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A Mass Transfer Model for Simulating VOC Emissions from Building Materials

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Abstract:

Based on heat and mass transfer hypothesis and existing theoretical models, a mathematical ideal for volatile organic compounds (VOC) emission was established to estimate the evolution of pollutant concentration inside wet building materials. The dynamic distribution characteristics of VOC concentration with multi-pollution sources in an actual building were simulated. The results show that the specific distribution form of indoor VOC concentration is related to its own density and the arrangement of obstacles. It will significantly promote/inhibit VOC emission from indoor building materials.

***Keywords**: Mass transfer, VOC, Simulation, Building materials.*

I. INTRODUCTION

Indoor gaseous pollutants represented by formaldehyde emission from building materials are proven to have considerable affects the indoor comfort, human health and productivity [1]. In China, humans spend close to 90% of their occasion in these indoor environments with relatively narrow space and complex air components [2], and the levels of indoor pollution can be serious [3]. With the development of new urbanization and building materials industry, especially the upsurge of full decoration, volatile organic compounds (VOCs) released in the whole life cycle of building materials cannot be ignored. VOC emission from building materials, such as furniture, paint, wallpaper and thermal insulation material, as well as from the adhesives used in some wood products [4]. In addition, the emphasis on air tightness from the perspective of energy conservation has led to a sharp reduction in fresh air entering indoor environment. Among regularly monitor indoor gaseous pollutants, VOCs volatilize slowly and are not easy to attract human attention [5]. How to effectively reduce indoor VOC pollution emission from building materials is an urgent problem to be solved.

In the early stage, the VOC emission from building materials was summarized through a large number

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of experiments, from the classical first-order attenuation model or double first-order attenuation model to the semi empirical model represented by the surface sink model [6]. These models are simple in form and easy to apply, but they lack mechanism support and cannot reflect the physical mechanism of VOC emission. Then, the focus turned to the mass transfer model with clearer physical concept and the treatment method of model parameters with physical significance. The early Little model proposed that VOC emission is diffusion controlled process, ignoring the convective mass transfer resistance. It was assumed that the initial concentration and indoor concentration in building materials are single values [7]. Aiming at Little model problem, Yang [8], Huang and Haghighat [9] began to consider the boundary convective mass transfer resistance, Xu and Zhang [10] further considered the comprehensive influence of convective mass transfer resistance and initial concentration, making the calculation results closer to the measured data. The above models are mostly aimed at the single-sided emission of single-layer materials. Hu [11] proposed the double-sided emission model of multi-layer materials considering the internal concentration heterogeneity. Thereafter, the multilayer material emission model [12] and the space fraction diffusion model [13] considering the material chemical reaction were proposed respectively. Li [14] studied the influence of surface radiation on indoor gas pollutant emission and diffusion process using K- ω model.

In recent years, with the in-depth insight of the VOC emissions mechanisms of porous building materials, some research have gradually focused on the emission model based on adsorption/desorption and wet building materials. Yang et al. [8] considered the VOC adsorption/desorption characteristics of air-building materials interface earlier. In order to simplify the model, it was assumed that the diffusion coefficient and distribution coefficient of building materials remained unchanged. Zhou [15] deeply analyzed the multi-scale mechanism of VOC desorption of porous building materials and gave the calculation formula of adsorption potential energy. Zhu [16] proposed an integrated model of VOC adsorption/desorption, and obtained a semi analytical solution through generalized integral transformation. At the same time, the test object is also changed to wet material under complex conditions. Li [17] proposed specific process for controlling VOC emission process of building materials in different stages.

The research on the propagation characteristics of VOC multi-sources emission in indoor decoration and furniture has important theoretical and practical significance for guiding the removal of indoor VOC in hot and humid areas. The mathematical model that takes into account the multi-sources on VOC diffusion can be used to analyze the objective characteristic of VOC emissions from indoor materials [18]. In this work, a original VOC diffusion model in building materials is established and the distribution characteristics of pollutant concentration in buildings are explored.

II. MATHEMATICAL MODEL OF VOC EMISSION

To express VOC emission operation, some theory models have been studied to forecast VOC emission from indoor building materials [19]. Based on the research status of existing VOC pollutant emission models and mass diffusion theory [20], this paper establishes a mathematical model for the VOC emission process of indoor building materials. The VOC emission model considers three procedures: the diffusion

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and mass transfer in building materials, convection diffusion and mass conservation in the indoor air, and convection and mass transfer on the material/air boundary [21].

In order to simplify the physical model, the following assumptions have been made. (i) The amount of coating used per unit area is very minute, so the coating is rapidly absorbed by the carrier and a wet layer with uniform VOC concentration is formed on the surface of the carrier. The topmost surface of the wet layer is exposed to the air environment, and the under surface is the bearing surface, which is not affected by the wet layer at the initial stage of volatilization. (ii) The coating and the carrier are macroscopically homogeneous. Therefore, the effective diffusion coefficient of VOC can be defined. (iii) In the volatilization process, VOC volatilization is only carried out on the surface of the coating and air. (iv) The concentration gradient of VOC is considered to be the only mass transfer power. (v) The mass transfer rate among coating and air is extremely low, so the heat absorption/release related to volatilization can be ignored. (vi) After VOC leaves the coating and enters the air, it will be evenly mixed with the surrounding air in a short time.

2.1 Diffusion in the Coating

Depending on Fick's law and the mass transfer theory using the above assumptions, the governing equation of VOC diffusion in the coating can be given as follows:

$$\frac{\partial C_m(x,\tau)}{\partial \tau} = \frac{\partial}{\partial x_i}\left(D_m \frac{\partial C_m(x,\tau)}{\partial x_i}\right) \tag{1}$$

Where, $C_m(x,\tau)$ is the VOC concentration in the coating (mg/m^3); D_m is the diffusion coefficient of VOC in the coating (m^2/s); x_i is diffusion direction (m); τ is the time, (s).

Since the coating is assumed to be homogeneous, the VOC emission process can be simplified to a one-dimensional diffusion, the above formula can be simplified to

$$\frac{\partial C_m(\tau)}{\partial \tau} = \frac{\partial}{\partial x}\left(D_m \frac{\partial C_m(\tau)}{\partial x}\right) \tag{2}$$

2.2 Carrier

Using Fick's law, the diffusion process of VOC in the carrier can be expressed as

$$\frac{\partial C_s(\tau)}{\partial \tau} = \frac{\partial}{\partial x}\left(D_s \frac{\partial C_s(\tau)}{\partial x}\right) \tag{3}$$

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Where, $C_s(\tau)$ is the VOC concentration in the carrier (mg/m^3).

2.3 Coating-air Surface

On the surface of the coating and air, VOC changes from liquid or solid to gaseous. The main mass transfer mechanisms in this process are evaporation and convection. As long as the concentration gradient exists, surface volatilization will occur. Henry's law can be used to relate the concentration of volatile substances on the coating surface to the VOC emission concentration in the gas phase on the coating surface. Although Henry's law is only applicable to low concentration solutions, some studies have shown that it is also applicable to most VOC studies. Therefore, the following equation holds:

$$C_m(x,\tau) = K_{ma} C_a(\tau) \tag{4}$$

Where, $C_a(\tau)$ is the VOC emission concentration in the gas phase on the coating surface, (mg/m^3); K_{ma} is the separation factor between material and air.

2.4 Ambient Air

The concentration equation of VOC in the air of the main flow area is as follows [22].

$$V\frac{dC_\infty}{d\tau} = Q(C_{in} - C_\infty) + S \cdot E - R_s \tag{5}$$

$$E = -D_m \frac{\partial C_m}{\partial x} \tag{6}$$

Where, C_∞ is the concentration of VOC in the air of the mainstream area (mg/m^3); C_{in} is the concentration of outdoor air pollutants (μg/m^3); S is the surface area of the coating (m^2); Q is ventilation volume (m^3/h); V is the effective volume of room (m^3); R_s is the absorption rate of VOC (mg/ h); E is the emission rate of VOC from pollution source (mg/m^2·h).

2.5 Initial Condition

$$C_{a,0} = C_{\infty,0} \tag{7}$$

$$C_{m,0} = C_{l,0} / h \tag{8}$$

$$C_{s,0} = 0 \tag{9}$$

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Where, h is mass transfer coefficient (m/s).

2.6 Boundary Condition

Interface between coating and air:

$$-D_m \frac{\partial C_m}{\partial x}\bigg|_{x=L} = h_m (C_a - C_\infty),\ \tau > 0 \tag{10}$$

Interface between coating and carrier:

$$-D_m \frac{\partial C_m}{\partial x} = -D_s \frac{\partial C_s}{\partial x}, C_m = C_s,\ \tau > 0 \tag{11}$$

The other side of the load without coating:

$$C_{s,x=0} = 0,\ \tau > 0 \tag{12}$$

III. DISTRIBUTION SIMULATION OF INDOOR VOC

3.1 Simulation Model

The simulation object is a newly decorated building in Ningbo. The room size is 10.4 m ×8 m ×3.6 m. The geometric model is established according to the internal layout of the building plan, as shown in Fig. 1.

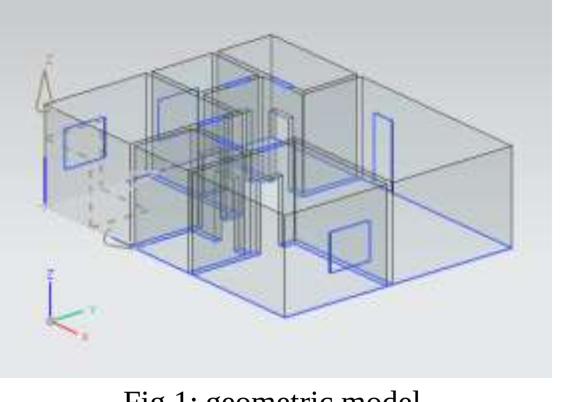

Fig 1: geometric model

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The governing differential equation of indoor air turbulent flow can be described in following form [23].

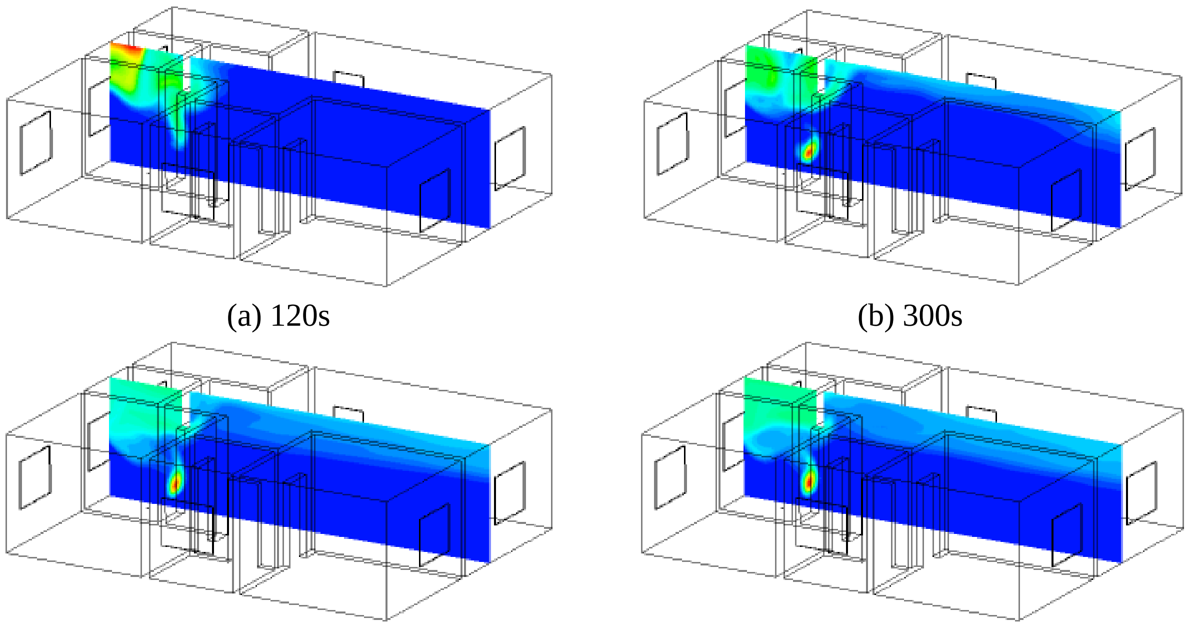
$$\frac{\partial(\rho\phi)}{\partial t}+div(\rho u\phi)=div(\Gamma_{\phi}grad\phi)+S_{\phi} \tag{13}$$

Where ϕ is a general variable; Γ_{ϕ} is the generalized diffusion coefficient and S_{ϕ} is the generalized source term.

The standard k-ε turbulence equation was used in the simulation, and the flow field in the simulated indoor environment was calculated by the simple algorithm.

3.2 Simulation Results

In order to obtain the diffusion law of pollutants when a single pollution source releases VOC, the release of pollutants from walls as a single source is simulated, as shown in Figure 2. It can be seen from Figure 2, VOC is continuously emitted, but due to the existence of pressure outlets on both sides, the fluctuation of air flow affects the jet movement. From 120s to 300s period, the jet movement is unstable and swings to the left and right sides. Until 480s, the jet movement tends to be stable and lasts until 600s. In fact, pollutant emission is a slow process, and its indoor pollutants will exist for a long time. The longer the ventilation time or the greater the ventilation speed, the faster the diffusion of pollutants.



(a) 120s (b) 300s

(c) 480s (d) 600s

Fig 2: indoor VOC diffusion with time

Indoor air quality is closely linked indoor pollution sources, as well as there are usually multiple indoor

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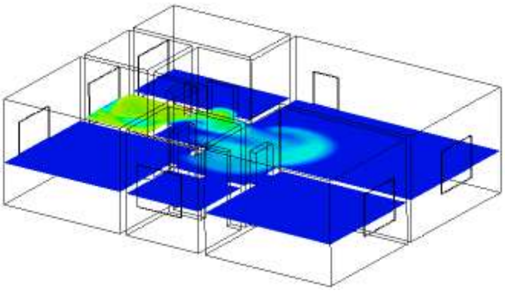
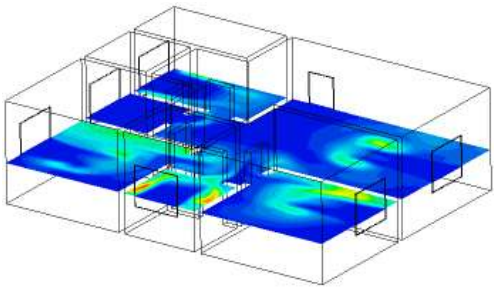
VOC pollution sources. At present, a lot of studies are concentrate on the impact of a single source on the built environment [24], but the indoor VOC pollutant concentration distribution is closely related to the emission conditions of pollution sources, especially the impact on the indoor pollutant concentration distribution when multiple pollution sources interact, Especially when the interaction makes the indoor pollutant concentration change, it is particularly of utmost importance to study the indoor VOC concentration diffusion under the action of multiple pollution sources.

In order to acquire the influence of multi-sources on indoor VOC diffusion, the simultaneous emission characteristics of four side walls + ground were analyzed, and the distribution law of indoor pollutant concentration at different room heights was observed. As can be seen from Figure 3, in the process of simultaneous emission of VOC from multiple pollution sources, the VOC concentration reduce with the develop of height, and the concentration distribution is different at dissimilar heights. When VOC diffusion plays a dominant role, the specific distribution form of indoor pollutants is related to its own density and the arrangement of obstacles.



(a) single pollution source



(b) multi-pollution sources

Fig 3: effect of pollution sources on VOC distribution

IV. CONCLUSION

In this work, wet materials were selected as the research object, and a new VOC diffusion model in building materials is established by comprehensively considering the internal diffusion and surface emission process of flat materials. The distribution characteristics of pollutant concentration in buildings under the characteristics of dynamic process and multiple pollution sources are explored. In the process of VOC diffusion, its diffusion rate will be affected by pollution parameters. Multi pollution parameter diffusion will make the diffusion rate of pollutants larger than that of single pollution parameter. The complete diffusion of VOC in building materials takes a long time. Therefore, for the sake of personnel health, more environmentally friendly materials should be selected during decoration, and furniture should be added in batches.

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