

# *Simulation Analysis of Out-of-control Reason of Vehicle Interior Air Quality*

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**Abstract:** To determine the main reasons of out-of-control of vehicle interior air quality (VIAQ) during mass production, we constructed a three physical field coupling simulation model, which included dilute matter transfer, volatile organic compounds (VOCs) distribution across temperature ranges, and VOCs convective flow. Effects of storage temperature, ventilation rate, ventilation pollution, storage time, and emission difficulty on the VOCs concentration of a sample of interior materials were quantitatively analyzed. Simulation results showed that storage temperature fluctuation could cause an emittable concentration increase of up to 71% at 25°C, which was the most likely out-of-control reason of VIAQ; ventilation pollution can significantly contribute to uncontrolled vehicle air quality with up to 82% concentration increase; fluctuations in ventilation rate and interior materials that are less likely to emit VOCs would not cause the VIAQ to be out of control; higher heating devolatilization temperatures can result in a faster reduction of emittable concentration in the interior materials at 25 °C.

## **1. Introduction**

The concentration of VOCs and odor intensity are the leading indicators of vehicle interior air quality (VIAQ). They are a vital concern in the development of each vehicle model. They are controlled in terms of interior raw materials selection and process of optimization of auto parts to make the VOCs and odors of the prototype vehicle meet the requirements of the industry standards and health indicators<sup>[1,2,3]</sup>. In principle, once the raw materials and methods are determined, it could maintain similar levels of VIAQ in vehicle at the mass production stage and the prototype vehicle at the development stage. However, numerous original equipment manufacturers (OEMs) have found that the VIAQ of the same vehicle is not as stable as expected during the mass production of the vehicle<sup>[4,5]</sup>.

For example, an OEM conducted sampling tests of the in-vehicle VOCs of a vehicle based on the standard HJ/T 400-2007 "*Determination of Volatile Organic Compounds and Carbonyl Compounds in Cabin of Vehicles*"<sup>[6]</sup> in July and December 2021. The results of benzene were 4 µg/m<sup>3</sup> in July and 74 µg/m<sup>3</sup> in December, toluene was 79 µg/m<sup>3</sup> and 516 µg/m<sup>3</sup>, formaldehyde was 35 µg/m<sup>3</sup> and 56 µg/m<sup>3</sup>, and acetaldehyde was 65 µg/m<sup>3</sup> and 243 µg/m<sup>3</sup>. The concentrations of a variety of VOCs showed lower values in summer and higher in winter, with increases ranging from 60% to 1750%, and the acetaldehyde concentration had significantly exceeded the control limits of the standard GB/T

27630-2011 "Guideline for Air Quality Assessment of Passenger Car"<sup>[7]</sup>, indicating of the out-of-control of VIAQ.

There is no systematic quantitative analysis of the out-of-control reasons of VIAQ in the vehicle mass production phase, which is closely related to the emission properties of VOCs from the interior of materials or auto parts, suppliers cutting corners, the ambient temperature, storage phase, ventilation rate, ventilation pollution and storage time during the transportation, as well as the random use of interior repair adhesives<sup>[8]</sup>. These factors will affect the concentration of VOCs in the interiors of vehicles, leading to uncontrolled VIAQ. Since the main out-of-control reasons have not yet to be clarified, it is impossible to design a targeted air quality control process, making it difficult for OEMs to control VIAQ in the mass production phase.

In this work, we constructed a three-physics field coupling simulation and analysis method that includes dilute matter transfer, VOCs distribution across temperature ranges, and convective flow, based on the simulation study of the mass transfer and emission of interior VOCs dilutes<sup>[9,10,11,12,13]</sup>. We quantitatively analyzed the effects of storage temperature, ventilation rate, ventilation pollution, storage time, and the degree of emission difficulty on the concentration of auto interior VOCs. This allows us to determine the main reasons of uncontrolled VIAQ, which can further provide references for the OEMs to design more optimal air quality control processes.

## 2. Simulation Methods

### 2.1. Design of Geometric Model

We plotted off an interiors material with a length of 10 cm and a height of 1 cm at the left-to-bottom position in an emission space, as shown in Figure 1. The finite element mesh was divided into 15,403 mesh vertices to obtain a two-dimensional geometric model for the simulation of the VOCs emission from the interiors.

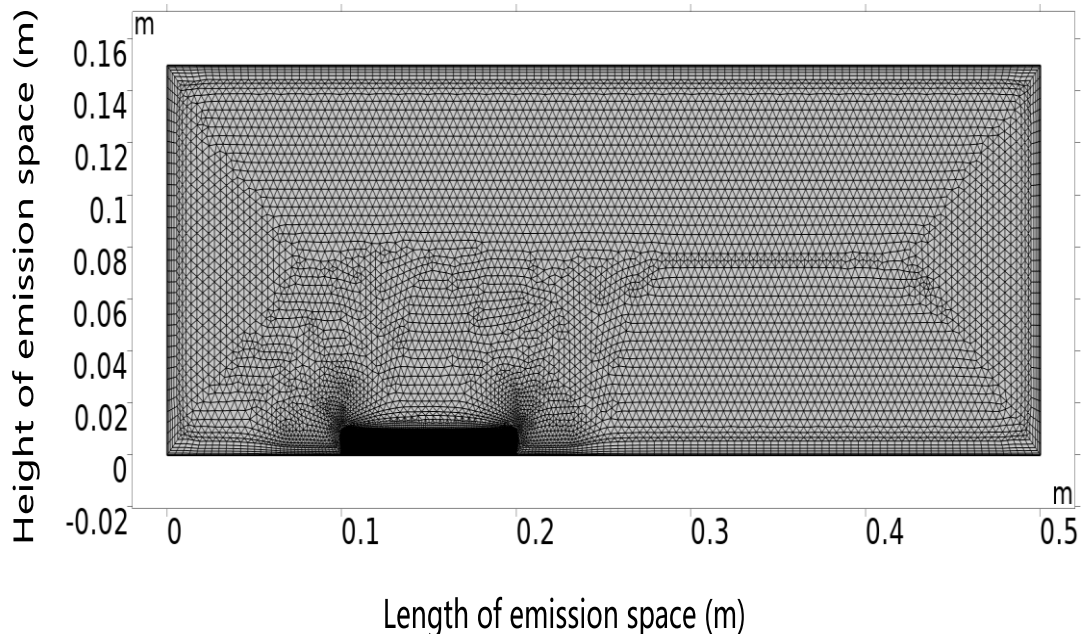


Figure 1: Geometric model of VOCs emission from the interiors within an emission space.

## 2.2. Constructing the Control Equations

Based on the law of mass conservation, Fick's second law of diffusion, adsorption potential theory, Henry's law, and hydrodynamic theory[14,15,16], we constructed a three-physics field coupling simulation model considering the diluted matter transfer, distribution of VOCs across different temperatures, and convective flow of VOCs. The simulation model was then applied to the geometric model shown in Figure 1.

In this case, the laminar steady-state equations for incompressible fluids is used to describe the traditional VOCs' convective flow occurred in the emission space outside the interiors[17]. The distribution of VOCs across different temperature ranges occurs only in the auto interiors. It has a complex coupling with the mass transfer of the diluted materials because the emission of VOCs within interior materials into the surrounding air is driven by concentration gradients and non-monotonically affected by storage temperature. On the one hand, the higher the temperature is, the higher the diffusion coefficients of VOCs in the material and the air are, the lower the partition coefficient at the materials/air interface is, the easier it is for VOCs to diffuse from the interior materials into the air, thus the faster the concentration of VOCs within the materials decreases. On the other hand, the higher the temperature, the easier it is for the adsorbed VOCs within the material to overcome the adsorption barriers and convert into the dispersed VOCs, leading to increase of the emittable concentration of VOCs within the material. The control equation for the above non-monotonic effect and the derivation process are described in detail in the Chinese invention application "Non-isothermal Emission Simulation and Calculation Method of Volatile Organic Compounds in Automobile Interior Materials"[18]. Emission coefficient  $Dm(C(t))$  and partition coefficient  $K(C(t))$  for VOCs in material are calculated respectively as

$$Dm(C(t)) = Dm_a \times (C(t) + 273.15)^{1.25} \times \exp\left(\frac{Dm_b}{C(t) + 273.15}\right) \quad (1)$$

$$K(C(t)) = K_a \times (C(t) + 273.15)^{0.5} \times \exp\left(\frac{K_b}{C(t) + 273.15}\right) \quad (2)$$

where  $Dm_a$  and  $Dm_b$  are the emission coefficients of VOCs in material,  $K_a$  and  $K_b$  are the emission coefficients of VOCs at the material-air interface. Emission coefficient  $Da(C(t))$  of VOCs in the air at 25 °C can be calculated as

$$Da(C(t)) = Da_{25} \times \left(\frac{C(t) + 273.15}{298.15}\right)^{1.81} \quad (3)$$

where  $Da_{25}$  is the emission coefficient of VOCs in the air at 25 °C. The average of the hourly emittable concentrations  $Cm_{avg}(t)$  of VOCs in material and  $Ca_{avg}(t)$  in the air at each mesh vertice can be calculated respectively as

$$Cm_{avg}(t) = \frac{\sum_{h=1}^{h=nx} Cm_h(t)}{x}, \quad t=0:t_{step}:t_{total} \quad (4)$$

$$Ca_{avg}(t) = \frac{\sum_{j=1}^{j=ay} Ca_j(t)}{y}, \quad t=0:t_{step}:t_{total} \quad (5)$$

where  $Cm_{h(t)}$  is the concentration of VOCs in material read on mesh vertices in the material mesh at moment  $t$ ,  $x$  is the number of mesh vertices in the material;  $Ca_{j(t)}$  is the concentration of VOCs in the air read on mesh vertices in the air mesh at moment  $t$ ,  $y$  is the number of mesh vertices in the air;  $t=0:t_{step}:t_{total}$  means the time variable  $t$  takes values from 0 to  $t_{total}$  in steps of  $t_{step}$ .

### 2.3. The Determination of Boundary Conditions and Initial Values of Simulation Parameters

We set boundary conditions for the geometric model shown in Figure 1 so that the fully developed ventilation flows vertically into the left boundary of the emission space and vertically from the right boundary at zero static pressure. The upper and lower boundaries of the emission space are defined as impermeable walls with no slip.

Table 1 shows the initial values of the parameters assigned to the simulation model of Figure 1. The initial emittable concentration and the diffusion coefficient were assigned to each grid vertex of the interior material. The diffusion coefficient in the air was assigned to each grid vertex of the dispersed space. The distribution coefficient was assigned to the grid vertices at the junction of the interior material and the dispersed space. The ventilation rate and the ventilation pollution were assigned to the grid vertices at the left boundary of the dispersed space. The storage temperature was assigned to all the grid vertices of the geometrical model. The time of simulation calculation was set as the storage time.

Table 1: Main parameters of simulation analysis.

Parameter name	Easily emittable materials	Difficult-to-emit materials
Initial emittable concentration of interior VOCs at 25 °C	100 mg/m <sup>3</sup>	
Initial emittable concentration of interior VOCs at 65 °C	800 mg/m <sup>3</sup>	
Diffusion coefficient of VOCs in air at 25 °C	1e-5 m <sup>2</sup> /s	
Diffusion coefficient of VOCs in interiors at 25 °C	1e-11 m <sup>2</sup> /s	1e-13 m <sup>2</sup> /s
Diffusion coefficient of VOCs in interiors at 65 °C	5e-9 m <sup>2</sup> /s	5e-12 m <sup>2</sup> /s
Partition coefficient of VOCs at the solid-gas interface at 25 °C	130	500
Partition coefficient of VOCs at the solid-gas interface at 65 °C	100	300
Ventilation rate	0.01, 1 or 100 L/min	1 L/min
Ventilation contamination	0, 0.1, 0.5 or 1 mg/m <sup>3</sup>	0 mg/m <sup>3</sup>
Storage temperature	Weather station monitoring data	
Storage time	Nine consecutive days in summer or winter	

Among them, the storage temperature recorded by the weather station is the ambient temperature in Guangzhou in summer and winter every three hours for nine consecutive days, as shown in Figure 2. We used a linear interpolation method to complement the unmonitored temperature values during the simulation calculations.

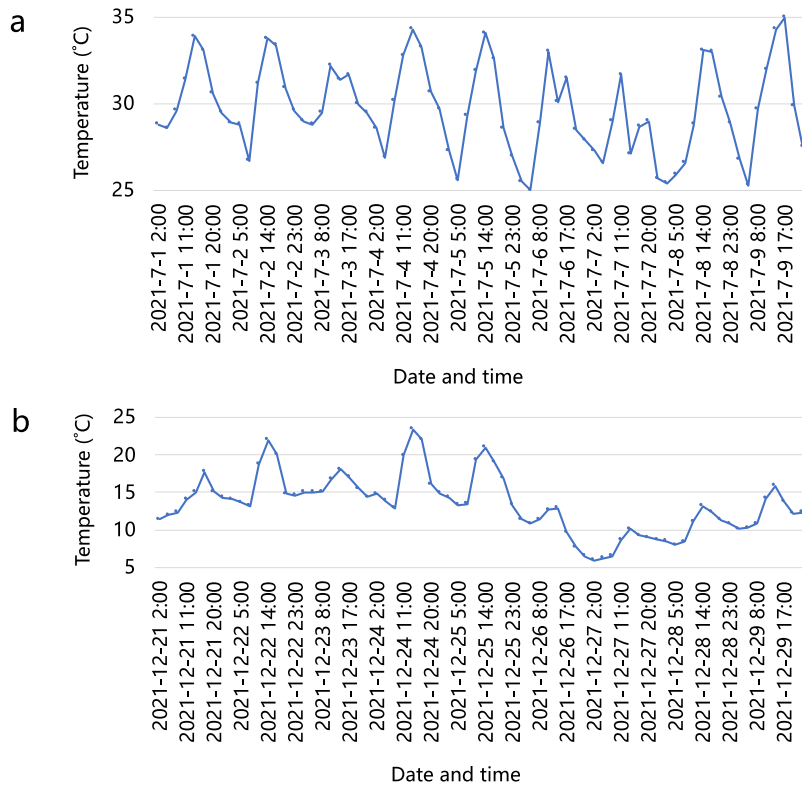


Figure 2: Celsius temperatures in Guangzhou for nine consecutive days in (a) summer and (b) winter.

## 2.4. Defining the Amount of Simulation Analysis Attention

The purpose of this paper is to quantitatively analyze the effects of storage temperature, ventilation rate, ventilation pollution, storage time, and emission difficulty on the VOCs concentration of interior materials through simulation, focusing on four groups of quantities of attention calculated during the simulation process, namely: (1) The hourly VOCs emittable concentration averaged over the vertexes of the grid within the material for each 1 °C temperature range, abbreviated as the emittable concentration at each temperature range,  $\text{mg}/\text{m}^3$ ; (2) the sum of the emittable concentrations for each temperature range in each simulation time step which is not higher than the temperature at that time step is the hourly temperature emittable concentration,  $\text{mg}/\text{m}^3$ ; (3) the sum of the emittable concentrations of temperature ranges not higher than 25 °C in each simulation time step is the emittable concentration at 25 °C,  $\text{mg}/\text{m}^3$ ; (4) the average of the concentration of VOCs in the right boundary of the emitting space at the vertexes of each grid is denoted as ventilation outlet concentration,  $\mu\text{g}/\text{m}^3$ .

## 3. Results and Discussion

### 3.1. Verification of the Validity of the Simulation Model

We conducted simulation calculations using the data of the easily emittable materials in Table 1, under the condition of 1 L/min ventilation rate, 0  $\text{mg}/\text{m}^3$  ventilation pollution, and the storage temperature of nine consecutive days of weather station monitoring data in summer in Guangzhou (Figure 2). The time-range change curve of the emittable concentration in each temperature range in the summer of Guangzhou was obtained as shown in Figure 3.

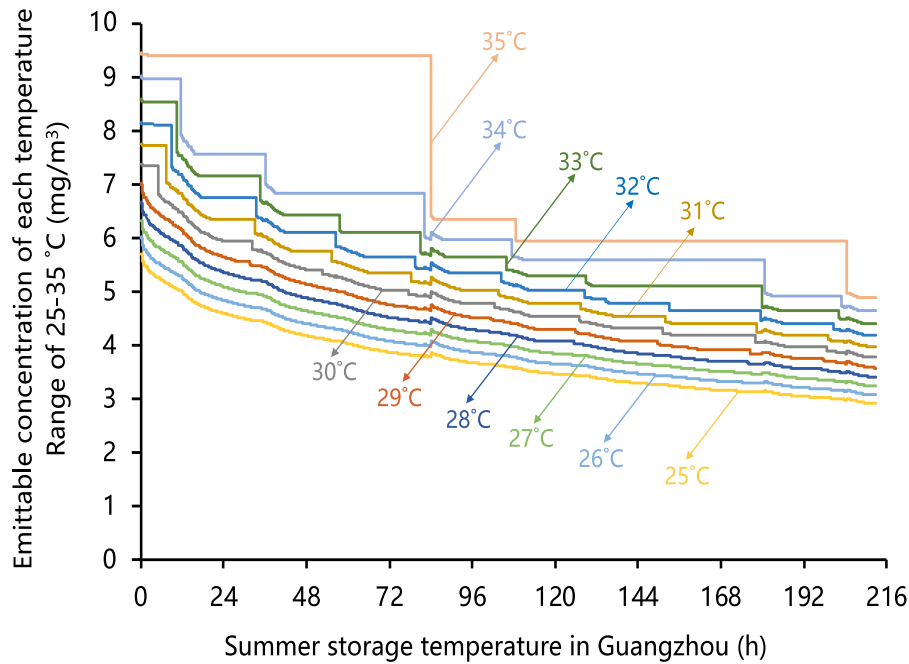


Figure 3: Simulation results of emittable concentration in each temperature range at summer storage temperature in Guangzhou.

From the topmost emittable concentration curve of the 35 °C temperature range in Figure 3, we found that the concentration of VOCs in this temperature range is almost constant until the storage time reaches 84 h, which means the VOCs in this temperature range are stationary phase VOCs that do not participate in the emission; then the concentration decreases significantly at 84 h, which means they are transformed into dispersed phase VOCs that participate in the emission; then the concentration keeps constant until the temperature reaches 108 h, which means they are transformed into stationary phase VOCs that do not participate in the emission. The curve shows that the concentration decreased significantly at 84 h, 108 h, and 204 h and remained constant at other times. This matches the time of entering the 35 °C temperature range for nine consecutive days of temperature monitoring data in Guangzhou during summer in Figure 2 at 84 h (2021-7-4 14:00), 108 h (2021-7-5 14:00), and 204 h (2021-7-9 14:00), while the temperature was lower than 34 °C at other times. The emittable concentration profiles in Figure 3 at temperatures ranging from 25-34 °C are consistent with Guangzhou's summer temperature monitoring data in Figure 2.

In addition, in contrast with the significant decrease in the emittable concentration at 84 h and 35 °C in Figure 3, the emittable concentration at each temperature (25-34) °C shows a significant increase in a specific proportion, indicating that some of the VOCs transformed from the stationary phase to the dispersed phase at the higher temperatures are not only emit into the emission space, but also replenish into the lower temperatures. This phenomenon is consistent with the fact that VOCs in the dispersed phase can redistribute across different temperatures between lower temperature ranges.

The above analysis indicates the VOCs distribution of cross-temperature range and VOCs emission characteristics associated with the coupling of dilute matter transfer with two-physical-field have been effectively demonstrated. Therefore, the three-physical-field coupling simulation model, which includes dilute matter transfer, cross-temperature VOCs distribution, and convective flow of VOCs is also effective.



### 3.2. Effect of Storage Temperature on Interior VOCs

Using the data of easily emittable materials in Table 1, we conducted simulation calculations under the conditions of 1 L/min ventilation rate, 0 mg/m<sup>3</sup> ventilation pollution, and storage temperature of nine consecutive days based on the monitoring data from weather stations in Guangzhou in summer and winter (Figure 2), Figure 4a shows the simulated emittable concentration curves as a function of storage time during the nine days of storage of interior materials in summer and winter in Guangzhou and the emittable concentration curves at 25 °C as shown in Figure 4b.

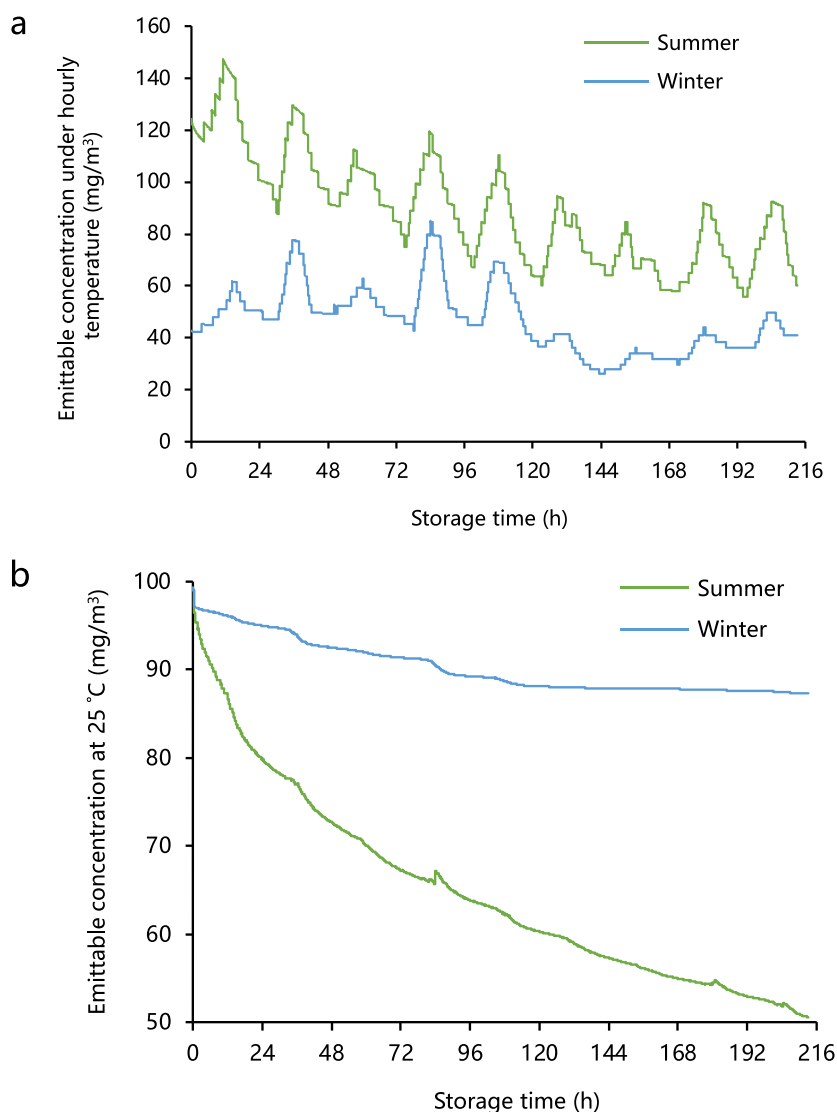


Figure 4: (a) The emittable concentration of easily emittable interior materials as a function of storage time under hourly temperature during the nine days of storage in Guangzhou in summer and winter. (b) The emittable concentration of easily emittable interior materials as a function of storage time at 25 °C.

From the simulation results of the emittable concentration under hourly temperature in Figure 4a and the temperature change monitoring data in Figure 2, we found that the change of emittable concentration under the hourly temperature of interior materials is consistent with the rise and fall of temperature in the warehouse, i.e., the emittable concentration is higher when the temperature is higher in the daytime, and is lower when the temperature is lower at night. Moreover, the summer

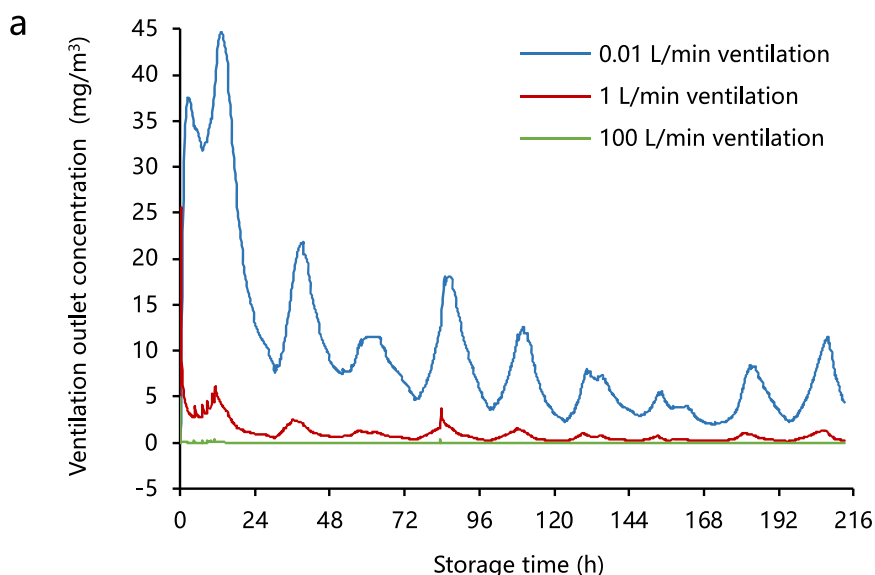
temperature in Guangzhou is generally higher than the winter temperature. Thus, the simulation results of the emittable concentration under the hourly temperature in summer are correspondingly higher than those in winter.

The higher the emittable concentration at the hourly temperature, the more VOCs are emitted to the emission space around the interior materials, and the lower the emittable concentration at 25 °C inside the interior materials, as shown in Figure 4b. The 25 °C is the testing temperature of VOCs inside the car commonly adopted by the OEMs as specified in the standard HJ/T 400-2007. As a result, the lower the emittable concentration of interior materials at the end of storage, the lower the emittable concentration of materials that can be emitted at 25 °C in the whole vehicle after assembly, and the more controllable the VIAQ is.

The simulation results of emittable concentration at 25 °C during the storage in summer and winter as shown in Figure 4b show that the simulation value in summer gradually decreased from 100 mg/m<sup>3</sup> at the beginning of storage to 51 mg/m<sup>3</sup> after nine days, while the simulation value in winter gradually reduced from 100 mg/m<sup>3</sup> at the beginning of storage to 87 mg/m<sup>3</sup> after nine days of storage. In other words, at the same storage ventilation rate, ventilation pollution, and storage time, the VOCs in the same interior material can be emitted 71% more in winter at 25 °C than in summer. These VOCs trapped in the interior due to the lower storage temperature will be involved in the vehicle's final assembly, an essential out-of-control reason of VIAQ in winter.

### 3.3. Effect of Ventilation Rate on Interior VOCs

Using the data of easily emittable materials in Table 1, we conducted simulation calculations at a ventilation rates of 0.01, 1, or 100 L/min, respectively, ventilation pollution of 0 mg/m<sup>3</sup>, and storage temperatures based on the nine consecutive days of monitoring data from weather stations in Guangzhou summer as shown in Figure 2. We obtained ventilation outlet concentration curves and emittable concentration curves at 25 °C for interior materials under three ventilation rates during nine days of storage in summer in Guangzhou, as shown in Figure 5, and the distribution of VOCs concentration in the emission space after storage for 84 h as shown in Figure 6.





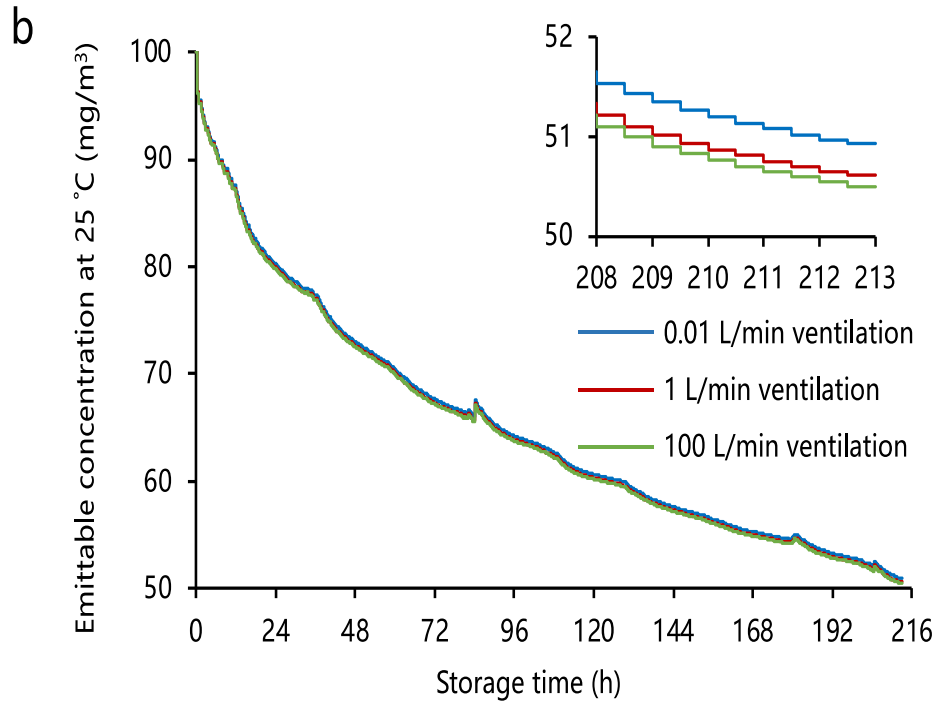
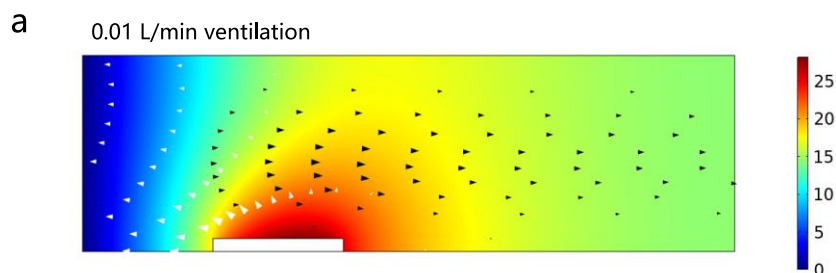


Figure 5: Influence of ventilation rate on ventilation outlet concentration and emittable concentration at 25 °C during nine days of storage of interior materials in Guangzhou summer season. (a) Ventilation outlet concentration curves; (b) Emittable concentration curves at 25 °C.

As shown in the ventilation outlet concentration profile in Figure 5, increasing the ventilation rate from 0.01 L/min (maximum linear rate of 0.0119 mm/s, approximately stationary) to 1 L/min (maximum linear rate of 1.19 mm/s) or 100 L/min (maximum linear rate of 114 mm/s), the concentration of VOCs at the right boundary of the emission space reduced significantly. The above change in concentration is because greater ventilation rates can dilute and remove the VOCs emitted from the interior materials from the emission space more quickly, as shown in Figure 6.

As shown in the emittable concentration curve at 25 °C in Figure 5, increasing the ventilation rate from 0.01 L/min to 1 L/min or 100 L/min within the range of simulation parameters only reduces the emittable concentration at 25 °C after nine days of storage of interior materials by 0.6% or 0.8%. This is due to the interior materials VOCs emitted by the rate-limiting step is mainly the diffusion process within the material. For example, the diffusion coefficient of VOCs in the interior at 25 °C is generally lower than it in the air of 5 to 9 orders of magnitude, while increasing the ventilation rate in the air can only change the balance of VOCs concentration at the solid-air interface of the material, but cannot significantly accelerate the diffusion process of VOCs within the material. Therefore, fluctuations in ventilation rates are not a significant cause of uncontrolled VIAQ in the absence of ventilation pollution.



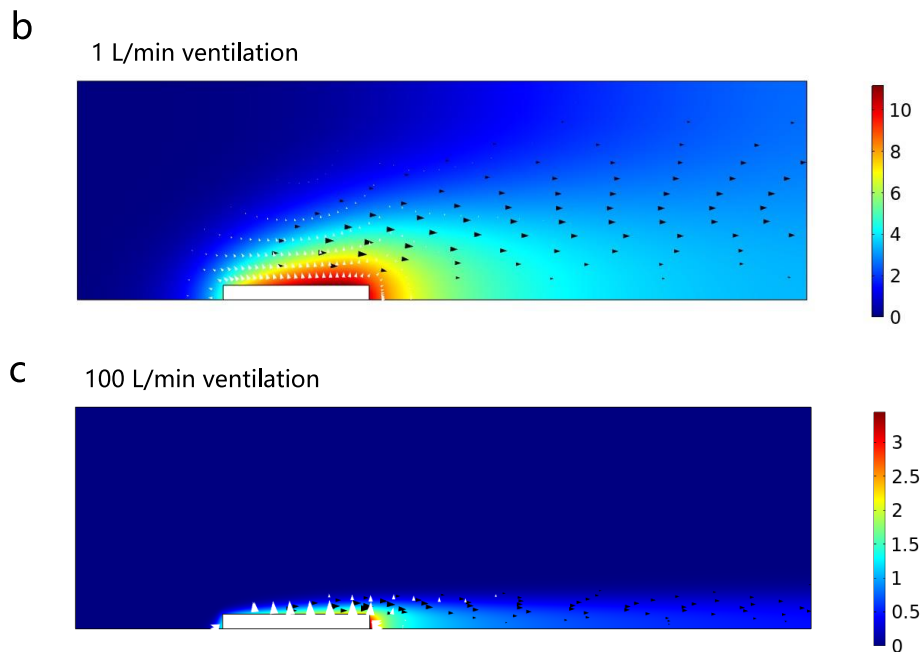


Figure 6: Distribution of VOCs concentration ( $\mu\text{g}/\text{m}^3$ ) under (a) 0.01 L/min ventilation and (b) 1 L/min ventilation and (c) 100 L/min ventilation in the emission space after storage for 84 h. The black and white arrows represent VOCs' convective and diffusive fluxes.

### 3.4. Impact of Ventilation Pollution on Interior VOCs

Using the data of easily emittable materials in Table 1, we conducted simulation calculations under the conditions of ventilation pollution of 0, 0.1, 0.5, or 1  $\text{mg}/\text{m}^3$ , ventilation rate of 1 L/min, and storage temperature of nine consecutive days based on the weather station monitoring data in Guangzhou summer as shown in Figure 2. We obtained the emittable concentration curves of the four kinds of ventilation pollution of interior materials at 25°C during nine days of storage in the summer of Guangzhou, as shown in Figure 7.

From Figure 7, ventilation pollution significantly affected the emittable concentration of the interior materials at 25 °C. Continuous pollution of 0.1, 0.5, or 1  $\text{mg}/\text{m}^3$  could respectively increase the emittable concentration of the interiors at 25 °C after nine days of storage by 8%, 42%, or 82%, compared with the non-polluted ventilation case. The more serious 0.5 or 1  $\text{mg}/\text{m}^3$  ventilation pollution inhibited the reduction of VOCs emitted from the material's interior and repeatedly increased the concentration curve instead of decreasing, i.e., the interior material absorbed the VOCs from the ventilation pollution in the reverse direction. These VOCs retained or even absorbed in the interior in the reverse direction due to the ventilation pollution of the storage will be involved in the total assembly on board and are a primary out-of-control reason of VIAQ.

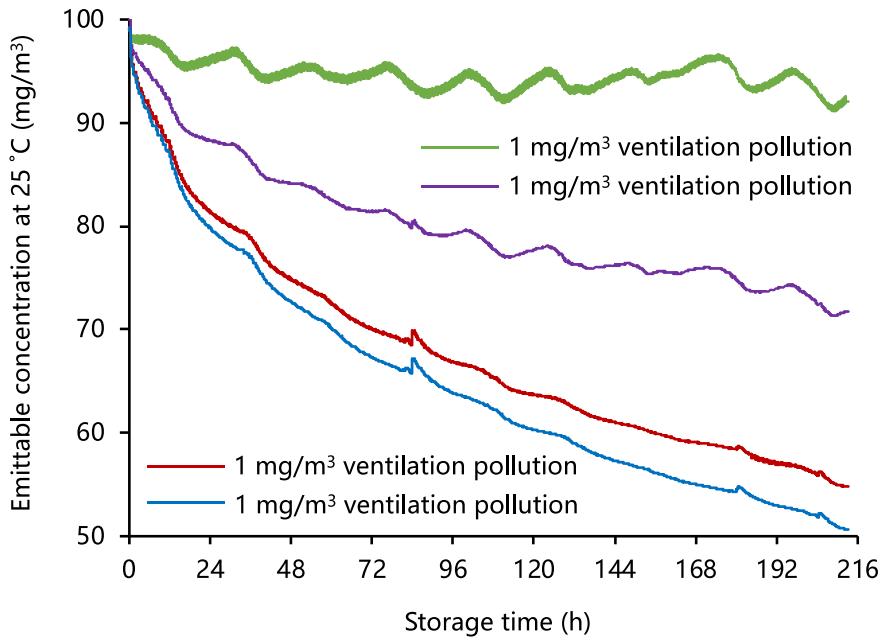


Figure 7: Effect of ventilation pollution on the emittable concentration at 25°C during nine days of storage of interior materials in Guangzhou summer season.

### 3.5. Influence of Properties of Emission of Interior VOCs

Using the data of difficult-to-emit materials in Table 1, we conducted simulation calculations under the storage temperature of nine consecutive days based on the weather station monitoring data in Guangzhou summer as shown in Figure 2. Figure 8 shows the emittable concentration curves of the difficult-to-emit interior materials at 25 °C during nine days of storage in Guangzhou in summer and winter.

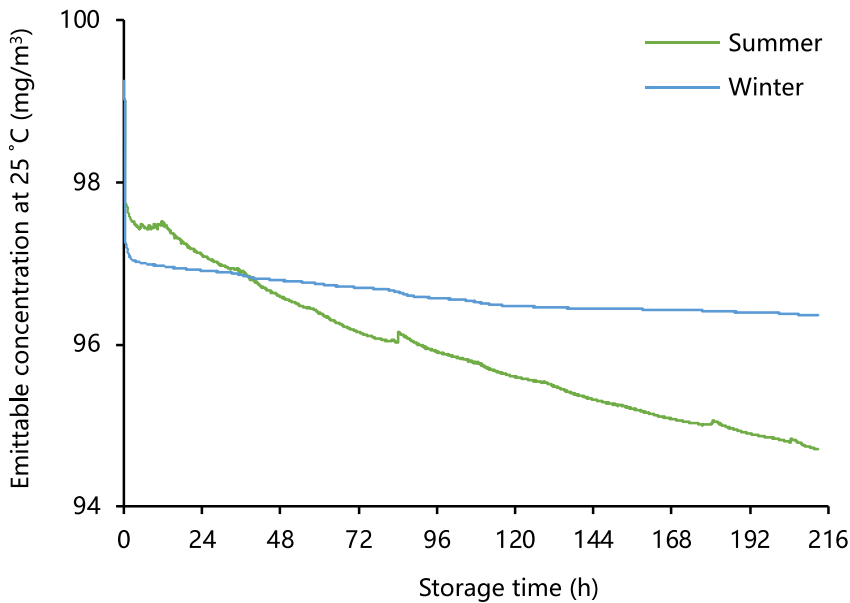


Figure 8: Effect of storage temperature on the concentration of difficult-to-emit interior materials at 25 °C during nine days of storage in Guangzhou in summer and winter.

In this paper, the difficult-to-emit materials are defined based on the crucial emission parameters of VOCs, mainly materials with smaller diffusion coefficients in the interiors and larger partition coefficients at the solid-gas interfaces, such as dense plastics. Smaller diffusion coefficients in the interior made the VOCs take more time to diffuse from the interior materials to the solid-gas interface. In comparison, larger partition coefficients at the solid-gas interface determine that a smaller proportion of VOCs are emitted from the solid-gas interface to the ambient air.

From Figure 8, after nine days of storage in summer or winter under the difficult-to-emit material parameters in Table 1, the emittable concentration at 25 °C of the materials slowly decreased from 100 mg/m<sup>3</sup> to 94.7 mg/m<sup>3</sup> or 96.4 mg/m<sup>3</sup>, with a decrease of about 5%. Compared with the winter and summer simulation results of easily emittable materials in Figure 4, the emittable concentration at 25 °C of difficult-to-emit materials was hardly affected by temperature changes, i.e., the VOCs performance was relatively stable. Therefore, interior materials that are more difficult to emit VOCs will not lead to uncontrolled VIAQ.

### 3.6. Simulation modeling expanded applications

Polymer devolatilization is the process of evaporation of volatile components from polymers at high temperatures. Currently, the most widely used VOCs treatment in the automobile industry is the polymer heating devolatilization process, and the heating temperature and time are the two most important parameters, which can be analyzed and optimized by simulation.

Setting the temperature and time of VOCs heating devolatilization, we conducted simulation calculations under the conditions of 1 L/min ventilation rate, no ventilation pollution, constant temperature at 25°C or heating devolatilization at 40°C, 55°C and 70°C for easily emittable materials. We obtained the emittable concentration curve at 25°C as shown in Figure 9.

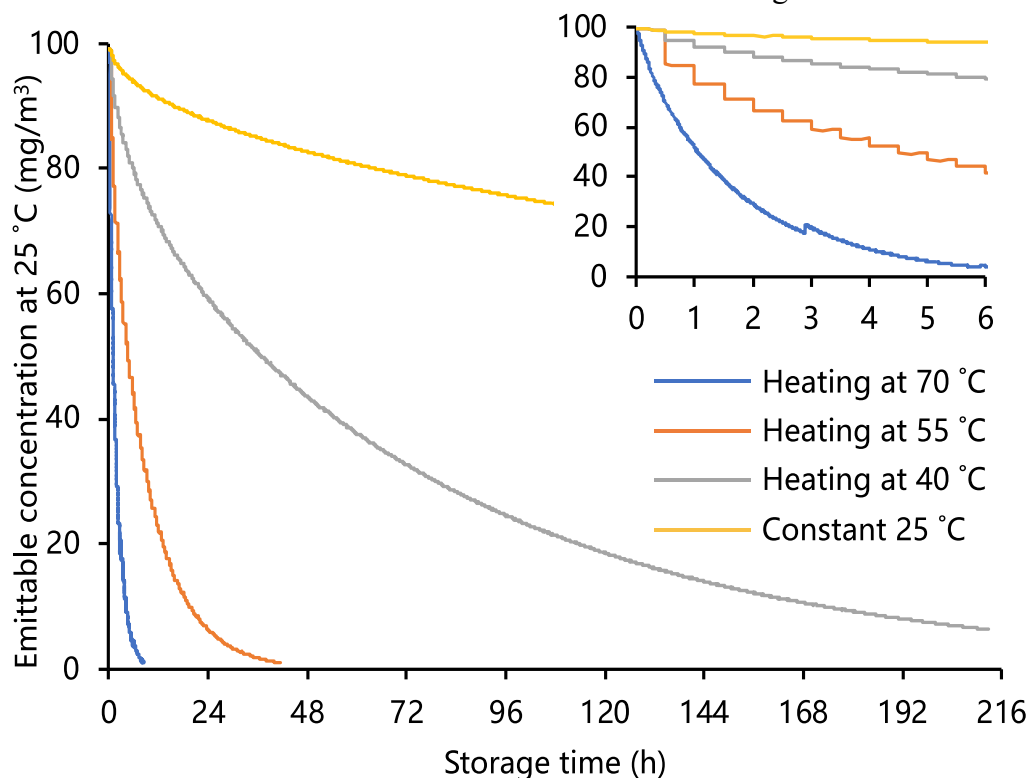


Figure 9: Effect of heating devolatilization temperature on the concentration of easily emittable materials at 25 °C during nine days of storage.

From Figure 9, higher heating devolatilization temperatures result in a faster reduction of emittable concentration in the interior materials at 25 °C. Heating devolatilization at 70 °C for 1 h can rapidly reduce the concentration from 100 mg/m<sup>3</sup> to 51 mg/m<sup>3</sup>. The results are the same as the natural devolatilization of the interior materials during nine days of storage in Guangzhou in summer.

## 4. Conclusion

The ambient temperature differences between winter and summer during the storage of interior materials can cause up to a 71% increase in emittable concentrations at 25 °C, which is the most likely out-of-control reason of the VIAQ. Ventilation pollution during storage of interior materials can significantly contribute to the out of control of VIAQ by as much as 82% of the increase in concentration, and pollution should be controlled at a low level of, for example, 0.1 mg/m<sup>3</sup>. In the absence of ventilation pollution, fluctuations in ventilation rates will not lead to uncontrolled VIAQ. Interior materials less likely to emit VOCs do not contribute to uncontrolled VIAQ, and the use of easily emittable interior materials should be controlled. Higher heating devolatilization temperatures will result in a faster reduction of emittable concentration in the interior materials at 25 °C.

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