Computational fluid dynamics simulation of formaldehyde emission characteristics and its experimental validation in environment chamber

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Abstract: We investigated the effect of supply air rate and temperature on formaldehyde emission characteristics in an environment chamber. A three-dimensional computational fluid dynamics (CFD) chamber model for simulating formaldehyde emission in twelve different cases was developed for obtaining formaldehyde concentration by the area-weighted average method. Laboratory experiments were conducted in an environment chamber to validate the simulation results of twelve different cases and the formaldehyde concentration was measured by continuous sampling. The results show that there was good agreement between the model prediction and the experimental values within 4.3% difference for each case. The CFD simulation results varied in the range from 0.21 mg/m³ to 0.94 mg/m³, and the measuring results in the range from 0.17 mg/m³ to 0.87 mg/m³. The variation trend of formaldehyde concentration with supply air rate and temperature variation for CFD simulation and experiment measuring was consistent. With the existence of steady formaldehyde emission sources, formaldehyde concentration generally increased with the increase of temperature, and it decreased with the increase of air supply rate. We also provided some reasonable suggestions to reduce formaldehyde concentration and to improve indoor air quality for newly decorated rooms.

Keywords: formaldehyde concentration; environment chamber; computational fluid dynamics simulation; supply air rate; temperature

I Introduction

Acceptable indoor air quality (IAQ) is very important to human health and comfort because most people spend most of their time in indoor environment. In recent years, the awareness of potential IAQ problems has prompted active studies of IAQ. Indoor pollutants, which cannot be perceived, do great harm to occupants’ health. Large quantity of chemical substances are emitted during the initial period of occupancy in newly decorating rooms. Some studies have indicated that these emissions have resulted in headaches, mucous membrane irritations, and dryness of the throat, eyes and nose [1-3]. One of the most common substances in the indoor environment, formaldehyde, has been a matter of concern for over decades. Formaldehyde mean values could be in the range of 334 mg/m³ to 193 mg/m³ and of 86 mg/m³ to 58 mg/m³ in new and old buildings, respectively. This results from the frequent use of this compound as a component of many resins and as preservative [4]. Personal exposure to formaldehyde may cause dizziness, vomiting, and headaches, and in severe cases can lead to dermatitis and asthma [5-6], which can stimulate the mucous membranes of the eyes, nose, and

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throat. Since the formaldehyde has so much harm to the occupants’ health [7], it is necessary to investigate the objective characteristics of formaldehyde emission so as to protect the occupants’ health by reducing the exposure level.

Though various studies have been performed to estimate the emission rate of formaldehyde using the environment chamber [8-9], the effect of supply air velocity and temperature on formaldehyde emission characteristics is still unknown thoroughly. In this paper, we developed a three-dimensional (3D) transient computational fluid dynamics (CFD) model for simulating formaldehyde emission at first, and presented the formaldehyde emission characteristics. Laboratory experiments in 12 different working conditions were conducted in an environment chamber to validate these results. The results indicate that there was a good agreement between the experimental results and the CFD model predictions. Some conclusions can be used in reducing the formaldehyde concentration.

2 CFD simulation

2.1 CFD model

The environmental inner chamber of 9 m in length, 8 m in width, and 5 m in height had a variable air volume (VAV) air-conditioning and mechanical ventilation (ACMV) system, which can control the air temperature, relative humidity (RH), and supply air velocity. The chamber had one velocity inlet and one outlet on its outer surface of chamber. Two cubes (1.3 m×1.3 m×0.4 m) were set inside the chamber, of which the upper surfaces were defined as formaldehyde emission sources (Fig. 1).

![Fig. 1 Schematic of CFD model](image)

Models used in the study were the standard k-ε turbulence model and species model, and the simulation was carried out by Fluent 6.3.26. A uniform hex mesh system was used in all the region of chamber. The interval size was taken as 0.1 unit. The boundary condition of upper surfaces of the two cubes was defined as the mass flow inlet [10], and the formaldehyde concentration was taken as 4.05 mg/m³, which was equal to the concentration caused by 0.5% formaldehyde concentration solution in the experiment. The controlling equations were as follows.

The formaldehyde mass conservation equation is

\[ V \frac{d c_i}{dt} = [V(1 - F_s)u c_i + S dt + F t q c_i] dt, \]

where \( c_i \) is the formaldehyde concentration of indoor air, \( c_o \) is the formaldehyde concentration of outdoor air and was taken as zero, \( V \) is the effective volume of environment chamber, \( F \) is the removal efficiency of purification, \( F_s \) is the removal efficiency of abstersion process, \( u \) is the indoor rate of ventilation, \( S \) is the formaldehyde emission rate, \( t \) is the time, and \( q \) is the volumetric airflow through the purification devices. \( F \) was taken as 0, because there were no purification devices in the environment chamber.

The continuity equation is

\[ \frac{\partial V_i}{\partial X_i} = 0, \]

where \( V_i \) is the unit volume, and \( X_i \) is the unit distance.

The momentum equation is

\[ \frac{\partial \rho V_i}{\partial t} + \frac{\partial (\rho V_i V_j)}{\partial X_j} = - \frac{\partial P}{\partial X_i} + \frac{\partial}{\partial X_j} \left[ \mu_{eff} \left( \frac{\partial V_i}{\partial X_i} + \frac{\partial V_j}{\partial X_j} \right) \right], \]

where \( \mu_{eff} \) is the viscosity coefficient, and \( \mu_{eff} = \mu + \mu_k. \rho \) is the mass density, \( V_i \) is the unit volume of j-direction, \( X_j \) is the unit distance of j-direction, \( X_i \) is the unit distance of i-direction, and \( P \) is the pressure.

\[ \frac{\partial \rho K}{\partial t} + \frac{\partial (\rho V_i K)}{\partial X_i} = \frac{\partial}{\partial X_j} \left[ \left( \mu + \frac{\mu_k}{\sigma_s} \right) \frac{\partial V_i}{\partial X_i} \right] + \mu_k \frac{\partial V_i}{\partial X_j} \left( \frac{\partial V_j}{\partial X_j} + \frac{\partial V_i}{\partial X_i} \right) - \rho \varepsilon, \]

where \( K \) is the dissipation capacity per unit weight, \( \sigma_s \) is the energy dissipation coefficient, and \( \mu \) is the turbulent viscosity.

The equation of viscosity energy dissipation (\( \varepsilon \) equation) is
\[ \frac{\partial \rho e}{\partial t} + \frac{\partial (\rho V K)}{\partial X_j} = \frac{\partial}{\partial X_j} \left[ (\mu + \frac{\mu_s}{\sigma_k}) \frac{\partial V}{\partial X_j} \right] + c_1 \frac{e}{K} \frac{\partial V}{\partial X_j} \left( \frac{\partial V}{\partial X_j} + \frac{\partial V}{\partial X_i} \right) - c_2 \frac{\rho e^2}{K} , \quad (5) \]

where \( c_1 \) and \( c_2 \) are constant coefficients that are 1.44 and 1.92, respectively.

The energy equation is
\[ \frac{\partial \rho T}{\partial t} + \frac{\partial (\rho V T)}{\partial X_j} = \frac{\partial}{\partial X_j} \left[ (k + \frac{\mu_s}{\sigma_T}) \frac{\partial T}{\partial X_j} \right] , \quad (6) \]

where \( T \) is the temperature, \( k \) is the coefficient of heat conduction, \( c_p \) is the specific heat capacity, and \( \sigma_T \) is the energy dissipation coefficient.

### 2.2 Determination of pollutant emission physical model

Pollutant emission physical model was based on the mass transfer theory. The process of pollutant emission can be summarized as follows: Internal material pollutant emission was drove by the grades of pressure, temperature and concentration, which could be described by the Fick’s second diffusion law [11-12]. The exterior pollutant emission was induced by evaporation, convection and diffusion. The physical model is distinguished from the pollutants internal and exterior emission factors. The common pollutants emission models are list in Table 1 and newly renovating material pollutants emission model was chosen as the pollutant emission physical model.

### 2.3 CFD simulation process and results

Twelve different simulation cases (Table 2 shows specific parameters for each case) were simulated. Representative iso-surface \((x = 0)\) was extracted to display the formaldehyde concentration. The contours of formaldehyde concentration on iso-surface \((x = 0)\) for twelve different cases are shown in Fig. 2. The area-weighted average formaldehyde concentration can be calculated in each case by Fluent software, and the results are listed in Table 3.

<table>
<thead>
<tr>
<th>Model name</th>
<th>Expression</th>
<th>Fields of using</th>
</tr>
</thead>
<tbody>
<tr>
<td>Vasquez-Beggs model</td>
<td>[ R = h_0 \left( C_c - C_c^0 \right) ]</td>
<td>Evaporation</td>
</tr>
<tr>
<td>Newly renovating material pollutants emission model</td>
<td>[ \frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} ]</td>
<td>Mass transfer, evaporation and diffusion</td>
</tr>
<tr>
<td>The dry material emission model</td>
<td>[ \frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} ]</td>
<td>Mass transfer and diffusion</td>
</tr>
<tr>
<td>John little model</td>
<td>[ V \frac{\partial C}{\partial t} = -D \frac{\partial^2 C}{\partial x^2} ]</td>
<td>Mass transfer and diffusion</td>
</tr>
</tbody>
</table>

Notes: \( R \) : emission rate; \( M_0 \) : original quantity of emission source; \( \tau \) : time; \( h_0 \) : convective mass transfer coefficient; \( C_V \) : initial vapor pressure; \( M \) : residual quantity of emission source; \( D \) : diffusion coefficient; \( C \) : mass concentration of inner material; \( \rho \) : air density; \( x_j \) : linear dimension of diffusion direction; \( \Phi \) : model variable; \( u_j \) : velocity; \( \Gamma_0 \) : diffusion coefficient; \( S_0 \) : source; \( V \) : room volume; and \( Q \) : ventilation air rate
Fig. 2 Contours of formaldehyde concentration for iso-surface ($x = 0$) in Cases 1 to 12
Table 3 indicated that formaldehyde concentration in Case 12 was the highest compared with the others. From Case 1 to Case 6, it was clear that the formaldehyde concentration got down when the supply air rate increased. From Case 7 to Case 12, the formaldehyde concentration increased with the increase of supply air temperature. The results were consistent with that in Refs [13] to [15].

Table 2  Specific parameters for Cases 1 to 12

<table>
<thead>
<tr>
<th>Case</th>
<th>Supply air temperature/°C</th>
<th>Supply air rate/(m/s)</th>
<th>Relative humidity/%</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>22</td>
<td>0.2</td>
<td>60</td>
</tr>
<tr>
<td>2</td>
<td>22</td>
<td>0.3</td>
<td>60</td>
</tr>
<tr>
<td>3</td>
<td>22</td>
<td>0.4</td>
<td>60</td>
</tr>
<tr>
<td>4</td>
<td>22</td>
<td>0.5</td>
<td>60</td>
</tr>
<tr>
<td>5</td>
<td>22</td>
<td>0.6</td>
<td>60</td>
</tr>
<tr>
<td>6</td>
<td>22</td>
<td>0.7</td>
<td>60</td>
</tr>
<tr>
<td>7</td>
<td>16</td>
<td>0.3</td>
<td>60</td>
</tr>
<tr>
<td>8</td>
<td>20</td>
<td>0.3</td>
<td>60</td>
</tr>
<tr>
<td>9</td>
<td>24</td>
<td>0.3</td>
<td>60</td>
</tr>
<tr>
<td>10</td>
<td>28</td>
<td>0.3</td>
<td>60</td>
</tr>
<tr>
<td>11</td>
<td>32</td>
<td>0.3</td>
<td>60</td>
</tr>
<tr>
<td>12</td>
<td>36</td>
<td>0.3</td>
<td>60</td>
</tr>
</tbody>
</table>

Table 3  CFD simulation results for Cases 1 to 12

<table>
<thead>
<tr>
<th>Case</th>
<th>Average formaldehyde concentration/(mg/m³)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.68</td>
</tr>
<tr>
<td>2</td>
<td>0.55</td>
</tr>
<tr>
<td>3</td>
<td>0.42</td>
</tr>
<tr>
<td>4</td>
<td>0.23</td>
</tr>
<tr>
<td>5</td>
<td>0.29</td>
</tr>
<tr>
<td>6</td>
<td>0.21</td>
</tr>
<tr>
<td>7</td>
<td>0.45</td>
</tr>
<tr>
<td>8</td>
<td>0.47</td>
</tr>
<tr>
<td>9</td>
<td>0.61</td>
</tr>
<tr>
<td>10</td>
<td>0.71</td>
</tr>
<tr>
<td>11</td>
<td>0.67</td>
</tr>
<tr>
<td>12</td>
<td>0.94</td>
</tr>
</tbody>
</table>

3  Laboratory validation

3.1 Experiment

The test facility included environment chamber and measuring system. The tests were conducted in China Academy of Building Research, Beijing. Fig. 3 shows a schematic drawing of the environment chamber with the ventilation system for the validation experiment. The chamber was surrounded by another environment-controlling room to keep the environment parameters stable. The chamber was made of stainless steel so that adsorption by the surface can be ignored, and there was a steady formaldehyde emission source in the chamber. Tightness should be checked before conducting experiments. Figs. 4 to 6 are pictures of chamber’s outline, dynamic sampling instruments, and inner formaldehyde concentration sampling devices. The formaldehyde concentration of indoor air came from the 0.5% formaldehyde solution, so the emission of formaldehyde could be regarded as a constant emission process.

Fig. 3  Schematic diagram of environment chamber

HEPA filter: high efficiency particulate air filter

Fig. 4 Environment chamber outline

3.2 Air duct system of environment chamber

The duct design conforms to ASHRAE Standard 52.2-2007 [16]. The duct was a closed-loop wind
tunnel through which air can be continuously circulated. The test ducts were constructed of galvanized iron sheet with the cross 1.5 m×1.5 m. The whole air ducts were constituted with two straight pipes and an elbow of 0.5 m radius. The air duct system was composed of the high efficiency particulate air filter, humidifier, orifice meter, fan, cooler and so on. Fig. 3 clearly display the air duct system.

3.3 Measuring method for formaldehyde

Continuous sampling method was used to obtain the formaldehyde concentration. The representative iso-surface \((x=0)\) of environment chamber was divided into 15 small pieces. The sampling point was located at the intersection of diagonal of each small rectangle. Complying with the regulations as prescribed by GB50325-2001 [17], each location must be sampled for 4 times. The sampling locations are as shown in Fig. 7. The measuring instrument was portable automatic absorption of formaldehyde gas detector (XP-308 II) with a measuring range of 0.00 mg/m\(^3\) to 3.00 mg/m\(^3\) and a minimum resolution of 0.01 mg/m\(^3\), which complied with ISO 16000-9, 2006 [18].

3.4 Experiment process and results

Twelve different experiment cases were conducted. Similarly, the representative iso-surface \((x=0)\) was chose to determine the formaldehyde concentration. Table 4 lists the measuring results. Each case was sampled for 60 times on iso-surface \((x=0)\). Each point was sampled for 4 times though Acceptable Indoor Air Quality guideline required three times samplings [19]. The average formaldehyde concentration was obtained by using area-weighted average calculations.

<table>
<thead>
<tr>
<th>Case</th>
<th>Average formaldehyde concentration/(mg/m(^3))</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.72</td>
</tr>
<tr>
<td>2</td>
<td>0.53</td>
</tr>
<tr>
<td>3</td>
<td>0.41</td>
</tr>
<tr>
<td>4</td>
<td>0.32</td>
</tr>
<tr>
<td>5</td>
<td>0.26</td>
</tr>
<tr>
<td>6</td>
<td>0.17</td>
</tr>
<tr>
<td>7</td>
<td>0.44</td>
</tr>
<tr>
<td>8</td>
<td>0.46</td>
</tr>
<tr>
<td>9</td>
<td>0.62</td>
</tr>
<tr>
<td>10</td>
<td>0.74</td>
</tr>
<tr>
<td>11</td>
<td>0.77</td>
</tr>
<tr>
<td>12</td>
<td>0.87</td>
</tr>
</tbody>
</table>

From Case 1 to Case 6, the supply air temperature and RH were respectively kept at 22 °C and 60%. When the supply air rate varied from 0.2 m/s to 0.7 m/s, the formaldehyde concentration showed a decreasing trend (Fig. 8). Good ventilation was favorable to the formaldehyde diffusion, which was consistent with the experiment result of Ref. [20].

From Case 7 to Case 12, the supply air rate and RH...
were respectively kept at 0.3 m/s and 60%. When the supply air temperature varied from 16 °C to 36 °C, the formaldehyde concentration showed an increasing trend (Fig. 9). Liu et al. [21], Gustafson et al. [22], and Meckler [23] demonstrated that the supply air temperature had effect on formaldehyde emission, but they did not mention the formaldehyde concentration variation regulation with the supply air temperature. High temperature was conducive to solution evaporation and could enhance pollutant molecular motion.

Fig. 8 Formaldehyde concentration variation trend as supply air rate increasing in environment test chamber

Fig. 9 Formaldehyde concentration variation trend as supply air temperature increasing in environment test chamber

4 Comparison between CFD simulation and experimental results

In the experimental investigation, the formaldehyde concentration in each case was measured by portable automatic absorption of formaldehyde gas detector (XP-308 II). The measuring errors of the detector for formaldehyde concentration are ±0.01 mg. Fig. 10 shows that CFD simulation results of formaldehyde concentration were in accord with the experimental results obtained in environment chamber experiment. High temperature was conducive to the release of formaldehyde and good ventilation could dilute the formaldehyde concentration. Therefore, it provided potential methods to reduce formaldehyde concentration of newly renovating buildings quickly. From Fig. 10, it can also be observed that there is a good agreement between the model prediction and the experimental values within difference of 4.3%. The CFD simulation results varied in the range of 0.21 mg/m³ to 0.94 mg/m³, and the measuring results in the range of 0.17 mg/m³ to 0.87 mg/m³. The variation trend of formaldehyde concentration in CFD simulation and measuring was consistent as supply air rate and temperature varied.

Fig. 10 Comparison between measuring and CFD simulation results for 12 cases

5 Conclusions

A 3D CFD model was developed to simulate the formaldehyde emission characteristics in an environment chamber. The CFD model gave good agreement with the experimental results for simulating formaldehyde emission characteristics. Based on the analysis of simulation and experiment results, we presented the following conclusions:

1) The simulation and experiment results revealed the effect of supply air rate and temperature on the formaldehyde emission characteristics. Formaldehyde concentration presented a decreasing trend when the
supply air rate increased, and it presented a increasing trend when the supply air temperature increased. When the supply air rate increased, violent air turbulence was contributed to formaldehyde diffusion. High temperature was conducive to solution evaporation and could enhance formaldehyde molecular motion.

2) Maintaining a higher temperature and higher wind speed was favorable to the rapid release of formaldehyde for indoor air. Good ventilation should be employed to avoid high pollutant concentration. Before moving into a new renovating house, high temperature should be kept for some time so that pollutants can quickly emit. Decorating materials containing high level formaldehyde should not be used to reduce pollutant sources.

3) The constant emission rate of formaldehyde was used in the experiment, which may not be justified in terms of actual emission conditions in decorated buildings. Therefore, research should focus on the no-constant emission rate of formaldehyde characteristics in the future.

Nomenclature

- $c_i$: formaldehyde concentration of indoor air, mg/m$^3$
- $c_0$: formaldehyde concentration of outdoor air, mg/m$^3$
- $V$: effective volume of environment chamber
- $F$: effective volume of environment chamber
- $u$: indoor rate of ventilation, times/h
- $S$: formaldehyde emission rate, mg/m$^3$
- $q$: volumetric airflow through the purification devices, m$^3$/h
- $K$: dissipation capacity per unit weight
- $F_r$: removal efficiency of abstersion process
- $t$: time
- $V_r$: unit volume
- $X$: unit distance
- $\rho$: mass density
- $X_i$: unit distance of i-direction
- $X_j$: unit distance of j-direction
- $P$: pressure
- $c_i$: constant coefficient (1.44)
- $c_s$: constant coefficient (1.92)
- $T$: temperature
- $k$: coefficient of heat conduction
- $c_p$: specific heat capacity

Greek symbols:
- $\varepsilon$: turbulence dissipation rate
- $\nu$: kinematics viscosity of air, m$^2$/s

$\mu$: turbulent viscosity, m$^2$/s
$\mu$: steady flow viscosity, m$^2$/s
$\mu_{eff}$: viscosity coefficient, $\mu_{eff} = \mu + \mu_t$, m$^2$/s
$\sigma_i$: turbulence energy Prandtl number
$\sigma_f$: energy dissipation coefficient

References


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