

1 **A numerical model predicting indoor volatile organic compounds emissions**
2 **from multiple building materials**

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12

13 **Abstract**

14 There have been many studies on the model of volatile organic compounds (VOCs)
15 emissions from individual dry building material and have been validated in the chamber.

16 Actually, VOCs emitted from multiple dry building materials simultaneously indoor. The
17 concentration of VOCs indoor increases and will inhibit the VOCs emission of dry building
18 materials indoor. This paper developed a new model predicting indoor VOCs concentrations
19 caused by simultaneous emissions from multiple dry building materials, with a consideration

20 of impact from dynamic VOCs concentrations on the emission rate. The model has been used
21 to predict the VOCs emissions from a combination of medium density fiberboard (MDF) and
22 consolidated compound floor (CCF) simultaneously. The study demonstrated a good prediction
23 performance of the newly proposed model, against field experimental data. The study also
24 showed that when multiple dry building materials emit pollutants in a common space, a mutual
25 inhibition effect could be observed. Furthermore, when multiple dry building materials emit
26 VOCs simultaneously, the change of VOCs concentrations in the air followed the trends of
27 VOCs emissions from building materials with higher initial concentration (C_0), diffusion
28 coefficient (D_m) and the partition coefficient (K_{ma}).

29

30 **Keywords:** Volatile Organic Compounds; Multiple dry building materials; Dynamic model;
31 Initial concentration; Diffusion coefficient; Partition coefficient

32

33 **Highlights:**

- 34 ● The model can predict VOCs concentration indoor.
- 35 ● The mutual inhibition effect can be reflected
- 36 ● The influence of three key parameters on indoor concentration of VOCs are
37 analyzed.
- 38 ● Can therefore reduce the health risks of people exposed to VOCs.

39

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58 **1: Introduction**

59 People spending long time in rooms with poor indoor air quality would exhibit a variety of
60 pathological reactions, such as Sick Building Syndrome (SBS), mainly due to the emitted
61 Volatile Organic Compounds (VOCs) from building construction materials and furniture(J. TEN
62 BRINKE. 1998). To provide comfortable and healthy living/working environment, indoor air
63 quality has become a key research area globally.

64

65 VOCs have clear adverse effects on human's respiratory, cardiovascular and nervous systems,
66 and may even cause cancer(L. Mølhav. 1989). To improve indoor air quality, it is necessary to
67 gain a better understanding on the mechanism and characteristics of VOCs emissions from
68 building construction materials. This formed a basic need for calculating indoor VOCs
69 concentration and determining required fresh air volume, airflow organization and air
70 purification equipment.

71

72 Accurate models predicting indoor VOCs emissions are essential for determining indoor
73 pollutant concentrations and occupant exposure(WANG 2006). Existing emission models are
74 typically belonging to one of the following types: empirical, semi-empirical or mass transfer.
75 Based on a large number of experiments on VOCs emissions, researchers have established
76 many empirical or semi-empirical models to describe VOCs emissions from different
77 materials(Matthews T G 1987; Colombo A 1987; Clausen P A 1993), represented by either first-order

78 attenuation models or exponential decay models(Zhu J P 2001). The former models were the
79 most widely used empirical models(Clausen P A 1993; Dunn L E. 1987). Empirical models are
80 generally with simple forms but with limitations from experimental conditions. Therefore when
81 being used for predictions, correction coefficients are usually needed(Zhao D 2002).

82

83 Entering the new century, analytical models based on mass transfer mechanism have become
84 the most popular and widely used method to form VOCs emission models. Little et al.(Little
85 J C 1994) firstly proposed an analytical model for predicting VOCs emissions from Single-
86 layer homogeneous material. The model, however, neglects the convective mass transfer
87 resistance between building materials and surrounding air, which gave prediction errors(Xu Y
88 2003). Huang and Haghigat (Huang and Haghigat 2002) took the convective mass transfer
89 resistance into account in their model; they assumed the VOC concentration in the air to be
90 zero to derive an analytical solution. This is not always justified under real conditions; they
91 also provide a numerical solution based on finite difference method. Xu and Zhang (Xu Y
92 2003) develop a new model without the two preceding models assumption from a mass transfer
93 perspective, and obtained an analytical solution. However, Xu and Zhang's solution is not fully
94 explicit analytical solution. Deng and Kim (Deng B Q and Kim C N 2004) developed a fully
95 analytical model considering both diffusion in the materials and mass transfer through the air
96 boundary layer. VOC emissions from building materials that conform to the model assumptions
97 can therefore be calculated by explicit formulae.

98

99 In addition to these models for single-layer homogeneous material with one surface that emits
100 VOC to air, some researchers (Wang and Zhang, 2006; Kumar and Little, 2003 ; Li and Niu,
101 2007 60; Qian et al. 2007 ; Yuan et al. 2007; Deng et al. 2010) developed models for multi-
102 layer homogeneous material, some researchers(Wang et al. 2006; Hu et al. 2007) developed
103 models for materials with two emission surfaces and some researchers(Murakami et al. 2003;
104 Lee et al. (2005); Xiong et al. 2008) developed models for materials with porous materials.

105

106 All models mentioned above were developed for predicting VOCs emissions of single building
107 material. In actual buildings, however, there will be many different dry building materials
108 existing in the same room. When a variety of dry building materials are releasing VOCs at the
109 same time, the indoor VOCs concentration will increase, and in reverse this increased
110 concentration will inhibit the VOCs release from individual building materials. Therefore, the
111 whole process is dynamically changing. Therefore, if the above-mentioned models developed
112 for predicting VOCs emissions from a single building material are used to separately solve the
113 VOCs concentration emitted by each dry building material and the VOCs concentration of
114 indoor obtained by superposition will be too large. Therefore, the final indoor VOCs
115 concentration should not be obtained by simply superimposing the concentrations of pollutants
116 emitted from individual dry building materials(Cheng T 2002).

117

118 In this paper, the simultaneous emission of VOCs from multiple single-layer materials
119 coexisting in indoor environment is developed. A numerical solution of the indoor
120 concentration is derived using the finite difference method. The accuracy of the numerical
121 solution was verified by measuring VOCs emission of MDF and CCF in the chamber. In
122 addition, C_0 , D_m and K_{ma} of different dry building materials affecting concentration of
123 VOCs indoor have been discussed.

124

125 **2: Model Development**

126 In the model proposed in this study, the number of thin layer materials were defined as i . The
127 mass transfer equations were combined with the mass conservation equations. Since the initial
128 concentration of this model was assumed to be a constant, which would not last for a long time,
129 the model is applicable for short-term predictions only. The model can be used as a quick and
130 useful tool for predicting indoor VOCs concentrations at any time in newly
131 refurbished/decorated homes, giving occupants ideas on the indoor pollutant level of their
132 living environment. When developing the model, it was also necessary to determine the
133 partition coefficient (K), the diffusion coefficient (D) and the initial concentration(C_0) in each
134 material, and this was done using the C-History method(Xiong J 2011).

135

136 ***2.1 Model formation***

137 The model developed here assumed that VOCs were simultaneously emitted from several thin
138 homogeneous materials. The VOCs diffusion in dry material was assumed to be one-
139 dimensional, i.e. from the material to the air. For a homogeneous material with uniform initial
140 VOCs concentration, the transient VOCs diffusion could be described by the following
141 diffusion equation,

142
$$\frac{\partial C_m}{\partial t} = D_m \frac{\partial^2 C_m}{\partial y^2} \quad (1)$$

143 where C_m was the concentration of the VOCs in the thin layer material; t was time; y was
144 linear distance; D_m was diffusion coefficient of the thin layer material.

145

146 The number of thin layer materials were defined as i in the proposed model. Eq. (1) was used
147 for each thin layer material by Equation 2,

148
$$\frac{\partial C_{m,i}}{\partial t} = D_{m,i} \frac{\partial^2 C_{m,i}}{\partial y^2} \quad (2)$$

149 where i represented the i^{th} thin layer material, with initial condition given as:

150
$$C_{m,i|t=0} = C_{0,i} \text{ for } 0 \leq y \leq \delta_i \quad (3)$$

151 where $C_{0,i}$ was the VOCs concentration at $t=0$ for the i^{th} thin layer material and δ_i was the
152 thickness of the i^{th} thin layer material. For thin layer materials placed on the stainless steel floor
153 of the chamber, the boundary condition was assumed to have no flux from the bottom of the
154 thin layer materials. Therefore, since Equation (2) is subject to the boundary condition:

155 $\frac{\partial C_{m,i}}{\partial y} \Big|_{y=0} = 0$ (4)

156 For the material-air interface, the emission of VOCs from the thin layer materials was

157 determined by Equation 5,

158 $-D_{m,i} \frac{\partial C_{m,i}}{\partial y} \Big|_{y=\delta_i} = h(C_{ai,i} - C_a)$ (5)

159 where h was the mean gas-phase mass transfer coefficient, assumed to be the same for all

160 materials; $C_{ai,i}$ was the VOCs concentration of material-air interface in the i^{th} thin layer

161 material ($\mu\text{g m}^{-3}$), and C_a was the average VOCs concentration in the chamber.

162

163 Equilibrium was assumed to exist between the VOCs concentrations at the surface of thin layer

164 materials and that in the chamber. At the boundary, Equation 6 existed:

165 $C_{m,i} \Big|_{y=\delta_i} = K_{ma,i} C_{ai,i}$ (6)

166 where $K_{ma,i}$ was the i^{th} material-air partition coefficient.

167

168 C_a in equation (5) could be derived from the mass balance of VOCs in the chamber. Because

169 the inlet VOCs concentration was assumed as zero, the mass balance equation was written as,

170 $V \frac{\partial C_a}{\partial t} = -AD_m \frac{\partial C_m}{\partial y} \Big|_{y=\delta} - QC_a$ (7)

171

172 When VOCs are simultaneously emitted from multiple dry building materials, C_a changes

173 significantly. According to Equation (5), the value of C_a also affects the state of VOCs inside

174 the building materials. Therefore, the VOCs concentration in the chamber cannot be calculated
175 by mathematically superimposing the VOCs emissions from individual building materials. The
176 governing equation describing the transient mass balance for all thin layer materials was
177 defined as follows:

$$178 V \frac{\partial C_a}{\partial t} = -QC_a - A_1 D_{m,1} \left. \frac{\partial C_{m,1}}{\partial y} \right|_{y=\delta_1} - A_2 D_{m,2} \left. \frac{\partial C_{m,2}}{\partial y} \right|_{y=\delta_2} \dots - A_i D_{m,i} \left. \frac{\partial C_{m,i}}{\partial y} \right|_{y=\delta_i}, i = 1, 2, 3 \dots$$

179 (8)

180 where V was the volume of the chamber (m^3); Q was the ventilated quantity ($m^3 h^{-1}$), and A_i
181 was the area of the i^{th} building material.

182

183 The initial concentration (C_0) was assumed to be constant in this model. Since this assumption
184 is only applicable for short time periods, this model is only suitable for short-term predictions.

185

186 **2.2 Numerical solutions**

187 The solution was coupled with the concentration in the air, which was an unknown function of
188 time. The concentration in the material and the mass balance equation in the air must be solved
189 simultaneously by finite difference technique. Saul'ev finite difference method has a semi-
190 implicit format, which not only solves the problem that the explicit format is not easy to
191 stabilize, but also avoids the complicated calculation of the implicit format. In the article, the
192 Saul'ev finite difference method was used to solve the above model, and Equations (2) to (7)

193 were transformed into following equations,

194

195 (a) VOCs concentration in the material:

196 Based on the Saul'ev finite difference method, equation (2) was converted into:

$$197 \quad C_{m,1}^{k+1} = \frac{1-D_{m,1}\lambda}{1+D_{m,1}\lambda} C_{m,1}^k + \frac{D_{m,1}\lambda}{1+D_{m,1}\lambda} (C_{m,1}^{k+1} + C_{m,1}^k); \quad k = 0, 1, \dots; j = 1, 2, \dots, n_1 - 1;$$

$$198 \quad C_{m,2}^{k+1} = \frac{1-D_{m,2}\lambda}{1+D_{m,2}\lambda} C_{m,2}^k + \frac{D_{m,2}\lambda}{1+D_{m,2}\lambda} (C_{m,2}^{k+1} + C_{m,2}^k); \quad k = 0, 1, \dots; j = 1, 2, \dots, n_2 - 1;$$

199 ...

$$200 \quad C_{m,i}^{k+1} = \frac{1-D_{m,i}\lambda}{1+D_{m,i}\lambda} C_{m,i}^k + \frac{D_{m,i}\lambda}{1+D_{m,i}\lambda} (C_{m,i}^{k+1} + C_{m,i}^k); \quad k = 0, 1, \dots; j = 1, 2, \dots, n_i - 1; \quad (8)$$

201 (b) VOCs concentration in indoor air:

202 Based on Trapezoidal method, equation (2) was converted into:

$$203 \quad \frac{\partial C_a}{\partial t} = -NC_a - L_1(hC_a - h \frac{C_{m,1}|_{y=\delta_1}}{K_{ma,1}}) - L_2(hC_a - h \frac{C_{m,2}|_{y=\delta_2}}{K_{ma,2}}) \dots - L_i(hC_a - h \frac{C_{m,i}|_{y=\delta_i}}{K_{ma,i}})$$

$$204 \quad = -(N + L_1h + L_2h + \dots + L_ih)C_a + \frac{L_1h}{K_{ma,1}} C_{m,1}|_{y=\delta_1} + \frac{L_2h}{K_{ma,2}} C_{m,2}|_{y=\delta_2} + \dots + \frac{L_ih}{K_{ma,i}} C_{m,i}|_{y=\delta_i}$$

$$205 \quad \rightarrow \quad C_a^{k+1} - C_a^k = \frac{\tau}{2} \left[\frac{L_1h}{K_{ma,1}} C_{m,1}^{k+1} + \frac{L_2h}{K_{ma,2}} C_{m,2}^{k+1} + \dots + \frac{L_ih}{K_{ma,i}} C_{m,i}^{k+1} - (N + L_1h + L_2h + \dots + L_ih)C_a^{k+1} \right]$$

$$206 \quad \dots + L_ih)C_a^{k+1} + \frac{L_1h}{K_{ma,1}} C_{m,1}^k + \frac{L_2h}{K_{ma,2}} C_{m,2}^k + \dots + \frac{L_ih}{K_{ma,i}} C_{m,i}^k - (N + L_1h + L_2h + \dots + L_ih)C_a^k;$$

$$207 \quad L_ih)C_a^k];$$

$$208 \quad \rightarrow \quad \left[1 + \frac{\tau}{2} (N + L_1h + L_2h + \dots + L_ih) \right] C_a^{k+1} = \left[1 - \frac{\tau}{2} (N + L_1h + L_2h + \dots + L_ih) \right] C_a^k +$$

$$209 \quad \frac{\tau}{2} \times \frac{L_1h}{K_{am,1}} (C_{m,1}^{k+1} + C_{m,1}^k) + \frac{\tau}{2} \times \frac{L_2h}{K_{am,2}} (C_{m,2}^{k+1} + C_{m,2}^k) + \dots + \frac{\tau}{2} \times \frac{L_ih}{K_{am,i}} (C_{m,i}^{k+1} + C_{m,i}^k)$$

$$210 \quad C_{m,i}^k)$$

$$211 \quad k = 0, 1, 2 \dots \quad (9)$$

212 (c) VOCs concentration at the surface of the material:

213 According to formula (3) and formula (5), assuming that the diffusion equation is also true on

214 the boundary, the difference format of the inner point can be extended to the boundary.

215 Considering the previous difference format:

$$216 \quad C_{m,1}^{k+1}_0 = (1 - 2\lambda_1 D_{m,1}) C_{m,1}^k_0 + 2\lambda_1 D_{m,1} C_{m,1}^k_1$$

$$217 \quad C_{m,2_0}^{k+1} = (1 - 2\lambda_2 D_{m,2}) C_{m,2_0}^k + 2\lambda_2 D_{m,2} C_{m,2_1}^k$$

218 ...

$$219 \quad C_{m,i_0}^{k+1} = (1 - 2\lambda_i D_{m,i}) C_{m,i_0}^k + 2\lambda_i D_{m,i} C_{m,i_1}^k; k = 0, 1, \dots$$

$$220 \quad C_{m,1}{}_{n_1}^{k+1} = \left[1 - 2\lambda_1 D_{m,1} \left(1 + \frac{h_1 \times h}{D_{m,1} K_{ma,1}} \right) \right] C_{m,1}{}_{n_1}^k + 2\lambda_1 D_{m,1} C_{m,1}{}_{n_1-1}^k + 2\lambda_1 h_1 \times h C_a{}^k$$

$$221 \quad C_{m,2}{}_{n_2}^{k+1} = \left[1 - 2\lambda_2 D_{m,2} \left(1 + \frac{h_2 \times h}{D_{m,2} K_{ma,2}} \right) \right] C_{m,2}{}_{n_2}^k + 2\lambda_2 D_{m,2} C_{m,2}{}_{n_2-1}^k + 2\lambda_2 h_2 \times h C_a{}^k$$

$$222 \quad C_{m,i}^{k+1} = \left[1 - 2\lambda_i D_{m,i} \left(1 + \frac{h_2 \times h}{D_{m,i} K_{ma,i}} \right) \right] C_{m,i}^k + 2\lambda_i D_{m,i} C_{m,i}^k + 2\lambda_i h_i \times h C_a^k$$

223 where $\lambda_i = \tau/h_i^2$, $h_i = \delta_i/n_i$ (10)

224

225 *2.3 Estimation of key parameters*

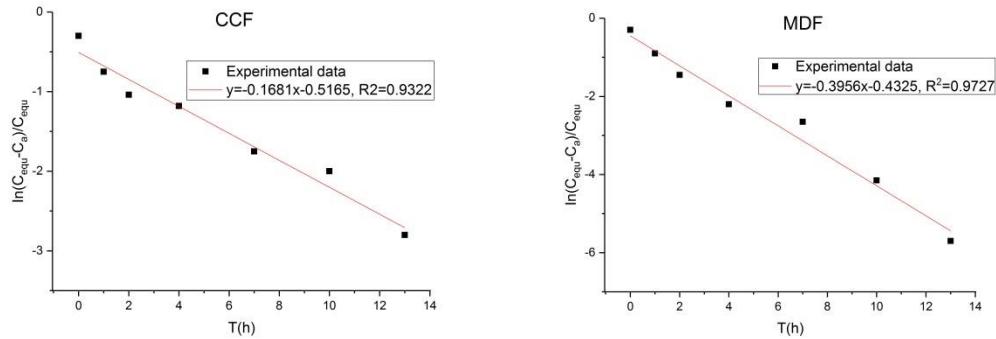
226 To use the model proposed in this study, there were four key parameters: K_{ma} , D_m , C_0 and h

227 in the material, and in existing studies the former three have been determined using different

228 methods (Wang X 2009; Xiong J 2011; Huang, Xiong J 2013; Li F 2005). In this study, the C-history

method proposed by Xiong et al. (Xiong J 2011) was adopted. The C-history method involves some steps: 1) placing the building materials in a chamber; 2) recording the curve of concentration change in the chamber; 3) solving the emission characteristic parameters (C_0 , D_m and K_{ma}) for the dry building materials through the least squares fitting method. Since wood-based panels are the main source of indoor VOC, and this experiment studied the emission law of multiple dry building materials, MDF and CCF which are widely used in furniture and decoration were chosen as subjects. Before the experiments, MDF and CCF were processed according to the method specified in (ISO 16000-11). As required by the C-History method, one specimen of each building material was placed in a chamber respectively.

According to (ISO 12460-1), a chamber with a volume of $1m^3$ has been used for testing formaldehyde emissions from CCF and MDF in this study. The measurement method adopted here for formaldehyde was known as the MBTH (3-methyl-2-benzothiazolinone hydrazine) spectrophotometric method, as defined in the Chinese GB/T 18204.26 standard(GB/T18204.26-2000). The formaldehyde emission was monitored with fitted linear curves shown in Fig. 1. From the correlation coefficient (R^2) listed in Fig. 1, it could conclude that the both fitted linear models have adequate performance, according to (ASTM Standard D5157-97). Table 1 lists the values for C_0 , D_m and K_{ma} from the experiment.



247

248 **Fig. 1:** Fitted linear curves of chamber formaldehyde concentrations for CCF and MDF separately

249

250 **Table 1:** Characteristic parameters for formaldehyde in the test specimens

Material	C_0 ($\mu\text{g m}^{-3}$)	D ($\text{m}^2 \text{s}^{-1}$)	K
CCF	2.89×10^6	8.9×10^{-11}	1033
MDF	1.32×10^7	2.32×10^{-10}	820

251

252 Some empirical relations can be adopted to solve h . For laminar flow, these exists:

253
$$Sh = 0.664 Sc^{1/3} Re^{1/2}$$

254 Where $Sh = hl/D_a$, $Sc = \nu/D_a$, $Re = ul/\nu$ 255 Sh is Sherwood number, Sc is Schmidt number, Re is Reynolds number, l was the256 characteristic length of the material, ν was the kinematic viscosity of the air, and u was the257 velocity of the air over the material. According to this empirical relation, h was used in the258 present model to be 2.3×10^{-3} m/s.

259

260 **3: Model Validation**

261 ***3.1 Experimental materials and conditions***

262 Due to the wide usage of wooden boards in furniture, floors and decorative materials in China,
263 two common board types, i.e. MDF and CCF were chosen for the analysis, as tested in the
264 above section. The specimens were cut into the same dimensions as $0.5 \times 0.5 \times 0.012\text{m}^3$. Both
265 types of experimental materials required proper treatment prior to and during the test according
266 to (ISO16000-9). Before the experiment, both MDF and CCF were sealed in a bag using tin
267 foil for approximately 20 days to give a uniform distribution of pollutants inside the building
268 materials. As described in Section 2, their C_0 , D_m and K_{ma} values were obtained and
269 calculated based on experiments. ISO standards(ISO16000-9., ISO12460-1.) have suggested a
270 method testing formaldehyde and VOCs in environmental chambers with various sizes.
271 According to (ISO 12460-1), a chamber with a volume of 1m^3 has been used for testing
272 formaldehyde emissions from CCF and MDF in this study. During the experiment, temperature,
273 relative humidity (RH) and air exchange rate in the chamber were maintained at $23\pm0.5\text{ }^\circ\text{C}$,
274 $50\%\pm5\%$ and 1 ACH, respectively(ISO16000-9.).
275 Formaldehyde was selected as the target chemical pollutant for this study, as it is a major
276 pollutant found in building materials and a common indoor air pollutant in many
277 countries(Zhang L 2009). The measurement method adopted here for formaldehyde was known
278 as the MBTH (3-methyl-2-benzothiazolinone hydrazine) spectrophotometric method, as

279 defined in the Chinese GB/T 18204.26 standard(GB/T18204.26-2000). During the experiment,
280 the flow rate was measured at 0.5L/min for both pre-sampling and post-sampling, based on a
281 sampling time of 20min. Chemical analysis was carried out right after each sampling work.
282

282 The whole experiment was consisted of three different VOCs emission tests, which were:

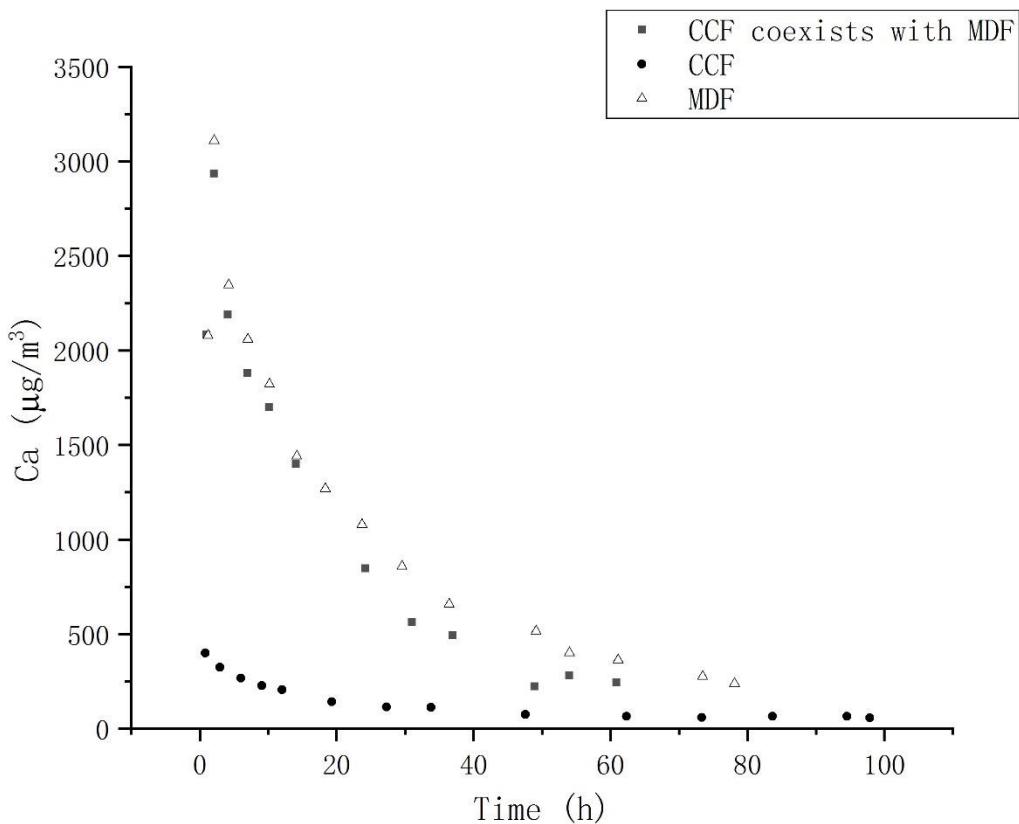
- 283 1. One piece of MDF was placed in the chamber and the concentration of formaldehyde
284 in the chamber was measured and recorded, until the data trend became stable;
- 285 2. One piece of CCF was placed in the chamber and the concentration of formaldehyde
286 in the chamber was measured and recorded, until the data trend became stable;
- 287 3. One piece of MDF and one piece of CCF were placed in the chamber and the
288 concentration of formaldehyde in the chamber was measured and recorded, until the data
289 trend became stable.

290 The first two experiments were designed to validate the model's performance on single material
291 and the last experiment was designed to validate its performance on multiple materials.

292

293 The experimental results of the three experiments are shown in Fig. 2. The test duration is about
294 100 hours. The concentration of formaldehyde became stable after 100 hours approximately. It
295 is found from the experimental results that although the concentration of formaldehyde
296 emission by MDF is much higher than CCF, in the case of integrated emission, significant
297 inhibition is still produced when CCF and MDF emitted formaldehyde together. In most cases,

298 the concentration of formaldehyde in chamber emitted by CCF coexists with MDF is slightly
299 lower than the concentration emitted by MDF alone.



300

301

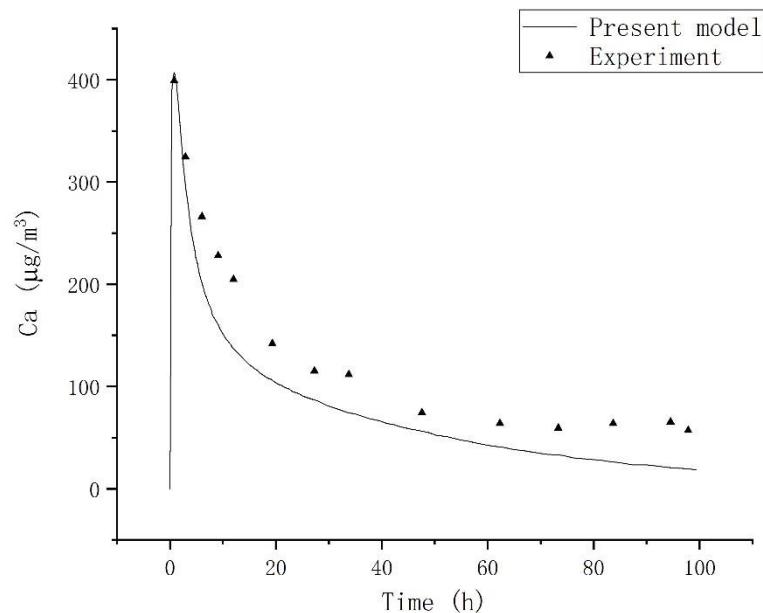
Fig. 2: Summary of experimental results

302

303 **3.2 Results**

304 The present model has been applied to the formaldehyde emission from CCF and MDF. The
305 building materials for both the Deng&Kim's model and the present model are single-layer
306 homogeneous materials, and the assumptions used in both models are the same. In addition to

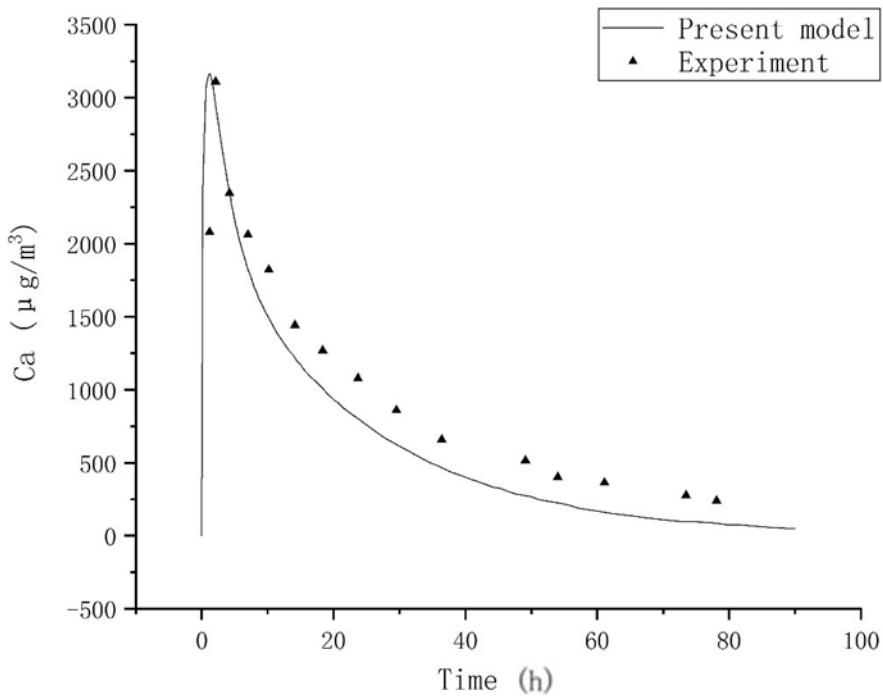
307 this, the Deng&Kim's model obtained a fully analytical solution which is more accurate than
308 the numerical solution. Therefore, the solution of Deng&Kim's model (Deng B Q and Kim C N
309 2004) is selected and compared with the experimental data and the solution of the present model.
310 The indoor concentration of formaldehyde emission from CCF and MDF respectively are
311 presented in Figs.3-4. It can be found that the predicted values from the present model had a
312 good fit with the real measured values. Numerical solution of this model is in good agreement
313 with experimental results. Therefore, the problem of pollutant emission of various building
314 materials cannot be ignored.



315

316 **Fig. 3:** Chamber concentration of formaldehyde emitted from CCF with time

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318

319

Fig. 4: Chamber concentration of formaldehyde emitted from MDF with time

320

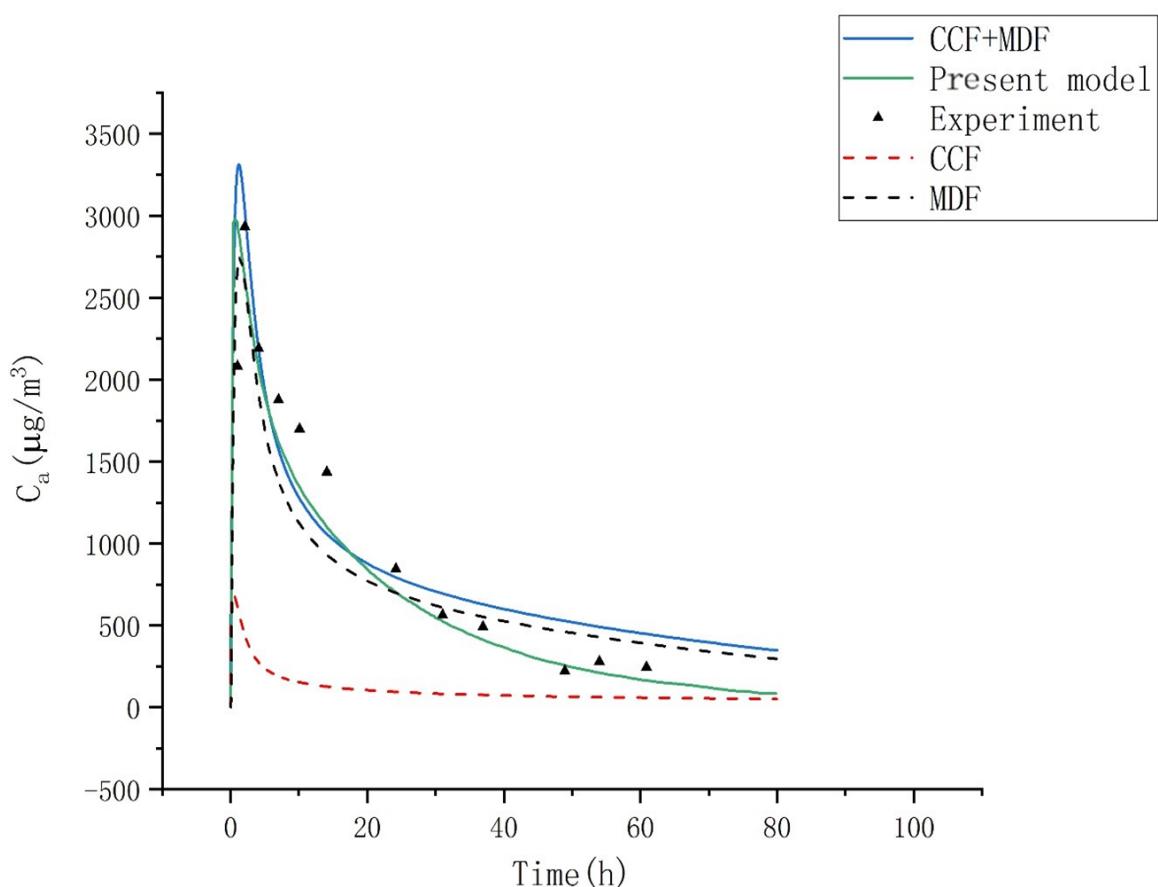
321 Fig.5 compares the results of the present model, the experimental results, and the results of
 322 mathematical superposition using the Deng&Kim model(Deng B Q and Kim C N 2004) when the
 323 CCF and MDF emitted formaldehyde together.

324

325 It can be seen from the figure that the application of the Deng&Kim model(Deng B Q and Kim
 326 C N 2004) for a single building material to calculate the formaldehyde emission of the CCF and
 327 MDF respectively, and the results of emission by CCF coexists with MDF obtained by
 328 mathematical superposition cannot reflect the mutual inhibition of the existence of various

329 building materials. The results of the present model are in line with the experimental results.
330 The present model can reflect the inhibition of formaldehyde emission from multiple building
331 materials together.

332



333

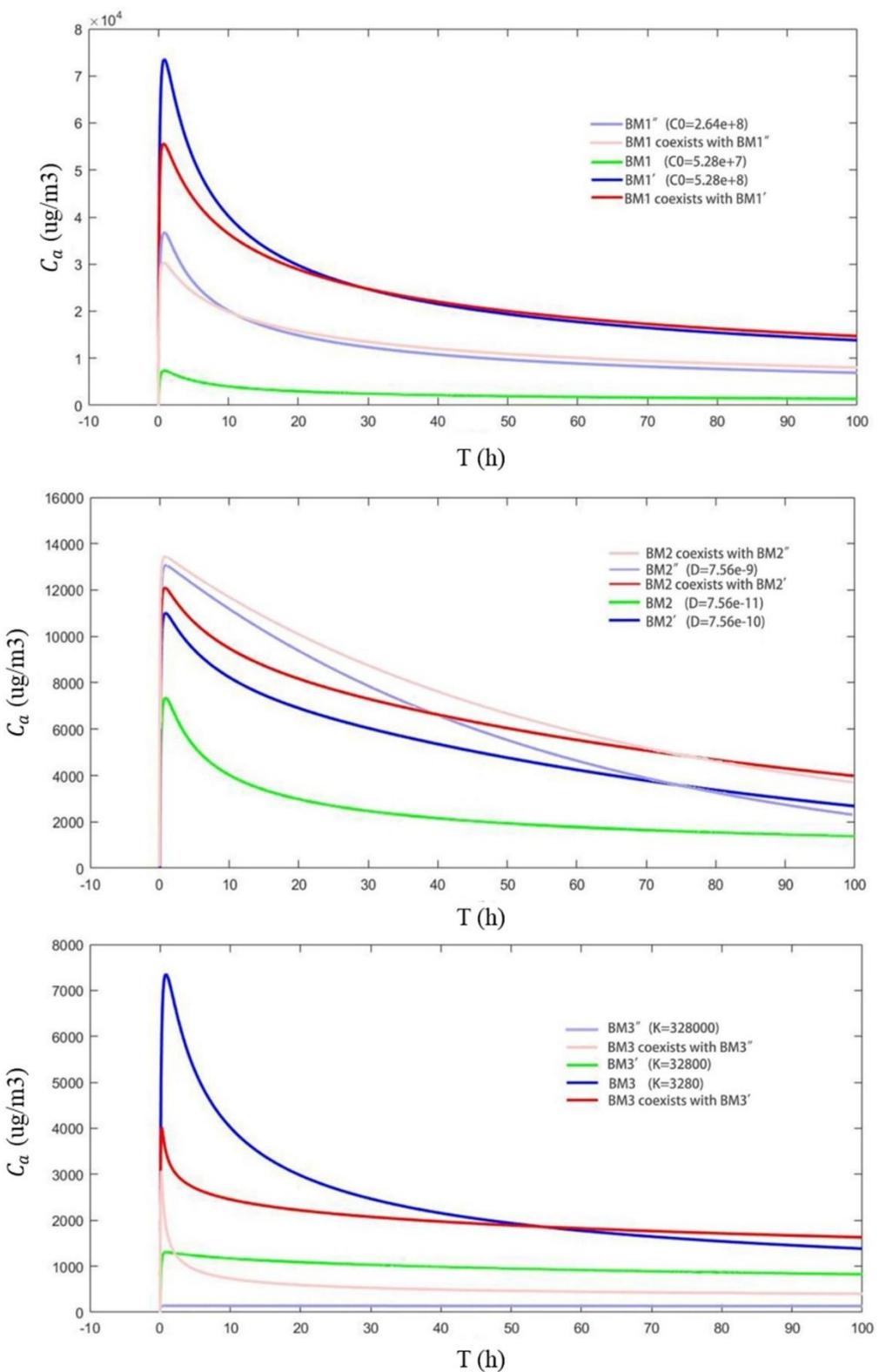
334 **Fig. 5:** chamber concentration of formaldehyde emitted from CCF and MDF with time. “CCF” and
335 “MDF” are the simulation results of Deng&Kim for two kinds of plates respectively. “CCF+MDF” is the
336 mathematical superposition of the results of CCF and MDF, and “Present model” is the simulation
337 results of the coexistence of CCF and MDF by the present model

338

339 **4: Discussions**

340 Partition coefficient (K_{ma}), diffusion coefficient (D_m) and initial concentration (C_0) are main
341 factors influencing VOCs emissions from building materials(Yang X 2001). In this study, three
342 sets of simulations were carried out to determine the influences of these parameters on the
343 VOCs concentrations from multiple dry building materials. In each experiment, both size and
344 emission surface area were kept constant for the two types of building materials under
345 investigation, but with varying key parameters. For both types, C_0 , D_m and K_{ma} were set to
346 $5.28 \times 10^7 / 5.28 \times 10^8 / 2.64 \times 10^8 \mu\text{g/m}^3$, $7.56 \times 10^{-11} / 7.56 \times 10^{-10} / 7.56 \times 10^{-9} \text{ m}^2/\text{s}$, and
347 $3280 / 32800 / 328000$, respectively. Fig. 6 shows the results from the simulations. According to
348 Fig. 6, higher C_0 and D_m would lead to increased VOCs concentrations in the air, and higher
349 K_{ma} gave lowered VOCs concentrations. When there were more than one type of dry building
350 materials existing, the change of VOCs concentrations in the air would be closer to that of the
351 dry building material with higher C_0 , higher D_m and lower K_{ma} , especially at later stages.
352 Furthermore, existence of other dry building materials would partly decrease the VOCs
353 emission of a single building material, when it existed alone. Additionally, a material with
354 lower VOCs emission could act as a pollutant balancer at early stages of VOCs emissions, as
355 reflected by Figs. 6 (a) and (c).

356



357

358 **Fig. 6** Comparison of VOC concentrations over time for different values of a) C_0 (BM1), b) D_m (BM2),

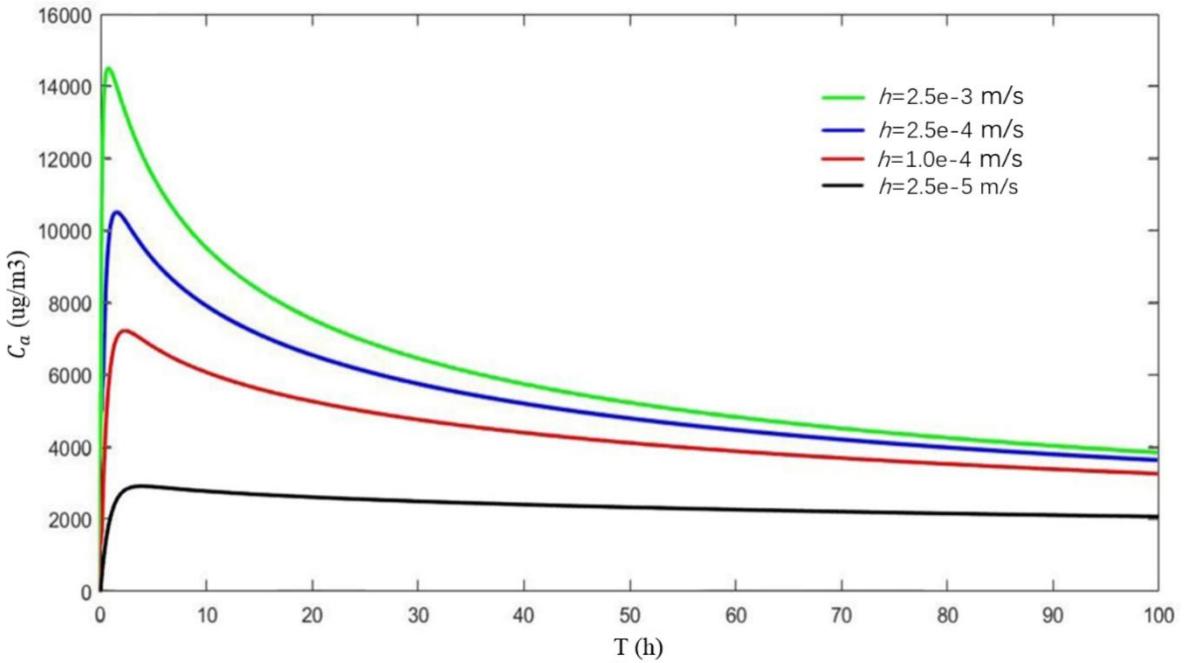
359 and K_{ma} (BM3)

360

361 Using the model developed, the effects of both convective mass-transfer coefficient (h) and air
362 exchange rate (N) on VOCs emissions from multiple building materials were analyzed as well.

363 Using two types of building materials as an example, it was found that h only had significant
364 influences at the start of the VOCs emission process but at later stages the influences from this
365 parameter can be neglected. When the magnitude of h was less than 10^{-4} , the VOCs emission
366 would reach steady state quickly (Fig. 7). Different values of N would affect the whole VOCs
367 emission process of multiple dry building materials (Fig. 8). At the late stages of VOCs
368 emission, it was observed that the VOCs concentration in the air performed a linear correlation
369 with N.

370

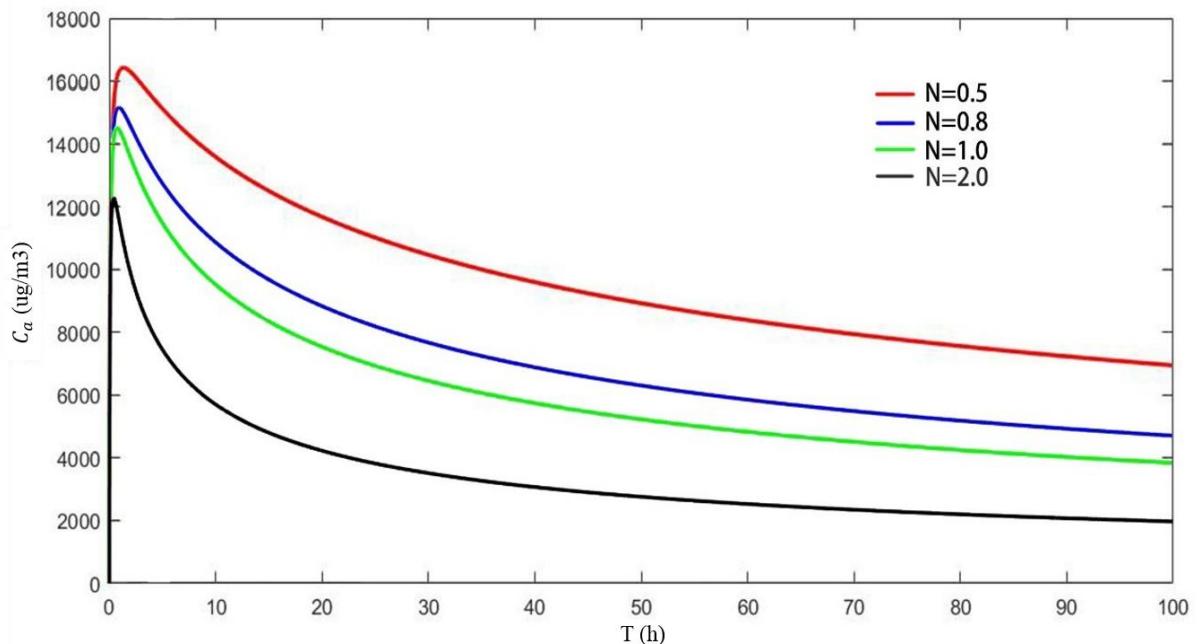


371

372

Fig. 7 Comparison of VOC concentrations with varying convective mass-transfer coefficient (h)

373



374

375

Fig. 8 Comparison of VOC concentrations with varying air exchange rate (N)

376

377 **5: Conclusion**

378 As indoor building materials release a large amount of pollutants into the air, the increase
379 in indoor air pollutant concentration will endanger people's health. Therefore, it is necessary to
380 predict the indoor VOCs concentration emitted by indoor building materials. At present, the
381 indoor air quality prediction platform generally adopts the empirical formula or the emission
382 model. But the empirical coefficient in the empirical formula is obtained by fitting the
383 experimental data of emission experiment in the chamber. In the actual environment, the
384 correction coefficient needs to be considered. The emission model only considers the mass
385 transfer process of a single building material, and does not consider the suppression between
386 various building materials. Using the emission model to calculate the VOCs emissions of each
387 building material and superimposing will directly lead to huge deviation of indoor VOCs
388 concentration.

389

390 A mathematical model and a new numerical solution were established to predict the
391 concentration of VOCs indoor emitted from multiple materials in buildings. The model
392 considers the inhibitory effect that occurs when various building materials emit VOCs at the
393 same time and proposes a numerical solution for this problem. The model predictions show a
394 good agreement with experimental data for two VOCs emission sources (MDF and CCF). The

395 proposed model can be used to predict VOCs concentrations in the air for a newly decorated
396 room, thereby reducing the health risks of exposure to VOCs.

397

398 When multiple dry building materials emit pollutants in the same space, a mutual inhibition
399 effect is observed; this effect requires further attention. Additionally, when multiple dry
400 building materials emit VOCs simultaneously, the VOCs concentration change is similar to the
401 VOCs emission trend of building materials with higher C_0 , D_m , and K_{ma} values. The emission
402 of VOCs from building materials with lower C_0 values is inhibited, and the VOCs in the air is
403 even adsorbed. D_m does not significantly affect the inhibition of different building materials,
404 but it does affect the maximum concentration of VOCs. The K_{ma} value also has a significant
405 impact on the inhibition of different building materials; VOCs emission is significantly
406 inhibited at a low K_{ma} value and an adsorption effect may even be observed. The N value has
407 a more obvious impact on the coexistence of multiple dry building materials, especially in the
408 later stage of VOCs emission, which indicates a linear relationship. The h value does not have
409 a significant impact on the later stage of VOCs emission from multiple building materials.

410

411 **Declaration of interest**

412 The authors report no conflicts of interest.

413

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