



Evaluation and investigation of the effects of ventilation layout, rate, and room temperature on pollution dispersion across a laboratory indoor environment

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Abstract

The presence of chemicals in laboratories and research centers exposes the staff working at such indoor environment to health risks. In this piece of research, a study was performed on the indoor environment of the Center for Environmental Engineering Research at Sahand University of Technology (Tabriz, Iran). For this purpose, the parameters affecting the dispersion of volatile organic compounds (VOCs), including ventilation rate, room temperature, pollution emission time, venting location, air flow regime within the indoor environment, and the number of vents, were simulated via CFD modeling. The CFD modeling was performed three-dimensionally in unsteady state. In case of turbulent flow within the indoor environment, $k-\epsilon$ turbulence model was used to obtain air velocity profile. Experimental data was used to validate the model. Results of the present research showed that when the venting location is on the ceiling, pollution concentration of 25 ppm can be achieved at some low temperature under a particular set of conditions. However, when the venting location was on the walls close to the pollution source, concentrations as low as 5 ppm and lower were observed within the laboratory indoor environment.

Keywords Indoor air quality · CFD · Ventilation · Laboratory · VOC

Introduction

People spend most of their time in indoor environments. This is while, according to studies performed by numerous researchers, the level of pollution in indoor environments is in many cases higher than that in outdoor environments (Goyal and Kumar 2013; Krugly et al. 2014; Lee et al. 1999; Loupa et al. 2007; Patnaik et al. 2018; Zhang et al. 2018). Being exposed to chemicals, laboratories are often more polluted than other indoor environments (e.g., residents, offices, schools, etc.) by several folds. Accordingly, the laboratory staff are exposed to a high level of health risk (Davardoost and Kahforoushan 2018; Gammage 2018; Lerner et al. 2018).

Volatile organic compounds (VOCs) are among the most widely used chemicals in laboratories. Due to their high vapor pressure, low boiling point at room temperature, and high coefficient of diffusion into air, VOCs such as benzene, toluene, and formaldehyde tend to disperse through indoor environment air readily, thereby affecting indoor air quality (IAQ) (Edwards et al. 2001; Lewis 1991; Salthammer et al. 2018; Wolkoff 1995; Wolkoff and Nielsen 2001; Wolkoff et al. 2006). Exposure to chemicals such as VOCs, particularly benzene, can end up with numerous health problems (Bono et al. 2003; Capleton and Levy 2005; Norton et al. 2018; Sarigiannis et al. 2011). As such, it is necessary to evaluate the diffusion of such compounds in laboratory indoor environment accurately. Given the wide spectrum of already discovered VOCs, it is very difficult and time-intensive to consider every single one of them separately. Accordingly, in this research, in order to develop an understanding of the amount and dispersion mechanism of VOCs, benzene was selected as a representative VOC.

Following the same line of research, some researchers have concluded that smoking, surfactants, chemical solvents, dyes, sterilizing agents, and combustion products are among the

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sources of VOC emission (Annesi-Maesano et al. 2013; Baya et al. 2004; Begum et al. 2009; Fromme et al. 2008; Lagoudi et al. 1996; Lerner et al. 2018; Lewis 1991; Norton et al. 2018; Su et al. 2018; Wolkoff 1995; Yoon et al. 2011).

Investigation and evaluation of air quality within different types of indoor environment have been the subject of numerous research works. Among others, a research performed in Norway explored the exposure to organic solvents in seven offset printing houses based on NIOSH-1501. The results indicated that the concentration of toluene and exposure to benzene were two to four and one to two times larger than the limits set in the NIOSH standard, respectively. Given that the organic solvent used in this study was alcohol-based, 10% isopropanol was identified as the third dominant pollutant emitted when washing the printing rolls in the printing house (Svendsen and Rognes 2000). A research performed by Baya et al. to measure and evaluate the concentration of 16 VOCs in indoor environment of 25 houses in Athena, mean, median, maximum, and minimum values of the concentration of the 16 VOCs were estimated using a total of 324 samples on seasonal, daily, and hourly bases. The obtained results indicated that 16 VOCs (including aliphatic and branched alkanes, aromatic and cyclic compounds) comprised 50% of the measured VOCs; it was further found that concentration of the VOCs was maximal in winter time (Baya et al. 2004). Guo et al. evaluated the health risk associated with exposure to VOCs in indoor environment in Hong Kong. For this purpose, four groups of people were selected, including the staff working at restaurant, office staff, housewives, and pupils. The main objective of their research was to identify the most risky location for the staff. The authors ended up concluding that the staff working at restaurant suffered from the highest risk of cancer when exposed to chloroform (Guo et al. 2004). Ramos et al. examined the contents of CO₂, CO, VOC, and O₃ at 11 fitness gyms across the city of Lisbon using a WolfSense apparatus. The results indicated that, in order to reduce the athletes' exposure to air pollutants as they practice, the HVAC system and ventilation rate shall be optimized (Ramos et al. 2014). Lee et al. evaluated the rate of pollutions emitted from office equipment, such as fax set, laser printers, inkjet printers, scanners, and photocopiers. The measured pollutants included VOCs, TVOC, ozone, PM₁₀, m,p-xylene, and styrene. According to the results, among other VOCs, toluene, ethyl benzene, and styrene exhibited high concentrations. In addition, emission rate of ozone and VOC was higher from laser printers rather than inkjet ones (Lee et al. 2001). In a research where indoor air quality (IAQ) was investigated and compared between museums, printing industry, and offices, it was concluded that PM_{2.5}, benzene, toluene, SO₂, and NO₃ exhibit the highest concentrations in printing industry. Formaldehyde exhibited the highest concentration at museums, and O₃ was the most concentrated pollutant in non-smoking offices. This was while the lowest concentration in

printing industry was that of O₃. It is worth mentioning that, in addition to the activities, machineries, and equipment used in these industries, the location within each environment is of paramount importance when it comes to the indoor air pollution (Saraga et al. 2011). Zhuang et al. presented a validated CFD model where IAQ was investigated within an office room with different ventilation and furniture layouts. According to the results presented based on this model, furniture layout inside the building acts as an important factor affecting the ventilation effectiveness and IAQ. Therefore, adjustment of the furniture layout can be very useful for improving air quality within breathing zone (Zhuang et al. 2014).

Working with chemicals, the staff working at research centers and laboratories are at serious health risks (Convertino et al. 2018; Spurgeon et al. 1997; Su et al. 2018). However, based on the abovementioned studies, it is inferred that, in contrary to the numerous research works performed on air pollution monitoring in indoor environments, smaller deals of attention have been paid to research centers and laboratories. As such, the present research discusses the factors affecting the dispersion of benzene, as an example of high-risk chemicals negatively impacting human health, in laboratory indoor environment. Using CFD modeling, effects of different parameters including openness/closeness of openings, ventilation rate, number of vents, venting location, and temperature on the dispersion of pollution were investigated. The $k-\epsilon$ turbulence model was used to model air flow under turbulent regime.

Methodology

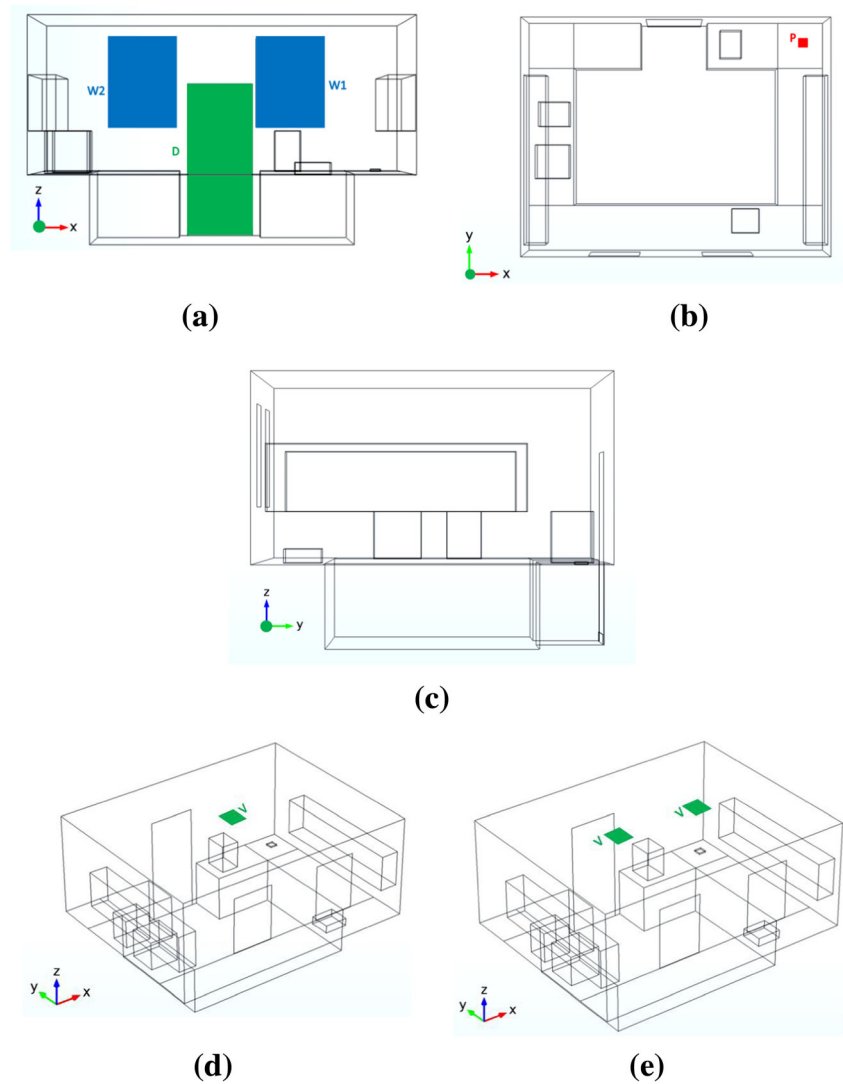
Geometry of case study

Figure 1 depicts the studied geometry. Dimensions of the room, door, windows, pollution source, and ventilation are given in Table 1. The symbols P, W₁, W₂, D, and V in Fig. 1 denote pollution source, window #1, window #2, door, and ceiling vent. It should be noted that the dimensions herein considered for the contamination source were not equal to the dimensions of the laboratory dishes containing the VOCs, but rather part of the cross-sectional area of the laboratory dishes and also compared to the test environment (the place into which the contamination is dispersed); the test pollutant source's dimensions were negligible in terms of environment dimensions, and given that the alteration of dimensions for various test equipment is very small, then minor changes in the dimensions of leakage may not impose any significant effect on the amount and dispersion of VOCs.

Governing equations

Pollution dispersion proceeds mainly through molecular diffusion and convection mechanism. In order to simulate air flow

Fig. 1 Geometry of case study (a) Z-X view, no ventilation; (b) Y-X view, no ventilation; (c) Z-Y view, no ventilation; (d) 3D view, one ventilation; and (e) 3D view, two ventilations



under turbulent flow regime, $k-\varepsilon$ turbulence model was used (Eqs. (1)–(5)) (Anderson and Wendt 1995; Bergman and Incropera 2011; Cussler 2009; Hirsch 2007; Hoffmann and Stein 2002; Kassomenos et al. 2008; Panagopoulos et al. 2011; Stathopoulou and Assimakopoulos 2008; Treybal 1980; Wendt 2008; Wilcox 1998; Wilcox 2008; Zhang and Niu 2004).

Continuity equation:

$$\frac{\partial u_i}{\partial x_i} = 0 \quad (1)$$

Table 1 Dimensions of different parts of the studied indoor environment

| | |
|------------------|--------------------------|
| Room | 4.85 m × 3.75 m × 2.91 m |
| Pollution source | 0.14 m × 0.14 m × 0.03 m |
| Door | 2.10 m × 1.00 m |
| Windows | 1.10 m × 0.80 m |
| Ventilations | 0.3 m × 0.3 m |

Momentum conservation equation

$$\rho \frac{\partial u_j}{\partial t} + \rho u_i \frac{\partial u_j}{\partial x_i} = -\frac{\partial p}{\partial x_j} + \mu \frac{\partial^2 u_j}{\partial x_i^2} + \rho g_j \quad (2)$$

Equation of continuity for species of benzene

$$C \frac{\partial x_\alpha}{\partial t} + C u_i \frac{\partial x_\alpha}{\partial x_i} = C D_{\alpha\beta} \frac{\partial^2 x_\alpha}{\partial x_i^2} + r_\alpha \quad (3)$$

Transport conservation equation for k and e

$$\rho \frac{\partial k}{\partial t} + \rho u_i \frac{\partial k}{\partial x_i} = \frac{\partial}{\partial x_i} \left[\frac{\mu_t}{\sigma_k} \frac{\partial k}{\partial x_i} \right] + G_k + G_b - \varepsilon \quad (4)$$

$$\rho \frac{\partial \varepsilon}{\partial t} + \rho u_i \frac{\partial \varepsilon}{\partial x_i} = \frac{\partial}{\partial x_i} \left[\frac{\mu_t}{\sigma_\varepsilon} \frac{\partial \varepsilon}{\partial x_i} \right] + C_{\varepsilon 1} \frac{\varepsilon}{k} (G_k + G_b) - C_{\varepsilon 2} \frac{\varepsilon^2}{k} \quad (5)$$

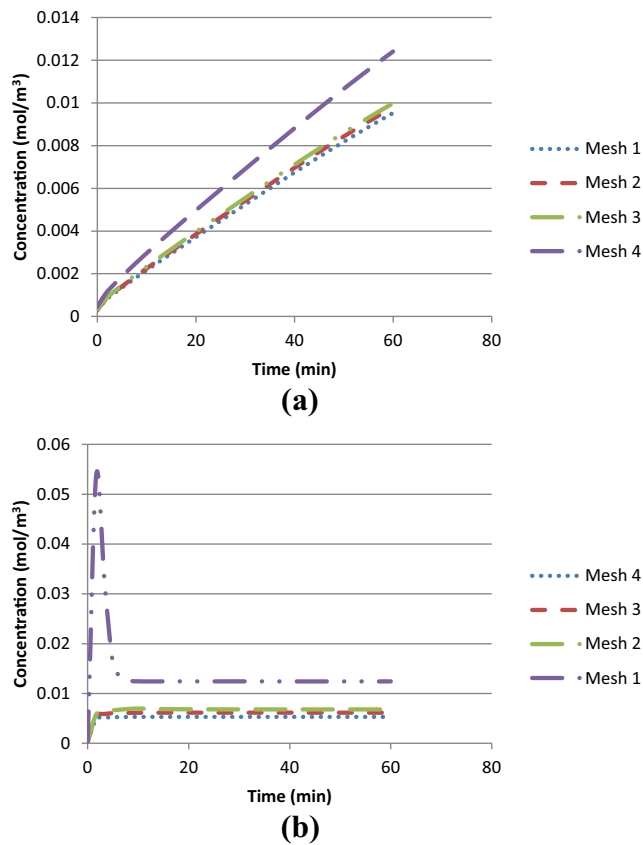


Fig. 2 Average concentration of acetone in room versus time. (a) CFD modeling results for laminar flow when only one of the windows is open and the door is closed with no ventilation. (b) CFD modeling results for turbulent flow inside the room when all windows and door are open and still there is no ventilation. Mesh 1: 1,075,112 elements, mesh 2: 2,440,389 elements, mesh 3: 7,495,534 elements, and mesh 4: 9,793,942 elements

where u_i is the air flow velocity along x_i direction, ρ is air density, u_j is air flow velocity along x_j direction, t is time, p is air pressure, μ is viscosity, g_j is gravitational acceleration along x_j direction, C is molar concentration of air-benzene mixture, x_α is molar fraction of benzene in air, $D_{\alpha\beta}$ is diffusion coefficient of benzene into air, r_α is volumetric reaction rate, k is turbulence kinetic energy (TKE), ε is TKE loss rate, μ_t is turbulent viscosity, G_k is the kinetic energy produced by buoyancy, and the constants $C_{\varepsilon 1}$ and $C_{\varepsilon 2}$ are herein assumed as 1.44 and 1.92, respectively (Anderson and Wendt 1995; Hoffmann and Stein 2002; Sada and Ichikawa 1993; Teodosiu et al. 2016; Wilcox 1998; Wilcox 2008).

The velocity equation was solved under steady state and no slip condition. In the meantime, continuity equation for

benzene was solved in unsteady state considering the chemical reaction term, because of the assumption of no reaction between benzene and air compounds. Initial and boundary conditions are presented in the following (Eqs. (6)–(12)):

$$C_\alpha|_{t=0} = 0 \tag{6}$$

$$\frac{\partial C_\alpha}{\partial x_i} \Big|_{wall} = 0 \tag{7}$$

$$C_\alpha|_{pollution\ source} = C_\alpha^{sat} \tag{8}$$

$$u|_{wall} = 0 \tag{9}$$

$$Q_{air}|_{window(s)} = Q_i \tag{10}$$

$$Q_{air,outlet}|_{ventilation} = Q_j \tag{11}$$

$$\Delta P|_{door} = 0 \tag{12}$$

Equations (6)–(12) express the following, respectively: zero initial pollution, no pollution diffusion into walls, equality of the concentration on pollution source-air interface and the saturated concentration, zero velocity on the walls, input flow rate through the windows equal to Q_i , output flow rate through vent(s) equal to Q_j (13 m³/h), and zero pressure difference between the room and outdoor environment when the door is open. It is worth noting that, in some cases, the modeling was performed with the door close. In such cases, the air flow infiltrates from the room toward the outdoor environment through a very narrow gap between the door and the ground (~7 cm).

Meshing

In order to investigate the grid number independence of the results, four meshing layouts with different numbers of elements were considered to simultaneously solve the equations of momentum, continuity, and mass transfer. According to Fig. 2, no significant difference was observed in the results between the third and fourth meshing layouts. Figure 2a shows the CFD modeling results for laminar flow when only one of the windows is open and the door is closed with no ventilation. Figure 2b demonstrates the CFD modeling results for turbulent flow inside the room when all windows and door are open and still there is no ventilation. More details on the number and layout of the meshes are reported in Table 2.

CFD modeling was performed using COMSOL software (Guide 1998; Multiphysics 2012). Mass transfer and momentum equations were solved in fully coupled mode. In order to

Table 2 Number and layout of the computational mesh used in CFD model

| Number of elements | Element type | Minimum element quality | Average element quality | Maximum growth rate | Average growth rate |
|--------------------|--------------|-------------------------|-------------------------|---------------------|---------------------|
| 2,440,389 | Tetrahedral | 0.01602 | 0.6251 | 13.95 | 1.823 |

Table 3 Number of runs, symbols related to each run, and conditions considered for each run when the ventilation system is equipped at ceiling

| Run number | Temperature (K) | W2 (m ³ /s) | W1 (m ³ /s) | D | Ventilation (number) | Air flow regime | Symbols |
|------------|-----------------|------------------------|------------------------|-------|----------------------|-----------------|---------|
| 1 | 298 | 0.01 | 0.01 | Open | 0 | Laminar | LWWD0 |
| 2 | 298 | 0 | 0.01 | Open | 0 | Laminar | L0WD0 |
| 3 | 298 | 0 | 0.01 | Close | 0 | Laminar | L0W00 |
| 4 | 298 | 0.01 | 0.01 | Close | 0 | Laminar | LWW00 |
| 5 | 298 | 0.01 | 0 | Open | 0 | Laminar | LW0D0 |
| 6 | 298 | 0.01 | 0 | Close | 0 | Laminar | LW000 |
| 7 | 298 | 0.01 | 0.01 | Close | 1 | Laminar | LWW01 |
| 8 | 298 | 0.01 | 0.01 | Close | 2 | Laminar | LWW02 |
| 9 | 298 | 0.01 | 0 | Close | 1 | Laminar | LW001 |
| 10 | 298 | 0.01 | 0 | Close | 2 | Laminar | LW002 |
| 11 | 298 | 0 | 0 | Close | 1 | Laminar | L0001 |
| 12 | 298 | 0 | 0 | Close | 2 | Laminar | L0002 |
| 13 | 298 | 0.05 | 0.05 | Open | 0 | Turbulent | TWWD0 |
| 14 | 298 | 0 | 0.05 | Open | 0 | Turbulent | T0WD0 |
| 15 | 298 | 0 | 0.05 | Close | 0 | Turbulent | T0WD0 |
| 16 | 298 | 0.05 | 0.05 | Close | 0 | Turbulent | TWW00 |
| 17 | 298 | 0.05 | 0 | Open | 0 | Turbulent | TW0D0 |
| 18 | 298 | 0.05 | 0 | Close | 0 | Turbulent | TW000 |
| 19 | 298 | 0.05 | 0.05 | Close | 1 | Turbulent | TWW01 |
| 20 | 298 | 0.05 | 0.05 | Close | 2 | Turbulent | TWW02 |
| 21 | 298 | 0.05 | 0 | Close | 1 | Turbulent | TW001 |
| 22 | 298 | 0.05 | 0 | Close | 2 | Turbulent | TW002 |
| 23 | 298 | 0 | 0 | Close | 1 | Turbulent | T0001 |
| 24 | 298 | 0 | 0 | Close | 2 | Turbulent | T0002 |
| 25 | 268 | 0.01 | 0.01 | Open | 0 | Laminar | LWWD0 |
| 26 | 268 | 0 | 0.01 | Open | 0 | Laminar | L0WD0 |
| 27 | 268 | 0 | 0.01 | Close | 0 | Laminar | L0W00 |
| 28 | 268 | 0.01 | 0.01 | Close | 0 | Laminar | LWW00 |
| 29 | 268 | 0.01 | 0 | Open | 0 | Laminar | LW0D0 |
| 30 | 268 | 0.01 | 0 | Close | 0 | Laminar | LW000 |
| 31 | 268 | 0.01 | 0.01 | Close | 1 | Laminar | LWW01 |
| 32 | 268 | 0.01 | 0.01 | Close | 2 | Laminar | LWW02 |
| 33 | 268 | 0.01 | 0 | Close | 1 | Laminar | LW001 |
| 34 | 268 | 0.01 | 0 | Close | 2 | Laminar | LW002 |
| 35 | 268 | 0 | 0 | Close | 1 | Laminar | L0001 |
| 36 | 268 | 0 | 0 | Close | 2 | Laminar | L0002 |
| 37 | 268 | 0.05 | 0.05 | Open | 0 | Turbulent | TWWD0 |
| 38 | 268 | 0 | 0.05 | Open | 0 | Turbulent | T0WD0 |
| 39 | 268 | 0 | 0.05 | Close | 0 | Turbulent | T0W00 |
| 40 | 268 | 0.05 | 0.05 | Close | 0 | Turbulent | TWW00 |
| 41 | 268 | 0.05 | 0 | Open | 0 | Turbulent | TW0D0 |
| 42 | 268 | 0.05 | 0 | Close | 0 | Turbulent | TW000 |
| 43 | 268 | 0.05 | 0.05 | Close | 1 | Turbulent | TWW01 |
| 44 | 268 | 0.05 | 0.05 | Close | 2 | Turbulent | TWW02 |
| 45 | 268 | 0.05 | 0 | Close | 1 | Turbulent | TW001 |
| 46 | 268 | 0.05 | 0 | Close | 2 | Turbulent | TW002 |
| 47 | 268 | 0 | 0 | Close | 1 | Turbulent | T0001 |
| 48 | 268 | 0 | 0 | Close | 2 | Turbulent | T0002 |

check the effects of different parameters on pollution dispersion in indoor environment, the model was run under different sets of conditions. Table 3 provides a list of the symbols and conditions investigated in each run.

The backward differential formula (BDF) was used to solve unsteady modeling. In this method, the values of initial step, maximum step, maximum BDF order, minimum BDF order, and fraction of initial step for backward Euler were found to be 0.001, 0.1, 2, 1, and 0.001, respectively.

Along the last column of Table 3 (the symbols), each run is designated by a five-character code. The characters indicate flow type (L = laminar, T = turbulent), openness/closeness of the window W1 (0 = closed, W = open), openness/closeness of the window W2 (0 = closed, W = open), openness/closeness of the door (0 = closed, D = open), and number of vents (0 = without ventilation, 1 = one ventilation at roof, 2 = two ventilations at roof).

Validation

In order to validate the model, acetone was used as a representative pollutant, because exposure to and working with benzene is known to raise serious health risks. Moreover, acetone is a VOC with volatility (diffusion coefficient and saturated concentration) close to benzene, widely available, and vastly used in different laboratories, making it a good candidate for validating the model. Governing equations (Eqs. (1)–(5)), boundary conditions, and initial conditions used to model the dispersion of acetone are the same as those adopted for benzene. In other words, similar to benzene, acetone is a volatile organic compound (VOC); the only differences were that, compared to benzene, the acetone was much safer in terms of testing and exposure. Experiments were performed in the temperature

range of 25–27 °C (room temperature) under four sets of conditions representing different air flow regimes, ventilation rates, and numbers of vents in an indoor environment. Air flow and room temperature measurements were performed using hot wire anemometer, and acetone concentration was measured using an online VOC concentration measurement tool (PID) with the capability of storing the recorded data and transferring them to a PC. Measurements were performed at three points: (A) center of the room, (B) a point at 1-m distance to the point A along positive x-axis, and (C) a point at 1-m distance to the point A along positive y-axis. The three points were at the breathing height (1.5 m).

For solving Eqs. (1)–(12), diffusion coefficient of acetone into air and saturated concentration of acetone were considered as $0.1049 \times 10^{-4} \text{ m}^2/\text{s}$ and $11 \text{ mol}/\text{m}^3$ (Lugg 1968; Pashley et al. 1998), respectively. Each test was conducted in three or four replications, and average values were reported. Moreover, experimental data were modeled and compared following 30 and 60 min of start of the pollution emission in indoor environment, with the results reported in Table 4. The results tabulated in Table 4 indicate that the experimental data and modeling results are in agreement. As such, the proposed model can be used to predict benzene concentration distribution in laboratory indoor environment.

Using Eqs. (13) and (14), the agreement between the model results and corresponding experimental data was examined based on R^2 and normalized mean square error (NMSE) (Abdoli et al. 2018a, b; Roy 2010).

$$R^2 = \frac{\sum_{i=1}^N (C_i^{exp} - C_a^{exp})^2 - \sum_{i=1}^N (C_i^{exp} - C_i^{model})^2}{\sum_{i=1}^N (C_i^{exp} - C_a^{exp})^2} \tag{13}$$

Table 4 Comparison of modeling results and experimental data

| Symbols | Ventilation rate (m ³ /s) | Point | Experiment | | | Model | | |
|---------|--------------------------------------|-------|------------|-------------------|-------------------|----------------------|-------------------|-------------------|
| | | | u (m/s) | c (ppm) at 30 min | c (ppm) at 60 min | u (m/s) | c (ppm) at 30 min | c (ppm) at 60 min |
| LWWD0 | 0.014–0.016 | A | 0.00–0.00 | 38.11 | 902.10 | 0.00178 | 41.00 | 937.89 |
| | | B | 0.00–0.01 | 201.05 | 715.36 | 0.00499 | 193.76 | 747.71 |
| | | C | 0.00–0.01 | 3.54 | 68.88 | 0.00321 | 03.93 | 72.57 |
| LW000 | 0.007–0.01 | A | 0.00–0.02 | 4.35 | 321.39 | 0.00128 | 06.77 | 370.94 |
| | | B | 0.00–0.01 | 23.36 | 174.96 | 6.0×10^{-4} | 30.016 | 183.01 |
| | | C | 0.00–0.01 | 7.19 | 159.74 | 0.00140 | 05.41 | 165.312 |
| TWWD0 | 0.07–0.1 | A | 0.00–0.02 | 111.32 | 114.59 | 0.00685 | 121.50 | 122.44 |
| | | B | 0.00–0.04 | 238.38 | 244.01 | 0.01881 | 252.22 | 255.37 |
| | | C | 0.02–0.04 | 169.15 | 175.23 | 0.01655 | 176.51 | 180.32 |
| TOW00 | 0.03–0.05 | A | 0.00–0.03 | 87.97 | 100.04 | 0.00844 | 99.23 | 109.54 |
| | | B | 0.01–0.04 | 451.05 | 459.63 | 0.02638 | 441.06 | 437.70 |
| | | C | 0.01–0.03 | 71.73 | 82.94 | 0.01187 | 60.70 | 69.22 |

Table 5 R^2 and NMSE values in four different conditions

| Symbol | R^2 | NMSE |
|--------|-------------|-------------|
| LWWD0 | 0.996804717 | 0.00374248 |
| LW000 | 0.967630512 | 0.002968099 |
| TWWD0 | 0.965736633 | 0.002910174 |
| TOW00 | 0.993935878 | 0.004355468 |

$$\text{NMSE} = \frac{1}{N} \sum_{i=1}^N \frac{(C_i^{\text{model}} - C_i^{\text{exp}})^2}{C_a^{\text{model}} C_a^{\text{exp}}} \quad (14)$$

In the above equations, C_i^{exp} refers to the concentrations measured via experimentation, C_a^{exp} is average value of measured concentrations, C_i^{model} is the concentration predicted by the CFD model, and C_a^{model} is average value of the concentration predicted by the CFD model. The data given in Table 5 indicate the agreement between the experimental data and modeling results. That is, the proposed CFD model can be used to predict the dispersion of various VOCs under different operating conditions.

The simulation for benzene (based on the diffusion coefficient of benzene in the air = $0.0932 \times 10^{-4} \text{ m}^2/\text{s}$ (Lugg 1968)) was performed under the same conditions as those applied for acetone, and the results are presented in Table 6. By comparing the data provided in Table 4 (experimental data and simulation results for acetone) against that in Table 6 (simulation results for benzene), one may observe that, with increasing the ventilation rate, the pollution concentration decreased, as per the simulation results, for both benzene and acetone. Moreover, the pollution concentration increased with time in both of the cases. In general, similar trends of changes in pollution concentration were seen both along the offset (the points A, B, and C) and time axes. The difference between the data reported in Tables 4 and 6 stems from the corresponding difference between diffusion coefficients of acetone and

benzene through air as well as the difference between saturation concentrations of the two substances.

Results and discussion

The amount and evolution of pollution dispersion were investigated for 1 h. In order to investigate the factors affecting benzene dispersion in indoor environment, the proposed CFD model was run for 48 conditions.

Figure 3 shows the influence of closeness/openness of the windows, door, number of the vents at a temperature of 25 °C (298 K), and laminar flow on benzene pollution level at breathing height (1.5 m from the ground). According to Fig. 3, with increasing the number of vents on the ceiling of the laboratory, the level of pollution within breathing height was seen to increase; as such, a change guides the pollution toward the ceiling. The effect is less significant when the door is closed, because the air infiltration through the gap below the door leads the pollution downward to the ground. This parameter was more significantly observed when no vent is incorporated into the ceiling. Based on the results presented in Fig. 3, the pollution would be minimal with LW0D0 ventilation layout, with the pollution level reaching about 30 ppm after 1 h of the start of the emission.

According to OSHA standard, OEL-C, OEL-STEL, and OEL-TWA (indicating short-term exposure limit, 15-min exposure limit, and 8-h exposure limit) for benzene are 25, 5, and 1 ppm, respectively (Capleton and Levy 2005; Hygienists 1986; Values 1996; Williams 2014). Comparing the benzene concentration in the LW0D0 layout with the allowed limits, it is seen that the staff are at health risk upon either short-term or long-term exposure.

Based on Fig. 4, one can see the effects of closeness/openness of the windows, door, number of the vents at a temperature of 25 °C (298 K), and turbulent flow on benzene

Table 6 Modeling results (benzene)

| Symbols | Ventilation rate (m^3/s) | Point | c (ppm) at 30 min | c (ppm) at 60 min |
|---------|--|-------|---------------------|---------------------|
| LWWD0 | 0.014–0.016 | A | 12.55 | 298.27 |
| | | B | 52.57 | 212.22 |
| | | C | 2.78 | 19.18 |
| LW000 | 0.007–0.01 | A | 5.78 | 114.02 |
| | | B | 7.63 | 34.57 |
| | | C | 5.30 | 52.19 |
| TWWD0 | 0.07–0.1 | A | 407.29 | 410.11 |
| | | B | 67.07 | 67.71 |
| | | C | 60.15 | 61.46 |
| TOW00 | 0.03–0.05 | A | 29.71 | 31.41 |
| | | B | 131.14 | 130.85 |
| | | C | 19.36 | 21.08 |

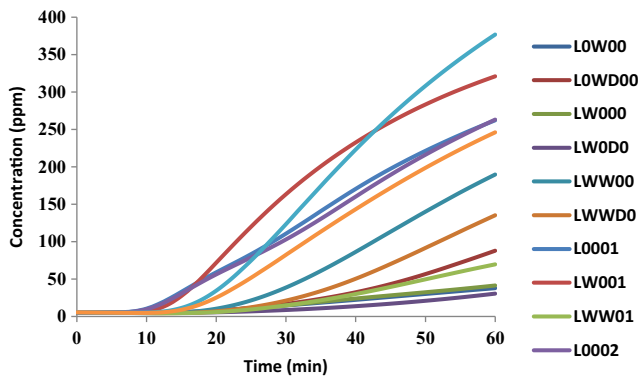


Fig. 3 CFD modeling results for laminar flow ($T=25\text{ }^{\circ}\text{C}$)

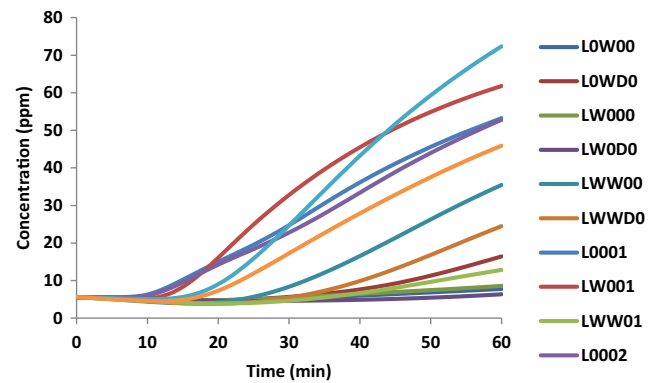


Fig. 5 CFD modeling results for laminar flow ($T=-5\text{ }^{\circ}\text{C}$)

pollution level at breathing height (1.5 m from the ground). The figure indicates that the minimum benzene concentration within breathing zone is seen in the TWW02 layout (56 ppm), which is still higher than the allowed limits. As such, this ventilation layout cannot provide the laboratory with suitable working conditions for the staff.

By comparing Figs. 3 and 4, one can see the effect of air flow on pollution dispersion at 298 K. Upon changing the flow regime from laminar to turbulent, average concentration became uniform rapidly; that is, under turbulent flow regime, variations of average pollution concentration with time are hardly subtle.

Effects of closeness/openness of the windows, door, number of the vents at a temperature of $-5\text{ }^{\circ}\text{C}$ (268 K), and laminar flow on benzene pollution level at breathing height (1.5 m from the ground) can be observed in Fig. 5. According to the figure, the minimum benzene concentration within the indoor environment is seen in the LW0D0 layout (about 6 ppm, OEL-STEL), in which case it is still hard to definitely confirm desirable working conditions for the staff.

The reason behind the similarity between the trends of changes in concentration with time in Figs. 3 and 5 is the similarity in air flow field in the two cases. This is while average concentration at $25\text{ }^{\circ}\text{C}$ is higher than that at $-5\text{ }^{\circ}\text{C}$ under the same air flow regime, which can be explained by the

reduction in coefficient of diffusion and saturated concentration of benzene with decreasing the temperature.

Figure 6 shows the influence of closeness/openness of the windows, door, number of the vents at a temperature of $-5\text{ }^{\circ}\text{C}$ (268 K), and turbulent flow regime on benzene pollution level at breathing height (1.5 m from the ground). According to Fig. 6, the lowest benzene concentration across the laboratory was obtained with TWW01 layout, in which case the benzene content of air reduced to 12 ppm. Comparing Figs. 4 and 6, it can be concluded that an increase in room temperature affects indoor air pollution directly.

According to Figs. 3, 4, 5, and 6, average concentration of the pollution was lower than the allowed limit per OEL-Ceiling (25 ppm) only at 268 K and with L0W00, L0WD0, LW000, LW0D0, LWWD0, LWW00, T0W00, TW000, TW0D0, TWW00, TWWD0, TW001, and TWW01 layouts; that is, short-term exposure under the abovementioned conditions is free of health risk for the staff. Given that the pollution concentration within breathing zone was not below the OEL-TWA and OEL-STEL in all of the layouts, another exhausted ventilation layout is considered in the following.

According to Fig. 7, vents were considered on the two walls close to the pollution source. In order to investigate the effect of layout change in different air flow regimes and at various temperatures, modeling was performed according to

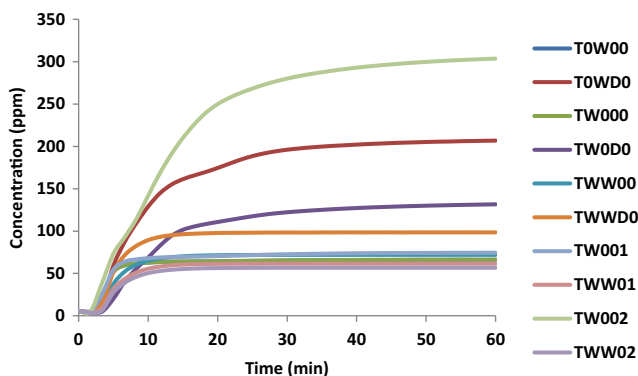


Fig. 4 CFD modeling results for turbulent flow ($T=25\text{ }^{\circ}\text{C}$)

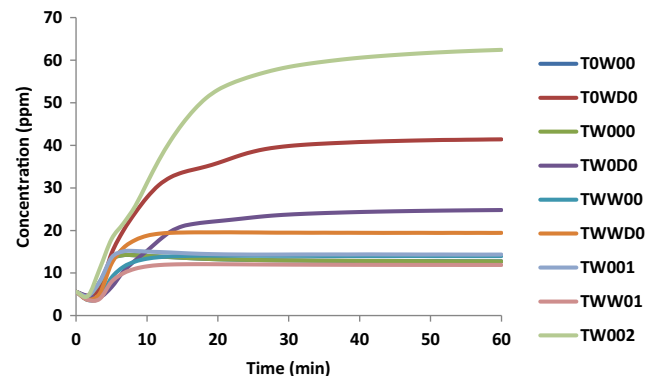


Fig. 6 CFD modeling results for turbulent flow ($T=-5\text{ }^{\circ}\text{C}$)

Fig. 7 Geometry of case study (a) 3D view, vent at ZX plane, and (b) 3D view, vent at YZ plane

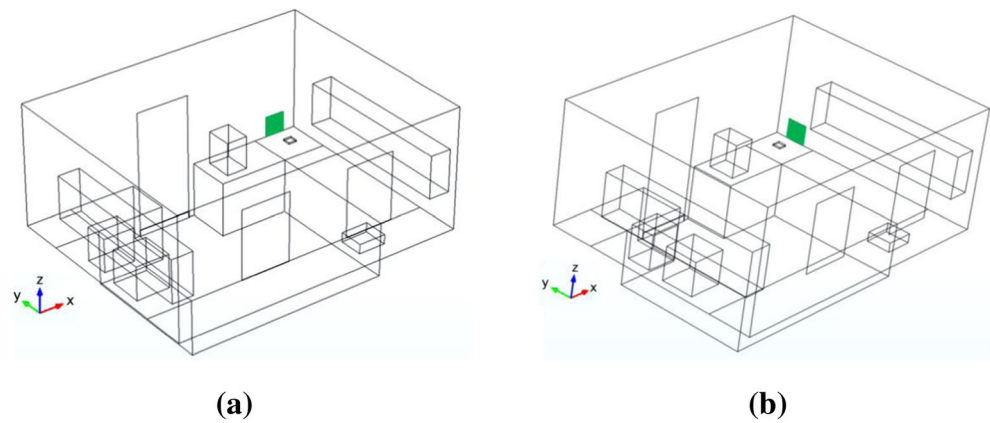


Table 7. The designation practiced in Table 7 follows the same rules used in Table 3, except that the last character in Table 7 refers to the normal vector of the plane in which the exhausted ventilation resides.

Table 8 provides the modeling results when the ventilation is located on the walls close to the pollution source (Fig. 7). The concentrations in breathing zone (1.5 m from the ground) presented in Table 8 refer to 30 and 60 min after the start of emission at 298 and 268 K. According to Table 8, it is observed that, in all layouts where laminar flow is developed in the room, the pollution concentration is less than OEL-STEL (5 ppm).

Comparing the results obtained from Figs. 3, 4, 5, and 6 and those reported in Table 8, it is observed that the change of exhausted ventilation position from the ceiling to the walls close

to the pollution source decreases the pollution content within the breathing zone. If the exhausted ventilation layout is similar to that demonstrated in Fig. 7, the presence and activities of the staff and students in the laboratory will be free of health risk for limited time spans (about 15 min); however, since the pollution concentration is still above OEL-TWA (1 ppm), the presence and activities of the staff and students in the laboratory for long times may end up with health risks for them.

Conclusions

In the present research, in order to investigate the effects of temperature, ventilation layout, number of vents, time, and air

Table 7 Number of runs, symbols related to each run, and conditions considered for each run when the ventilation system is equipped at wall

| Symbol | Air flow regime | Temperature (K) | W2 (m ³ /s) | W1 (m ³ /s) | D | Ventilation plane position |
|--------|-----------------|-----------------|------------------------|------------------------|---|----------------------------|
| L000Y | Laminar | 298 | 0 | 0 | 0 | ZX |
| LW00Y | Laminar | 298 | 0.01 | 0 | 0 | ZX |
| LWW0Y | Laminar | 298 | 0.01 | 0.01 | 0 | ZX |
| TW00Y | Turbulent | 298 | 0.05 | 0 | 0 | ZX |
| TWW0Y | Turbulent | 298 | 0.05 | 0.05 | 0 | ZX |
| L000Y | Laminar | 268 | 0 | 0 | 0 | ZX |
| LW00Y | Laminar | 268 | 0.01 | 0 | 0 | ZX |
| LWW0Y | Laminar | 268 | 0.01 | 0.01 | 0 | ZX |
| TW00Y | Turbulent | 268 | 0.05 | 0 | 0 | ZX |
| TWW0Y | Turbulent | 268 | 0.05 | 0.05 | 0 | ZX |
| L000X | Laminar | 298 | 0 | 0 | 0 | ZY |
| LW00X | Laminar | 298 | 0.01 | 0 | 0 | ZY |
| LWW0X | Laminar | 298 | 0.01 | 0.01 | 0 | ZY |
| TW00X | Turbulent | 298 | 0.05 | 0 | 0 | ZY |
| TWW0X | Turbulent | 298 | 0.05 | 0.05 | 0 | ZY |
| L000X | Laminar | 268 | 0 | 0 | 0 | ZY |
| LW00X | Laminar | 268 | 0.01 | 0 | 0 | ZY |
| LWW0X | Laminar | 268 | 0.01 | 0.01 | 0 | ZY |
| TW00X | Turbulent | 268 | 0.05 | 0 | 0 | ZY |
| TWW0X | Turbulent | 268 | 0.05 | 0.05 | 0 | ZY |

Table 8 Modeling results when the ventilation is located on the walls close to the pollution source

| Symbols | T = 268 K | | T = 298 K | |
|---------|-----------------------------------|-----------------------------------|-----------------------------------|-----------------------------------|
| | Concentration at t = 30 min (ppm) | Concentration at t = 60 min (ppm) | Concentration at t = 30 min (ppm) | Concentration at t = 60 min (ppm) |
| L000Y | 4.942 | 4.257 | 4.933 | 4.235 |
| LW00Y | 4.135 | 3.439 | 4.134 | 3.417 |
| LWW0Y | 2.862 | 1.994 | 2.874 | 2.000 |
| TW00Y | 10.540 | 10.312 | 52.149 | 52.848 |
| TWW0Y | 4.054 | 3.968 | 21.275 | 21.233 |
| L000X | 4.937 | 4.231 | 4.928 | 4.214 |
| LW00X | 4.125 | 3.412 | 4.113 | 3.388 |
| LWW0X | 2.839 | 1.990 | 2.858 | 1.980 |
| TW00X | 12.972 | 12.744 | 65.401 | 66.264 |
| TWW0X | 15.517 | 15.664 | 79.090 | 80.111 |

flow velocity within a room, three-dimensional CFD modeling was performed in unsteady state. The Environmental Engineering Research Center at Sahand University of Technology (Tabriz, Iran) was selected as an experimental indoor environment, representing similar laboratories and research centers. Moreover, knowing that the governing equations for the selected indoor environment hold true for other indoor environments, the results of this research can be generalized to other laboratories and research centers. Differences in the dimensions of similar laboratory environments, as compared to Environmental Engineering Research Center at University of Sahand, may solely affect the geometry rather than the theories and equations governing the dispersion of contamination in the laboratory environment. As such, one can use the governing equations, boundary conditions, modeling approach, and the general results obtained herein for other laboratories and research centers.

Once finished with simulating the model using experimental data, the model results were used to compare the obtained concentrations with the allowed limits by OSHA.

Results of the present research show that, when the vents are located on the ceiling of a room and air flows within the room under either laminar or turbulent regime, pollution concentration within breathing zone may not decrease, due to the driving force generated in such layout. Moreover, with increasing the temperature and air flow velocity in an indoor environment, concentration of pollution within breathing zone increases. In order to achieve pollution concentrations below the OEL-Ceiling (25 ppm), the room temperature should set at 268 K and the ventilation layout should be one of the following: L0W00, L0WD0, LW000, LW0D0, LWW00, LWW01, T0W00, TW000, TW0D0, TWW00, TWW01, TW001, and TWW01. This is while, under none of the mentioned layouts, average pollution concentration within breathing zone does not fall below OEL-TWA or OEL-STEL. As such, another exhausted ventilation layout was considered in this study.

Results of the present research can be used to develop occupational health standards for various types of laboratories and research centers, so as to present not only allowable exposure limits for different occupations but also safe positions within indoor spaces.

According to the results of the present research, if the exhausted ventilation layout is positioned on the walls close to the pollution source, average pollution concentration within breathing zone will be less than 5 ppm, so that the presence and activities of the staff and students in the laboratory will be free of health risk for limited time spans (about 15 min); however, since the pollution concentration is still above OEL-TWA (1 ppm), the presence and activities of the staff and students in the laboratory for longer periods are not recommended.

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