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Integration of Indoor Air Quality to the Life Cycle Assessment of Buildings

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Abstract. Pollutants – gases or particles – are emitted in indoor air by different sources such as building materials, furniture, occupants and their activities. Spending over 80 % of our time indoors, we are directly exposed to substances that are potentially harmful to our health. Through measurements and simulation tools, the concentrations of these substances in air can be evaluated. However, today, Indoor Air Quality (IAQ) is not taken into account in the Life Cycle Assessment of buildings (LCA). The aim of this study is to calculate and compare the damage of IAQ on occupants' health with the damage over the whole building life cycle, expressed in the same unit as in LCA: Disability-Adjusted Life Years (DALY), in order to propose a decision-making tool. Volatile organic compounds (VOCs) are emitted by building materials or furniture and then are assimilated by occupants. A model describing their emissions including unknown or uncertain parameters is calibrated using existing emission data. Secondly, emission data on occupants and their activities are used to simulate indoor concentrations of VOCs. The assimilation and consequent health damages are then calculated. According to a case study of an office, health damages related to the emissions of gypsum-covered walls were of 1.32×10^{-6} DALY.year⁻¹, about 2 orders of magnitude lower than those of the other life stages of the building (from fabrication and transport of products, construction, use, until end-of-life processes) which correspond to 1.2 to 4.5×10^{-3} DALY.year⁻¹. Those related to regular office activities were of 3.7×10^{-26} DALY.year⁻¹. This methodology can help in eco-design of buildings by identifying main sources of impacts. It can help to choose between materials or to dimension the ventilation for the evacuation of pollutants.

1. Introduction

Indoor air quality (IAQ) is a matter of crucial concern since humans spend more than 90% of their time indoors (U.S. Environmental Protection Agency 1989) and are directly exposed to substances that can be harmful to their health. These substances, called pollutants, are either in the form of particulate matter (PM) or gases and are either emitted directly by indoor sources (materials used in construction and furniture, human activities and humans themselves) or brought from outdoors through ventilation. Since people spend a lot of their time indoors, most of the intake takes place there, even when considering



outdoor pollution. Several studies have documented the burden of indoor air pollution on occupant health (Mainka and Fantke 2022; Karr et al. 2021; Ali et al. 2021; Smith and Mehta 2003; Bardana 2001). The presence of several of these substances can be influenced by the building's design. However, at present, building eco-design is mainly based on its life cycle assessment (LCA) and IAQ is evaluated using different, uncorrelated tools. It is hence important to assess the effects of IAQ and integrate them to building eco-design as a means of avoiding IAQ-related impacts right at the design phase. For this, it is required to model emissions of pollutants indoors and calculate their damage on human health with the same unit as that of LCA.

One of the design choices that affects indoor pollutant concentrations, is that of the ventilation system (Poirier et al. 2021; Norhidayah et al. 2013; Shaw 2004). It can be dimensioned to evacuate a maximum of indoor gaseous or particulate pollutants. Another important design choice that is a contributor to indoor chemical concentrations is that of the materials (Huang et al. 2022; Shaw 2004). The composition of the material determines the substances that can be emitted due to their volatility, but this composition is often unknown, though average values can be found for some material categories in the Pharos database (Friar and Vittori 2017). Different parameters define the emission dynamics, including the chemical properties of the substance and properties of the material. While chemical properties are well-known and readily available in literature, material-specific properties have been computed from large datasets of about 1000 measurements (Huang and Jolliet 2019; Huang et al. 2017) and contain uncertainties. These reference values can be used in order to simulate average indoor concentrations when no specific emission data is available. On the other hand, different studies have aimed at measuring the emission of VOCs from specific materials (Wilke et al. 2004; Won et al. 2003; Shaw 2004; James and Yang 2005). Furthermore, since 2011, it is mandatory for manufacturers to measure VOC emissions of construction and wall and flooring materials under the regulatory labelling scheme in France (Journal officiel 'Lois et Décrets' 2011).

Since current VOC emission models contain uncertainties, a coupling between the model and available data can be realised to fix the model parameters. This paper presents the methodology developed for the model-data coupling and a framework to quantify the health impacts related to the intake of these pollutants is proposed. The health damages on building occupants are calculated in DALYs (Disability-Adjusted Life Years), which is a measure of the number of healthy life years lost due to sickness or premature death, a unit of toxicity recommended by the World Health Organisation (Murray et al. 1996) and currently used as an endpoint indicator in LCA.

The pathway from source leading to impacts can be separated into four main blocks as represented in Figure 1.

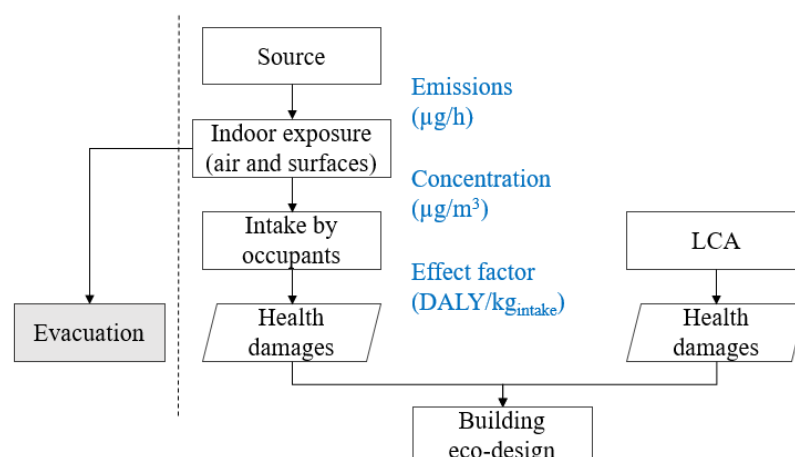


Figure 1: Pollutant pathway from source to health damages

2. Materials and methods

The calibration method developed is based on an existing emission model and emission data. The main steps are summarised in Figure 2.

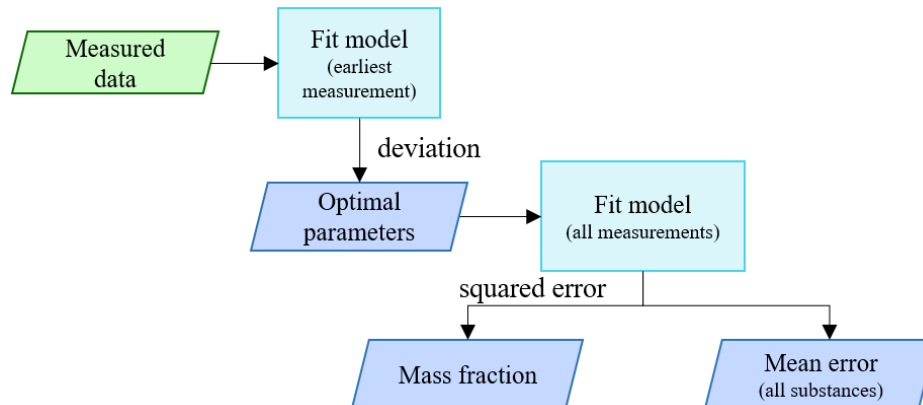


Figure 2: Calibration framework

2.1. Emission model

The multilayered material emission model discussed in this paper, applied by Micolier (2019), has been developed by Yan et al. (2009) and modified by Guo (2013). It is based on the mass balance of substances at different nodes within the material and in air. The material is divided into several layers, with each considered to have a uniform concentration of the substance and each represented by a single node. The emission rate depends on the initial mass fraction of the substance in the material, MF_0 . It also depends on D_m and K_{ma} , expressed below, which themselves depend on material-specific coefficients.

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

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

MW (g/mol) is the molecular mass of the substance, T (K) is the absolute temperature of the room and b , τ (K) and β are material-specific coefficients with reference values computed by Huang et al. (2017) and Huang and Jolliet (2019), ∇H_v (J/mol) the enthalpy of vaporisation and K_{oa} is the chemical's dimensionless octanol-air partition coefficient at 25 °C. Coefficients b and β are obtained from measured data and contain uncertainties.

2.2. Emission data

Emission data are available in literature or from manufacturers, and are obtained through the measurement of emitted substances in test chambers. These chambers are conditioned with specific ventilation rates, relative humidity and temperatures. The surfaces of the room are made of materials that have very low absorption or emission, such as glass or stainless steel, in order not to interfere with the tested material. The material is placed inside the chamber with only one face emitting substances, the other being covered in an impermeable material. Measurements of the concentration of several VOCs in the chamber air are then taken at different times, for example, 3, 28, 35 and 42 days.

2.3. Choice of substances

As discussed earlier, b and β contain uncertainties and the initial mass fraction of the substance in the material, MF_0 , is most often unknown. In order to fix these parameters and initial masses, a calibration is realised using available VOC emission data. The data used are for mono-layered materials with information on the test chamber conditions and at least two measurement points for at least three

substances. This is because emission data for at least two substances are used for calibration and the model is validated with at least one other substance. The choice of substances is based on their diffusion and partition coefficients: those having different emission dynamics are selected. At least one substance that is D-limited and one substance that is K-limited are selected according to the cut-off criteria described by Huang et al. (2020).

$$D_m^{0.61} \cdot K_{ma} < 0.40 \quad (3)$$

If all substances are limited by only D_m or only K_{ma} , the ones having the highest and the ones having the lowest difference and sum between $D_m^{0.61}$ and K_{ma} are selected.

2.4. Calculation of optimal parameters

First of all, b and β are varied in their range of uncertainty. For each combination of b and β called x , the initial mass fraction MF_0 of the substance s under study is determined by an iterative process so that the model predicts the correct earliest measurement¹. For example, for two readings C_{t_1} and C_{t_2} at times t_1 and t_2 , the model has to predict the correct concentration C_{t_1} . This is done to evaluate the deviation of the predicted value from the measured value of C_{t_2} . We call the deviation, d_{x_s} , the ratio expressed below, based on the first and second measurements of s at given times t_1 and t_2 and for a given couple x :

$$d_{x_s} = \text{abs} \left(\log_{10} \left(\frac{C_{t_1, m_s} / C_{t_2, m_s}}{C_{t_1, p_{sx}} / C_{t_2, p_{sx}}} \right) \right) \quad (4)$$

where C represents the concentration in air and subscripts t_1 and t_2 indicate the time of the measurement, m , or prediction, p . The log is taken in order to avoid giving higher importance to higher readings. For each couple x , the mean deviation for all substances is calculated as \bar{d}_x .

To this deviation, a penalty for diverting from the reference D_m and K_m values is applied to each x . The penalty p_x is given using the log of the ratio between the reference and model coefficients x as shown below:

$$p_x = \text{abs}(\log_{10}(K_{ma,x}/K_{ma,ref})) + \text{abs}(\log_{10}(D_{m,x}/D_{m,ref})) \quad (5)$$

The sum of the deviation and penalty, ε , is made for all b and β couple x and is given by the expression below:

$$\varepsilon_x = \bar{d}_x + \frac{p_x}{10} \quad (6)$$

The weight of 0.1 adds more importance to the measurements as compared to the reference values. The optimal parameters are those that minimise the sum of ε_x for all selected substances and all b and β couple x .

2.5. Calculation of mass fraction

The optimal parameters determined through the above method are then used in the calculation of the initial mass fraction of the substance in the material. For this, the total squared error e for all n readings at i times of each substance is calculated and the MF_0 that yields the lowest mean squared error is selected.

¹ It is to be noted that this step only serves the purpose of optimisation but does not determine the actual mass fraction of the substance in the material. For this, all readings are going to be used, as described in Calculation of mass fraction.

$$e_{MF_0} = \frac{1}{n} \sum_{i=1}^n (C_{t_i, m_s} - C_{t_i, p_s, MF_0})^2 \quad (7)$$

This method allows for all measurement points to be used in the determination of the unknown parameter MF_0 .

2.6. Hypotheses

The model is valid under the following hypotheses: 1) the concentration of the substance is initially identical inside all layers of the same material, 2) the concentration of the substance in each layer is uniform at any point in time, 3) the substances emitted are volatile, 4) the calculated MF_0 corresponds to the time at which measurements in the chamber have begun and this could differ from the initial mass fraction of the substance in the material corresponding to its composition right after manufacture, 5) D_m and K_{ma} are unique to all layers of the same material and 6) emissions occur under stable atmospheric conditions with constant pressure, relative humidity and temperature.

2.7. Health damage

The intake of substances can occur through four different pathways and the exposure factors are used to calculate the volume of exposure through each pathway. The calculation of the exposure factors XF for each pathway, inhalation, gaseous dermal uptake, dust ingestion and direct dermal contact are calculated according to Huang et al. (2017) using parameters recommended by the Exposure Factors Handbook of the Environmental Protection Agency (US EPA 2011).

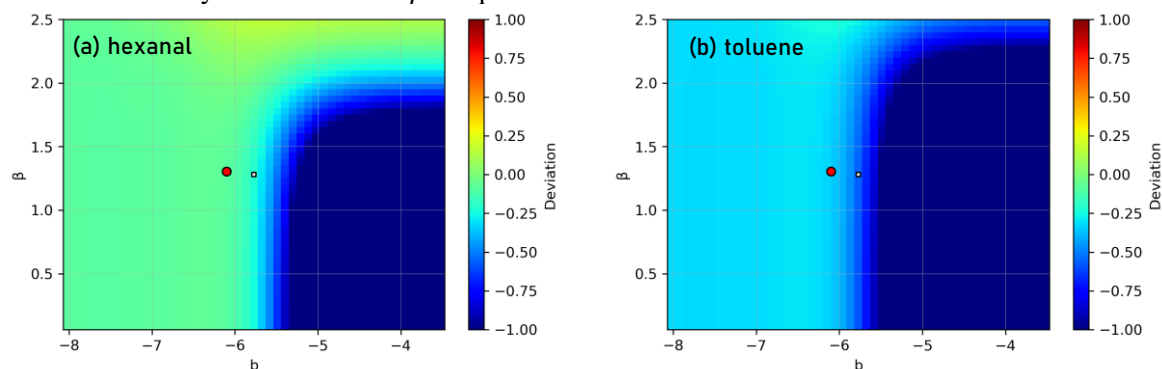
Health damages are calculated for VOCs according to the USEtox model and effect factors are calculated from the 50% effect dose ED_{50} (Fantke et al. 2017).

3. Results and discussion

The above framework is tested on gypsum board with data collected the manufacturer emission sheet. The board is 12.5 mm thick and its density is 1150 kg.m^{-3} . The chamber has a volume of 0.123 m^3 with an air change rate of 0.5 vol.h^{-1} at $23 \text{ }^\circ\text{C}$ with a relative humidity of 50 %. The loading ratio (surface area of material divided by the volume of the room) is $1 \text{ m}^2.\text{m}^{-3}$. Emission data is available for 20 substances, but only 5 of them have two measurements recorded: at 3 days (t_1) and at 28 days (t_2). No uncertainty or error on the measurements were given. According to the method described based on equation (3), the selected substances out of these 5 are hexanal, toluene and n-hexadecane. The b and β reference values for gypsum board are -5.77 and 1.28 respectively (Huang et al. 2017; Huang and Jolliet 2019).

3.1. Optimal parameters.

The heat maps below present the deviation of the model from the predicted concentration at 28 days when fitted at 3 days for each b and β couple for the three selected substances.



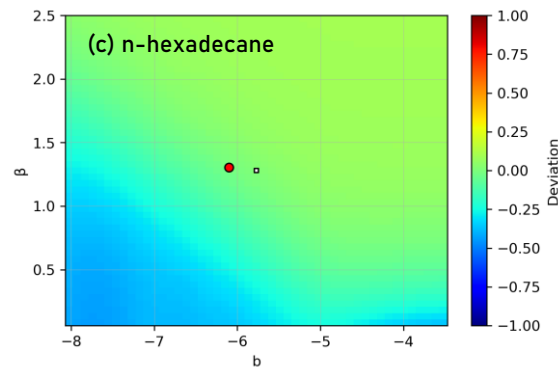
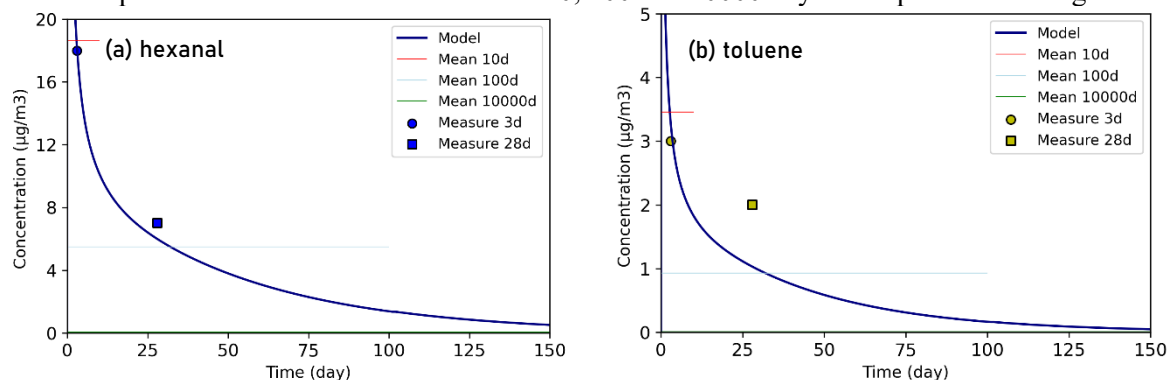


Figure 3: Heat maps of the deviation of predicted concentrations from observed values for (a) hexanal, (b) toluene and (c) n-hexadecane emissions from gypsum board with the reference values indicated by a yellow dot at the centre and optimal values by a larger red dot

It can be noted that for hexanal, the model agrees with the prediction for values of b ranging from -5.7 to -8, corresponding to the lower end of the uncertainty range and β ranging from 2.3 to 2.5, corresponding to the higher uncertainty range. The material-air partition coefficient, determined by β , has less influence on the deviation. For toluene, no b and β couple yields low deviation values. The substance is nevertheless more sensitive to a change in diffusion, determined by a change in b . Finally, n-hexadecane shows sensitivity to both b and β , with a higher sensitivity related to β . Higher values of β yield lower, close to zero, deviations. The final solutions for b and β are hence those giving the lowest ε_x when considering all three substances with the deviations and penalties and correspond to -6.10 and 1.30 respectively.

3.2. Calculation of mass fraction and concentrations.

Once the optimal parameters are defined using the two measurement points, the initial mass of each substance is calculated according to (7). The predicted concentration curves, the measurement points as well as the predicted mean concentrations over 10, 100 and 10000 days are represented in Figure 4.



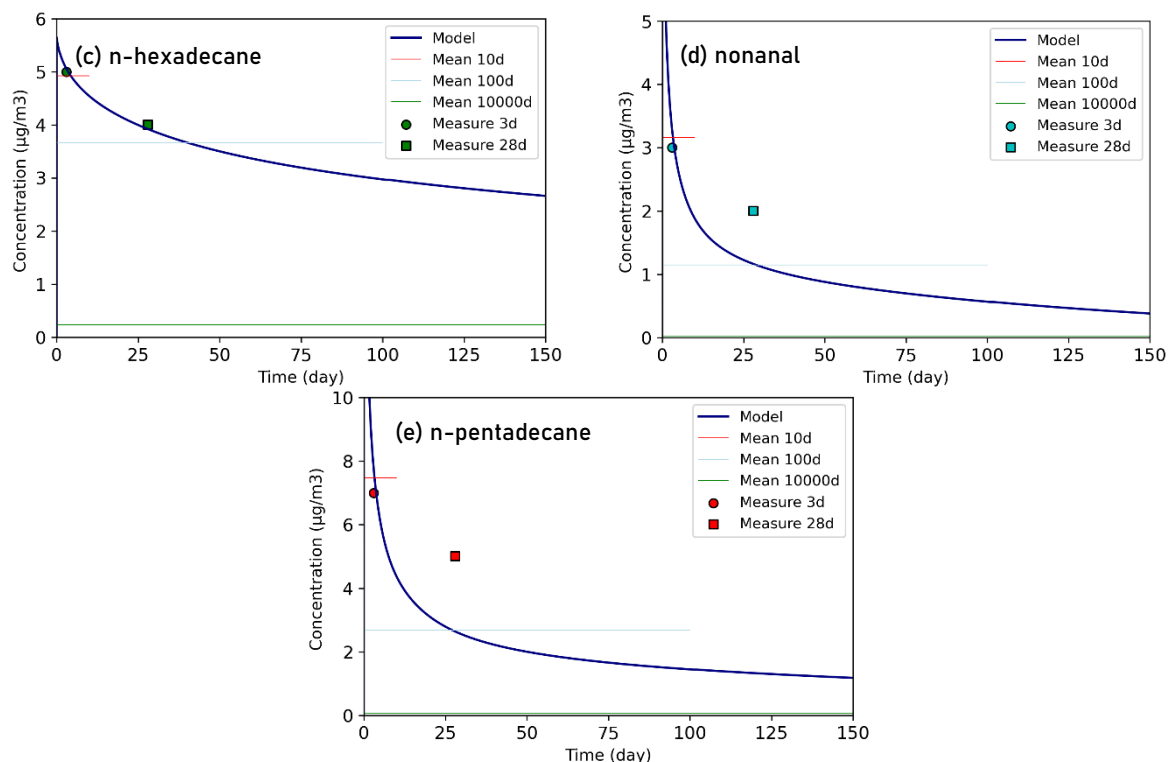


Figure 4: Predicted concentration curves of the 5 substances, (a) hexanal, (b) toluene, (c) hexadecane, (d) nonanal and (e) n-pentadecane, containing 2 measurement points and the predicted mean concentration over 10, 100 and 10000 days

The volatile nature of the substances can be noted from the mean concentrations that decrease with an increased time frame, until they tend towards zero after a very long period of time (about 25 years in the present study). Furthermore, it can be noted that the optimal curve with the calculated MF_0 tends to be closer to the first value. This is because a change in MF_0 changes by the same proportion all concentration points. Hence, the difference between predicted and measured values also change proportionally: for higher readings, the difference tends to be higher. This is accentuated by the fact that the squared difference is taken (7). The optimal MF_0 is the one that is sufficiently close to the second reading to decrease the error, but closer to the first, larger measurement which can give high error values. The mass fractions of the other substances (those having only one measurement point) are also calculated using the optimal parameters by fitting the model to the single measurement.

3.3. Validation

The results are presented in Figure 8. Readings closest to the dotted green line are those where predictions match the measurements. The colours represent the same substances as in Figure 5, with round markers representing 3-day measurements and squared markers representing 28-day measurements. The results are presented in log-scale in order to visualise the smaller readings with the same amplitude as the larger ones.

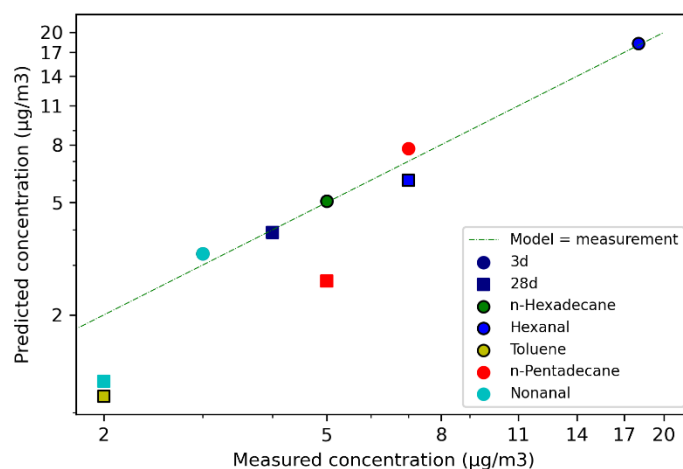


Figure 5: Measured v/s predicted concentrations for 3-day and 28-day measurements from gypsum board

The percentage error, the root mean squared error (RMSE) and the mean absolute log deviation (MALD) are calculated for each of the five substances. The MALD is given by the expression below:

$$MALD = \frac{1}{n} \sum_{i=1}^n Abs(\log_{10}(C_{m,i}) - \log_{10}(C_{p,i})) \quad (8)$$

The percentage error gives a relative evaluation of the error, the RMSE gives an absolute evaluation in the unit of the concentrations while MALD indicates, when considering 10^{MALD} , the ratio of the measured value to the predicted value without giving more weight to higher measured values. Table 1 shows the values of the different validation methods when considering all substances, only validation points or only substances selected for calibration.

Table 1: Validation of the model with measurement values using percentage error, RMSE and MALD

	All substances including selected	Validation points	Only selected
% Error	18.70	27.50	12.90
% Error 3d	6.72	9.96	5.91
% Error 28d	30.76	41.80	28.00
RMSE ($\mu\text{g}\cdot\text{m}^{-3}$)	1.82	3.48	0.72
RMSE %	7 – 66	16 – 148	6 – 54
MALD	0.20	0.30	0.14
MALD ratio	1.60	1.99	1.38

When considering all substances, the percentage error is of 18.7% the RMSE equals to $1.82 \mu\text{g}\cdot\text{m}^{-3}$ (corresponding to 7 to 66% of the highest and lowest reading) while the MALD is of 0.20, corresponding to a ratio of 1.60 between the observed and predicted values. When considering only the two validation points, nonanal and n-pentadecane, the error indicators are higher and, as expected, when considering only substances selected for optimisation, the error indicators are lower.

3.4. Office case study

The above results are applied to a case study of a 15 m² office having walls covered in gypsum board. In the case study, the office is occupied by 3 persons, 8 hours per working day. The air renewal rate is of 1 vol.h⁻¹. The concentrations of the VOCs emitted by the walls are modelled using the calculated optimal parameters b and β of the material and MF_0 of each substance. The contribution of regular office activities (use of cleaner, desktop, printer and air freshener) to the VOC concentrations are also included. They were modelled using the INCA-Indoor computing machine (Octopus Lab 2017) coupled with emissions from regular office activities obtained in the PANDORA database (Abadie and Blondeau 2011). Relevant data used in the simulations are presented in annex. The intake is then calculated according to the exposure which itself depends on the indoor concentrations. In order to calculate the health damages, all substances with known toxicity data are considered. A total of 17 substances out of the 22 have known toxicity data in the case of gypsum board and 19 out of 57 in the case of activities. However, the intake quantities of VOCs from activities are over 12 orders of magnitude lower as compared to those related to material emissions, except for one substance, 3-carene, that is emitted from air-fresheners.

The intake and consequent health damage on a time-scale of 10, 100 and 10000 days are presented in Figure 6 for the 17 substances emitted by the wall and 3-carene emitted by air-fresheners.

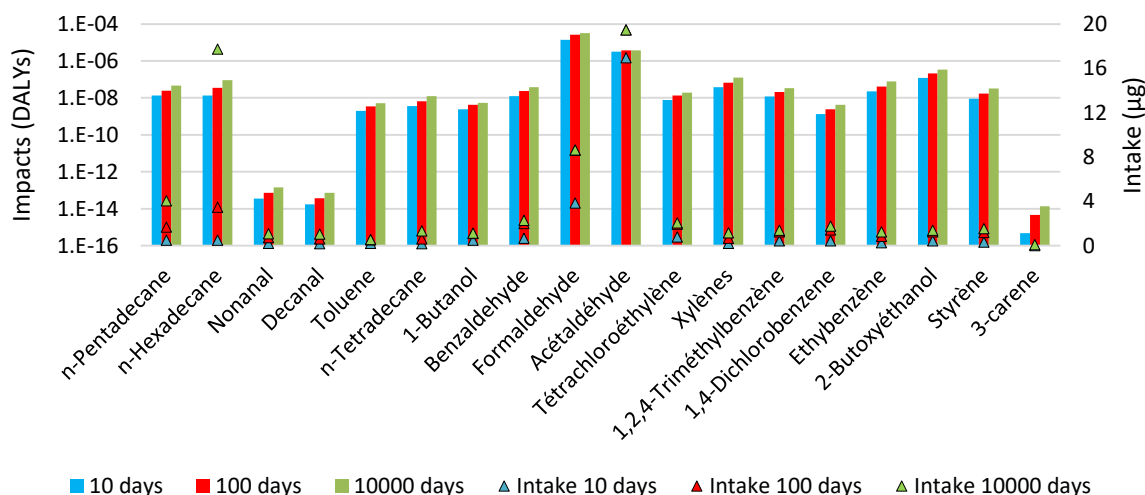


Figure 6: Health damages in DALYs related to the emission and intake of 17 substances on the health of three office occupants

The total impact of the gypsum-covered walls related to the emission of the 17 substances for which toxicity data are known is 1.76×10^{-5} , 3.05×10^{-5} and 3.62×10^{-5} DALY respectively when considering a time frame of 10, 100 and 10000 days (27.4 years). Considering the presence of three persons, the surface area of 15 m² and the duration of 27.4 years, the damages are equal to 8.80×10^{-8} DALY/m²/year or 4.40×10^{-7} DALY/p/y (DALY per person per year). The VOCs emitted by office activities are responsible for 4.62×10^{-15} DALY/p/y, several orders of magnitude lower than material emissions.

Different substances having different effect factors, their concentration or intake quantity do not determine the health damages they are responsible for. Figure 6 indicates that impacts are very different for similar intake quantities, or that they can be higher for substances with lower intake quantities. For example, formaldehyde has an intake quantity of 8.64 µg while acetaldehyde has an intake quantity of 19.46 µg. Their respective health damages are 31.65 µDALY and 3.68 µDALY. Formaldehyde hence has over eight times the impact of acetaldehyde on the health of the occupants despite having almost half of the intake quantity, since formaldehyde has a higher effect factor than acetaldehyde.

These results can be compared to the health damages related to the LCA of a typical office, which have been evaluated as 8×10^{-5} to 3×10^{-4} DALY/m²/year (Wurtz and Peuportier 2021) or to the estimate of

the chronic health impacts of indoor air pollutants (IAPs) which amounts to 1.1×10^{-2} DALY/p/y (Logue et al. 2012).

4. Conclusions and perspectives

This work demonstrated a methodology of calibration of an emission model that depends on parameters that are either unknown or contain uncertainties. The calibration can be realised in order to adapt the model parameters to a specific material with known emission data. The methodology has been applied to the context of the evaluation of the health damage related to VOC emissions from materials as a step towards the integration of IAQ in building eco-design. VOC emission data from office activities were also considered and the concentrations were simulated with INCA Indoor. However, it was found that health damages related to VOC from activities were several orders of magnitude lower than those emitted from gypsum board.

In the present case study of the office with gypsum-covered walls, the health damage related to VOC emissions was of 4.40×10^{-7} DALY/p/y. However, the following facts are to be noted. 1) Current LCA results provide damages on the health of populations at the level of a region, country or continent, while the present framework provides direct health damage to building occupants, so the two results should be interpreted with this in mind. 2) The present method is highly dependent on data, either material emission data or chemical toxicity data. There is, at present, only limited data since emission data are often confidential or incomplete and toxicity data are dependent on observations, but substances certainly cannot be tested for their toxicity on humans. Health damages are thus likely to be underestimated. As an effort to characterise more chemicals, machine learning models can be used to convert toxic chemicals into LCA impact characterisation factors based on their physicochemical properties (Hou et al. 2020). 3) Only one material has been assessed in this case study and only VOCs were considered. The higher estimation of the burden of IAPs by Logue et al. (2012) indicates that the contribution of more materials and the presence particulate matter (PM), estimated as being responsible for the highest number of DALYs lost, should be assessed.

Perspectives of this work thus include the addition of more toxicity and emission data when they become available, the integration of more materials to the study and the evaluation of concentrations of indoor PM and their effects on occupant health.

5. Annex

The data used for the calibration of the emission model is presented in Table 2 and those used for the office activities are presented in Table 3.

Table 2: Substances emitted by gypsum board and their measured concentrations in air at 3 and 28 days

Chemical	Concentration at 3 days ($\mu\text{g}/\text{m}^3$)	Concentration at 28 days ($\mu\text{g}/\text{m}^3$)	Chemical	Concentration at 3 days ($\mu\text{g}/\text{m}^3$)	Concentration at 28 days ($\mu\text{g}/\text{m}^3$)
112-31-2	2	3	64-19-7	3	
124-19-6	3	2	127-18-4	-	2
108-88-3	3	2	1330-20-7	-	2
544-76-3	5	4	95-63-6	-	2
629-62-9	7	5	106-46-7	-	2
66-25-1	18	7	100-41-4	-	2
100-52-7	10		111-76-2	-	2
71-36-3	7		100-42-5	-	2
67-63-0	7		75-07-0	-	3
123-38-6	4		50-00-0	-	6
629-59-4	3				

Table 3: Emission rates for different substances obtained from PANDORA (Abadie and Blondeau 2011), emitted by indoor office activities and the duration considered in the case study

Source	Chemical	Emission value ($\mu\text{g/h}$)	Duration (min)
Air freshener	100-52-7	267.08	15
Air freshener	100-51-6	3671.55	15
Air freshener	122-63-4	1331.98	15
Air freshener	76-49-3	178.60	15
Air freshener	125-12-2	9291.65	15
Air freshener	138-86-3	3678.50	15
Air freshener	80-56-8	2828.70	15
Air freshener	127-91-3	2514.20	15
Air freshener	79-92-5	953.23	15
Air freshener	13466-78-9	551.33	15
All-purpose cleaner	138-86-3	17000.00	20
All-purpose cleaner	80-56-8	956.25	20
All-purpose cleaner	79-92-5	1487.50	20
All-purpose cleaner	127-91-3	106.25	20
All-purpose cleaner	99-83-2	425.00	20
All-purpose cleaner	99-86-5	1700.00	20
All-purpose cleaner	5989-27-5	17000.00	20
All-purpose cleaner	99-85-4	1806.25	20
All-purpose cleaner	586-62-9	19125.00	20
All-purpose cleaner	586-82-3	3931.25	20
All-purpose cleaner	138-87-4	1912.50	20
All-purpose cleaner	562-74-3	1593.75	20
All-purpose cleaner	98-55-5	24437.50	20
All-purpose cleaner	586-81-2	2656.25	20
All-purpose cleaner	99-87-6	2656.25	20
All-purpose cleaner	470-82-6	4781.25	20
Photocopier*	100-41-4	33.00	[20]
Photocopier*	106-42-3	27.00	[20]
Photocopier*	100-42-5	20.00	[20]
Desktop	106-42-3	0.01	540
Desktop	629-62-9	0.03	540
Desktop	100-42-5	0.03	540
Desktop	108-88-3	0.02	540
Desktop	100-52-7	0.01	540
Desktop	5989-27-5	0.08	540
Desktop	80-56-8	0.02	540
Desktop	108-95-2	0.01	540

* In the case of the photocopier, emission values are given in $\mu\text{g/unit}$ and the duration is given in [units]

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