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1 **Integrated empirical and modelled determination of the human health impacts of**  
2 **building material VOCs**

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18

## 19 **1. Introduction**

20 Indoor air quality (IAQ) is of crucial concern since humans spend more than 90% of  
21 their time indoors[1] and are directly exposed to substances that can be harmful to their health.  
22 These substances, called pollutants, are either in the form of gases or are adsorbed to  
23 particulate matter (PM) and are either emitted directly by indoor sources (materials used in  
24 construction and furniture, human activities and humans themselves) or transferred from the  
25 outdoor environment through ventilation, infiltration and airing. Since people spend a lot of  
26 their time and get most of their intakes indoors, it is crucial to assess indoor pollutant  
27 concentrations and to identify their main sources in order to limit IAQ-related intake and  
28 health damage.

29 Materials have been identified as important continuous sources of chemicals present in  
30 indoor environments [2–4], which can directly affect human health or react with other  
31 substances such as ozone to form new harmful substances in the gas or particle phase [4].  
32 Thus, a high number of studies have measured the emission of volatile organic compounds  
33 (VOCs) from specific materials [3,5–7]. Furthermore, since 2011, it is mandatory for  
34 manufacturers to measure VOC emissions of construction, wall and flooring materials under  
35 the regulatory labelling scheme in France[8]. However, measured data are only available and  
36 valid at a few specific points in time, during a restricted timespan of a few days to a few  
37 weeks. In order to obtain a complete emission profile and assess the cumulative intake of  
38 these VOCs, concentrations have to be extrapolated. Linear extrapolations cannot be applied  
39 since emissions themselves vary with the time dependent mass of the substance left in the  
40 material. Simple fit of decay exponential curves has also limited validity to reflect the  
41 potential increase of initial air concentration. Moreover, air chamber measurements and  
42 emissions depend on the actual ventilation rate and surfaces to volume ratio, and therefore  
43 need to be scaled up to real building usage conditions[9–11]. Thus there is a need to couple  
44 measurements with more elaborated emission models to determine the emission and resulting  
45 concentration profiles as a function of time.

46 Emission models of VOCs from materials are based on the mass balance of the  
47 substance emitted from the material and depend on chemical, material and building  
48 parameters. Two main parameters characterize the combined influence of material and  
49 chemical properties and are unique to each material-chemical combination: 1) the diffusion of  
50 these substances through the material, determined by the diffusion coefficient,  $D_m$  and 2) the  
51 material-air partition coefficient,  $K_{ma}$ , which is the ratio at equilibrium of the concentration of

52 the chemical at the surface of the material and in the boundary air layer at material surface.  
53 QPPRs (Quality Property-property Relationship) have been developed to compute material-  
54 specific properties such as  $D_m$  and  $K_{ma}$ , for multiple material types from chemical properties  
55 more commonly available such as molecular weight and  $K_{oa}$  [12,13]. Developed from large  
56 datasets of about 1000 measurements, these QPPRs reference values can be used to simulate  
57 average indoor concentrations when no specific emission data are available, but are associated  
58 with relatively large uncertainties of a factor 10 to a 100. Another key parameter is the mass  
59 fraction of volatile substances in the material,  $MF_0$ , which determines the amount that can be  
60 emitted in air. Material compositions are often unknown, except for the average values that  
61 can be found for some material categories in e.g. the Pharos database, aggregating  
62 information on chemicals in building materials and associated human and environmental  
63 health hazards [14].

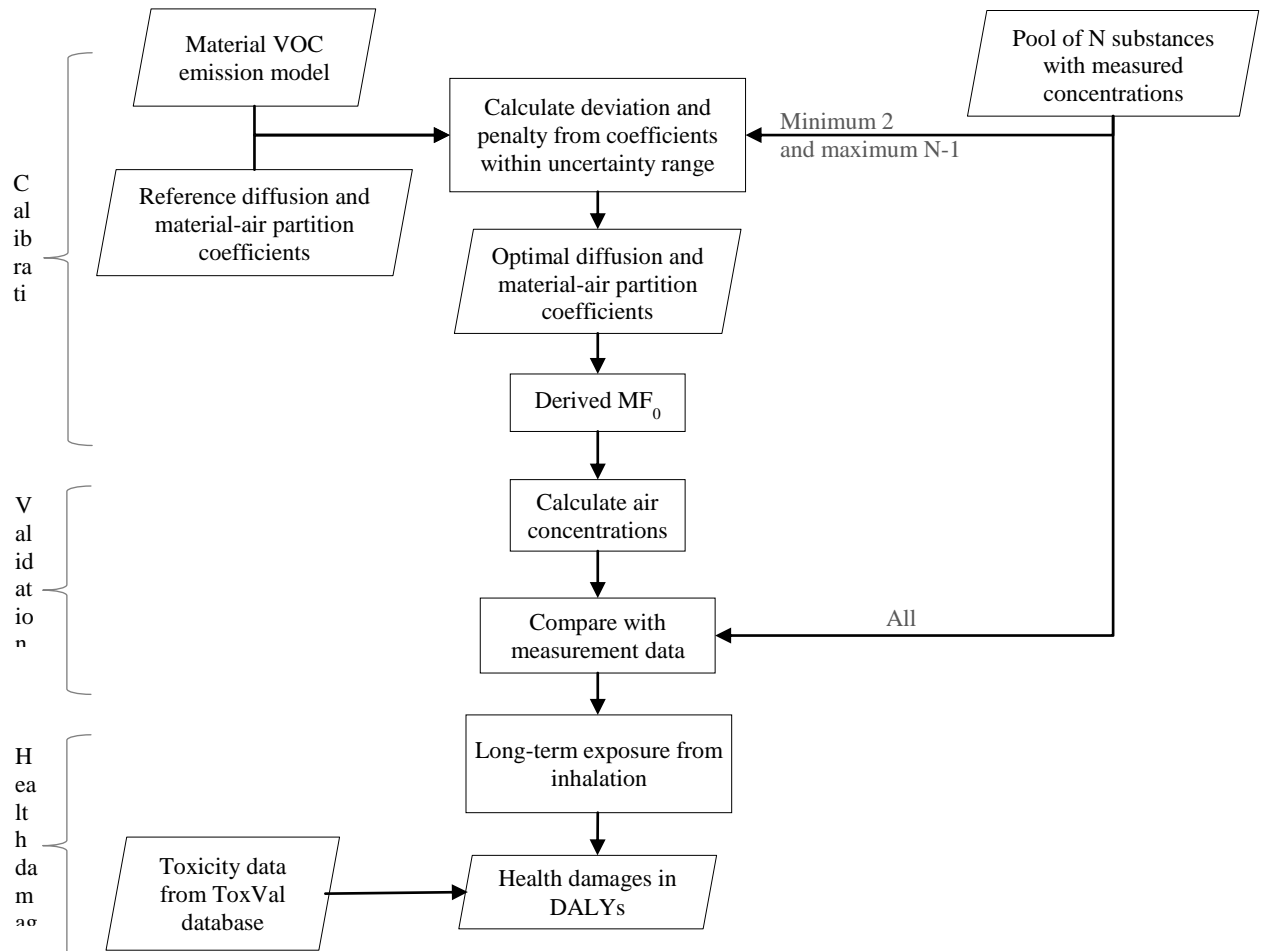
64 Measurements do not represent real-life occupied indoor environments and are only  
65 available at specific points in time, while models contain uncertainties and unknowns. The  
66 combination of the measurements to emission models could take advantage of the respective  
67 strengths of these approaches and help to predict more precisely the evolution of indoor VOC  
68 concentrations. Furthermore, since VOCs can have serious adverse effects on health, it is  
69 beneficial to model intake and health damages on building occupants in order to make  
70 judicious choices right at the design stage. The present paper therefore aims to propose and  
71 apply a framework combining measured emission data with a mass balance model of VOCs  
72 emission from materials. More specifically, the different objectives are:

- 73 1. Develop a framework to use multi-layered emission model for interpreting and  
74 generalising measured emission data from building materials
- 75 2. Perform a parameter optimisation and evaluate the quality of the approach based on  
76 sets of chemicals in gypsum board and bamboo flooring
- 77 3. Determine long-term chemical intakes and related human health impacts and compare  
78 across chemicals

79 First, we will present the framework developed to calibrate an emission model with  
80 emission data. The framework will then be applied to two mono-layered materials: gypsum  
81 board and bamboo flooring. In a case study, we will evaluate the health damages related to the  
82 intake of VOCs emitted by the gypsum board and bamboo flooring.

## 83 **2. Material and methods**

84 In this study, the driving input parameters of an emission model will be adjusted using  
 85 available measured concentrations from chamber experiments to simulate continuous VOC  
 86 emissions from materials. The framework will be applied to two materials: gypsum board and  
 87 bamboo flooring. The main steps are summarised in Figure 1.



88  
 89 *Figure 1: Methodology for extrapolating VOC emission data with an emission model:*  
 90 *calibration, application and validation on different materials with measured data and*  
 91 *determination of health damages from exposure*

92 From a test chamber measurement pool of N substances emitted by the material under  
 93 study, a minimum of 2 and maximum of N-1 substances are selected and coupled with an  
 94 existing emission model and reference coefficient values in order to estimate the optimal  
 95 diffusion and material-air partition coefficients unique to the material that best fit the  
 96 measurements. The initial mass fraction,  $MF_0$ , of each substance, specific to each material,  
 97 that yield the lowest error of the predicted compared to the measured concentrations are then  
 98 derived. The framework is validated by comparing the predicted concentrations to measured  
 99 data for all N substances. Using the determined optimal parameters, the inhalation exposure to

100 material VOCs can be determined by the model and combined with exposure-response data to  
101 evaluate corresponding health damages.

## 102 **2.1 Measured air concentration data in test chamber**

103 Air concentration measurements of different substances emitted at different points in  
104 time by materials, for instance by material manufacturers. Since these measurements are made  
105 in test chambers, the following chamber characteristics are considered: 1) the chamber walls  
106 are made of very low absorption or emission materials such as glass or stainless steel, in order  
107 not to interfere with the tested material and 2) only one face of the material emits substances,  
108 the other being covered by an impermeable material. The ventilation rate and temperature  
109 during measurements must also be known.

110 In this study, we used data on two mono-layered materials: gypsum board and bamboo  
111 flooring. Air concentration data are available at 3 days ( $t_1$ ) and/or 28 days ( $t_2$ ) for the two  
112 materials from the manufacturer's data sheet (created in response to the regulatory labelling  
113 scheme [8]), with no uncertainty range available. For all two materials, the tests were carried  
114 out with an air change rate of  $0.5 \text{ vol.h}^{-1}$  at  $23 \text{ }^\circ\text{C}$  and a relative humidity of 50 %. A summary  
115 of relevant information is presented in [Table 1](#).

116 *Table 1: Main characteristics of the measurement of VOCs emissions from gypsum*  
117 *board and bamboo flooring*

	<b>Gypsum board</b>	<b>Bamboo flooring</b>
Number of substances measured (at both $t_1$ and $t_2$ )	21 (5)	11 (3)
Thickness of material (mm)	12.5	38
Density ( $\text{kg.m}^{-3}$ )	1150	1150
Chamber volume ( $\text{m}^3$ )	0.123	0.25
Loading ratio ( $\text{m}^2.\text{m}^{-3}$ )	1	0.4

118 Out of the total number of chemicals measured, only those having two measurement  
119 points (at  $t_1$  and  $t_2$ ) were chosen for calibration and validation: 5 for gypsum board and 3 for  
120 bamboo flooring. Calibration substances were selected based on their emission dynamics,  
121 defined by their diffusion  $D_m$  ( $\text{m}^2/\text{s}$ ) and material-air partition  $K_{ma}$  (-) coefficients, as

122 explained in paragraph 2.3: hexanal, toluene and n-hexadecane for gypsum board, and acetic  
123 acid and phenol for bamboo flooring.

## 124 **2.2 Emission model and main parameters of influence**

125 The multi-layered material emission model used in this paper has been developed by  
126 Yan et al. [15], modified by Guo [16], and further adjusted by Micolier [17]. The material is  
127 divided into several layers. Each layer is considered to have a uniform substance  
128 concentration and is represented by a single node. The emission rate is obtained from the  
129 mass balance of substances at different nodes within the material and in air, as a function of  
130 the initial mass fraction of the substance in the material,  $MF_0$  ( $\text{kg}_{\text{chemical}}/\text{kg}_{\text{material}}$ ). The mass  
131 balance equations for each node are given in SI S.1. VOC emissions are driven by two major  
132 parameters, i.e. the diffusion coefficient on  $D_m$  and the material partition coefficients  $K_{ma}$  and  
133 this emission can be limited by its diffusion through the material (D-limited) or by its partition  
134 from the material to the boundary layer (K-limited).

135 These two parameters have been estimated from material and substance specific  
136 coefficients [12,13] as follows:

$$D_m = 10^{6.39 + \frac{\tau - 3486}{T} - 2.49 \log_{10} MW + b} \quad (1)$$

$$K_{ma} = 10^{-0.38 + 0.63 \log_{10} K_{oa} + 0.96 \frac{1.37 \nabla H_v - 14}{2.303 R} \left( \frac{1}{T} - \frac{1}{298.15} \right) + \beta} \quad (2)$$

137  $MW$  (g/mol) is the molecular mass of the substance,  $T$  (K) is the absolute temperature  
138 of the room and  $b$ ,  $\tau$  (K) and  $\beta$  are material-specific coefficients,  $\nabla H_v$  (J/mol) the enthalpy of  
139 vaporisation and  $K_{oa}$  is the chemical's dimensionless octanol-air partition coefficient at  
140 25 °C.

141 Coefficients  $b$  and  $\beta$  have several reference values as a function of the type of material  
142 independently of the considered chemical. These values have been obtained by Huang et al.  
143 (2017) and Huang and Joliet (2019) based on the analysis of more than 1000 measured  
144 diffusion coefficients and material-air partitioning coefficients, with high  $R^2$ , but still  
145 substantial remaining uncertainties: SE on  $\log_{10} D$  and  $\log_{10} K$  amount to  $\pm 2.30$  and  $\pm 1.22$   
146 respectively, corresponding to uncertainty factors of 200 and 17. It is therefore interesting to  
147 take advantage of the measured concentrations to calibrate these parameters within their  
148 uncertainty range to the specific considered material.

## 149 **2.3 Selection of substances for main parameter calibration**

150 In order to optimise the parameters  $b$  (material-specific coefficient for diffusion) and  
 151  $\beta$  (material-specific coefficient for partition), a calibration is realised for each material using  
 152 data for part of  $N$  substances for which measurements at two points in time ( $t_1$  and  $t_2$ ) are  
 153 known, the other substances (at least one) being kept for the validation step. Excluding one  
 154 substance for validation (from  $N-1$ ), we select at least two and up to four substances for  
 155 calibration, with the broadest range possible in their diffusion ( $D_m$ ) and partition coefficients  
 156 to cover various emission dynamics: the substance having the highest  $D_m$  and highest  $K_{ma}$ ,  
 157 and the one with the lowest  $D_m$  and lowest  $K_{ma}$  are chosen. If more than one substance  
 158 remains, up to two additional substances are selected: the one(s) having the highest absolute  
 159 difference between  $D_m$  and  $K_{ma}$ . Any remaining substance is kept for validation. A detailed  
 160 description of the selection process is given in SI section S.2.

## 161 2.4 Parameters calibration

162  $b$  and  $\beta$  are first varied within their range of uncertainty using a 50 x 50 grid, yielding  
 163 2500 combinations of  $D$  and  $K$ . For each of these combinations  $b$ - $\beta$ , we perform the  
 164 following iterative process: a) We first back-calculate the initial mass fraction  $MF_{0,b-\beta}$  of the  
 165 substance  $s$  under study<sup>1</sup> that correctly predicts the concentration at time  $t_1$ ,  $C_{t_1}$ . b) We then  
 166 evaluate for each  $b$ - $\beta$  combination the deviation ( $d_{b-\beta_s}$ ) between the log of observed and  
 167 predicted ratios of  $C_{t_1}/C_{t_2}$  calculated as :

$$d_{b-\beta_s} = \left| \left( \log_{10}(C_{t_1,m_s}) - \log_{10}(C_{t_2,m_s}) \right) - \left( \log_{10}(C_{t_1,p_{s_{b-\beta}}}) - \log_{10}(C_{t_2,p_{s_{b-\beta}}}) \right) \right| \quad (3)$$

168 c) We calculate for each  $b$ - $\beta$  combination, the mean deviation ( $\bar{d}_{b-\beta}$ ) across all calibration  
 169 substances

170 d) We also determine for each  $b$ - $\beta$  combination a penalty for diverging from the reference  $D_m$   
 171 and  $K_m$  values is applied to each  $b$ - $\beta$  couple, calculated as:

---

<sup>1</sup> This step only serves the purpose of calibration. The actual mass fraction of the substance in the material is determined later based on all available measurements (see section below).



$$p_{b-\beta} = 0.1 \times (abs(\log_{10}(K_{ma,b-\beta}) - \log_{10}(K_{ma,ref})) + abs(\log_{10}(D_{m,b-\beta}) - \log_{10}(D_{m,ref}))) \quad (4)$$

172 The optimal  $b-\beta$  combination is selected as the one minimizing  $\varepsilon_{b-\beta_{tot}}$ , the sum of the  
 173 obtained average deviation plus the penalty  $p_{b-\beta}$  :

$$\varepsilon_{b-\beta_{tot}} = \sum_{s=1}^n \bar{d}_{b-\beta_s} + p_{b-\beta_s} \quad (5)$$

## 174 2.5 Mass fraction and resulting air concentration

175 Since initial mass fractions of substances inside the measured materials ( $MF_0$ ) are  
 176 usually unknown, we use the optimal parameters from the calibration step to determine  $MF_0$   
 177 as the mass that minimizes the root mean squared log error (RMSLE) on all concentrations for  
 178 all times ( $i=1,n$ ) and substances ( $s=1,x$ ):

$$e_{MF_0} = \sqrt{\frac{1}{n} \sum_{i=1}^n \sum_{s=1}^x (\log_{10}(C_{t_i,m_s} + 1) - \log_{10}(C_{t_i,p_s,MF_0} + 1))^2} \quad (6)$$

179 We then apply the emission model from Micolier (2019) to yield predicted air  
 180 concentrations.

## 181 2.6 Health impacts calculation

182 Health impacts  $HI$  (DALY) are calculated in DALYs (disability-adjusted life years), a  
 183 measure of the number of healthy life years lost due to sickness or premature death  
 184 recommended by the World Health Organisation (Murray et al. 1996), currently used as an  
 185 endpoint indicator in life cycle assessment (LCA), from the severity factor (DALY/cases),  
 186 effect factor  $EF$  (cases/kg<sub>intake</sub>), product intake fraction  $PiF$  (kg<sub>intake</sub>/kg<sub>in product</sub>) and the initial  
 187 mass of substance in the material  $M_0$  (kg<sub>in product</sub>).

$$HI_{rep/dev} = (SF_{rep/dev} \times EF_{rep/dev} + SF_{general\ non\ cancer} \times EF_{general\ non\ cancer} + SF_{cancer} \times EF_{cancer}) \times PiF \times M_0 \quad (7)$$

188 With

$$PiF = \frac{XF_{inh} \times V_{room} \int_{t=0}^T C_{in} dt}{M_0} \quad (8)$$

189           Where  $XF$  (1/s) is the exposure factor representing the fraction of the air volume that  
 190 is taken in by the occupants per time unit.

## 191 **2.7 Case study**

192           We selected as a case study a room with of 38.75 m<sup>2</sup> gypsum-covered walls and 15 m<sup>2</sup>  
 193 bamboo flooring. The room is ventilated at 1 ACH and occupied by 3 persons 8 hours per  
 194 working day and indoor temperature is set at 20°C.

## 195 **2.8 Applicability and assumptions**

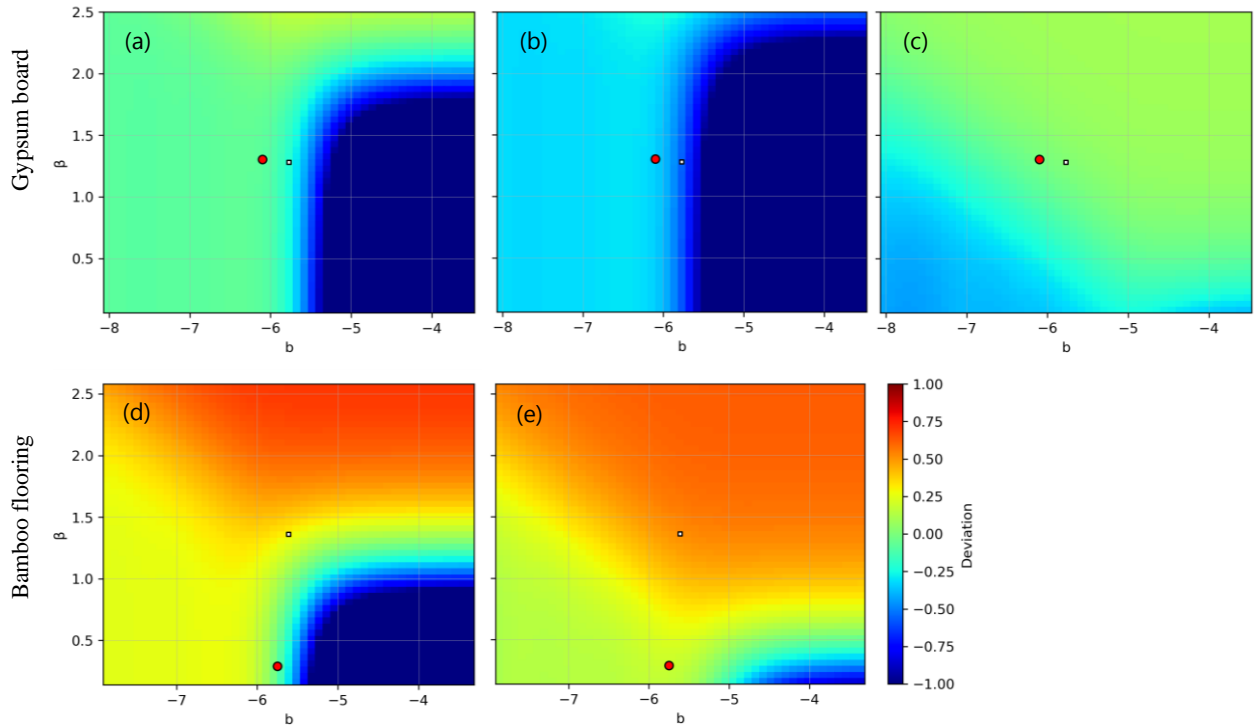
196           The framework is applicable under the following conditions: 1) data is available on  
 197 test chamber conditions, namely volume, air change rate and temperature, 2) dimensions of  
 198 the material are known and 3) at least two measurement points for at least three substances are  
 199 available, since emission data for at least two substances are used for calibration and the  
 200 model is validated with at least one other substance.

201           The model is applied under the following assumptions: 1) the concentration of the  
 202 substance is initially identical for all layers of the same material, 2) the concentration of the  
 203 substance in each layer is uniform at any point in time, 3) the substances emitted are volatile,  
 204 4)  $D_m$  and  $K_{ma}$  are unique to all layers of the same material and 5) emissions occur under  
 205 stable atmospheric conditions with constant pressure, relative humidity and temperature.

## 206 **3. Results**

### 207 **3.1. Deviation of predicted values from measured values**

208           The above framework is applied to the two mono-layered materials with available  
 209 measurement data: gypsum board and bamboo flooring. Hexanal, toluene and n-hexadecane  
 210 were selected for the calibration of the gypsum board parameters whereas acetic acid and  
 211 phenol were used for bamboo flooring calibration. [Figure 2](#) presents for each of these  
 212 chemicals-material combinations the deviation between the log of observed and predicted  
 213 ratios of concentrations  $C_{t_1}/C_{t_2}$ , as calculated by equation (3).



214 *Figure 2: Heat maps of  $d_{b-\beta_s}$ , the deviation between the log of observed and predicted*  
 215 *ratios of concentrations  $C_{t_1}/C_{t_2}$  for (a) hexanal, (b) toluene, (c) n-hexadecane emissions from*  
 216 *gypsum board and (d) acetic acid, (e) phenol from bamboo flooring as a function of the*  
 217 *material coefficient  $b$  for diffusion and  $\beta$  for material-air partition. The reference default*  
 218 *values of  $b$  and  $\beta$  are indicated by a yellow dot at the centre and optimal values by a larger*  
 219 *red dot. The scale of deviation, from -1 to 1, is given on the right side of (e).*

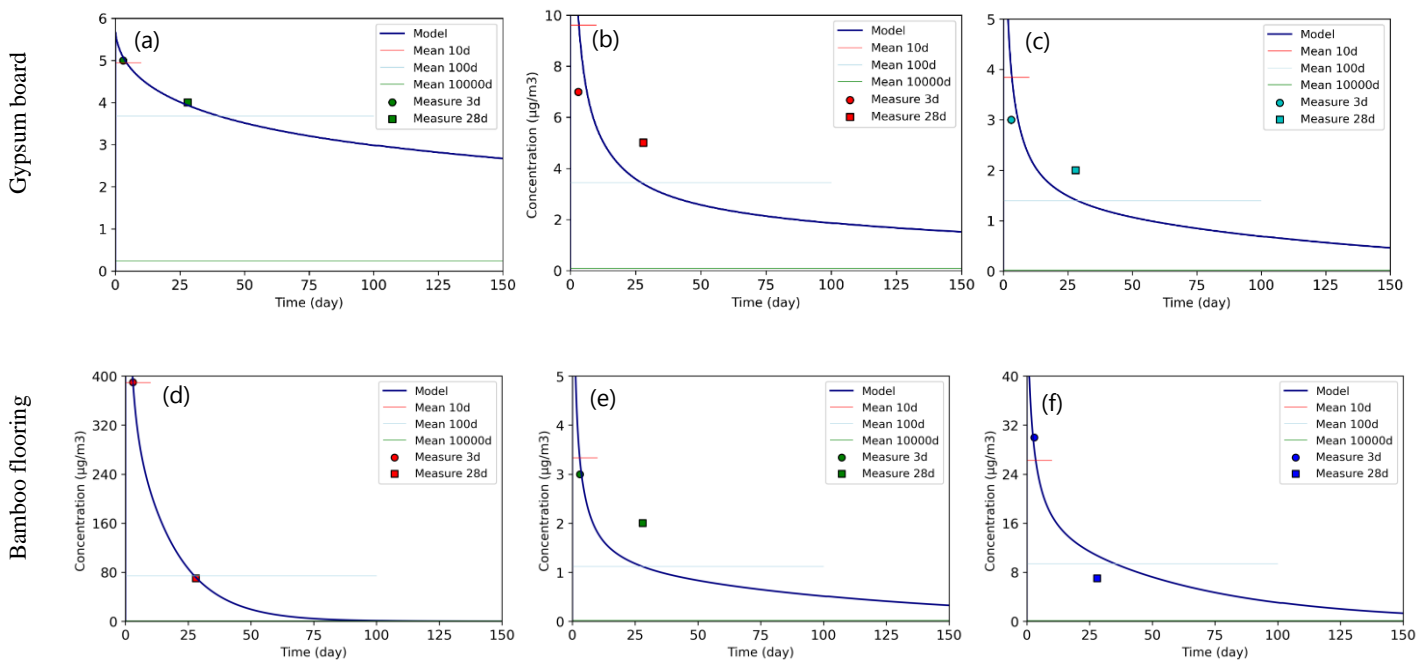
220 The optimal parameters  $b$  and  $\beta$  minimize the average deviation across chemicals as  
 221 determined by equation (5) (black-outlined red dots in Figure 2 and therefore fall in the light-  
 222 green or light blue areas that correspond to values that make the model best agree with  
 223 measurements and yield smallest deviations. For the gypsum board, the deviation primarily  
 224 depends on the diffusion coefficient  $b$ , with deviation of up to a factor 10 ( $d_{b-\beta_s} = -1$ , dark  
 225 blue area) between modelled and measured concentrations of hexanal and toluene at low  
 226 diffusion coefficient. The optimal  $b$  and  $\beta$  combination is obtained for  $b = -6.10$  and  
 227  $\beta = 1.3$ , which is close (within a factor 2 for the diffusion coefficient) to the reference values  
 228 of -5.77 and 1.26.

229 For the bamboo flooring, emissions are sensitive to both diffusion and material-air  
 230 partition coefficients when considering acetic acid and phenol. The low-deviation (light  
 231 green) regions are quite limited. Based on the deviation and penalty, the optimal solutions of

232  $b$  and  $\beta$  for bamboo flooring are -5.75 and 0.29, thus with a factor 10 lower on the material air  
 233 partition coefficient from the default reference value of -5.61 and 1.36.

234 **3.2. Predicted vs measured VOC air concentrations**

235 For each substance, the optimal parameters are used to determine  $MF_0$  based on  
 236 equation (6) are applied to the model, and obtain the air concentration of different emitted  
 237 substances as a function of time. Figure 3 compares the predicted concentration curves to the  
 238 measurement points and present the mean predicted concentrations over 10, 100 and  
 239 10000 days, showing a relatively good concordance between measured and modelled values.

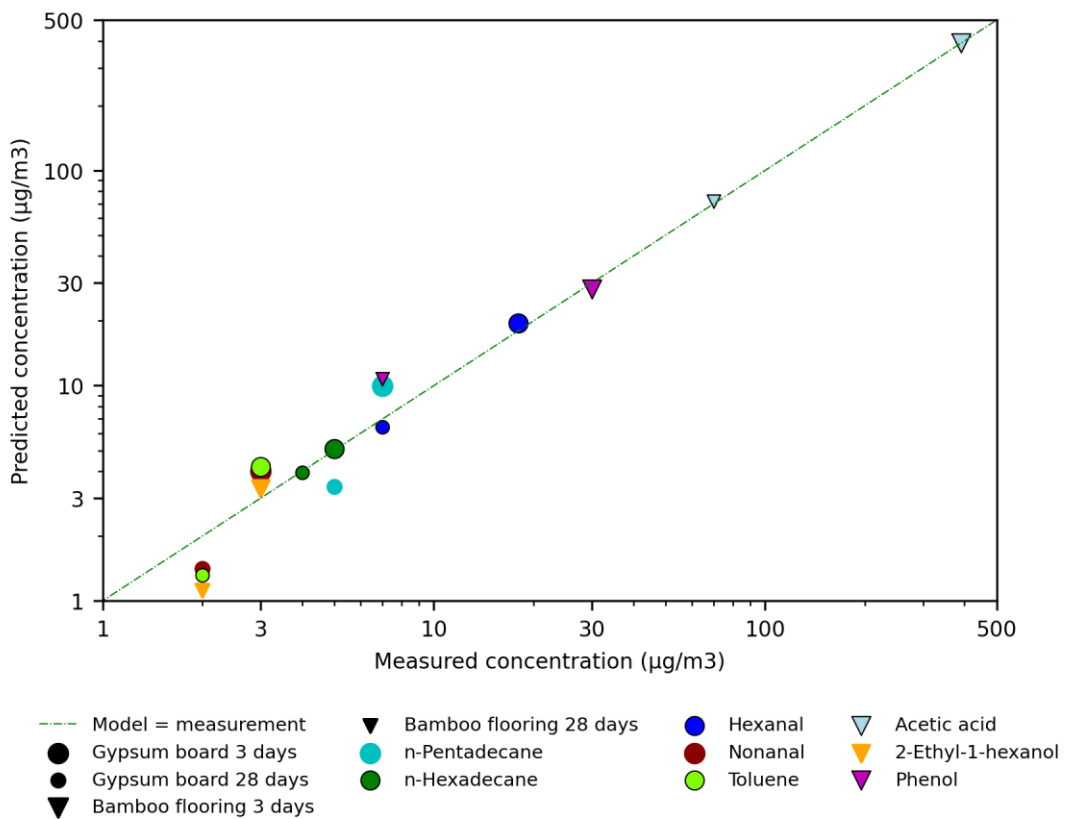


240 *Figure 3: Evolution of the predicted concentrations for (a) n-hexadecane, (b) n-*  
 241 *pentadecane, (c) nonanal emitted by gypsum board, and (d) acetic acid, (e) 2-ethyl 1-hexanol,*  
 242 *(f) phenol emitted by bamboo flooring: The mean predicted concentrations over 10, 100 and*  
 243 *10000 days are presented by red, light blue and green lines respectively.*

244 The volatile nature of the considered substances is reflected in the decrease in mean  
 245 concentrations with increasing time frame. Since the first measured point is higher, its squared  
 246 difference to the model tends to be higher as well and the concentration curves tend to be  
 247 closer to this first measured value, within a factor 1.4.

248 **3.3. Uncertainties**

249 The model is validated against the test substances calibration, estimating the  
250 percentage error, the root mean squared log error (RMSLE) and the mean absolute log  
251 deviation (MALD). Since predicted concentration different substances can vary over orders of  
252 magnitude, selecting the error on the log of concentrations gives equal importance to relative  
253 errors across the entire range of concentration and avoids a bias towards substances with  
254 higher concentrations. Figure 4 compares the predicted and measured air concentration, with  
255 circle markers for the gypsum board and triangles for the bamboo flooring mono-layered  
256 material.



257

258 *Figure 4: Measured v/s predicted concentrations for 3-day (bigger markers) and 28-*  
259 *day (smaller markers) measurements from gypsum board (circle markers) and bamboo*  
260 *flooring (triangle markers) for all substances with both measurements known. The substances*  
261 *with a black-outlined marker have been selected for the calibration process*

262 Figure 4 shows good agreement between measured and modelled data for both the  
263 calibration data and for the test data with less than a factor two for the test substances  
264 pentadecane and nonanal (cyan and brown circles) in the gypsum flooring and for 2-ethyl 1-  
265 hexanol in the bamboo flooring (orange triangle).

266 Table 2 summarises the errors (percentage error, RMSLE and MALD) for the  
 267 substances divided into three categories: all substances, only test substances and only  
 268 substances selected for the calibration process.

269 *Table 2: Relative error, Root Mean Squared Log Error, and Mean Absolute Log*  
 270 *Deviation (MALD) for all substances, only validation points and only substances selected for*  
 271 *the calibration*

	<b>All substances</b>	<b>Only test substances</b>	<b>Only calibration</b>
<b>% Error</b>	22%	32%	16%
<b>% Error 3d</b>	18%	29%	11%
<b>% Error 28d</b>	26%	35%	20%
<b>RMSLE</b>	0.02	0.05	0.02
<b>RMS uncertainty factor</b>	1.05	1.13	1.04
<b>MALD</b>	0.19	0.30	0.13
<b>MALD uncertainty factor</b>	1.56	1.99	1.34

272 As expected, the error indicators are lower for substances used in the calibration  
 273 procedure whereas, prediction remains within max a factor 2 of the observed value for the test  
 274 substances. Relative error, for all substances and all measurements, on the predicted values is  
 275 of 22%, corresponding to average errors on air concentration measurements, generally around  
 276 20%, but which could range from 5% to 25% [18,19].

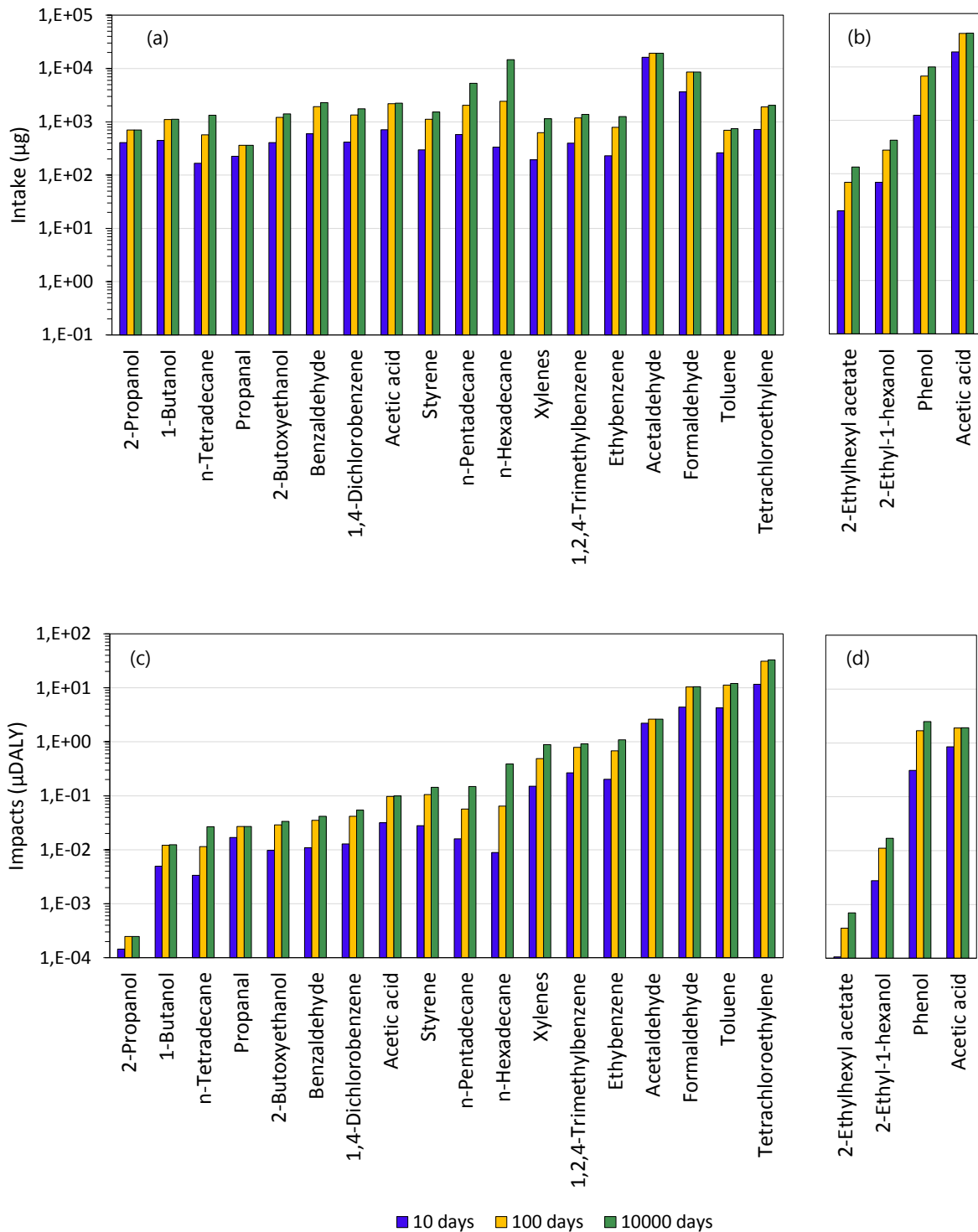
277 For the bamboo flooring, the predicted initial mass fractions of  $7.6 \times 10^{-7}$  for phenol  
 278 and  $8.4 \times 10^{-8}$  for toluene respectively 2 and 6 orders of magnitude lower than reported ones  
 279 in Pharos. Lower predictions could be explained by the difference between the composition of  
 280 the product under study and those referenced in Pharos. Calculated mass fractions correspond  
 281 to the amount of substance in the material at the beginning of chamber tests. Thus, low-end  
 282 values could also come from the time elapsed between the manufacture and the chamber tests,  
 283 and, consequently, partial emission of substances (especially highly volatile ones) before  
 284 measurements are taken.

### 285 **3.4. Application to the case study**

286 The case study parameters, optimal  $b$  and  $\beta$  and mass fractions calculated previously  
 287 for both materials are applied to the model for substances studied (those with two measured  
 288 data). For point with single measured data,  $MF_0$  is back-calculated from the measured  
 289 concentration using the same optimal  $b$  and  $\beta$  as for the other substances. The intake

290 fractions are calculated from equation (8) using concentrations and exposure fractions and the  
291 consequent health damages are evaluated using equation (7).

292 Figure 5 presents the intake ( $\mu\text{g}$ ) and health impacts ( $\mu\text{DALY}$ ) of substances emitted  
293 by gypsum board and bamboo flooring over short, medium and long-term exposure  
294 corresponding to 10, 100 and 10000 days respectively. 18 out of 21 substances emitted by  
295 gypsum board and 4 out of the 11 substances emitted by bamboo flooring have known  
296 toxicity data (effect factors).



297

298

299 *Figure 5: Intake quantities ( $\mu\text{g}$ ) for (a) 17 substances emitted by gypsum board and*  
 300 *(b) 6 substances emitted by bamboo flooring and health impacts for different substances*  
 301 *emitted by (c) gypsum board and (d) bamboo flooring over 10, 100 and 10,000 days*

302 **Figure 5** shows that the differences between short, medium and long-term exposures to  
 303 acetaldehyde emitted from gypsum board or acetic acid from bamboo flooring are not  
 304 significant since these substances are highly volatile and rapidly emitted. For some substances



305 such as n-hexadecane emitted from gypsum board, the short-term impacts can be lower but  
 306 long-term impacts higher than certain substances such as n-pentadecane, since their emission  
 307 dynamics are different.

308 It can also be noted that impacts can be different for similar intake quantities, or that  
 309 they can be higher for substances with lower intake quantities since there can be substantial  
 310 variations between effect factors of different substances. For example, the intake quantity of  
 311 acetic acid from bamboo flooring is of  $1.90 \times 10^4 \mu\text{g}$  while for phenol it is of  $1.24 \times 10^3 \mu\text{g}$ .  
 312 Their respective health damages are 1.91  $\mu\text{DALY}$  and 2.50  $\mu\text{DALY}$ . Despite having over 10  
 313 times the intake quantity of phenol, acetic acid is responsible for less health impacts due to its  
 314 lower effect factor. It can also be noted that the differences between the health damage from  
 315 different substances are several orders of magnitude high and that the substances of concern  
 316 in each material can be different. In the case of gypsum board, tetrachloroethylene is  
 317 responsible for 53% of the total damage from VOC emissions, toluene for 19% and  
 318 formaldehyde 17%. For bamboo flooring, phenol has the highest contribution, accounting for  
 319 52% of health impacts and acetic acid 48%. [Table 3](#) summarises the health damages related to  
 320 the exposure to VOCs emitted by the three materials for short, medium and long-term  
 321 exposures. The equivalent damage for 1 m<sup>2</sup> flooring area per year is also given based on the  
 322 long-term exposure.

323 *Table 3: Health damages related to the intake of substances with known toxicity data*  
 324 *for gypsum walls and bamboo floor for the office (3 persons in 15 m<sup>2</sup>) over three exposure*  
 325 *periods, per unit floor area per year and per kg of material*

<b>Health impacts</b>	<b>Gypsum walls</b>	<b>Bamboo floor</b>
10 days ( $\mu\text{DALY}$ )	23.18	1.16
100 days ( $\mu\text{DALY}$ )	57.60	3.60
10000 days ( $\mu\text{DALY}$ )	61.97	4.43
10000 days ( $\mu\text{DALY}/\text{m}^2/\text{year}$ )	0.15	0.01
10000 days ( $\mu\text{DALY}/\text{kg}$ )	0.11	0.01

326 From [Table 3](#), it can be noted that, for the functional unit of 1 m<sup>2</sup> floor area, gypsum  
 327 board leads to more health damage on occupants than bamboo floor.

## 328 **4. Conclusion**

329 A framework was developed to calibrate a material VOC emission model depending  
330 on parameters having relatively high uncertainties (factor 10 to 100), and to calculate  
331 unknown VOC mass fractions using measured air concentration data. It allows to extrapolate  
332 measurements, only valid at few points in time and for short time spans, scale concentrations  
333 to real building contexts, and calculate full exposure and long-term health impacts on  
334 occupants. The framework was tested on two mono-layered materials, yielding an uncertainty  
335 factor of 1.1 (RMSLE) and a relative error of 22% between measurements and predictions,  
336 corresponding to typical VOC air concentration measurement uncertainties. Calculated  
337 parameters were applied to a case study of an office to calculate short, medium and long-term  
338 health impacts from the exposure to VOCs: 24  $\mu$ DALY, 61  $\mu$ DALY and 66  $\mu$ DALY  
339 respectively. This framework, by providing full concentration profiles, can help  
340 manufacturers to devise material treatment strategies that aim at lowering impacts related to  
341 VOC off-gassing (e.g. artificial ageing). It can also help in decision-making process in the  
342 building sector: choice of low-impact materials and adequate ventilation rates to evacuate  
343 pollutants. The present method is dependent on emission data, but these are often confidential  
344 or incomplete. Due to regulations and growing concern regarding health implications of  
345 material VOCs, these data are expected to become more readily available in the future. Health  
346 impacts are possibly underestimated since toxicity data are lacking for a number of substances  
347 and should be updated when available, and also because, in real building contexts, gypsum  
348 board is often covered in paint which can lead to additional VOC emissions. Finally, chemical  
349 reactions in indoor air can consume existing chemicals or produce new ones and should be  
350 considered in IAQ health impact assessments [4].

## 351 **5. Data availability**

352 The ED10 and ED50 data used to support the findings of this study are included  
353 within the supplementary information files.

## 354 **6. Acknowledgement**

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356 Eco-design of buildings and infrastructure.

## 357 **7. Conflicts of interest**

358           The authors declare that there is no conflict of interest regarding the publication of this  
359 paper.

## 360 **8. Supplementary Materials**

361           The multilayered emission model is described in supplementary material S.1. Detailed  
362 description for the selection of substances based on their emission dynamics are given in S.2.  
363 In S.3. the equations used for the calculation of exposure factors  $XF$  and effect factors  $EF$  are  
364 given. The data used for the calculation of  $EF$  are given in Table S1 in S.4.

365

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