A mass transfer model for predicting emission of the volatile organic compounds in wet building materials

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A new mass transfer model is developed to predict the volatile organic compounds (VOCs) from fresh wet building materials. The dry section of wet materials during the process of VOC emission from wet building materials is considered in this new model, differing from the mass transfer-based models in other literatures. The mechanism of effect of saturated vapor pressure on the surface of wet building materials in the process of VOC emission is discussed. The concentration of total volatile organic compounds (TVOC) in the building materials gradually decreases as the emission of VOCs begins, and the vapor pressure of VOCs on the surface of wet building materials decreases in the case of newly wet building materials. To ensure the partial pressure of VOCs on the surface of wet building materials to be saturated vapor pressure, the interface of gas-wet layer is lowered, and a dry layer of no-volatile gases in the material is formed. Compared with the results obtained by VB model, CFD model and the experiment data, the results obtained by the present model agree well with the results obtained by CFD model and the experiment data. The present model is more accurate in predicting emission of VOC from wet building materials than VB model.

In recent years, indoor air quality has aroused the interests of many specialists. A lot of building materials can serve as the sources of VOCs (volatile organic compounds) which can cause indoor pollution\(^{[1]}\). But the mechanism of this problem is not clear yet. Therefore, it is important to find out the emission characteristics of these materials and the mechanism of VOCs transport so as to control VOC emissions and improve indoor air quality.

There has been a growing interest in the development of mathematical models to predict the process of VOC emissions. Currently, the methods of studying characterization of VOC emissions from building materials fall into two categories: the experimental approaches\(^{[2-4]}\) and the modeling approaches\(^{[5,6]}\). The former can provide most real results but requires expensive, well-controlled facilities. Furthermore, the results obtained under the test conditions may not be directly applicable to other conditions. Because of the limitation of the experimental approach, much interest has been paid to the development of mathematical models to predict the VOCs emissions in recent years. Generally speaking, there are two kinds of VOC emission models in the literature. The first type is the empirical model. The parameters of empirical models are determined by fitting experimental data to a predefined model. The typical examples are the first-order decay model\(^{[7]}\). The empirical method can provide most real results for a given model because the parameters of empirical models are defined by fitting experimental data. The main problem of these models is that the nonlinear regression curve fitting may lead to multiple solutions and it is difficult to extend empirical models to other geometry configuration different from the experimental configuration. The
second type of models is based on the mass transfer theory (diffusion, convection, and evaporation) and is called the physical model. Each parameter has its physical significance. The development of the physical model is important to understand the emission characteristics of building materials and the mechanism of VOCs transport. Guo et al.\cite{8,9} presented two typical physical models, i.e., VB (vapor pressure and boundary layer) model and VBX model. VB model and VBX model consider emission as a pure evaporation process and neglect internal diffusion. It has been found that such a model does not work for the entire emission process, especially when the material becomes relatively dry. The CFD model presented by Yang et al.\cite{10} considers the internal diffusion and VOC diffusion from the material film to the substrate. It is in good agreement with the experimental data.

In this paper, a new physical model based on dry process is presented. The new model considers the dry process in the material. Comparing the results with that of the VB model, CFD model and the experiment data show that the new model can predict VOC emission from wet building materials more accurately than VB model.

1 Model development

1.1 VB model and CFD model

VB model, shown as eq. (1), is a simple mass transfer model. It assumes that the concentration of TVOC in the mass boundary layer is in proportion to the concentration of TVOC in the material, and the concentration difference is the only driving force for the emission,

\[ E(t) = k_m \left( C_v \frac{M}{M_0} - C_a \right), \]

where subscript \( i \) represents component \( i \), \( \pi_i \) and \( \pi \) are the molar amounts (mol/m\(^2\)) in the source for component \( i \) and TVOC.

VB model and VBX model are physical models to predict emission of VOC from wet building materials. Each parameter has its physical significance, and the results are in good agreement with the experiment data in short time prediction. However, they are only for gas-phase-limited mass transfer. The internal-diffusion-controlled emissions cannot be predicted. The whole emission can be divided into three stages: evaporation controlled stage, transition stage and internal diffusion controlled stage. Both VB model and VBX model cannot be used in the internal diffusion controlled stage.

Yang et al.\cite{10} developed a CFD model which considers evaporation, movement of free and bound VOC, vapor flow and VOC diffusion from the material film to the substrate, and assumes the VOC diffusion coefficient in the material is in proportion to the concentration of TVOC in the material. It is in good agreement with the experimental data. In this paper, a new physical model is developed based on another point of view. The material film is divided into dry layer and wet layer in the whole drying process.

1.2 Drying model development

The process of drying and VOC emission of wet building material are schematically visualized in Figure 1, where Figure 1(a) is the initial state, (b) is the drying process, and (c) is the fully dried state. Each of these mechanisms is discussed in the following part.

![Figure 1](image_url)

In addressing this problem, the following assumptions are made:

(i) concentration difference is the only driving force for the emission;
(ii) partial pressure at the liquid-gas interface is the saturated vapor pressure in the initial state;
(iii) VOCs are the only volatile compounds in the wet building material;