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A study on the formaldehyde emission parameters of porous building materials based on adsorption potential theory

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ABSTRACT

The emission of formaldehyde from building materials is characterized by three key parameters: the initial emittable concentration, the partition coefficient, and the diffusion coefficient. Scholars have conducted considerable research to determine these three parameters. However, the experimental methods are mostly time consuming, and the experimental data cannot provide a mechanism to explain the influence of the main control factors on the emission parameters. Theoretical prediction models have been built to predict a certain parameter based on different theories and with different applicable scopes. Thus, it is necessary to establish a theoretical system that can analyze the formaldehyde emission process based on a fundamental theory and can simultaneously predict the emission parameters. Based on adsorption potential theory, this paper disassembled the pore structure of porous building materials and calculated the adsorption potential for a given pore diameter. According to the relationship between the molecular kinetic energy and the adsorption potential, the emittable ratios for each independent potential field were calculated. The initial emittable concentration of the whole material was finally obtained by reconstruction. Our previous study proposed a prediction model for the partition coefficient based on adsorption potential theory. Combining this proposed model with the effective diffusivity model, a new correlation between the diffusion coefficient and temperature was derived. Three types of medium density fiberboards and one type of particle board were used in the mercury intrusion porosimetry tests and the environmental chamber experiments of formaldehyde emission. The emission parameters calculated by the prediction models agreed well with the experimental data.

1. Introduction

Currently, people spend most of their time indoors; thus, indoor air quality (IAQ) has been attracting increasingly extensive attention [1–4]. As a factor that affects IAQ, formaldehyde is one of the main volatile organic compounds (VOCs) emitted from interior decorative materials. The increase in the manufacture and use of these materials has been accompanied by mounting public awareness of and concern about its detrimental effects on health and the environment. The guidelines for air quality published by the World Health Organization suggested that the deposition of inhaled chemicals from environmental media can have direct health consequences [5]. In addition, many studies revealed that long-term exposure to these compounds is associated with certain symptoms of sick building syndrome and multiple chemical sensitivities [6–9]. Therefore, controlling and harnessing VOC emission is a top priority for ensuring good IAQ.

The formaldehyde emissions of building materials can be characterized by three key parameters: the initial emittable concentration (C_{m0}), the partition coefficient (K_m), and the diffusion coefficient (D_m) [10–12]. These three parameters are very important for understanding the formaldehyde emission characteristics and predicting the indoor formaldehyde concentration. Among the three key parameters, C_{m0} is the most sensitive key parameter regarding the emission behaviors [13,14]; C_{m0} is defined as the total amount of the target VOC that can be emitted from the material when the environmental concentration is zero. However, gas emission from building materials is a long-term process. The time for the target VOC to be completely emitted approaches infinity; as a result, determining this parameter is difficult.

Chinese National Standards GB/T17657–1999 [15] and GB/T18580–2001 [16] and the European Standard EN120 [17] set the total formaldehyde concentration measured by the perforator

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Nomenclature

Symbols

A_m	surface area of the building material (m^2)
A_t	cross-sectional area of the porous media (m^2)
$C_a(t)$	formaldehyde concentration in the gas phase (mg/m^3)
C_{equ}	equilibrium formaldehyde concentrations in airtight environmental chamber (mg/m^3)
C_m	concentration at the surface of the adsorbent when equilibrium (mg/m^3)
C_{m0}	initial emittable concentration (mg/m^3)
$C_{0,total}$	total concentration (mg/m^3)
d_p	pore area fractal dimension
d_t	fractal dimension for tortuosity
D_e	effective diffusion coefficient (m^2/s)
D_m	diffusion coefficient (m^2/s)
D_r	mean diffusion coefficient of a capillary (m^2/s)
Fo_m	Fourier number
$F(\varepsilon_i)$	probability when the adsorption potential is ε_i
$g(\varepsilon_k)$	probability density of molecular kinetic energy distribution of ideal gas
K	partition coefficient at the pore surface in porous media model
K_m	partition coefficient
L	half thickness of the building material (m)
L_0	characteristic length of a capillary tube (m)
N_A	Avogadro's number
N_i	number of the pores with the diameter λi
p	balance pressure of the gas (Pa)
p_0	saturated vapor pressure (Pa)
R	universal gas constant (8.314 J/(mol K))
t	time (s)
T	thermodynamic temperature (K)
V	adsorbed volume per unit mass of adsorbent (m^3/mg)
V_i	pore volume of a certain pore diameter (m^3)
V_0	pore volume per unit mass of adsorbent (m^3/mg)
V_a	air volume in the experimental chamber (m^3)
$\overline{V}$	liquid molar volume of adsorbate (m^3/mol)
V_m	adsorbent volume per unit mass of adsorbent (m^3/mg)

Greek symbols

α	adsorption quantity per unit mass of adsorbent (mol/mg)
ε	adsorption potential (J)
φ	porosity of the material
λ_i	pore diameter (m)
λ_{max}	maximum pore diameter of the macropores (m)
λ_{min}	minimum pore diameter of the macropores (m)

Abbreviations

CLIMPAQ	chamber for laboratory investigations of materials, pollution and air quality
CTR-VVL	continuous temperature rising − variable volume loading
IAQ	indoor air quality
MDF	medium density fiberboard
MIP	mercury intrusion porosimetry
PB	particleboard
VOCs	volatile organic compounds

method as an indicator to evaluate and select building materials. However, the extraction temperature of the perforator method is much higher than the actual indoor temperature, which may result in some bound-state formaldehyde molecules transforming into emittable free-state molecules. The total concentration is much higher than the emittable concentration at room temperature. Therefore, it is necessary to design a reasonable method to determine C_{m0}.

The direct measurement methods of C_{m0} includes the fluidized bed desorption method [18] and the extraction method at room temperature [19,20]. Both of these methods require grinding the building materials into powder before the measurement. The destructive pore structure of the building material affects its potential field distribution; as a result, these methods cannot accurately measure C_{m0}. Wang et al. [21] proposed a multi-sorption equilibrium regression method based on the adsorption of building materials in which C_{m0} can be determined from the equilibrium concentrations after every sorption using the linear least-square regression. This method is rapid and has a high accuracy. However, the difference between C_{m0} and the total concentration ($C_{0,total}$) lacks quantitative analysis, and the functional mechanism of temperature also lacks in-depth systematic research. Xiong et al. [22,23] proposed a multi-emission/flush regression method to measure the C_{m0} of formaldehyde in a medium density board at different temperatures. They observed that C_{m0} increases significantly with increasing temperature and is far less than the value measured by the perforator method. However, theoretical analysis is still lacking on the relationship between C_{m0} and temperature, making it difficult to determine C_{m0} at temperatures other than those used in the experiments.

Huang et al. [24] derived a correlation between the emittable ratio and temperature by applying statistical physics theory. The adsorption energy is taken as a constant for the temperature range of interest in the derivation, and the impact of the non-uniform pore diameter distribution in the building materials is neglected. In fact, the non-uniformity of the pore diameter distribution of building materials results in the formation of different types of active centers. These active centers cause diverse affinities to gas molecules and different adsorption potentials. The adsorption potential is directly related to C_{m0}; thus, its heterogeneous distribution causes C_{m0} to vary inside building materials. A deeper relationship between C_{m0} and the adsorption potential needs to be explored.

The other two key parameters, D_m and K_m, also play important roles in analyzing of the VOC emissions characteristics of building materials. The main experimental methods for determining the two parameters can be divided into two categories. The first category involves the design of simple and easily controlled experiments based on the definition of parameters [25–28]. The second category uses a mathematical fitting method by establishing a mass transfer model [29–32]. However, the key parameters measured by the above experiments are the value of a single building material-VOC combination under specific experimental conditions. These methods are unable to analyze the functional mechanisms of the temperature, structural parameters, and VOC properties. Thus, the general applicability of predicting the key parameters under uncertain conditions is still needed.

Zhang et al. [33] derived an expression for K_m according to