



Effect of high-voltage electric field on formaldehyde diffusion within building materials



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ABSTRACT

An experimental study concerning the diffusion of formaldehyde within building material in different high-voltage electric fields was conducted. Formaldehyde concentration was tested under electric field intensities of 0, 33.3, 66.6 and 100 kV/m. The Capsule Concentration Footprint Method (CCFM) was proposed to analyse the resulting experimental data. It was found that both equilibrium concentration and emission rate increased under greater electric field intensity. In addition, the experimental data indicated that high-voltage electric fields have a significant effect on partition coefficient, little effect on initial concentration and nearly no influence on diffusion coefficient. The partition coefficient decreased remarkably, while initial concentrations increased slowly due to the increasing electric field intensity. A formula was obtained to explain the relationship between partition coefficient and electric field intensity. A simulation of the adsorption between the formaldehyde and building material was conducted to illustrate the decrease in adsorption potential due to the greater electric field intensity, which helps to understand the principle established by the experimental data. The results of this study confirmed the feasibility of a new method for the reduction of formaldehyde in the man-made boards.

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1. Introduction

Volatile organic compounds (VOCs) that are emitted from many building materials are considered to be a major cause of poor indoor air quality [1]. On average, people spend over 80% of their time indoors, and a major part of this is inside homes [2]. Poor indoor air quality can cause a variety of symptoms such as dry coughs; difficulty concentrating; tiredness; headaches; nose, eye or throat irritations; and dizziness and nausea [3–6]. Materials capable of depositing, adsorbing and/or accumulating pollutants can influence indoor air quality during the entire service life of a building [7]. Therefore, an accurate characterization of the sorptive properties of building materials and the impact of sorption on indoor air quality is important.

Several significant accomplishments have taken place over the past 20 years regarding the testing of formaldehyde emissions from wood products. On the one hand, there have been many studies using different testing methods to evaluate formaldehyde release or content in materials [8–11]. On the other hand, there have been studies on the impact factors leading to the release of formaldehyde from wood-based panelling [12], such as temperature, air velocity, humidity and board properties. Published approaches for studying the characteristics of VOC sources and sinks fall into two categories: modelling and simulation and experimental investigation [13]. Modelling and simulation studies of VOC diffusion within building materials have experienced significant developments. Xiong and Zhang used a theoretical approach to derive the correlation that characterizes the relationship between emission rate and temperature for formaldehyde emission [14]. Huang studied the impact of temperature on the ratio of initial emittable concentration to total concentration for formaldehyde in building material. They found a theoretical novel correlation that showed the logarithm of emittable ratio is multiplied by the power of 0.5 of temperature and is linearly related to the reciprocal of temperature. Experimental

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Nomenclature

A	emission area of building material (m^2)
C_0	initial concentration of formaldehyde in test chamber (mg/m^3)
$C_m(x, t)$	instantaneous concentration of formaldehyde in building material (mg/m^3)
$C_m(L, t)$	concentration of formaldehyde in building material adjacent to the interface (mg/m^3)
$C(t)$	concentration of formaldehyde in chamber (mg/m^3)
$C_s(t)$	concentration of formaldehyde in the air adjacent to the interface (mg/m^3)
$C_{equ}(t)$	equilibrium concentration of formaldehyde in test chamber (mg/m^3)
D	mass diffusion coefficient for formaldehyde in building material (m^2/s)
E	electric field intensity (kV/m)
h_m	convective mass transfer coefficient (m/s)
K	partition coefficient between building material and air (dimensionless)
L	thickness of building material slab (m)
M	emission rate (mg/s)
t	time (s)
U	electric voltage (kV)
V	volume of air in chamber (m^3)
x	linear distance (m)

results have indicated that emittable ratio increases significantly with increasing temperature, and this increase was 14-fold from 25.0 to 80.0 °C [15]. Ma and Chen applied a three-dimensional lattice Boltzmann method to simulate desorption and diffusion processes of VOCs in porous materials [16]. Although numerous researchers have focused on the modelling of VOC emissions from building materials and furnishings in ventilated space, it is more difficult to research the diffusion of VOCs experimentally; however, experimental studies have already obtained certain achievements. Parthasarathy studied the effects of temperature and humidity on formaldehyde emission from samples collected from temporary housing units [17]. Wei developed a liquid-inner tube diffusion-film-emission reference for quickly evaluating the performance of chamber systems for furniture/building material VOC emission tests [18]. Small-scale environmental chamber experiments have been performed using painted hardwood panels to evaluate the production of VOCs and formaldehyde at different ozone concentrations and reaction times by Huang [19]. Lin used a chamber to investigate the impact factors of temperature, relative humidity, air exchange rate and volatile organic compound properties on VOC specific emission rates and concentrations from wooden flooring [20]. Overall, the theoretical and experimental research on VOC emission has made great achievements.

However, VOC emissions from building materials have been rarely studied under the action of an external electric field. Electric fields have been used in many heat and mass transfer studies. Farmanzadeh performed a theoretical investigation of the adsorption of formaldehyde molecules onto the exterior surface of single-walled (8, 0) zinc oxide nanotubes and considered the effect of external electric fields on adsorptive properties. The results showed that the electric field can easily modulate the adsorptive energy of formaldehyde on zinc oxide nanotubes [21]. The effects of an electric field on CO and NO adsorption on a Pt (111) surface were studied by Koper [22]. The effects of an external electric field on the adsorption of O_2 molecules on the surface of Au-doped graphene

was studied using density functional theory calculations by Zhang, and the adsorption energy decreased under a positive electric field [23]. Lebovka investigated the influence of a pulsed electric field treatment on the convective drying of potato tissue and concluded that the effective moisture diffusivity increased with increasing strength of the pulsed electric field [24]. The application of electric fields in heating and mass transfer applications has a broad prospect for development. Therefore, the study of high-voltage electric fields applied to VOC emissions is essential.

Three emission characteristic parameters, initial concentration, diffusion coefficient and partition coefficient, were found to be useful for describing formaldehyde and VOC emissions from building material [25–29]. Therefore, in this study, these emission parameters were studied in detail under the action of different high-voltage electric fields. High-voltage electric fields were introduced for the removal of formaldehyde in man-made boards, which may be a highly useful method for formaldehyde reduction. Furthermore, research results from the diffusion of formaldehyde under the effects of an external electric field will make it easier to study the effects of high-voltage on other VOCs, experimentally and theoretically.

2. Experiments

2.1. Experimental principle

For one board of building material placed in an airtight chamber with inner volume V (Fig. 1), the following assumptions were made: (1) the building material is uniform; (2) VOC mass transfer is one-dimensional; (3) the initial VOC concentration is homogenous; (4) the partition coefficient K and the diffusion coefficient D are constant for a given voltage; (5) the VOC concentration in the chamber is uniform.

2.2. Experimental apparatus

The schematic diagram of the experimental apparatus used in this study is described in Fig. 2. It was mainly composed of five parts: airtight chamber, high-voltage electric field generation system, constant temperature control system, formaldehyde concentration sampler system and temperature and humidity monitoring system.

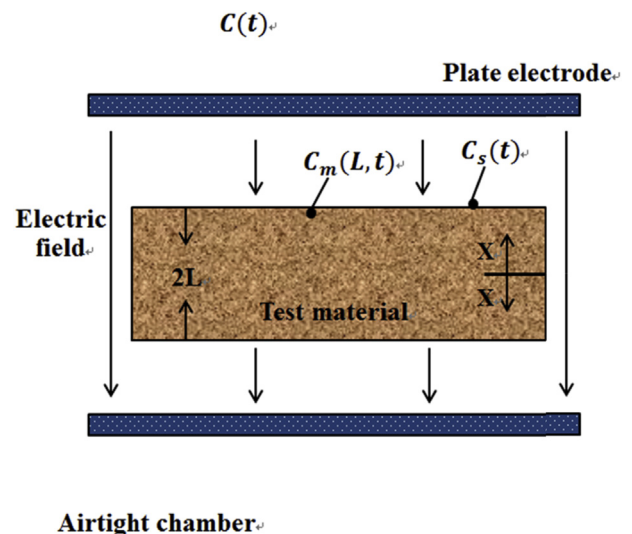


Fig. 1. Schematic diagram of the problem.

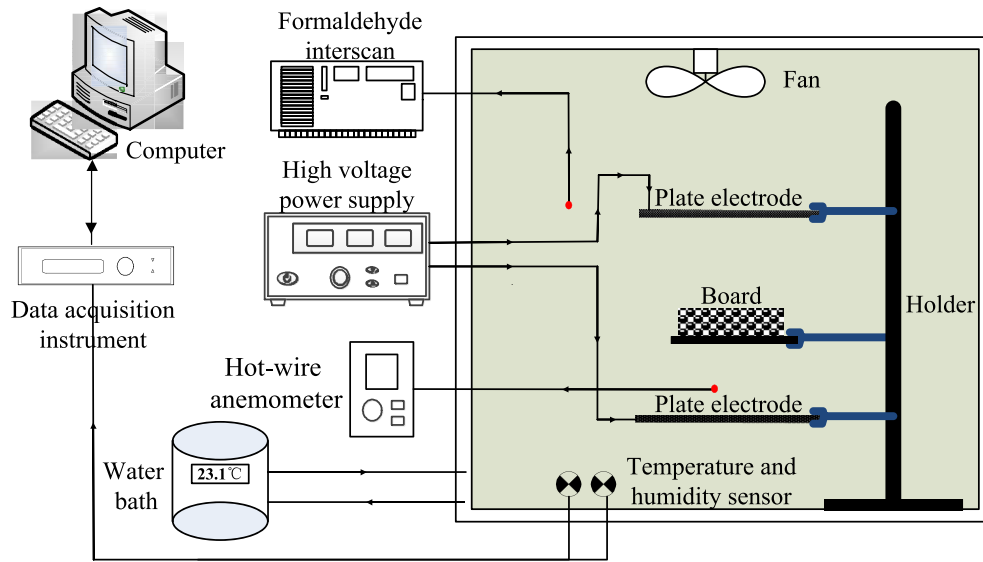


Fig. 2. The schematic diagram of experimental apparatus.

The test samples were placed in a stainless steel airtight chamber whose size was $0.35 \text{ m} \times 0.35 \text{ m} \times 0.5 \text{ m}$. The high-voltage electric field generation system included a plate electrode made of copper and a high-voltage power supply that could provide 0–50 kV of continuously adjustable constant voltage. By using a water bath, the chamber and air were maintained at a constant temperature. After the system reached thermal equilibrium, the samples were placed into the chamber and the instantaneous concentrations of formaldehyde were continuously recorded using an Interscan #4160–19.99 m portable analyser until an equilibrium concentration $C_{equ}(t)$ was reached. The precision of the Interscan #4160–19.99 m portable analyser was 0.05%. The temperature and humidity monitoring system included temperature and humidity sensors, an Agilent 34970A data acquisition instrument and a computer. In addition, the chamber was equipped with a small fan to ensure good gas mixing and a hot-wire anemometer was used to measure air speed.

2.3. Experimental material and environment

Samples of Medium Density Fibreboard (MDF) were tested in this experiment. For the test, to ensure that mass diffusion within the material was approximately one-dimensional, the side edges of each sample were sealed with aluminium foil. The size of MDF is listed in Table 1.

Tests were conducted at an air temperature in the chamber of $23 \pm 0.5 \text{ }^\circ\text{C}$, with air humidity in the range of $50 \pm 5\%$. The temperatures of the MDF surface under different electrical intensities were tested and exhibited in Fig. 3. As seen from the figure, the temperatures of the MDF surface were $23 \pm 0.7 \text{ }^\circ\text{C}$, $23.1 \pm 0.6 \text{ }^\circ\text{C}$, $22.9 \pm 0.7 \text{ }^\circ\text{C}$ and $22.8 \pm 0.8 \text{ }^\circ\text{C}$ at different electrical intensities. The biggest change in temperature was $0.8 \text{ }^\circ\text{C}$ and this was acceptable. Because the air temperature in the chamber was maintained at a constant desired temperature, the temperatures of the MDF surface

were also kept nearly constant. In this case, the influence of different electrical intensities on MDF temperature was eliminated within the margin of error. In addition, the air velocity was measured, and h_m was obtained to be 0.0015 m/s .

2.4. Airtightness test

The following test was performed to ensure the airtightness of the chamber. A dose of saturated formaldehyde vapour was injected into the sealed chamber. The instantaneous VOC concentration was recorded continuously after the VOC fully mixed with the air. The equation below measures the change in formaldehyde concentration in the chamber over time to assess the leakiness of the chamber:

$$V \cdot dC(t)/dt = Q[C_{in} - C(t)] \quad (1)$$

where Q is the air leakage rate. C_{in} is the formaldehyde concentration outside the chamber which is close to 0 here.

Thus, equation (1) can be written as follows:

$$\ln C(t) = -Q/V \cdot t + n \quad (2)$$

where n is a constant.

The test results were shown in Fig. 4. Air leakage per hour from the chamber was less than 1% of the chamber volume at different electric field intensities, which is negligible for the measuring period.

2.5. Determination of C_0 , K and D

Jiayin Xiong proposed a novel method for calculating C_0 , K and D called Capsule Concentration Footprint Method (CCFM) [30]. C_0 , K and D can be obtained by the following equations with CCFM:

$$\ln((C_{equ} - C(t))/C_{equ}) = Slope \cdot t + Intercept \quad (3)$$

$$Slope = -DL^{-2}q^2 \quad (4)$$

Table 1
Size of MDF.

Emission area A (m^2)	0.0625
Half thickness of each sample L (m)	0.009
$\beta = AL/V$	0.00918

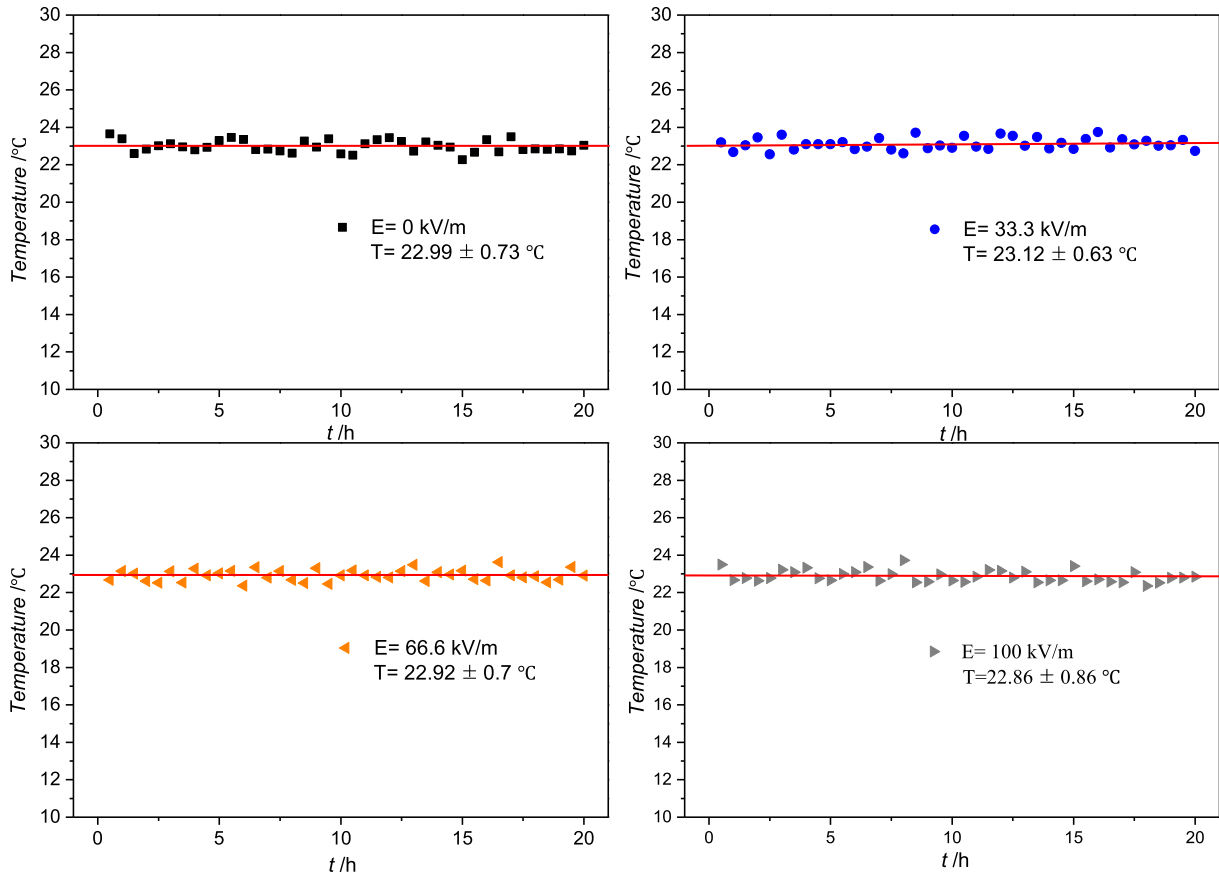


Fig. 3. Temperatures of MDF surface/time profiles under different electric intensity.

$$\text{Intercept} = \ln(-2(K\beta + 1)\sin q/(qa)) \quad (5)$$

where β is listed in Table 1 q and a can be obtained by Ref. [30].

3. Results and discussions

3.1. The instantaneous formaldehyde concentration and emission rate affected by different electric field intensities

The instantaneous formaldehyde concentrations in the chamber for building materials under different electric field intensities are shown in Fig. 5 to assess formaldehyde removal from man-made boards. In this figure, formaldehyde diffusion is strongly affected by the high-voltage electric field. The equilibrium concentrations increase over time, with an increase in electric field intensity from 0 to 100 kV/m. Equilibrium concentration at 100 kV/m was 2.236 mg/m³, approximately 36% greater than the 1.643 mg/m³ without an electric field. The increase in equilibrium concentration means more formaldehyde was emitted from the board when the electric field is present. This means that high-voltage electric fields contribute to formaldehyde diffusion, which can be used to reduce formaldehyde in building material.

The instantaneous formaldehyde concentrations in Fig. 5 are the average values of at least three sets of data under the same conditions, and the relative errors are also exhibited in this figure. Nearly all of the relative errors were below 10% to ensure the validity and accuracy of the data. The main source of error was the unique properties of the different samples. Although all of the MDF samples come from the same board, there are still some differences

among the samples, including pore structure, formaldehyde content and some other variable properties.

Fig. 6 presents the emission rates that resulted from different electric field intensities. The greatest emission rates under the four different electric field intensities occurred at the beginning of the test for all samples. The smallest emission rate of 0 kV/m was observed at 774×10^{-6} mg/s. In contrast, the greatest at 100 kV/m was 951×10^{-6} mg/s. What's more, although all of the emission rates decreased gradually, the emission rates under greater electric field intensity were always stronger. Based on these results, it may be stated that increases in electric field intensity were correlated to faster emission rates.

3.2. Three key parameters (D , C_0 , K) affected by different electric intensity

After applying the experimental data to equation (3) and performing linear curve fitting, the obtained results were depicted in Fig. 7. Based on the aforementioned procedure, the characteristic parameters (C_0 , K and D) were determined.

3.2.1. Determination of diffusion coefficients (D)

As shown in Fig. 8, there was a small change in the diffusion coefficient of the building material. The range of the diffusion coefficient was from 7.35×10^{-10} to 7.86×10^{-10} under different electric field intensities. Within the margin of error, D was within the normal range and the differences were negligible.

It should be mentioned that temperature generally has a significant effect on diffusion coefficients [31]. The high-voltage electric field may cause a local temperature rise. However, it was

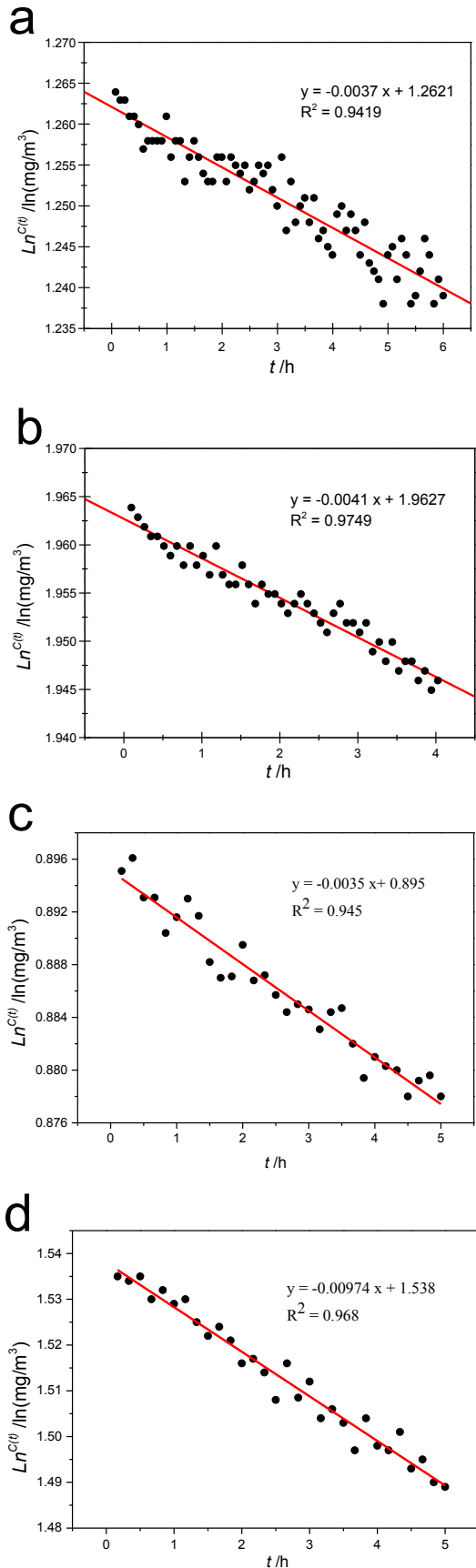


Fig. 4. The tested results for airtightness of the chamber. (a) $E = 0 \text{ kV/m}$; (b) $E = 33.3 \text{ kV/m}$; (c) $E = 66.6 \text{ kV/m}$; (d) $E = 100 \text{ kV/m}$.

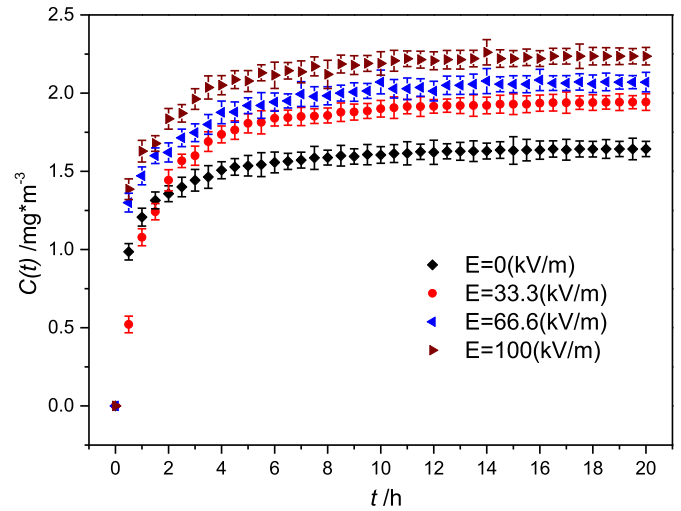


Fig. 5. Formaldehyde concentration and relative error/time profiles under different electric intensity.

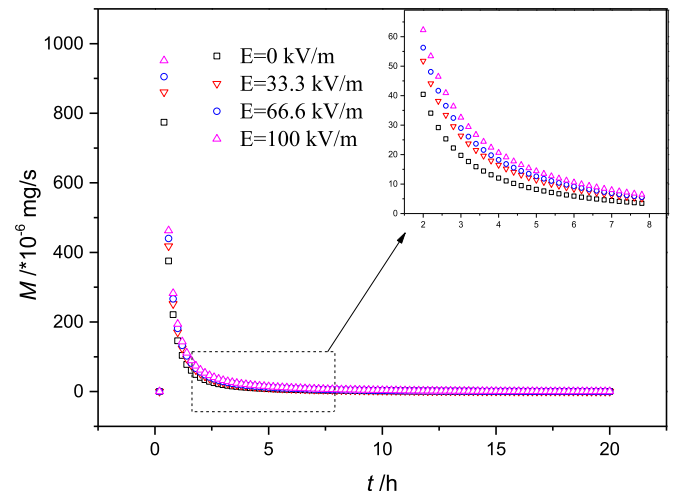


Fig. 6. Emission rate/time profiles under different electric intensity.

eliminated by the constant temperature of the experimental environment. In this case, it caused minimal change in the diffusion coefficient.

3.2.2. Determination of initial concentrations (C_0)

The formaldehyde initial concentrations are described in Fig. 9. It can be seen the smallest C_0 at 0 kV/m was $1820 \text{ mg}/\text{m}^3$. In contrast, the largest at 100 kV/m was $1920 \text{ mg}/\text{m}^3$. The linear relationship between C_0 and E is followed:

$$C_0 = 0.76 \times E + 1827 \quad (6)$$

Increases in electric field intensity (E) caused an increase in initial concentrations. This is because adsorption potential is one of the key factors affecting initial concentration. The desorptive condition is written as follows:

$$\varepsilon_a < \varepsilon_k \quad (7)$$

where ε_a is adsorption potential and ε_k is molecular kinetic energy.

When ε_k remains unchanged, the lower the adsorption potential, the more formaldehyde molecules will be desorbed. What's

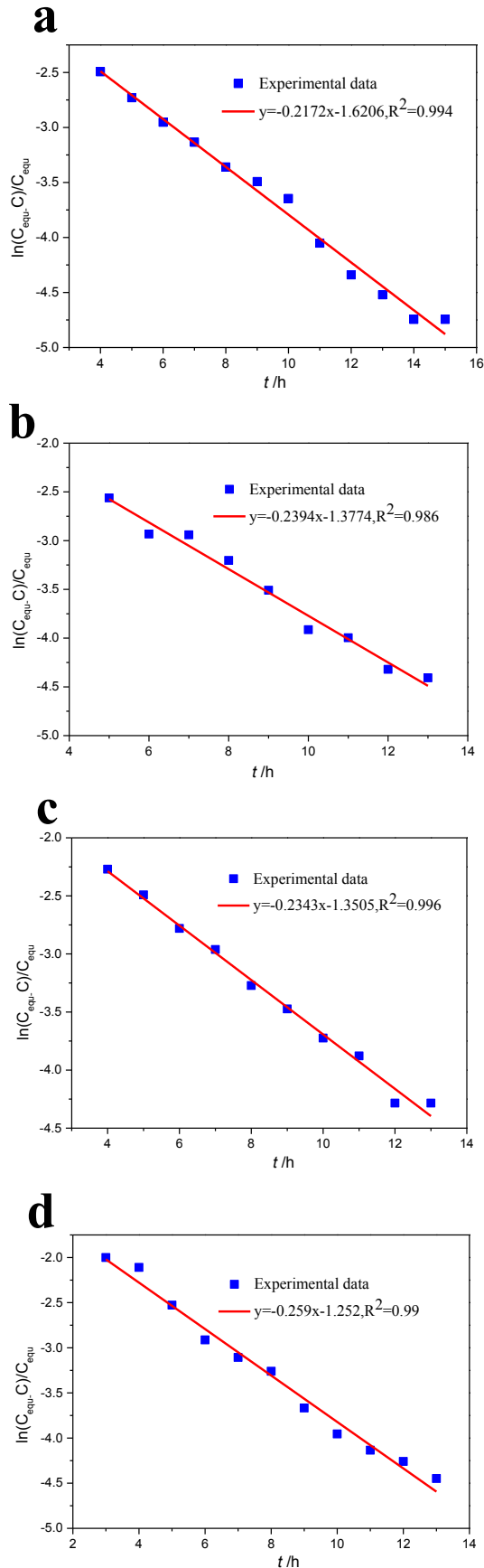


Fig. 7. Linear curve fitting applying Equation (3) for formaldehyde desorption in airtight chamber. (a) $E = 0$ kV/m; (b) $E = 33.3$ kV/m; (c) $E = 66.6$ kV/m; (d) $E = 100$ kV/m.

more, adsorption potential decreased with increased of electric field intensity, which is discussed in Section 3.3. Therefore, with greater electric field intensity, adsorption potential decreases and more formaldehyde molecules are desorbed, which results in an increase in initial concentration.

However, the rise in initial concentration was very slow. C_0 increased only 5% from 0 to 100 kV/m. Therefore, it can be concluded that initial concentration increases slowly with increases in electric field intensity. In this test, the samples were MDFs and electric intensity is limited to 100 kV/m. To verify the effect of high-voltage electric field on initial concentration, different material and higher electric field intensity are needed in future experiments.

3.2.3. Determination of the partition coefficients (K)

As described in Fig. 10, the partition coefficient was significantly influenced by electric field intensity. Increases in electric field intensity caused remarkable decreases in the partition coefficient. Additionally, when the electric field intensity approached 100 kV/m, the partition coefficient became close to 730, which was less than 70% of the partition coefficient of 1020 observed at 0 kV/m. It can be concluded that increases in electric field intensity caused a reduction in the partition coefficient. The most important explanation may be that the partition coefficient is also affected by adsorption potential. The increase in electric field intensity caused a decrease in adsorption potential, which resulted in a remarkable decrease in the partition coefficient.

A theoretical explanation of the relationship between the partition coefficient and electric field intensity is as followed:

$$K = \left(N_0 \Gamma_m a R T^{0.5} \exp(Q/RT) \right) / \left(k_1 v_s (2\pi MR)^{0.5} \right) \quad (8)$$

where Q is adsorption potential and the other parameters are assumed to be constant according to the literature [31].

Adsorption potential can be obtained by using the following equation [32]:

$$Q = a \cdot \exp(-b \cdot U) \quad (9)$$

where a and b are constant, and U is electric voltage and can be expressed as

$$U = E \cdot d \quad (10)$$

where d is the distance between two plate electrodes.

Combining Eq. (8) (9) (10) yields:

$$K = \left(N_0 \Gamma_m a R T^{0.5} \exp(a \cdot \exp(-b \cdot d \cdot E) / (RT)) \right) / \left(k_1 v_s (2\pi MR)^{0.5} \right) \quad (11)$$

For a given adsorbent and adsorbate, all parameters in Eq. (11) except the partition coefficient (K) are independent of electric field intensity (E). Therefore, Eq. (11) describes the relationship between the partition coefficient and the electric field intensity.

Finally, Eq. (11) can be written as followed:

$$K = A_1 \cdot \exp(A_2 \cdot \exp(A_3 \cdot E)) \quad (12)$$

where $A_1 = N_0 \Gamma_m a R^{0.5} T^{0.5} / (k_1 v_s (2\pi M)^{0.5})$, $A_2 = a / (RT)$ and $A_3 = -b \cdot d$ are constant for a given adsorbent and adsorbate.

Based on the formula, the correlations for the experimental results from the MDF were obtained (Fig. 10). The equation between K and E is followed:

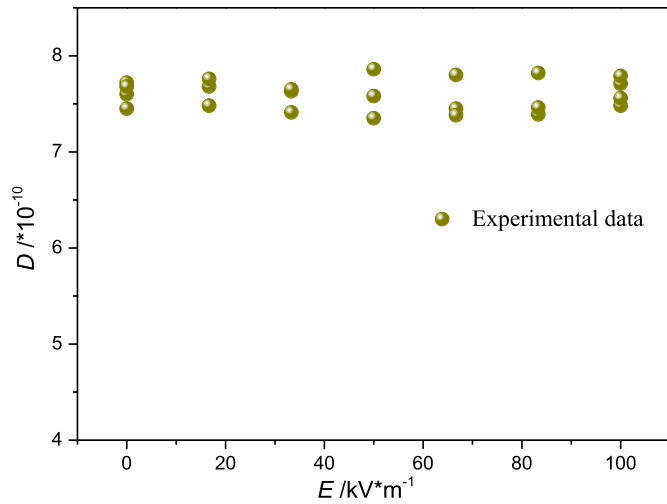


Fig. 8. D /time profiles under different electric intensity.

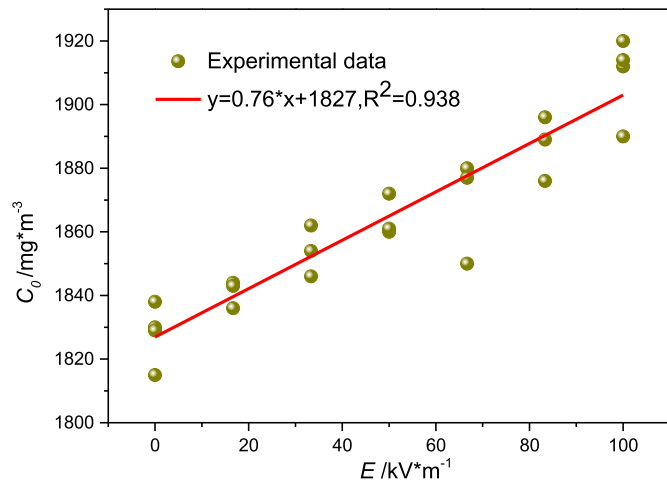


Fig. 9. C_0 /time profiles under different electric intensity.

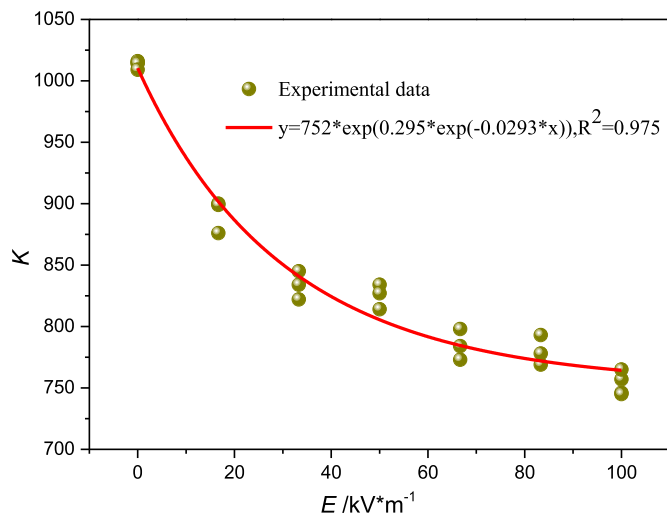


Fig. 10. K /time profiles under different electric intensity.

$$K = 752 * \exp(0.295 * \exp(-0.0293 * E)) \quad (13)$$

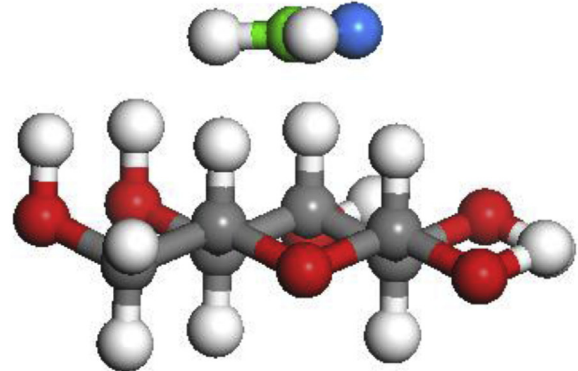
where $A_1 = 752$, $A_2 = 0.295$ and $A_3 = -0.0293$.

Eq. (13) is suitable for the MDF used in this experiment and the correlation agrees well with Eq. (12). However, to verify the relationship between partition coefficient and electric field intensity that was identified in MDF, more materials and further experimentation is needed.

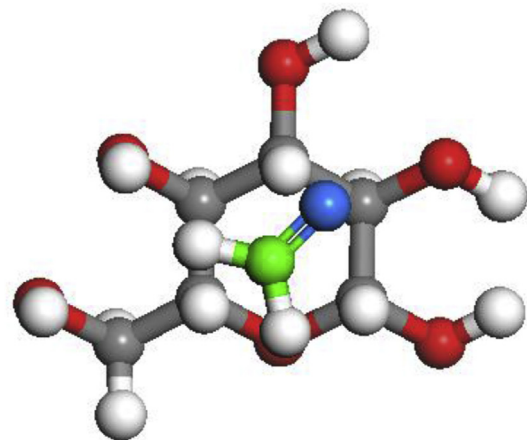
3.3. Simulation of formaldehyde adsorption within building materials

To more clearly illustrate formaldehyde adsorption within building materials, the adsorption process was simulated using density functional theory. Cellulose, an organic polymer, is the main organic constituent of wood. Therefore, the adsorption of formaldehyde within the board material should be equal to the adsorption of formaldehyde in the cellulose model.

The cellulose monomer was chosen as a typical adsorbent in this adsorption model. The optimization of structure model between the formaldehyde and the cellulose monomer was calculated by using the DMol³ code [33] embedded in the Materials Studio software and the most stable adsorption configuration was shown in Fig. 11. The adsorption processes for a formaldehyde molecule on



(a) Side View



(b) Top View

Fig. 11. Side view and top view of optimized adsorption structures of formaldehyde molecule on cellulose monomer.

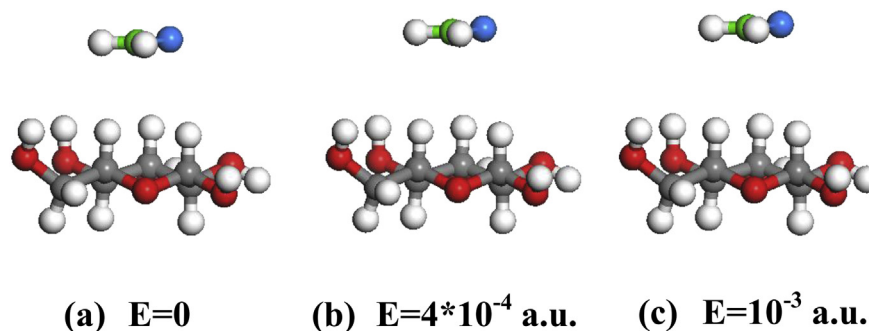


Fig. 12. Side view of adsorption structures under different electric field.

a cellulose monomer were investigated. The B3LYP [34–38] density functional combined with a basis set that included diffuse and polarization terms was used yielding accurate relative energies and structures of hydroxyl-containing compounds. The double numerical plus polarization (DNP) method, which has a computational precision comparable to the Gaussian split-valence basis set 6–31 g**, was applied to the expanded electronic wave function [39]. In addition, an all-electron core treatment was employed. To ensure high quality results, the self-consistent-field (SCF) density convergence threshold value of 1×10^{-5} Ha was specified. A Fermi smearing of 0.005 Ha was used to improve the calculation performance as well. The convergence criteria included threshold values of 1×10^{-5} Hartree (Ha), 0.002 Ha \AA^{-1} and 0.005 \AA for energy, force and displacement convergence, respectively. The uniform external electric field was varied from 2×10^{-4} to 10^{-3} a.u. ($1 \text{ a.u.} = 5.14224 \times 10^{11} \text{ V/m}$) with a step of 2×10^{-4} a.u. The electric field intensity in the simulation was much higher than in the experiment to compensate for the short time of simulation.

Using the aforementioned method, the bond length and bond angle of the formaldehyde molecule were calculated. The results are as follows: $d_{C=O} = 1.221 \text{ \AA}$, $d_{C-H} = 1.106 \text{ \AA}$, $\angle_{HCH} = 116.1^\circ$; these data correspond well to the experimental data [40] of 1.208 \AA , 1.116 \AA and 116.5° , respectively. As a consequence, the method mentioned above was considered to be effective and viable.

The results from simulation of the adsorptive process under different electric field intensities are exhibited in Fig. 12. The distance between the formaldehyde molecule and cellulose monomer increased as electric field intensity increased. The detailed distances can be seen clearly in Table 2, which also verifies the above results.

The Van der Waals (VDW) energy, due to interatomic interactions, can be described by Lennard-Jones's pair potential E_{LJ} [41,42].

$$E_{LJ}(\bar{d}) = 4\epsilon \left[\left(\frac{\sigma}{\bar{d}} \right)^{12} - \left(\frac{\sigma}{\bar{d}} \right)^6 \right] \quad (14)$$

where \bar{d} is the distance between the interacting atoms, ϵ is the depth of the potential, and σ is a parameter determined by the equilibrium distance.

Based on Equation (14), the VDW energy, which is the main energy of the adsorption potential, was reduced due to increases in distance between formaldehyde and cellulose. The simulation

results show that distance increases with greater electric field intensity, resulting in decreased interaction energy between molecules, which corresponds to the discussion between the partition coefficients and the electric field.

4. Conclusions

A series of experiments concerning formaldehyde diffusion within building material exposed to high-voltage electric field intensities of 0, 33.3, 66.6 and 100 kV/m was proposed. It can be concluded that both equilibrium concentrations and emission rates increased due to greater electric field intensity. In addition, high-voltage electric fields had a significant effect on partition coefficients, little effect on initial concentrations and nearly no influence on diffusion coefficients. The partition coefficient decreased remarkably, and initial concentration increased slowly due to the enhancement of electric field intensity. A formula was obtained to describe the relationship between partition coefficient and electric field intensity. The findings of this paper can be applied to the board production process in order to reduce formaldehyde content in man-made board. As a result, boards that have received treatment from a high-voltage electric field will be cleaner and more consumer-friendly.

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Table 2

The average distances between formaldehyde molecule and the cellulose monomer under different electric field.

Electric field ($\times 10^{-4}$ a.u.)	0	2	4	6	8	10
d (\AA)	4.0458	4.3284	4.3605	4.3749	4.3814	4.4247

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