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An Experimental and Modelling Study on the Adsorption Characteristics of Activated Carbon under Different Challenge Concentration Levels

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ABSTRACT
Applying air cleaning devices is an effective approach to control targeted indoor gaseous pollutants. It is important to understand the adsorption characteristics of filter media (e.g, activated carbon) at typical indoor application conditions as well as standard test conditions. Tests per ASHRAE Standard 145.1 for filter media performance evaluation can provide a relative comparison among different media. However, as the tests are conducted at elevated gas concentrations (1~100 ppm), they do not represent the media performance under lower concentrations typical of indoor applications (<0.1 ppm). Data are currently lacking for describing the correlation between the gas-phase filter media performance and the challenge concentration levels. In this study, single-pass adsorption tests were performed with smaller bed depth and pellet size than that specified in ASHRAE std 145.1 test protocol at four different concentration levels (50 ppb, 500 ppb, 5 ppm and 50 ppm). The data were used to determine the sorption isotherm and suggest a correlation between the partition coefficient and challenge concentration. Results revealed for the first time a linear correlation at log-log scale between the partition coefficient and the challenge concentration. Incorporation of this new correlation in a sorbent bed simulation model enabled the prediction of filter performance at low concentration based on the test data obtained from high concentration tests.

KEYWORDS
Indoor air quality, adsorption, partition coefficient, activated carbon.

INTRODUCTION
Poor indoor air quality has been statistically associated with occupants' health and performance (Seppänen & Fisk, 2006). Volatile organic compounds (VOCs) are found to be one of the major risk factors that are responsible for poor indoor air quality (Gallego et al, 2009). Ventilations, as a dilution method, has limitation in practice for removing targeted pollutants of interest because of its energy consumption and dependency on outdoor air quality. Thus, filtration through sorbent media (e.g., activated carbon) is considered as an effective alternative to reduce specific VOC concentration in an energy efficient manner (Fisk, 2008). Understanding and evaluating the performance of sorbent media become very important for designing a filtration system. ASHRAE standard 145.1-2015 has provided a laboratory test method to evaluate the performance of granular sorbent media (ASHRAE, 2008). However, the challenge concentration described in the test method is at 100±10 ppm, which is far above typical indoor concentration. Consequently, the results of the standard test cannot represent the actual performance of the sorbent media in the indoor environment. The goal of this study is to 1) investigate the performance of sorbent media at different concentration levels, from 100 pm down to 100 ppb (close to typical indoor concentration level of less than 50 ppb), and 2) develop a mechanistic model to simulate the sorbent media at real operation conditions.

METHODS

An air-cleaning technology test system (ACTTS) was used to investigate the performance of sorbent media at different challenge concentration levels. The design of the test system is illustrated in **Figure 1**. The ACTTS could control and provide the same test conditions, e.g., flow rate, temperature, humidity and challenge concentration to each test column (Figure 2). The diameter of the test column was consistent with ASHRAE 145.1 standard test but the height of sorbent media was reduced to L=1 cm to shorten the test period. Two test columns (sorbent column) were packed with sorbent media, and another one (reference column) was empty for inlet concentration monitoring.

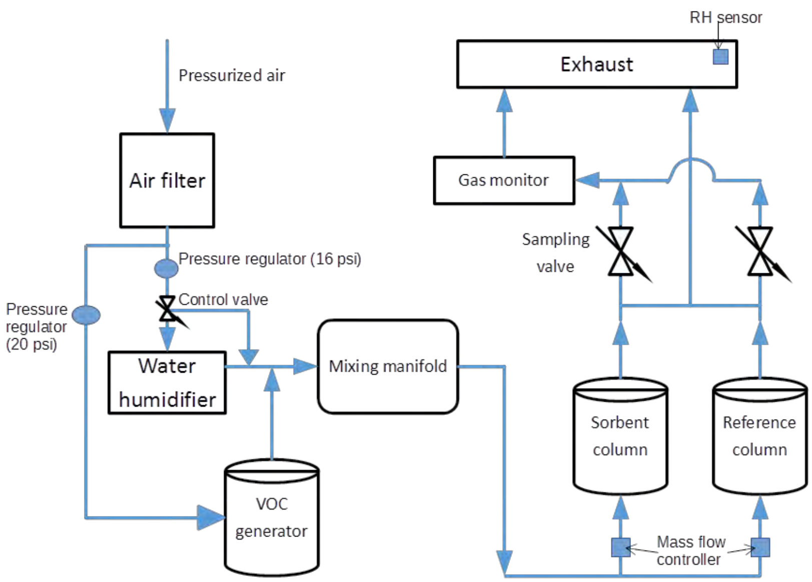

Figure 1 Schematics of the ACTTS

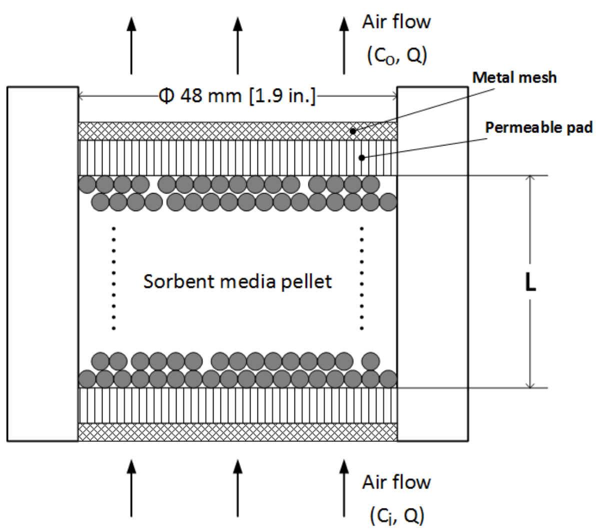

Figure 2 Schematic of the test column

Activated carbon is a widely used sorbent media in practice due to its high surface area and porous structure. Two types of virgin activated carbon were selected to test. The sorbent media were grounded into the particle size of 1 mm through ball-milling. The purpose of the grounding procedure is to ensure the packing of the sorbent bed is uniform. The specifications of the selected media are listed in Table 1.

Table 1 Specifications of test media

Media ID	M#1	M#2
Material	Coconut base virgin activated carbon	Coal base virgin activated carbon
Apparent density*	0.45 g/cc	0.49 g/cc
Pellet porosity*	0.3	0.4

* provided by manufactures

Toluene is one of the typical VOCs commonly found in the indoor environment. It has been widely used as a reference compound for total volatile organic compounds (TVOCs) in many studies. Bubbling method and heated permission tubes were used to generate high (≥5 ppm) and low concentrations of toluene, respectively. A portable device, ppbRAE 3000 (1ppb resolution; ±3% accuracy at calibration point), is used for toluene measurement. During the test, both the inlet concentration, C_i and outlet concentration C_o were monitored. The ratio between the adsorbed phase concentration and the gas-phase VOC concentration at equilibrium is defined as partition coefficient and used to represent the capacity of the activated carbon. The partition coefficient can be calculated through Eq-1.

$$K_{ma} = \frac{C_s}{C_i} = \frac{Q \cdot \int_0^t \left(C_i - C_o\right) dt}{\pi \cdot \frac{\phi^2}{4} \cdot L \cdot \left(1 - \varepsilon_b\right)} / C_i \tag{1}$$

where K_{ma} is the partition coefficient, C_s is the sorbent phase concentration, ε_b is the bed porosity, L is the height of the sorbent bed, and ϕ is the diameter of the sorbent bed. Tests were conducted in this study to provide the partition coefficients of the two types of activated carbon under 4 different concentration levels ranging from 100 ppb to 50 ppm.

MODELING AND SIMULATION

The mass transfer of VOC in the packed bed system includes: external convective mass transfer at the outer surface of sorbent particle, internal diffusion inside the pellet (within the pore air and on the internal surface) and adsorption of VOCs on the solid matrix of the sorbent, such as activated carbon. A mechanistic model has been developed to describe the mass transfer process in the sorbent bed in the previous study (He et al., 2014; Pei & Zhang, 2010). The same model was applied but a new method to determine the partition coefficient was used in the present study. Instead of using a constant partition coefficient gained from each experiment, the partition coefficient is considered as a variable that dependents on the gas-phase concentration. The correlation between the partition coefficient and the gas-phase concentration, namely, P-C correlation, was found to follow the form of:

$$K_{ma} = a\left(C_p\right)^b \tag{2}$$

where C_p is the gas-phase VOC concentration, which is equal to the inlet concentration at 100% breakthrough.

The parameters used in the simulation are listed in Table 2. The methods to determine the mass transfer coefficient and diffusion coefficient were introduced in the previous study (Pei & Zhang, 2012).

Table 2 Summary of the simulation parameters

Packed-bed	Bed diameter, D, cm	4.8	Measured
	Particle diameter, d_p, mm	1	
	Bed length, L, cm	1	
	bed porosity, ε_b	0.3	
	Pellet porosity, ε_p	0.3 (M#1), 0.4(M#2)	
	mass transfer coefficient, h_m, m/s	0.076	Sh, Re, Sc
Environment	Inlet concentration, C_i, ppm	42, 5, 0.58, 0.1	Measured
	Flow rate, Q, m^3/h	1.699	
	Superficial velocity, u_s, m/s	0.26	
Media	Pore diffusivity, Dp, m^2/s	8e-6	Literature (Do, 2011; Khazraei, 2014; Pei, 2011)
	Surface diffusivity, Ds, m^2/s	5e-10	
	P-C correlation	K_{ma}=2121.5*C_p^-0.728 (M#1) K_{ma}=1880.7*C_p^-0.70 (M#2)	Measured and regressed

RESULTS AND DISCUSSIONS

According to the experimental data from the breakthrough tests, the partition coefficient for two activated carbon at 4 different toluene concentration levels were obtained for Test M#1 and Test M#2 (**Figure 4**). The correlation of the partition coefficient and the corresponding challenge concentration was established by regression using Eq-2 (Figure 3). These two correlations for M#1 and M#2 were then used for determining the partition coefficient in each control volume in the simulation.

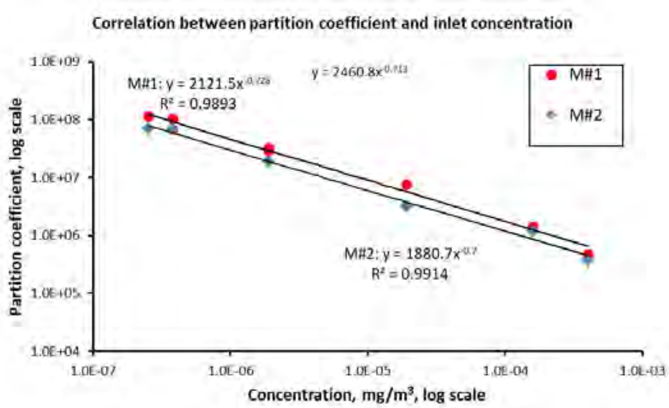

Figure 3 Correlation between the partition coefficient and the challenge concentration

In **Figure 4**, the simulation results were compared with the experimental data at 4 different concentration levels. The mechanistic model with the partition coefficient determined from the tests could generate results that have good agreement with the test data (R^2>0.9). The P-C correlation for each activated carbon media could be used to simulate the tests at both high concentration and low concentration.

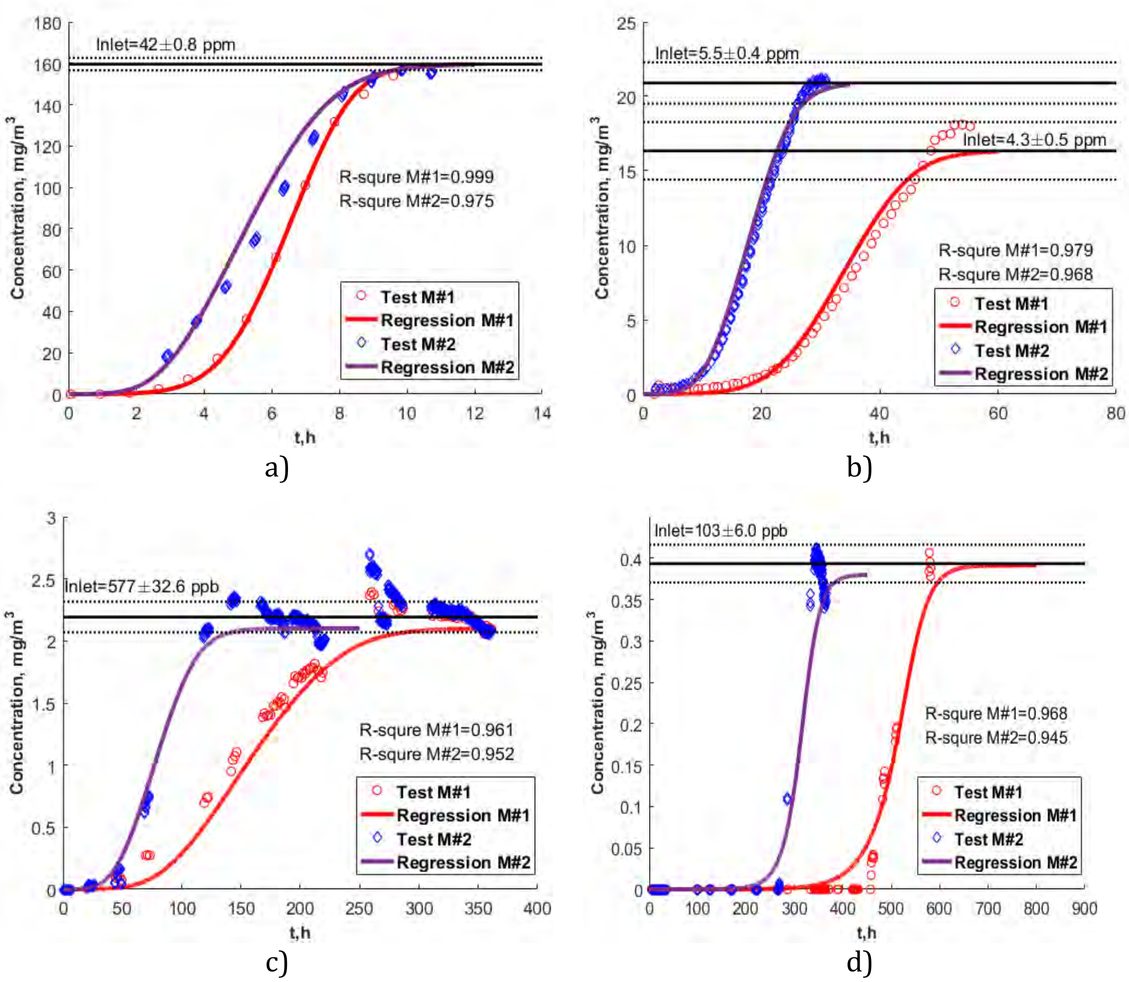

Figure 4 Breakthrough curve of toluene in activated carbon (M#1 and M#2) at four concentration levels

CONCLUSIONS

Based on the experimental investigation, the removal capacity at 100% breakthrough depends on the challenge concentration significantly. Tests of two types of activated carbon at 4 different concentration levels of toluene show that the partition coefficient increases with decreasing inlet concentration. The correlation between the partition coefficient and the concentration can be represented by a power-law empirical equation (i.e., a linear relationship in the log-log scale). The empirical equation can be used to determine the partition coefficient in the sorbent bed and applied in the mechanistic model to simulate performance of the activated carbon at both high and low concentration of toluene. As a result, it would enable the prediction of the filter performance at low concentration levels typical of indoor environment based on the standard accelerated tests at high concentration levels.

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