



Predicting VOC emissions from materials in vehicle cabins: Determination of the key parameters and the influence of environmental factors

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ABSTRACT

Emission of volatile organic compounds (VOCs) from materials in vehicle cabins is one of the main reasons for poor in-cabin air quality. The emission behaviors can be characterized by key parameters including the initial emittable concentration (C_0) and the diffusion coefficient (D_m). Determination of these parameters provides a foundation for predicting emissions and evaluating driver and passenger exposures. By analyzing VOC emissions from in-cabin materials under ventilated conditions, we propose a novel method to simultaneously determine C_0 and D_m . This method initially establishes a linear correlation between the logarithm of excess VOC concentration and emission time, then the key parameters C_0 and D_m are obtained by linear curve fitting and solving two equations. Using this method we determined the C_0 and D_m for five VOCs (benzene, toluene, p-xylene, ethylbenzene and styrene) emitted from a common in-cabin material under different environmental conditions. Good agreement between the predicted VOC concentrations based on the measured key parameters and experimental data demonstrates the effectiveness of this method. Moreover, the impact of temperature on C_0 was investigated for the five VOCs. Results indicated that C_0 of all the studied VOCs increased with an increase in temperature, and toluene showed the greatest increase. When the temperature increased from 25 °C to 50 °C at the relative humidity of 50%, the C_0 of toluene increased by 1.07 fold.

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1. Introduction

People spend a large portion of their time in buildings and in vehicles, so indoor and in-cabin air quality will significantly affect people's comfort, health and productivity [1–4]. Along with the indoor environment, the in-cabin microenvironment is now also recognized as a significant source of exposure to various pollutants. Although people only spend an average about 5.5% of their day in vehicles [5], the associated health risk is great in certain scenarios [6]. Many health concerns such as sick building/car syndrome, asthma and cancer have been shown to be related with poor indoor and in-cabin air quality [7–11]. In addition to fuel leakage and the infiltration of outside air pollution, the emissions of formaldehyde and volatile organic compounds (VOCs) contribute significantly to poor in-cabin air quality. These emissions result from interior materials used to equip the vehicle cabin, including leather, plastics, fabrics, carpets, sealants, adhesives, paints, foam

cushions, etc. [12–16]. Therefore, an understanding of the emission characteristics of formaldehyde and VOCs is a prerequisite to further study of emission mechanisms as well as providing the basis to effectively improve the in-cabin air quality.

Previous studies have primarily focused on the emission behaviors of VOCs from materials in the indoor environment, whereas studies for the in-cabin environment have seldom been reported. Studies on VOC emissions from building materials can be classified into two categories: modeling, and experimental measurement. For the former, empirical and physics-based models are developed to characterize the mass transfer process inside building materials [17–19]; for the latter, experiments are designed to measure the key parameters in the physics-based models, including the initial emittable concentration (C_0), the diffusion coefficient (D_m) and the partition coefficient (K) [20–23]. The main obstacle to model development is the lack of abundant experimental data for the key parameters used in equations. For this reason, many investigations have been undertaken to measure the three key parameters. The existing experimental methods used for determining the key parameters of VOC emissions from building materials can be

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Nomenclature

A	emission surface area (m^2)
Bi_m	Biot number for mass transfer
C_0	initial emittable VOC concentration ($\mu\text{g}/\text{m}^3$)
C_a	chamber VOC concentration ($\mu\text{g}/\text{m}^3$)
$C_{a,0}$	initial chamber VOC concentration ($\mu\text{g}/\text{m}^3$)
C_{in}	inlet VOC concentration ($\mu\text{g}/\text{m}^3$)
C_m	VOC concentration inside material ($\mu\text{g}/\text{m}^3$)
D_m	diffusion coefficient (m^2/s)
Fo_m	mass transfer Fourier number
h_m	convective mass transfer coefficient (m/s)
K	material/air partition coefficient
K_{oa}	octanol/air partition coefficient
Q	ventilation rate (m^3/s)

T	temperature (K)
t	time (s)
V	volume of environmental chamber (m^3)
y	coordinate (m)

Greek letters

α	dimensionless air exchange rate
β	ratio of the material volume to the chamber volume
δ	the half thickness of material (m)

Subscripts

a	air-phase
m	material-phase

divided into two categories: the closed chamber method [24,25] and the ventilated chamber method [26,27]. The ventilated chamber method can reflect the actual VOC emission process more accurately, as compared with the closed chamber method, in both indoor and in-cabin environments, and is thus preferred for routine tests. However, the current ventilated chamber methods are mainly used to determine D_m and K (e.g., the twin chamber method), but are seldom used to obtain C_0 , which is the most sensitive key parameter affecting emission behaviors [28,29]. Two recently developed methods can be used to measure C_0 but these still have some shortcomings. Li [30] proposed a non-fitting approach to determine C_0 and D_m . In this method, the convective mass transfer coefficient (h_m) along the material surface is ignored, which will result in some deviations when h_m is small. Huang et al. [31] developed a novel method to simultaneously measure C_0 , D_m and K . However, this approach includes tests taken under both closed and ventilated conditions, and is therefore not a purely ventilated chamber method. Materials found in buildings include wood-based boards (e.g., medium density fiberboard, particle board, oriented strand board) and furniture, which are very different to materials used in vehicles. The models describing VOC emission characteristics should be the same for different kinds of materials used in different environments, however the values of key parameters in the models will obviously differ. Taking this into consideration, if the key parameters, especially C_0 , of VOC emissions from in-cabin materials as well as indoor materials can be directly obtained from experiments performed only under ventilated conditions, such treatment will undoubtedly promote the development of laboratory tests and will be helpful for engineering applications.

Indoor or in-cabin environmental conditions such as temperature (T) and relative humidity (RH) frequently change with a change in outside conditions (weather, solar radiation, etc.), and this will cause a corresponding change in the key parameters. McLaren et al. [32] found that the temperature in a car cabin could reach a maximum of 67°C in a hot summer day. This is much higher than indoor temperature ranges, implying that the impact of environmental factors will be more significant in vehicle cabins than indoors. Zhang et al. [33] and Deng et al. [34] theoretically derived the correlations between D_m and T , and K and T , respectively. Xiong et al. [35] investigated the combined effect of T and RH on C_0 as well as on the emission rate. It should be noted that the latter study focused mainly on formaldehyde emissions. In addition, Crawford and Lungu [36] reported that C_0 of styrene from one kind of building material also changed with temperature. As far as we know, there is no report examining the impact of temperature on C_0 for VOC emissions from in-cabin materials. In the

Chinese guideline for assessing the air quality of passenger cars (GB/T 27630-2011) [37], some hazardous VOCs (e.g., benzene, toluene, ethylbenzene, styrene) are also labeled as the target pollutants in addition to formaldehyde. Therefore, further study is needed to investigate the effect of environmental factors on C_0 of VOCs from in-cabin materials.

In this study, we first developed an analytical model for characterizing VOC emissions from in-cabin materials. Based on this model we proposed a novel method to simultaneously measure C_0 and D_m in a ventilated chamber. Finally we examined the influence of environmental factors on C_0 and D_m for some typical VOCs in the in-cabin environment.

2. Development of the model and principle of the measurement method

When measuring the emission of VOCs from in-cabin materials in a real vehicle environment, we need to take into account the fact that the ventilation duct inlet air may contain a certain number of pollutants. In addition, the initial VOC concentration in the vehicle environment may be non-zero. Therefore, in this section we first develop an analytical model with different initial conditions, and we then introduce a new method for measuring the key parameters by virtue of this model.

A schematic of an in-cabin material placed in a ventilated chamber or in a vehicle environment is shown in Fig. 1. Both surfaces of the material are exposed to air allowing them to emit freely, and all the edges are sealed. Air with a constant VOC concentration (C_{in}) is introduced into the chamber, and a fan is placed at the top of the chamber to mix the air. The air in the chamber was well-mixed according to previous measurements [38,39]. Since the VOC concentration in the air is uniform, we can measure the concentration at the outlet of the chamber and take it as the chamber VOC concentration (C_a). To simplify the analysis of the problem, we make the following assumptions: (1) the VOC concentration inside the material at the beginning of the experiment is uniform; (2) the initial VOC concentration in the chamber is uniform and non-zero, recorded as $C_{a,0}$; (3) emission occurs from both surfaces of the material, and it can be treated as two single-sided emission processes from half of the material due to the symmetry of the material; (4) the material is uniform and is relatively thin, so that emission from the material can be regarded as one-dimensional; (5) the partition process at the material/air interface obeys Henry's linear adsorption isotherm.

Based on the above assumptions, the emission process of VOCs inside the material can be described by the one-dimensional diffusion equation:

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