

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. Mølhave. 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(Mathews 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 Haghghat (Huang and Haghghat 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  $i^{\text{th}}$  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  $i^{\text{th}}$  thin layer material and  $\delta_i$  was the  
152 thickness of the  $i^{\text{th}}$  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  $i^{\text{th}}$  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  $i^{\text{th}}$  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:

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

179 (8)

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

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

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

199 ...

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

201 (b) VOCs concentration in indoor air:

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

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

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

$$205 \quad \rightarrow C_a^{k+1} - C_a^k = \frac{\tau}{2} \left[ \frac{L_1h}{K_{ma,1}} C_{m,1n_1}^{k+1} + \frac{L_2h}{K_{ma,2}} C_{m,2n_2}^{k+1} + \dots + \frac{L_ih}{K_{ma,i}} C_{m,ini}^{k+1} - (N + L_1h + L_2h + \dots + L_ih)C_a^{k+1} + \frac{L_1h}{K_{ma,1}} C_{m,1n_1}^k + \frac{L_2h}{K_{ma,2}} C_{m,2n_2}^k + \dots + \frac{L_ih}{K_{ma,i}} C_{m,ini}^k - (N + L_1h + L_2h + \dots + L_ih)C_a^k \right];$$

$$206 \quad \dots + L_ih)C_a^{k+1} + \frac{L_1h}{K_{ma,1}} C_{m,1n_1}^k + \frac{L_2h}{K_{ma,2}} C_{m,2n_2}^k + \dots + \frac{L_ih}{K_{ma,i}} C_{m,ini}^k - (N + L_1h + L_2h + \dots +$$

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

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

$$209 \quad \frac{\tau}{2} \times \frac{L_1h}{K_{am,1}} (C_{m,1n_1}^{k+1} + C_{m,1n_1}^k) + \frac{\tau}{2} \times \frac{L_2h}{K_{am,2}} (C_{m,2n_2}^{k+1} + C_{m,2n_2}^k) + \dots + \frac{\tau}{2} \times \frac{L_ih}{K_{am,i}} (C_{m,ini}^{k+1} +$$

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

211  $k = 0, 1, 2 \dots$  (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  $C_{m,1_0}^{k+1} = (1 - 2\lambda_1 D_{m,1})C_{m,1_0}^k + 2\lambda_1 D_{m,1} C_{m,1_1}^k$

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

218 ...

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

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

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

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

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

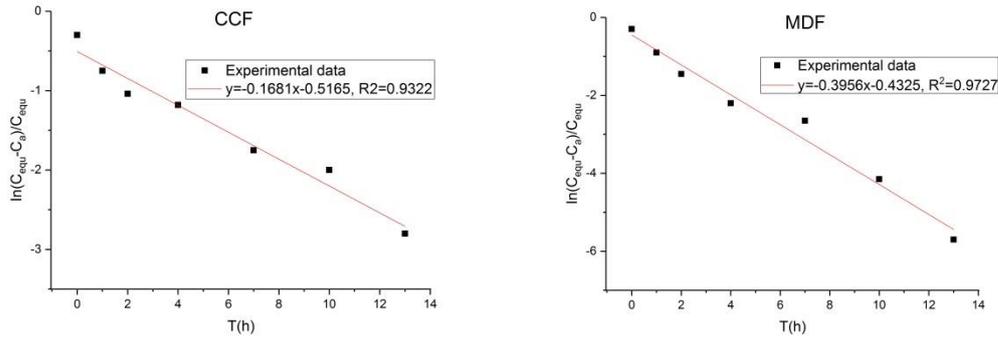
224

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

229 method proposed by Xiong et al. (Xiong J 2011) was adopted. The C-history method involves  
230 some steps: 1) placing the building materials in a chamber; 2) recording the curve of  
231 concentration change in the chamber; 3) solving the emission characteristic parameters ( $C_0$ ,  
232  $D_m$  and  $K_{ma}$ ) for the dry building materials through the least squares fitting method. Since  
233 wood-based panels are the main source of indoor VOC, and this experiment studied the  
234 emission law of multiple dry building materials, MDF and CCF which are widely used in  
235 furniture and decoration were chosen as subjects. Before the experiments, MDF and CCF were  
236 processed according to the method specified in (ISO 16000-11). As required by the C-History  
237 method, one specimen of each building material was placed in a chamber respectively.  
238 According to (ISO 12460-1), a chamber with a volume of  $1\text{m}^3$  has been used for testing  
239 formaldehyde emissions from CCF and MDF in this study. The measurement method adopted  
240 here for formaldehyde was known as the MBTH (3-methyl-2-benzothiazolinone hydrazine)  
241 spectrophotometric method, as defined in the Chinese GB/T 18204.26  
242 standard(GB/T18204.26-2000). The formaldehyde emission was monitored with fitted linear  
243 curves shown in Fig. 1. From the correlation coefficient ( $R^2$ ) listed in Fig. 1, it could conclude  
244 that the both fitted linear models have adequate performance, according to (ASTM Standard  
245 D5157-97). Table 1 lists the values for  $C_0$ ,  $D_m$  and  $K_{ma}$  from the experiment.

246



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	$2.89 \times 10^6$	$8.9 \times 10^{-11}$	1033
MDF	$1.32 \times 10^7$	$2.32 \times 10^{-10}$	820

251

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

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

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 the

256 characteristic length of the material,  $\nu$  was the kinematic viscosity of the air, and  $u$  was the

257 velocity of the air over the material. According to this empirical relation,  $h$  was used in the

258 present model to be  $2.3 \times 10^{-3}$  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  $1\text{m}^3$  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  $23\pm 0.5\text{ }^\circ\text{C}$ ,  
274  $50\%\pm 5\%$  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 The whole experiment was consisted of three different VOCs emission tests, which were:

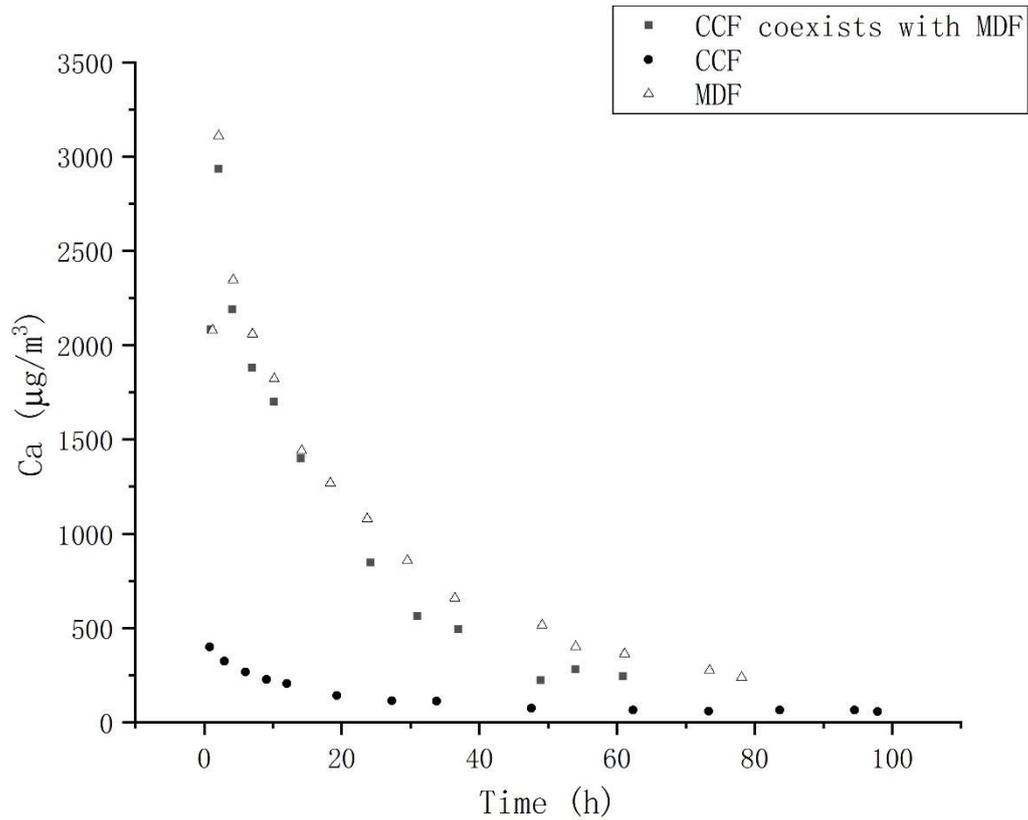
- 283 1. One piece of MDF was placed in the chamber and the concentration of formaldehyde  
284 in the chamber was measured and recorded, until the data trend became stable;
- 285 2. One piece of CCF was placed in the chamber and the concentration of formaldehyde  
286 in the chamber was measured and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



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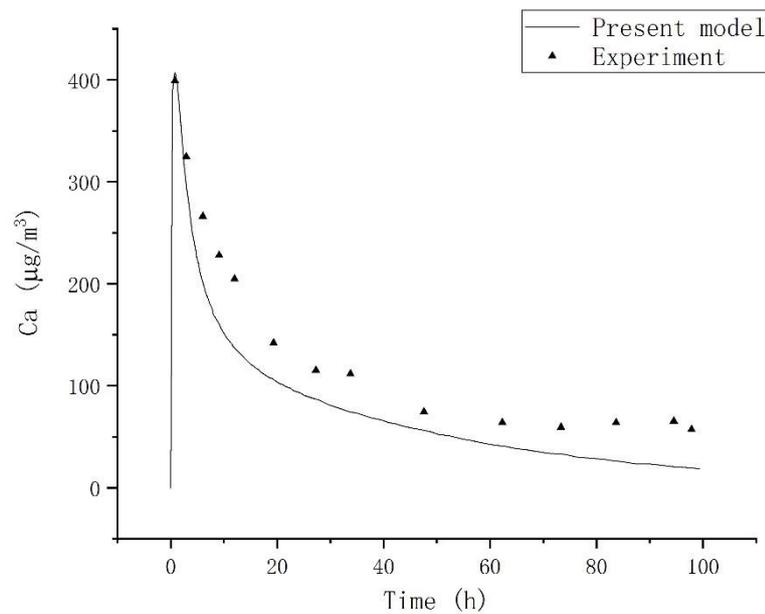
**Fig. 2:** Summary of experimental results

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

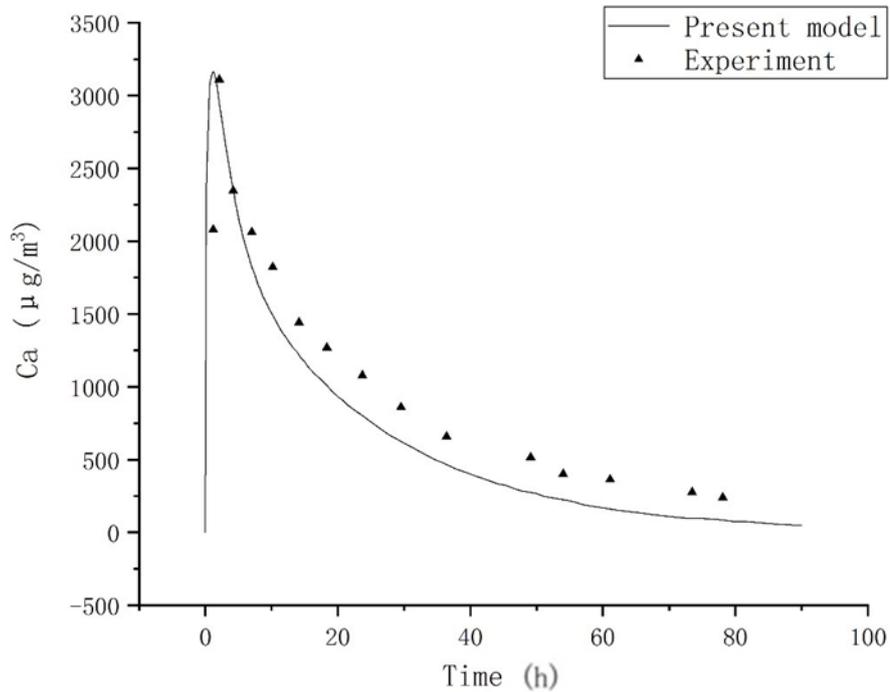
307 this, the Deng&Kim's model obtained a fully analytical solution which is more accurate than  
308 the numerical solution. Therefore, the solution of Deng&Kim's model (Deng B Q and Kim C N  
309 2004) is selected and compared with the experimental data and the solution of the present model.  
310 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

317



318

319

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

320

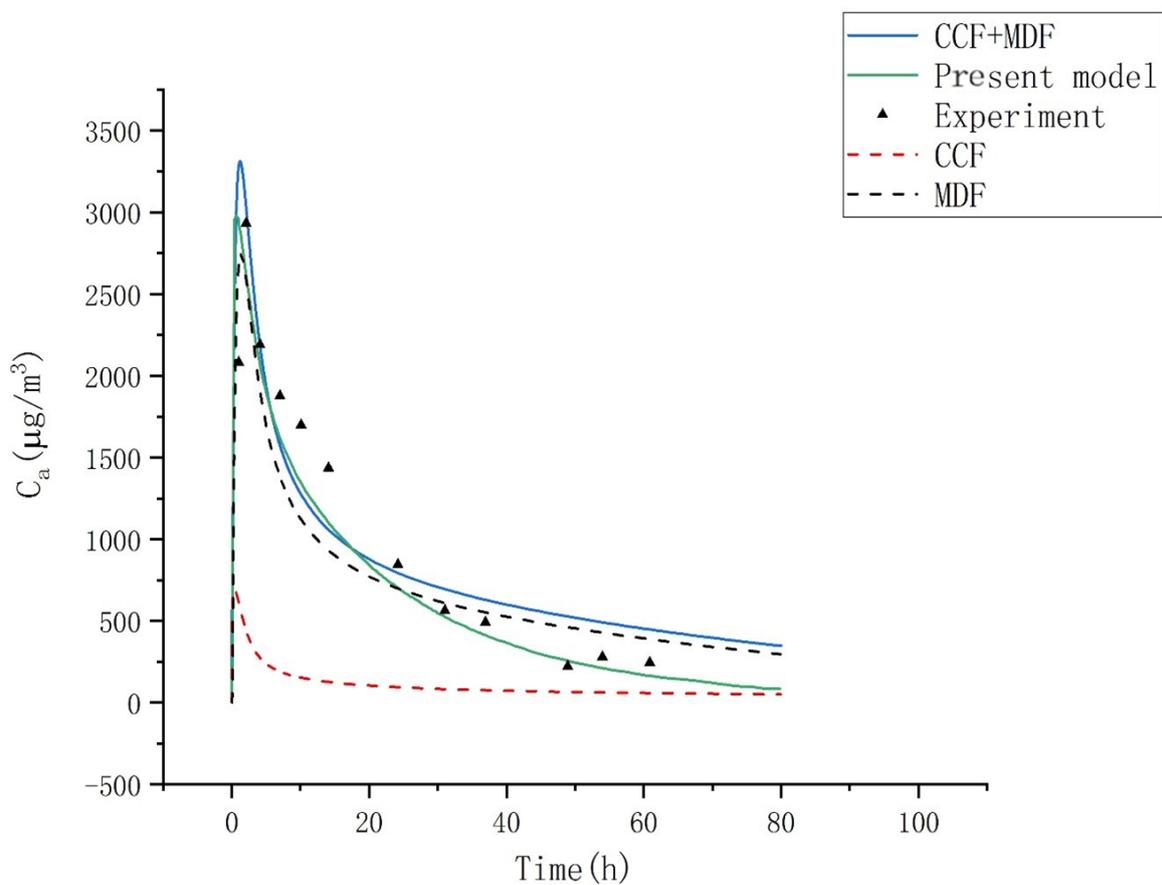
321 Fig.5 compares the results of the present model, the experimental results, and the results of  
 322 mathematical superposition using the Deng&Kim model(Deng B Q and Kim C N 2004) when the  
 323 CCF and MDF emitted formaldehyde together.

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

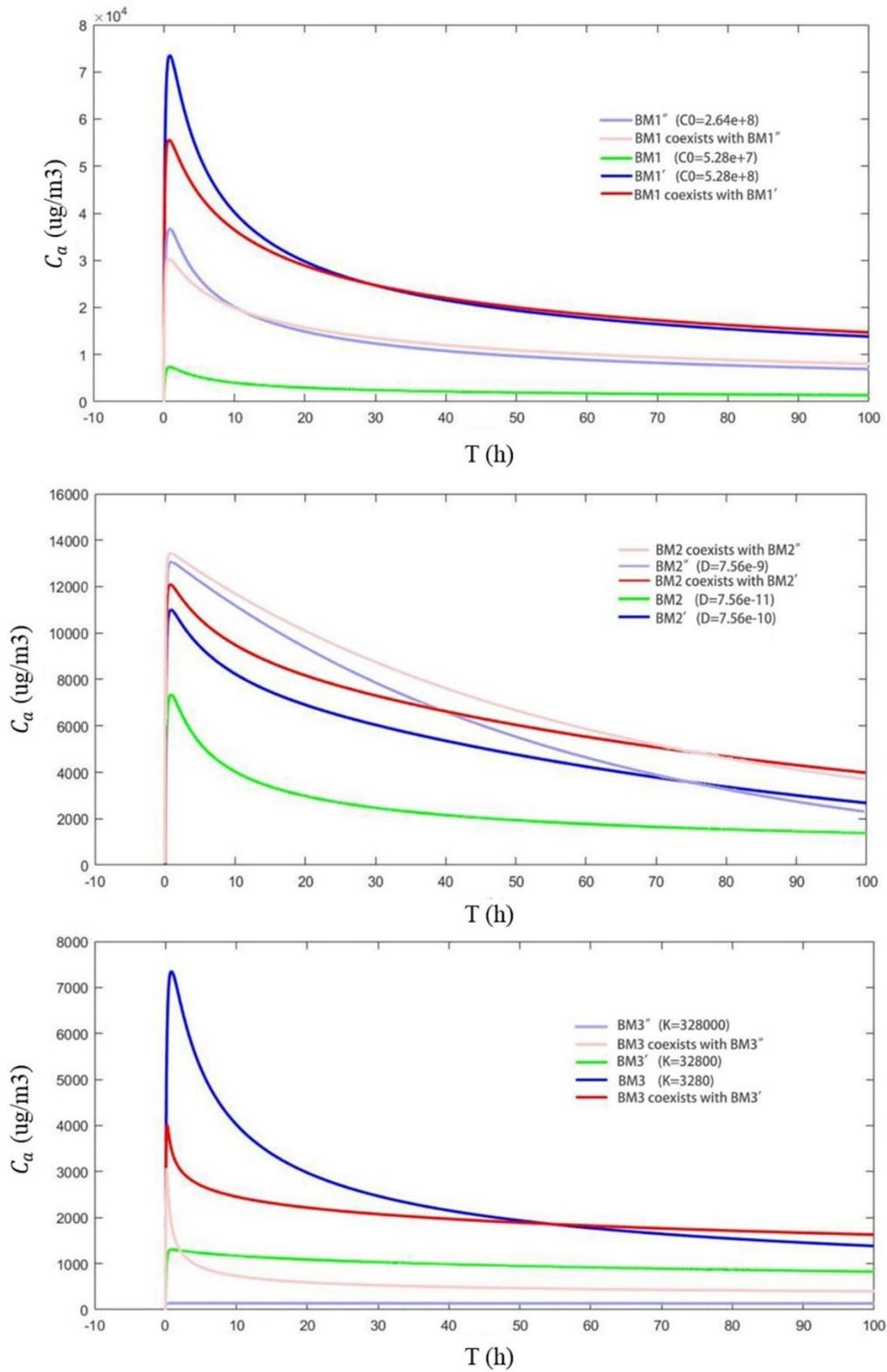
334 **Fig. 5:** chamber concentration of formaldehyde emitted from CCF and MDF with time. “CCF” and  
335 “MDF” are the simulation results of Deng&Kim for two kinds of plates respectively. “CCF+MDF” is the  
336 mathematical superposition of the results of CCF and MDF, and “Present model” is the simulation  
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  $5.28 \times 10^7 / 5.28 \times 10^8 / 2.64 \times 10^8 \text{ } \mu\text{g/m}^3$ ,  $7.56 \times 10^{-11} / 7.56 \times 10^{-10} / 7.56 \times 10^{-9} \text{ m}^2/\text{s}$ , 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.

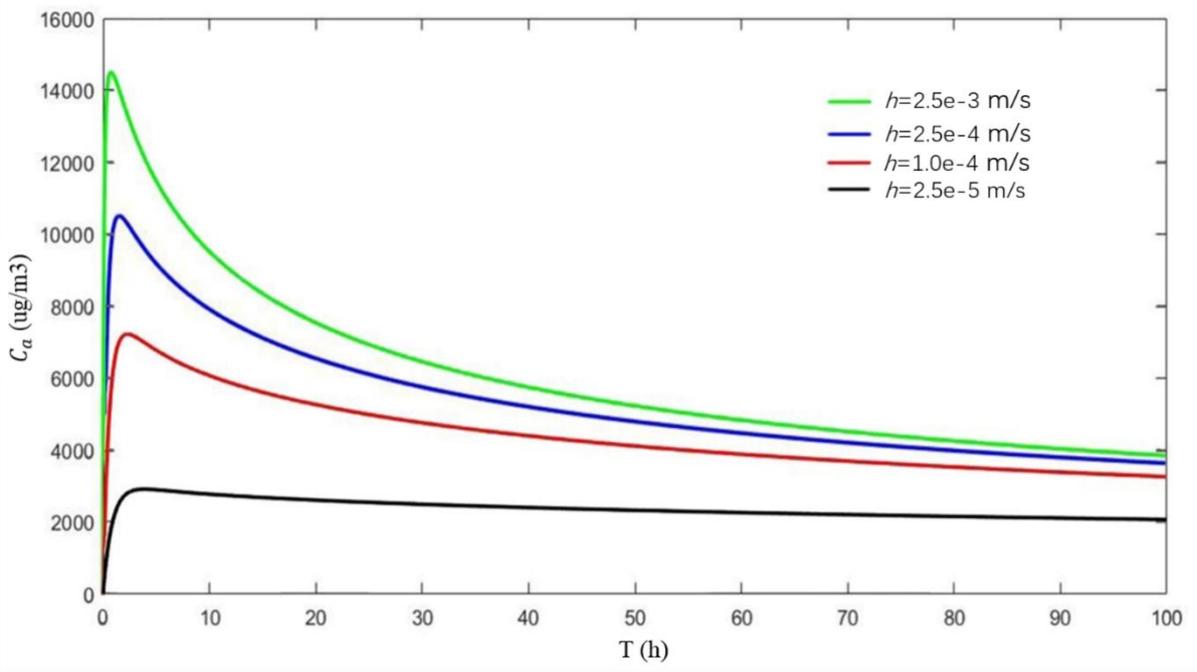
363 Using two types of building materials as an example, it was found that  $h$  only had significant  
364 influences at the start of the VOCs emission process but at later stages the influences from this

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

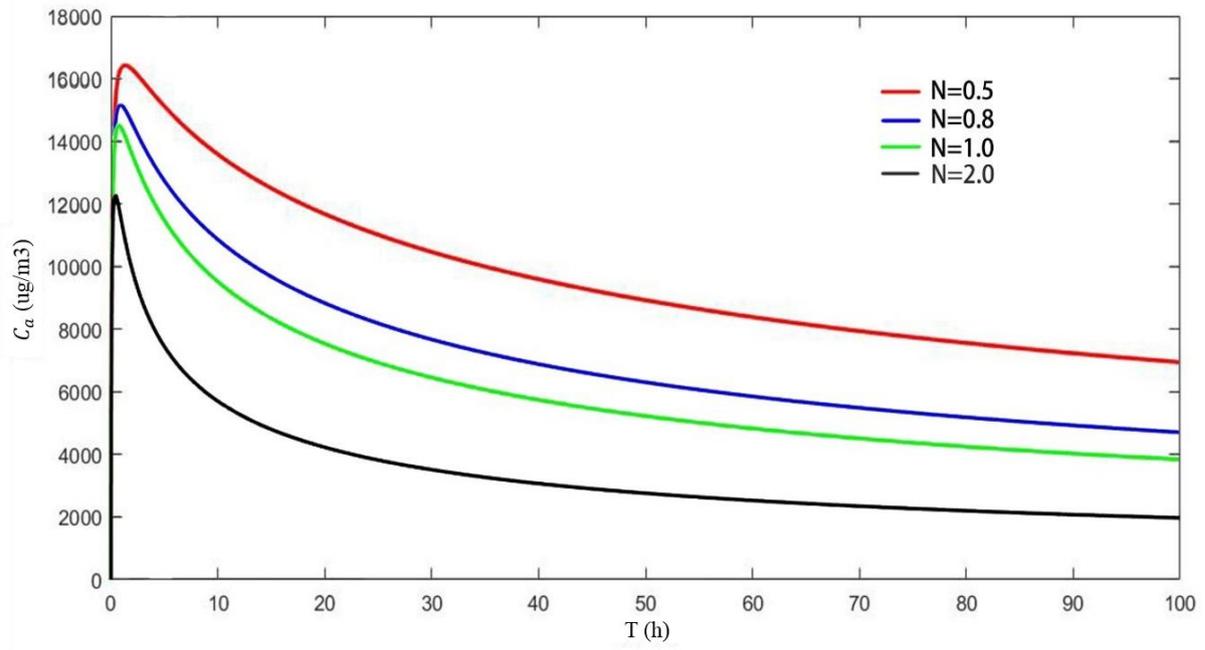


371

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

372

373



374

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

375

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

414 **References**

- 415 ASTM Standard D5157-97— Standard Guide for Statistical Evaluation of Indoor Air Quality Models
- 416 Cheng T , Jiang Y , Xu Y , et al. Mathematical model for simulation of VOC emissions and concentrations  
417 in buildings[J]. Atmospheric Environment, 2002, 36(32):5025-5030.
- 418 Clausen P A, Laursen B, Wolkoff P, et al. Emission of volatile organic compounds from vinyl floor covering.  
419 In: Nagda N L, ed. Modeling of Indoor Air Quality and Exposure ASTM STP1205. Philadelphia: American  
420 Society of Testing and Materials, 1993. 3—13
- 421 Colombo A, De Bortolli M, Pecchio E, et al. Chamber testing of organic emissions from building and  
422 furnishing materials.//[J] Sci Total Environ, 1987, 91: 237—249
- 423 Deng B Q and Kim C N. An analytical model for VOC emission from dry building materials. Atmospheric  
424 Environment, 2004, 38(8): 1173-1180.
- 425 Deng B, Tang S, Kim J, Kim C. Numerical modeling of volatile organic compound emissions from multi-  
426 layer dry building materials. Korean J Chem Eng 2010;27:1049e55.
- 427 Dunn L E. Models and statistical methods for gaseous emission testing of finite sources in well-mixed  
428 chambers.//[J] Atmospheric Environment, 1987, 21: 425-430.
- 429 GB/T18204.26-2000 — Methods for determination of formaldehyde in air of public places
- 430 Hu HP, Zhang YP, Wang XK, Little JC. An analytical mass transfer model for predicting VOC emissions  
431 from multi-layered building materials with convective surfaces on both sides. Int J Heat Mass Transfer  
432 2007;50:2069e77.
- 433 Huang H, Haghghat F. Modeling of VOC emission from dry building materials. Build Environ, 2002, 37:

434 1349—1360

435 Huang, Xiong J, Zhang Y. A rapid and accurate method, ventilated chamber C-history method, of  
436 measuring the emission characteristic parameters of formaldehyde/VOCs in building materials[J]. Journal  
437 of Hazardous Materials, 2013, 261:542-549.

438 ISO12460-1. Wood-Based Panels — Determination of Formaldehyde Release —Part 1: Formaldehyde  
439 Emission by the 1-Cubic-Metre Chamber Method. 2007.

440 ISO16000-11. Indoor Air—Part 11: Determination of the Emission of Volatile Organic Compounds from  
441 Building Products and Furnishing—Sampling, Storage of Samples and Preparation of Test Specimens. 2006.

442 ISO16000-9. Indoor Air —Part 9: Determination of the Emission of Volatile Organic Compounds from  
443 Building Products and Furnishing —Emission Test Chamber Method. 2006.

444 J. TEN BRINKE, S. SELVIN, A. T. HODGSON, et al. Development of New Volatile Organic Compound  
445 (VOC) Exposure Metrics and Their Relationship to "Sick Building Syndrome" Symptoms. Indoor Air,  
446 1998. 8: 140-152.

447 Kumar D, Little J C. Characterizing the source/sink behavior of double-layer building materials [J].  
448 Atmospheric Environment, 2003, 37(39-40):5529-5537.

449 L. Møhlhave. The sick buildings and other buildings with indoor climate problems [J]. Environment  
450 International, 1989, 15(1):65-74.

451 Lee C S, Haghghat F, Ghaly W S. A study on VOC source and sink behavior in porous building materials-  
452 analytical model development and assessment. Indoor Air, 2005, 15: 183—196

453 Li F, Niu J. Control of volatile organic compounds indoors Development of an integrated mass-transfer-

454 based model and its application. *Atmos Environ* 2007;41:2344e54.

455 Li F, Niu J. Simultaneous estimation of VOCs diffusion and partition coefficients in building materials via  
456 inverse analysis[J]. *Building & Environment*, 2005, 40(10):1366-1374.

457 Little J C, Hodgson A T, Gadgil A J. Modeling emissions of volatile organic compounds from new carpets.  
458 *Atmos Environ*, 1994, 28(2): 227—234

459 Matthews T G, Hawthorne A R, Thompson C V. Formaldehyde sorption and desorption characteristics of  
460 gypsum wallboard.//[J] *Environ Sci Tech*, 1987, 21: 629—634

461 Murakami S, Kato S, Ito K, Zhu Q. Modeling and CFD prediction for diffusion and adsorption within room  
462 with various adsorption isotherms. *Indoor Air* 2003;13:20e7.

463 Qian K, Zhang Y, Little JC, Wang X. Dimensionless correlations to predict VOC emissions from dry  
464 building materials. *Atmos Environ* 2007;41:352e9.

465 Wang X, Zhang Y. A New Method for Determining the Initial Mobile Formaldehyde Concentrations,  
466 Partition Coefficients, and Diffusion Coefficients of Dry Building Materials [J]. *Journal of the Air & Waste*  
467 *Management Association*, 2009, 59(7):819-825.

468 Wang X, Zhang Y, Zhao R. Study on characteristics of double surface VOC emissions from dry flat-plate  
469 building materials. *Chin Sci Bull* 2006;51: 2287e93.

470 Xiong J, Yao Y, Zhang Y. C-History Method: Rapid Measurement of the Initial Emittable Concentration,  
471 Diffusion and Partition Coefficients for Formaldehyde and VOCs in Building Materials[J]. *Environmental*  
472 *Science & Technology*, 2011, 45(8):3584-3590.

473 Xiong J, Zhang Y, Wang X, Chang D. Macroemeso two-scale model for predicting the VOC diffusion

474 coefficients and emission characteristics of porous building materials. *Atmos Environ* 2008;42:5278e90.

475 Xu Y, Zhang Y P. An improved mass transfer based model for analyzing VOC emissions from building  
476 materials.//[J]*Atmos Environ*, 2003, 37(18): 2497—2505

477 Yang X, Chen Q, Zhang J S, et al. Numerical simulation of VOC emissions from dry materials[J]. *Building  
478 & Environment*, 2001, 36(10):1099-1107.

479 Yuan H, Little J C, Marand E, Liu Z. Using fugacity to predict volatile emissions from layered materials  
480 with a clay/polymer diffusion barrier. *Atmos Environ* 2007;41:9300e8.

481 Zhang L, Steinmaus C, Eastmond D A, et al. Formaldehyde exposure and leukemia: a new meta-analysis  
482 and potential mechanisms. [J]. *Mutation Research/reviews in Mutation Research*, 2009, 681(2):150-168.

483 Zhao D, Little J C, Hodgson A T. Modeling the reversible, diffusive sink effect in response to transient  
484 contaminant sources.//[J] *Indoor Air*, 2002, 12: 184—190

485 Zhu J P, Zhang J S, Shaw C Y. Comparison of models for describing measured VOC emissions from wood-  
486 based panels under dynamic chamber test condition. *Chemosphere*, 2001, 44: 1253—1257