i'}$ – each VOC diffusion flux), while the right-hand side term $S_{i'}$ represents source/sink term.

Concerning the second term on the right-hand side of the Eq. (1), this term integrates in the numerical model both aspects of diffusion, molecular and turbulent:

$$\frac{\partial}{\partial x_i} J_{i',i} = \rho \frac{\partial}{\partial x_i}\left(D_{i',m} \frac{\partial m_{i'}}{\partial x_i} \right) - \frac{\partial}{\partial x_i}\left(-\overline{u_i' m_{i'}'} \right) \tag{2}$$

where $D_{i',m}$ stands for the molecular diffusion coefficient of each VOC and $u_i'm'_{i'}$ signifies the turbulent mass flux of each VOC, u_i' being the velocity fluctuation. The molecular diffusion is actually taking into account using Fick's first law: diffusion due to concentration gradients (by means of constant diffusion coefficient for each VOC). Concerning the turbulent diffusivity term from Eq. (2), in a manner correlated to that of the Reynolds analogy, we can associate the mixture turbulent diffusivity and the eddy viscosity μ_t by introducing the turbulent Schmidt number Sc_t:

$$-\overline{u_i' m_{i'}'} = \frac{\mu_t}{Sc_t} \frac{\partial m_{i'}}{\partial x} \tag{3}$$

As a result, this number is defined using the turbulent mass diffusivity D_t, the eddy viscosity and the mixture density:

$$Sc_t = \frac{\mu_t}{\rho D_t} \tag{4}$$

Finally, the value of the term source in Eq. (1) for each VOC is 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: ventilated office equipped with computers, monitors, and laser printers

The numerical model presented above is applied in this study for a small office (6.2 x 3.1 x 2.5 m^3), in the case of a 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 – Fig. 1).

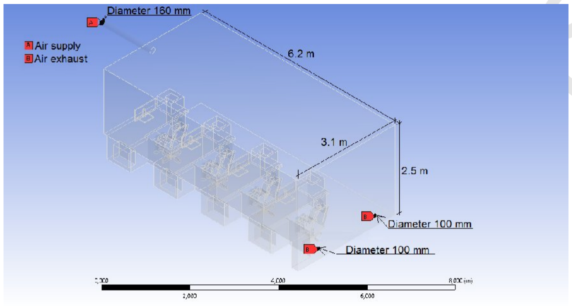


Fig. 1. Case study: office with mixing ventilation system

The simulations are carried out for low air flow rates with different air supply temperatures (isothermal air supply, cold air supply, and hot air supply), see Table 1.

Table 1. Case Study Conditions (Air Inlet Characteristics)

Test	Air flow rate (m^3/h)	Air changes per hour (h^{-1})	Temperature (°C)
T1: isothermal air supply	96.10	2.0	22.0
T2: isothermal air supply	144.15	3.0	22.0
T3: cold air supply	96.10	2.0	15.0
T4: cold air supply	144.15	3.0	15.0
T5: hot air supply	96.10	2.0	30.0
T6: hot air supply	144.15	3.0	30.0

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 Fig. 2).

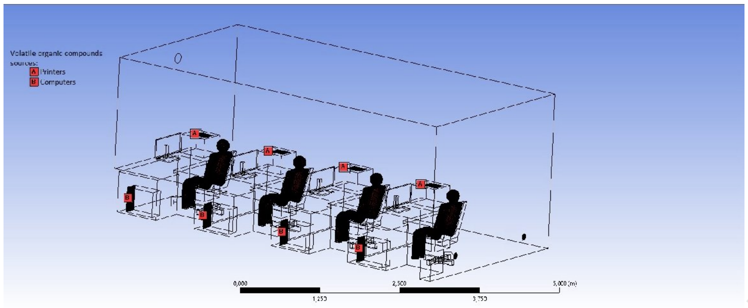


Fig. 2. VOCs sources

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 VOCs are considered suspected or confirmed carcinogens to humans by EPA.

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 2. VOC - Diffusion Coefficients in Air

VOC	benzaldehyde	ethylbenzene	o-xylene	styrene	toluene
diffusion coefficient x 10^{-6} (m^2/s)	7.3	7.5	7.5	7.1	8.7

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 taken into consideration. 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 3. VOC - Source Terms for Office Equipment

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

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

It should be noted that the proper choice of the turbulence model, associated to the characteristics of indoor airflows, is one of the major challenge for CFD simulations (van Hooff et al., 2013). In addition, the accurate description of the airflow has a straightforward effect on the pollutant transport and finally, on the contaminant concentrations in enclosures. Consequently, the choice of the turbulence model is particularly important in our study. As a result, the CFD approach proposed in this work takes into consideration a Shear Stress Transport (SST) turbulent kinetic energy-specific turbulent dissipation rate (k-ω), with low-Reynolds corrections turbulence model.

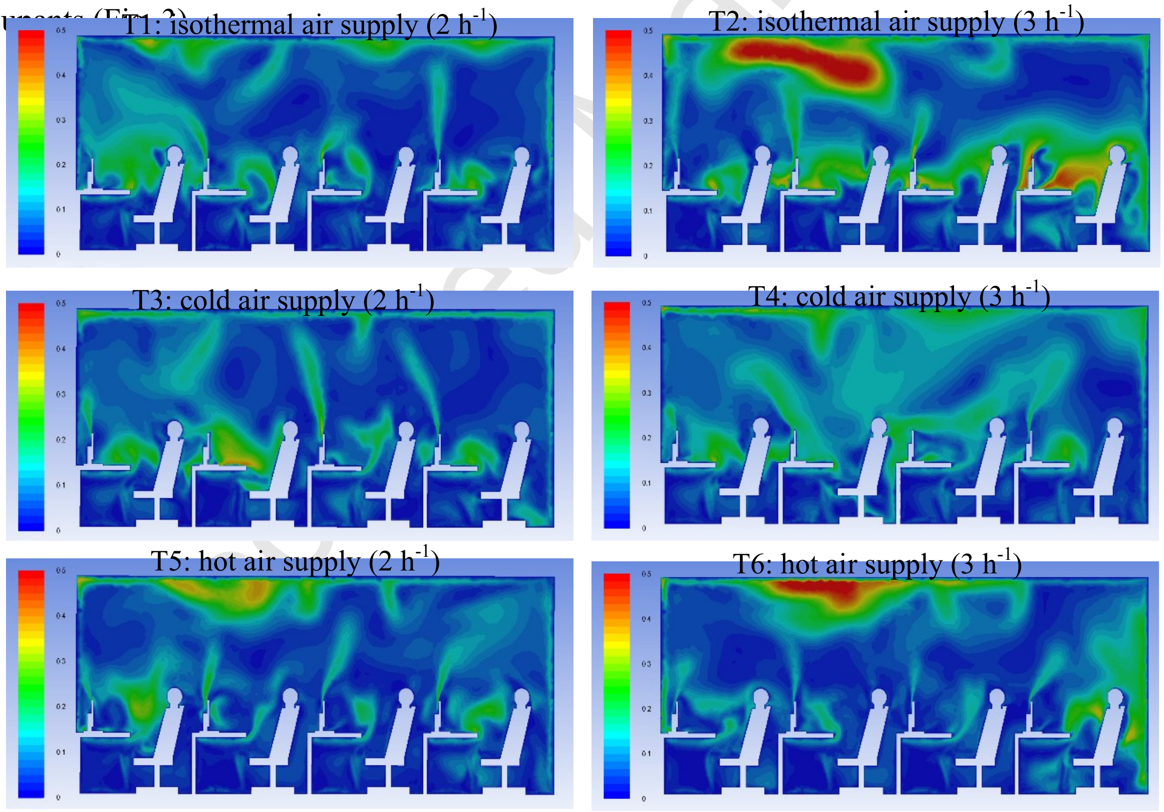
Based on a literature review, the application of k-ω turbulence models for indoor airflows has been generally characterized by good accuracy, numerical stability, and reasonable wall treatment for complex geometries (Hussain et al., 2012). Furthermore, the best behavior for internal convective airflows among k-ω models has been established by using SST k-ω turbulence models (Stamou and Katsiris, 2006). Finally, SST k-ω turbulence models have shown the better overall prediction of the airflow among 6 turbulence models investigated, in comparison with detailed experimental data for similar configurations to that in our study: airflows generated by mixing ventilation system in small rooms at low air changes per hour (Teodosiu et al., 2014).

Table 4. VOC Concentrations - CFD Model

Feature	Description
Fluid	air-VOCs mixture
Flow	three-dimensional, steady, non-isothermal, turbulent
Computational domain discretisation	finite volumes, unstructured mesh (tetrahedral elements): 5,744,884 cells for mixing ventilation
Turbulence model	Shear Stress Transport (SST) turbulent kinetic energy-specific turbulent dissipation rate (k-ω), with low-Reynolds corrections
Numerical resolution	second-order upwind scheme velocity-pressure coupling: SIMPLE algorithm convergence acceleration: algebraic multigrid
Convergence control (residuals)	continuity : 10^{-3} velocity components : 10^{-3} turbulent quantities : 10^{-3} energy : 10^{-5} VOCs : 10^{-4}
Convergence control (under-relaxation factors)	pressure: 0.3 momentum: 0.7 energy: 0.8 turbulent quantities : 0.8 VOCs : 0.8 other quantities : 1.0

4. Results

251659264251659264251659264As the airflow is one of the main factors influencing the VOCs concentration field in the office, we first present air mean velocity contours for all six cases taken into account (see Table 1). These results are reported in a vertical plane passing nearby the occupants (Fig. 2).



T1: isothermal air supply (2 h^{-1})

T2: isothermal air supply (3 h^{-1})

T3: cold air supply (2 h^{-1})

T4: cold air supply (3 h^{-1})

T5: hot air supply (2 h^{-1})

T6: hot air supply (3 h^{-1})

Fig. 3. Air velocity contours (m/s)

Concerning the isothermal air supply tests (T1 and T2 – Fig. 3), it can be clearly noticed the influence of the initial momentum forces of the supplied air jet on the development of the airflow in the room. Accordingly, in the case T2 (3 air changes per hour), compared to case T1 (2 air changes per hour), the jet region is more pronounced in the upper part of the office, leading to stronger induction mechanisms of surrounding air. This is expressed through higher air velocities in the occupied zone of the room (Awbi, 2008). As it will be shown further, this directly affects the VOCs level near the occupants.

For the more complex air flow which occurs in the case of a cold jet supplied in the room (T3 – and T4 – Fig. 3), it can be observed the impact of the ratio of the momentum forces to the buoyancy forces on the decay of the fresh air jet. Consequently, the contaminant fields nearby the occupants are strongly depending on the jet fall in the occupied zone of the office.

In winter situation (hot air supply, T5 and T6 – Fig. 3), the fresh air jet “sticks” to the ceiling due to the Coandă effect. In addition, in the case of test T6 (3 air changes per hour), the higher air flow rate leads to impinging jet phenomenon on the opposite wall. As a result, this has a direct influence on the VOCs level in that region (near the opposite wall to the air supply).

Concerning VOCs concentration fields in the office, the numerical model allows achieving values all over the computational domain. We present below results in terms of benzaldehyde, ethylbenzene, o-xylene, styrene, and toluene concentration contours in the same vertical plane as the one taken into consideration for the air velocity contours.

In the case of benzaldehyde (Fig. 4), it is obvious the effect of higher air flow rate on the level of this VOC in the room: whatever the situation (isothermal, cold or hot air supply), benzaldehyde concentrations are lower by approximately 50% for cases with 3 air changes per hour compared to cases with 2 air changes per hour. Therefore, the level of this VOC in the occupied zone of the room is around 9-10 $\mu g/m^3$ for ventilation configurations with 3 air changes per hour compared to roughly 6 µg/m^3 for 2 air changes per hour (see also Table 5). Nevertheless, as mentioned before, in the case of the cold jet supplied in the room, the jet fall in different regions of the occupied zone of the office (depending on the ratio of the momentum forces to the buoyancy forces) leads to lower benzaldehyde concentrations in the region nearby the first two occupants for the configuration T3 (2 air changes per hour), while the same phenomenon takes place in the area close to the second and third desk for the test T4 (3 air changes per hour). This is emphasised also by the values presented in Table 5.

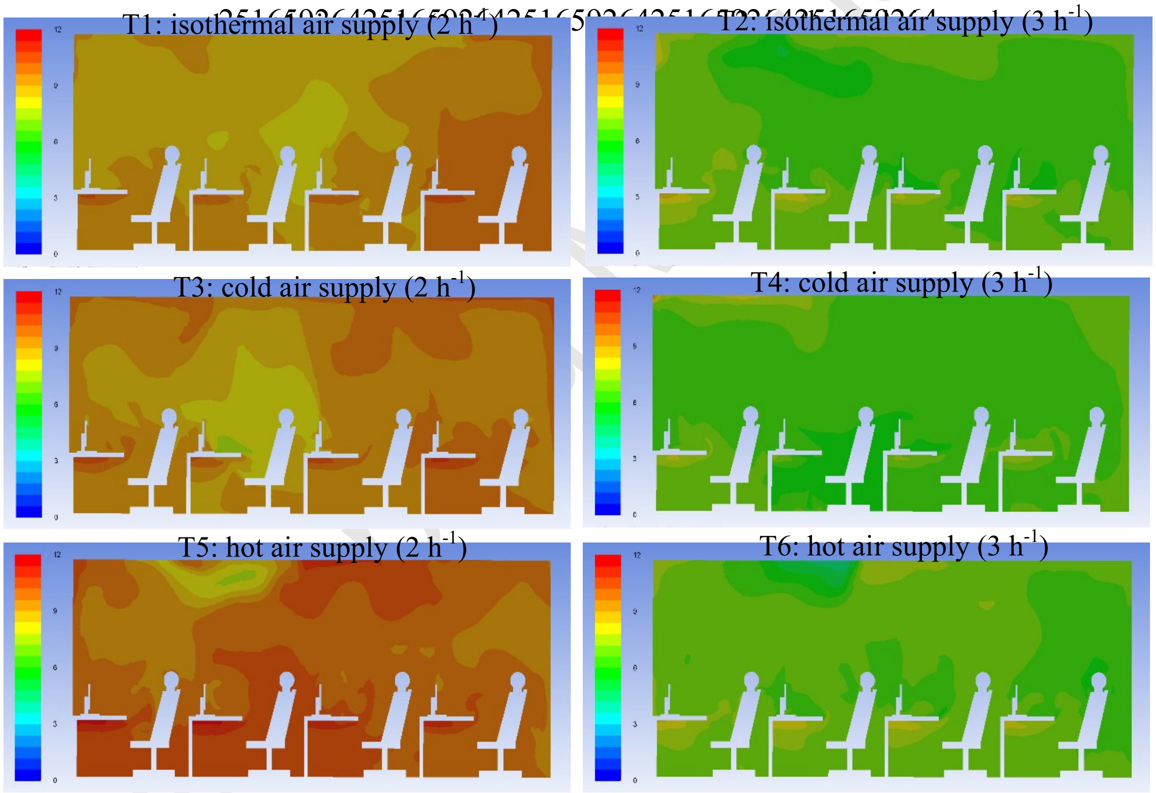


Fig. 4. Benzaldehyde concentrations (µg/m^3)

Regarding the ethylbenzene (Fig. 5), it can be noted the same behaviour as for benzaldehyde: concentrations reduced by 40%-50% for 3 h^{-1} ventilation air flow rates compared to values obtained for 2 h^{-1} ventilation air flow rates and lower levels in some areas near the occupants in the case of the cold jet, depending on the jet decay (see Table 5). However, it can be perceived a greater unevenness of ethylbenzene concentrations near the occupants compared to the values achieved for benzaldehyde. In addition, the impinging jet mechanisms on the opposite wall in the case of hot air supply (test T6 - 3 air changes per hour) lead to lower ethylbenzene concentrations in the region near the last desk in the office. On the other hand, higher concentrations are recorded under the desks (20-25 μg/m^3) in the case of ethylbenzene. This is mainly due to more important ethylbenzene emissions from computers, taken into account in the model (see Table 3).

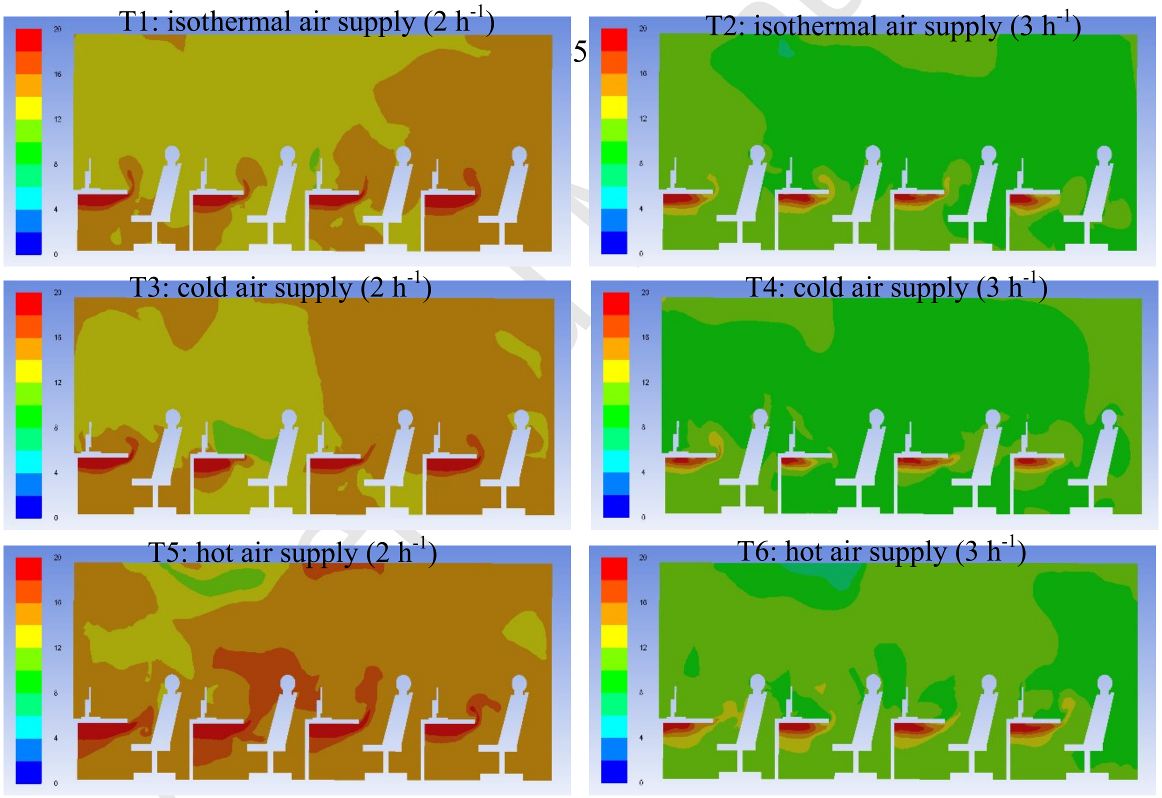

T1: isothermal air supply (2 h^{-1})
T2: isothermal air supply (3 h^{-1})
T3: cold air supply (2 h^{-1})
T4: cold air supply (3 h^{-1})
T5: hot air supply (2 h^{-1})
T6: hot air supply (3 h^{-1})

Fig. 5. Ethylbenzene concentrations (μg/m^3)

The o-xylene concentrations contours are shown in Fig. 6. Taking into account the fact that ethylbenzene and o-xylene have the same density and diffusion coefficients in air, as well as that these VOCs have similar total emissions from computers and laser printers (see Table 3), it is not surprising that their concentration fields in the office have the same characteristics. As a result, the o-xylene behaviour is comparable to that of ethylbenzene and the remarks done earlier for ethylbenzene are also valid for o-xylene.

Concerning the styrene concentrations (Fig. 7), the same main conclusions can be drawn, given that the distribution of this VOC is also influenced by the airflow established in the office. As a result, the average concentration of styrene in the occupied zone of the office is reduced from 12-14 µg/m^3 to 9-9.5 µg/m^3 when the ventilation rate is increased, regardless of the situation (iso th the 251 16 is reco

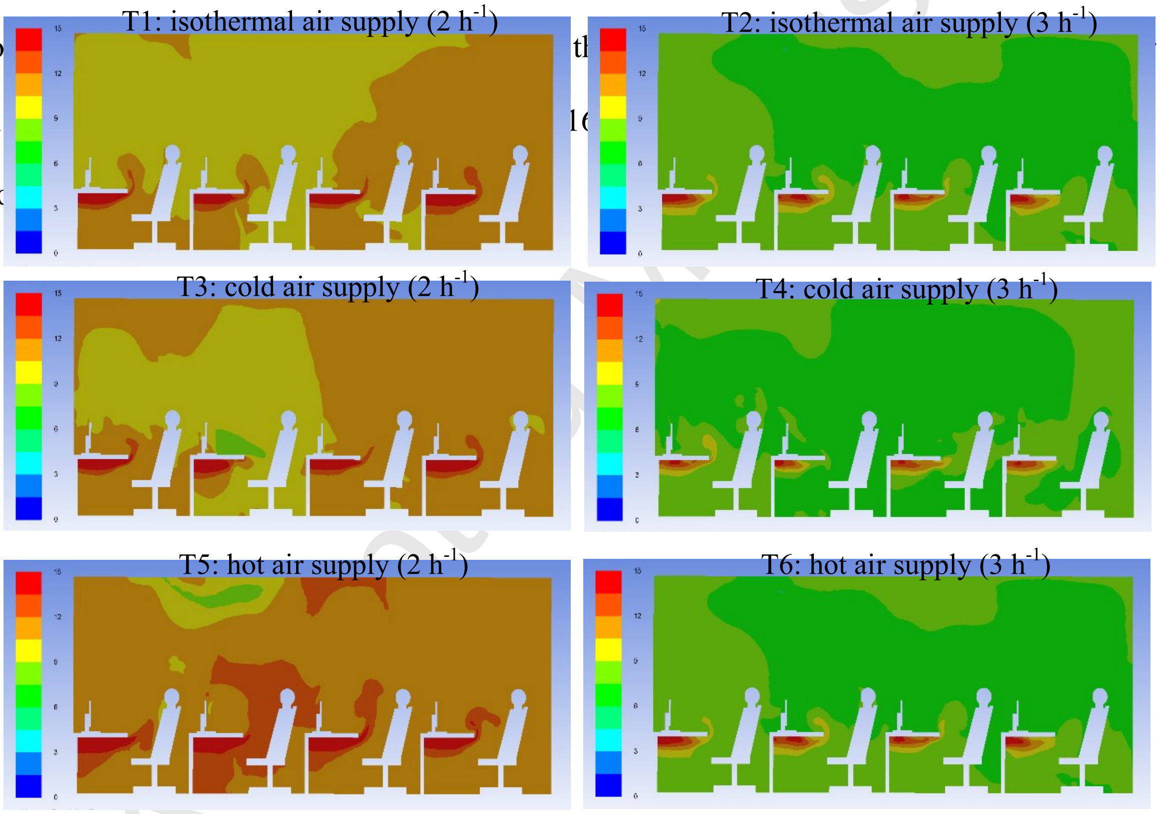

T1: isothermal air supply (2 h^{-1})
T2: isothermal air supply (3 h^{-1})
T3: cold air supply (2 h^{-1})
T4: cold air supply (3 h^{-1})
T5: hot air supply (2 h^{-1})
T6: hot air supply (3 h^{-1})

Fig. 6. O-xylene concentrations (µg/m^3)

Finally, the same comments can be made concerning the toluene dispersion in the office (Fig. 8). However, it is worth noting that in this case the concentrations in the occupied zone are the most homogenous and this occurs for all 6 configurations analysed. This can be explained by the fact that the toluene has the greatest diffusion coefficient in air of all 5 VOCs considered.

On the other hand, for all configurations taken into consideration, VOCs concentration levels in the occupied zone of the room (including peak values - Table 5) and even in the breathing zone of the occupants (Table 6) are well below the occupational exposure limits established by different organisms (Table 7): 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, 2015). In addition, these results confirm the experimental data summarised in (Levin and Hodgson, 2006).

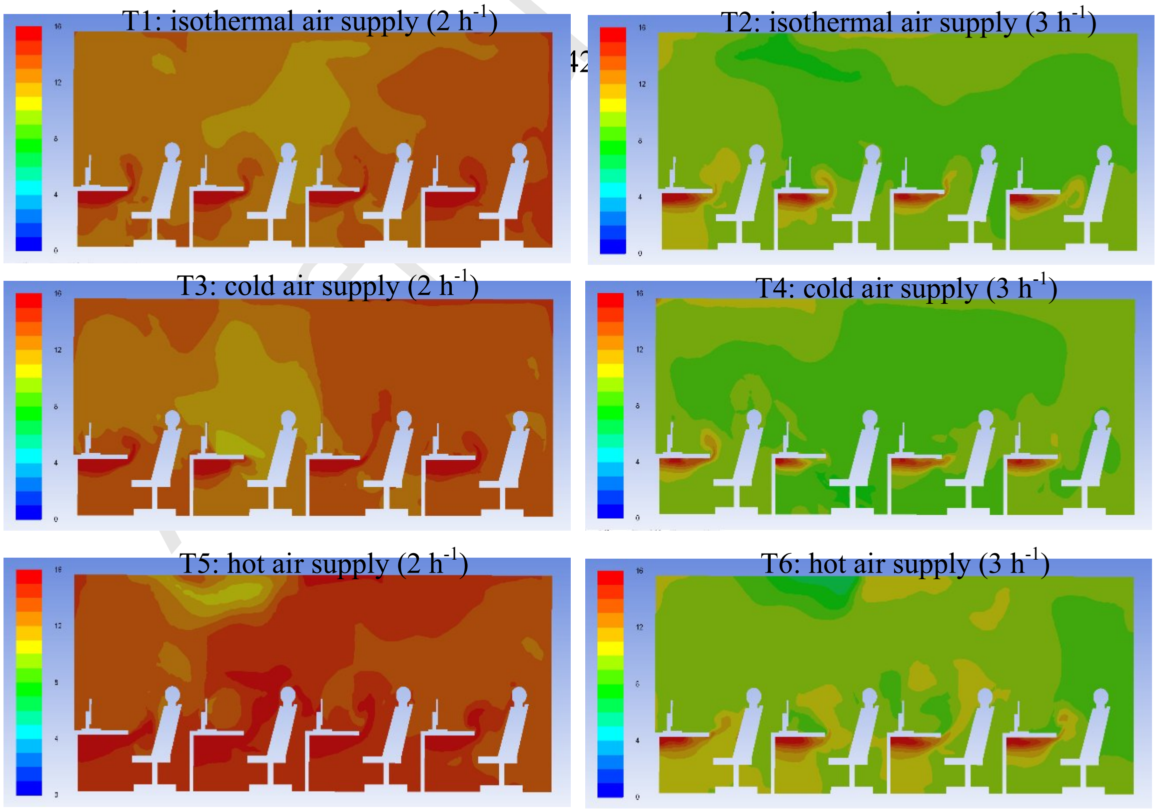
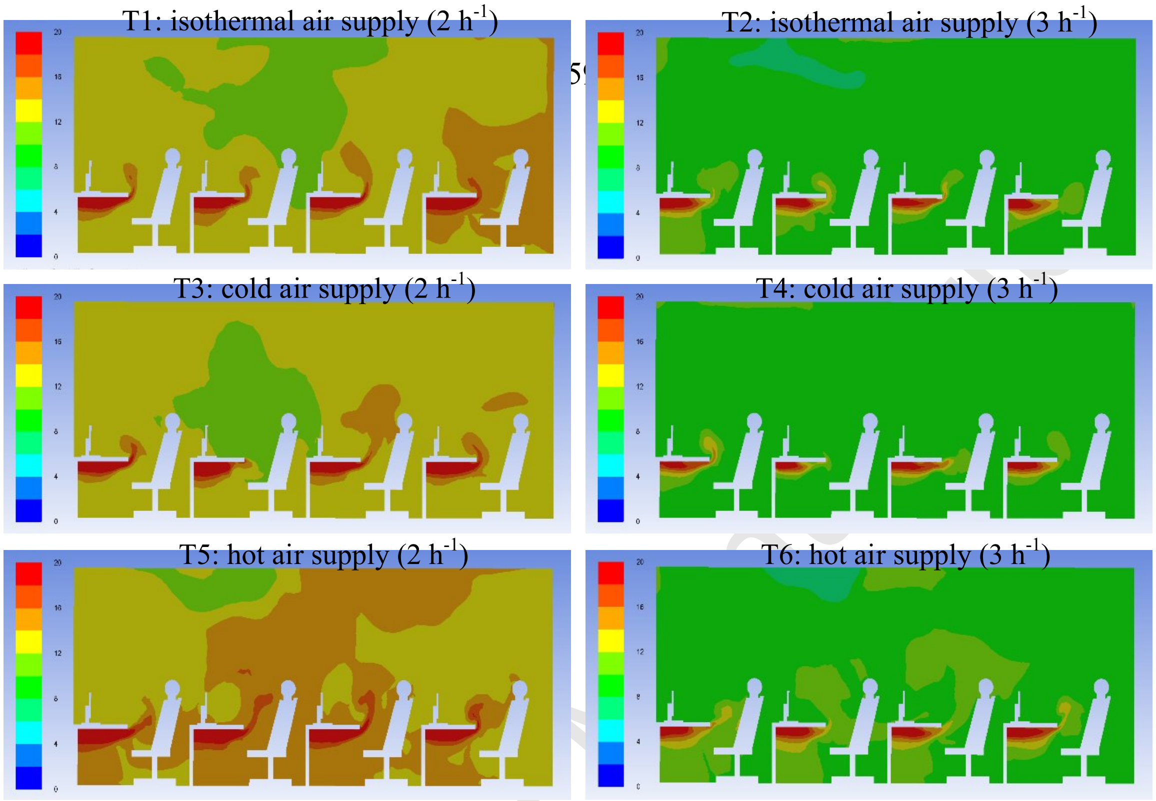


Fig. 7. Styrene concentrations (μg/m^3)


T1: isothermal air supply (2 h^{-1})

T2: isothermal air supply (3 h^{-1})

T3: cold air supply (2 h^{-1})

T4: cold air supply (3 h^{-1})

T5: hot air supply (2 h^{-1})

T6: hot air supply (3 h^{-1})

Fig. 8. Toluene concentrations (μg/m^3)

Table 5. Concentrations of VOCs in the occupied zone

Test	VOC	Average value ($\mu g/m^3$)	Maximum value ($\mu g/m^3$)
T1: isothermal air supply (2 air changes per hour)	benzaldehyde	9.0	16.4
	ethylbenzene	13.9	51.0
	o-xylene	10.6	34.8
	styrene	12.8	36.6
	toluene	13.0	59.8
T2: isothermal air supply (3 air changes per hour)	benzaldehyde	6.6	14.3
	ethylbenzene	10.0	55.1
	o-xylene	7.6	37.2
	styrene	9.3	38.4
	toluene	9.3	66.0
T3: cold air supply (2 air changes per hour)	benzaldehyde	9.0	17.8
	ethylbenzene	13.8	51.9
	o-xylene	10.4	35.6
	styrene	12.7	37.5
	toluene	12.8	60.7
T4: cold air supply (3 air changes per hour)	benzaldehyde	6.3	12.2
	ethylbenzene	9.8	46.0
	o-xylene	7.4	31.2
	styrene	9.0	32.4
	toluene	9.2	54.8
T5: hot air supply (2 air changes per hour)	benzaldehyde	10.0	17.8
	ethylbenzene	15.1	58.0
	o-xylene	11.5	39.6
	styrene	14.0	41.6
	toluene	14.0	67.9
T6: hot air supply (3 air changes per hour)	benzaldehyde	6.7	15.0
	ethylbenzene	10.3	52.2
	o-xylene	7.8	35.3
	styrene	9.5	36.5
	toluene	9.6	62.2

Table 6. Concentrations of VOCs in the breathing zone (10 cm. in front of the occupant's head)

Test	VOC	Occupant 1 (µg/m^3)	Occupant 2 (µg/m^3)	Occupant 3 (µg/m^3)	Occupant 4 (µg/m^3)
T1: isothermal air supply (2 air changes per hour)	benzaldehyde	9.1	8.5	9.0	9.8
	ethylbenzene	13.6	13.0	14.1	15.0
	o-xylene	10.3	9.9	10.7	11.4
	styrene	12.6	12.0	12.9	13.8
	toluene	12.5	12.1	13.2	14.0
T2: isothermal air supply (3 air changes per hour)	benzaldehyde	6.8	6.1	6.2	6.2
	ethylbenzene	10.3	9.2	9.4	9.3
	o-xylene	7.9	7.0	7.1	7.1
	styrene	9.6	8.6	8.7	8.6
	toluene	9.6	8.5	8.7	8.6
T3: cold air supply (2 air changes per hour)	benzaldehyde	8.6	8.1	9.6	9.6
	ethylbenzene	13.0	12.3	15.6	14.5
	o-xylene	9.8	9.3	11.7	11.0
	styrene	12.0	11.4	14.1	13.4
	toluene	11.9	11.3	15.0	13.3
T4: cold air supply (3 air changes per hour)	benzaldehyde	6.5	6.1	6.2	6.4
	ethylbenzene	9.9	9.3	9.6	10.1
	o-xylene	7.5	7.0	7.3	7.6
	styrene	9.2	8.6	8.8	9.2
	toluene	9.2	8.6	9.0	9.5
T5: hot air supply (2 air changes per hour)	benzaldehyde	9.6	10.4	10.0	9.8
	ethylbenzene	14.6	16.6	15.0	14.7
	o-xylene	11.1	12.5	11.5	11.2
	styrene	13.5	15.1	14.0	13.7
	toluene	13.5	15.7	14.0	13.5
T6: hot air supply (3 air changes per hour)	benzaldehyde	6.8	6.4	6.9	6.0
	ethylbenzene	10.2	9.7	11.5	8.9
	o-xylene	7.8	7.3	8.6	6.8
	styrene	7.7	7.3	8.6	6.8
	toluene	9.4	9.0	11.0	8.2

Table 7. VOCs occupational exposure limits

VOC	Permissible Exposure Limits – PELs (mg/m^3) (California, 2015)	Threshold Limit Values – TLVs (mg/m^3) (ACGIH, 2015)
benzaldehyde	-	-
ethylbenzene	435	86
o-xylene	435	434

styrene	420	86
toluene	37	75

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 carry out 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 the numerous indoor VOCs sources taken into account, limited dilution volume, and low ventilation rates. On the other hand, the reported maximum concentrations of VOCs taken into account (e.g. toluene) in the occupied zone approach to some extent the levels of concern with respect to odour or sensory irritation (discomfort). In addition, 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.

Acknowledgement

This work was supported by a grant of the Romanian Ministry of Education and Research, CNCS-UEFISCDI, project number PN-II-ID-JRP-RO-FR-2012-0071.

References

ACGIH, 2015	American Conference of Governmental Industrial Hygienists - ACGIH. Threshold Limit Values for Chemical Substances and Physical Agents & Biological Exposure Indices (1st ed.), ACGIH, Cincinnati, Ohio, USA (2015), ISBN-13: 978-1607260776
Alves et al., 2013	C. Alves, T. Nunes, J. Silva, M. Duarte. Comfort Parameters and Particulate Matter (PM$_{10}$ and PM$_{2,5}$) in School Classrooms and Outdoor Air. Aerosol and Air Quality Research, 13 (2013), pp. 1521-1535, ISSN: 1680-8584, doi: 10.4209/aaqr.2012.11.0321
Anderson and Albert, 1998	E.L. Anderson, R.E. Albert. Risk Assessment and Indoor Air Quality (1st ed.), CRC Press, Boca Raton (Fl), USA (1998), ISBN: 1-56670-323-9
Awbi, 2008	H.B. Awbi. Ventilation Systems: Design and Performance (1st ed.), Taylor & Francis, London, UK (2008), ISBN-13: 978-0-419-21700-8
de Blas et al., 2012	M. de Blas, M. Navazo, L. Alonso, N. Durana, M.C. Gomez, J. Iza. Simultaneous indoor and outdoor on-line hourly monitoring of atmospheric volatile organic compounds in an urban building. The role of inside and outside sources. Science of The Total Environment, 426 (2012), pp. 327-335, ISSN: 0048-9697, doi:10.1016/j.scitotenv.2012.04.003
California, 2015	California. Permissible Exposure Limits for Chemical Contaminants (State of California, USA – Department of Industrial Relations). Retrieved June 15, 2015 from https://www.dir.ca.gov/title8/5155table_ac1.html
Corgnati and Perino, 2013	S.P. Corgnati, M. Perino. CFD application to optimise the ventilation strategy of Senate Room at Palazzo Madama in Turin (Italy). Journal of Cultural Heritage, 14(1) (2013), pp. 62-69, doi: 10.1016/j.culher.2012.02.007
Dales et al., 2008	R. Dales, L. Liu, A.J. Wheeler, N.L. Gilbert. Quality of indoor

	residential air and health. Canadian Medical Association Journal, 179(2) (2008), pp. 147-152, doi: 10.1503/cmaj.070359
Helmis et al., 2007	C.G. Helmis, E. Adam, J. Tzoutzas, H.A. Flocas, C.H. Halios, O.I. Stathopoulou, V.D. Assimakopoulos, V. Panis, M. Apostolatou, G. Sgouros. Indoor air quality in a dentistry clinic. Science of the Total Environment, 377(2) (2007), pp. 349-365, doi:10.1016/j.scitotenv.2007.01.100
Hussain et al., 2012	S. Hussain, P.H. Oosthuizen, A. Kalendar. Evaluation of various turbulence models for the prediction of the airflow and temperature distributions in atria. Energy and Buildings, 48 (2012), pp. 18-28, doi: 10.1016/j.enbuild.2012.01.004
Kowalska et al., 2015	J. Kowalska, M. Szewczyńska, M. Pośniak. Measurements of chlorinated volatile organic compounds emitted from office printers and photocopiers. Environmental Science and Pollution Research, 22(7) (2015), pp. 5241-5252, doi: 10.1007/s11356-014-3672-3
Levin and Hodgson, 2006	H. Levin, A.T. Hodgson. VOC Concentrations of Interest in North American Offices and Homes. In: Proceedings of Healthy Buildings 2006, Lisbon, Portugal, vol. 3, pp. 233-238.
Maddalena et al., 2011	R. Maddalena, T. McKone, H. Destaillats, M. Rusell, A. Hodgson, C. Perino. Quantifying Pollutant Emissions from Office Equipment: A Concern in Energy-Efficient Buildings. California Energy Commission, PIER Energy-Related Environmental Research, CEC-500-2011-046 (2011)
Manivanan, 2006	R. Manivanan. Recycling of Industrial Effluents (1st ed.), New India Publishing Agency, New Delhi, India (2006)
Maroni et al., 1995	M. Maroni, B. Seifert, T. Lindvall. Indoor Air Quality a Comprehensive Reference Book (1st ed.), Elsevier, Amsterdam, The Netherlands (1995), ISBN: 0-444-81642-9
McGee, 2015	A. McGee. Potential Health Effects from Exposure to VOC Emissions (Institute of Neurotoxicology and Neurological Disorders). Retrieved June 4, 2015 from http://www.toxipedia.org/display/FOC/Potential+Health+Effects+from+Exposure+to+VOC+Emissions
New Jersey, 2015	New Jersey. Chemical Properties for Calculation of Impact to Ground Water Soil Remediation Standards (State of New Jersey, USA – Department of Environmental Protection). Retrieved June 10, 2015 from http://www.nj.gov/dep/srp/guidance/rs/chemproperties.pdf
van Hooff et al., 2013	T. van Hooff, B. Blocken, G.J.F. van Heijst. On the suitability of steady RANS CFD for forced mixing ventilation at transitional slot Reynolds

	numbers. Indoor Air, 23 (2013), pp. 236–249, doi:10.1111/ina.12010
Stamou and Katsiris, 2006	A. Stamou, I. Katsiris. Verification of a CFD model for indoor airflow and heat transfer. Building and Environment, 41(9) (2006), pp. 1171-1181, doi: 10.1016/j.buildenv.2005.06.029
Stathopoulou and Assimakopoulos, 2008	O.I. Stathopoulou, V.D. Assimakopoulos. Numerical Study of the Indoor Environmental Conditions of a Large Athletic Hall Using the CFD Code PHOENICS. Environmental Modeling & Assessment, 13(3) (2008), pp. 449-458, doi: 10.1007/s10666-007-9107-5
Teodosiu et al., 2014	C. Teodosiu, V. Ilie, R. Teodosiu. Appropriate CFD turbulence model for improving indoor air quality of ventilated spaces. Mathematical Modelling in Civil Engineering, 10(4) (2014), pp. 28-42, doi: 10.2478/mmce-2014-0020
Yang et al., 2009	D.S. Yang, S.V. Pennisi, K. Son, S.J. Kays. Screening indoor plants or volatile organic pollutant removal efficiency. HortScience, 44(5) (2009), pp. 1377-1381, ISSN: 0018-5345
Yang et al., 2014	L. Yang, M. Ye, B.J. He. CFD simulation research on residential indoor air quality. Science of the Total Environment, 472 (2014), pp. 1137-1144, doi: 10.1016/j.scitotenv.2013.11.118
Wang et al., 2011	Z.M. Wang, J. Wagner, S. Wall. Characterization of Laser Printer Nanoparticle and VOC Emissions, Formation Mechanisms, and Strategies to Reduce Airborne Exposures. Aerosol Science and Technology, 45(9) (2011), pp. 1060-1068, doi:10.1080/02786826.2011.580799
Zhuang et al,, 2014	R. Zhuang, X. Li, J. Tu. CFD study of the effects of furniture layout on indoor air quality under typical office ventilation schemes. Building Simulation, 7(3) (2014), pp. 263-275, doi: 10.1007/s12273-013-0144-5