VOC source and sink behaviour of porous building materials: Part II—effects of Reynolds number and temperature

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ABSTRACT
This study theoretically investigates the impact of air velocity and temperature on the source and sink behaviour of porous building materials, by applying the analytical model proposed in Part I. The impact of air velocity on the source and sink behaviour was investigated for various levels of material properties. The Reynolds number was varied from 10^2 to 10^5, which is equivalent to an air velocity from almost stagnant to 0.34 m/s when the material is 4.5 m long. The results of the extensive parametric study showed that the effect of air velocity depends on the effective diffusion coefficient and the thickness of the porous material. As the diffusion resistance of the material increases (effective diffusion coefficient decreases and/or the thickness increases), the effect of air velocity decreases up to a certain limit, beyond which no effect is observed.

Unlike air velocity, the temperature affects material properties and transport properties like gas diffusion coefficient and kinematic viscosity of air. The effects of temperature was investigated using the material properties of carpet obtained by Zhang *et al.* (2001) at three different temperature namely 10.5, 23 and 35°C. The effect of temperature was noticeable in all five VOCs considered, but the impact varied from one compound to another. The changes in the convective mass transfer coefficient relative to that of 23°C are less than 5%; hence, changes in the material properties are a major contributing factor.

KEYWORDS
VOC; Reynolds number effects; Temperature; Source/sink; Porous building materials

INTRODUCTION
Many experimental studies have been carried out to examine the effects of environmental conditions like temperature, air velocity and relative humidity on the emission and the sink effects of various building materials. The results however have not been conclusive due to the differences in sample preparation and preconditioning, test set-up, condition and duration, the range of the environmental parameter considered, VOCs measured, etc. For example, emission tests on carpets made of nylon fibre on a latex foam backing (Wolkoff, 1998; Knudsen *et al.*, 1999) and carpet/adhesive assembly made of nylon fibre with synthetic jute textured back (Low *et al.*, 1998) showed that air velocity generally affects the initial period of emission. However, Wolkoff (1998) reported that air velocity influences for the first week with the maximum difference in concentration less than 25% in the range of 0.01–0.09 m/s; Knudsen *et al.* (1999) concluded minor impact of air velocity, i.e. less than 10% change in concentration, in the range of 0.1–0.3 m/s. Low *et al.* (1998) observed no impact of air velocity after 30 h with the maximum difference in VOC concentration less than 25% in the range of 0.04–0.22 m/s. Since experimental studies provide restricted information, theoretical investigation is needed to complement these limitations and to provide more detailed comprehensive information.

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This paper investigates theoretically the effects of air velocity, expressed as Reynolds number, and temperature on the primary source and sink behaviour of porous building materials. An analytical model that considers internal diffusion, adsorption/desorption and generation within the porous material, and convection over the material was developed and assessed as presented in Part I. To investigate the effects on primary source and sink behaviour, the generation term for secondary emissions was not considered in this study. In the proposed model, the air velocity or Reynolds number affects only the convective mass transfer coefficient and the material properties are independent. Therefore, the effects of air velocity were carried out for a wide range of material properties. It is generally assumed that internal diffusion is the dominant process and convection, i.e. air velocity, is insignificant for dry building materials. This assumption has been adopted in modelling of source/sink behaviour (Little and Hodgson, 1996) and material property measurement (Bodalal *et al.*, 2000; Meininghaus *et al.*, 2000). The parametric study on the effects of Reynolds number can examine the validity of this assumption.

Even though the proposed model is developed for isothermal condition, the temperature affects the parameters like diffusion coefficient, sorption partition coefficient and the convective mass transfer coefficient. The effect of temperature on source/sink behaviour was investigated at 10.5, 23 and 35°C of the isothermal condition considering the changes in the temperature dependent parameters. The material properties, i.e. effective diffusion coefficient and sorption partition coefficient of carpet (olefin and nylon fibre on latex SBR backing) obtained by Zhang *et al.* (2001), were applied. Other temperature dependent parameters considered are molecular diffusion coefficient of VOC-air and kinematic viscosity of air, which affects the convective mass transfer coefficient.

EFFECT OF REYNOLDS NUMBER

The parameters were expressed in nondimensionalized form as follows:

- Diffusion coefficient of solid (D_s): D_a/D_s
- The thickness of the solid (b): b/L
- Air velocity (u_∞): $Re_L = (u_\infty \cdot L)/\nu$
- Time (t): $t^+ = t/t_{\text{diff}} = t/(b^2/D_s)$

where D_a is the molecular diffusion coefficient of VOC in the air (m^2/s), D_s is the effective diffusion coefficient of the material (m^2/s), b is the thickness of the material (m), L is the length of the material (m), Re_L is the Reynolds number as defined above, u_∞ is the air velocity outside the boundary layer (m/s), ν is the kinematic viscosity of air (m^2/s), t is the time (s), t_{diff} is the diffusion time defined as b^2/D_s (s). The basis of this nondimensionalization can be found in Lee *et al.* (2000). The porosity ε and the sorption partition coefficient K are defined as one parameter ($\varepsilon + K$).

D_a/D_s was assumed to vary in the range of 10–10^5. This range was decided based on the previous study, which showed the range of measured D_a/D_s for gas-phase diffusion of various building materials are from 4.42 to 1.55×10^4 (Haghighat *et al.*, 2002). ($\varepsilon + K$) varies from 10 to 10^5. The porosity ε is within the range of 0–1; however, K can be varied significantly. Cox *et al.* (2001) measured the sorption partition coefficients of various VOCs on the vinyl flooring and reported that they may vary from 810 to 4.2×10^5. The thickness to length ratio b/L was varied from 10^{-4} to 10^{-2}. The Reynolds number was varied from 10^2 to 10^5, which is equivalent to an air velocity from almost stagnant to 0.34 m/s when L is 4.5 m. The mass transfer coefficient h_D was obtained from the Sherwood number relation for the laminar forced convection over a flat plate as

$$Sh_L = 0.664 \cdot Re_L^{0.5} \cdot Sc^{1/3} \tag{1}$$

where Sh_L is the Sherwood number defined as $h_D \cdot L/D_a$, Sc is the Schmidt number defined as ν/D_a, h_D is the convective mass transfer coefficient (m/s).

The maximum mass of gas-phase VOCs that can be emitted from or be absorbed by a porous material per unit area m_{max} is

$$m_{max} = |C_0 - C_\infty| \times b \tag{2}$$

where m_{max} has the unit of (mg/m^2), C_0 is the initial gas-phase VOC concentration in the material (mg/m^3) and C_∞ is the VOC concentration outside the boundary layer, i.e. in the bulk air (mg/m^3). The total transfer time t_{total} is defined as the time required to emit/sink 99% of m_{max} from/into the material. The effects of Reynolds number and temperature were quantified using t_{total}.

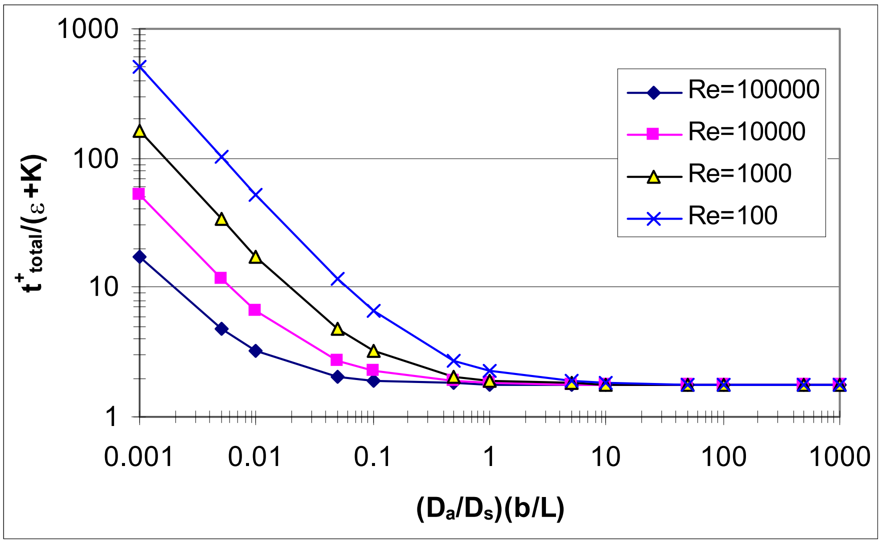

Figure 1 Effect of Reynolds number in t_{inf}.

All combinations of material parameters and Reynolds number were used to study the effects of these parameters on t_{total} and the trends observed are presented in Figure 1. t_{total} normalized by t_{diff}, denoted as t^+_{total} is shown in terms of $(D_a/D_s) \times (b/L)$ and $(\varepsilon + K)$ for various Reynolds numbers Re_L. $(\varepsilon + K)$ has linear impact on t^+_{total}: when $(D_a/D_s) \times (b/L)$ is 1 and $Re_L = 10^4$, t^+_{total} is 18.25 for $(\varepsilon + K) = 10$ and 1825 for $(\varepsilon + K) = 10^3$. For given material properties, t_{total} increases as Re_L decreases: when $(D_a/D_s) \times (b/L)$ is 0.01 and $(\varepsilon + K)$ is 100, t^+_{total} is 326.1 for $Re_L = 10^5$, while t^+_{total} is 5217.5 for $Re_L = 10^2$. This figure shows that as $(D_a/D_s) \times (b/L)$ increases the effect of Re_L decreases. When $(D_a/D_s) \times (b/L)$ is 0.01, t^+_{total} for $Re_L = 10^2$ is 16 times larger than that for $Re_L = 10^5$, while only 24% increases when $(D_a/D_s) \times (b/L)$ is 1.0. The influence of Re_L diminishes when $(D_a/D_s) \times (b/L)$ is larger than 1.0. In other words, the assumption of negligible convection is valid for $(D_a/D_s) \times (b/L)$ larger than 1.0.

To evaluate whether t_{total} can be a good index for this parametric study, the effect of Reynolds number on the emission rate (R) was investigated for cases of D_a/D_s = 10 and 10^3, $(\varepsilon + K)$=100, and b/L = 0.001. Figure 2 shows the big difference on the effect of Re_L depending on the D_a/D_s and the results agree with the results presented in Figure 1.

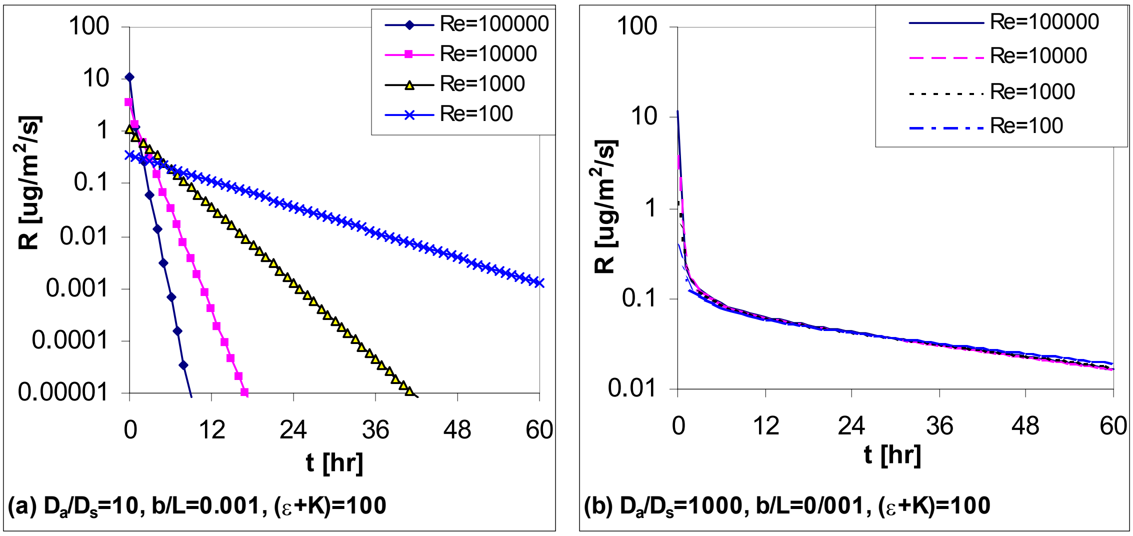

Figure 2 Effect of Reynolds number on emission rate.

EFFECT OF TEMPERATURE

Unlike air velocity, the temperature affects material properties and convective transport properties. Zhang *et al.* (2001) reported the material-phase diffusion coefficients and partition coefficients of an 8-mm thick carpet for five VOCs at temperatures of 10.5, 23 and 35°C. These reported material properties were applied to investigate the effect of temperature. In addition to the material properties, molecular diffusion coefficient of VOC-air D_a, density ρ and viscosity μ of air depend on the temperature. The density of air at different temperature was obtained using the ideal gas law. For the effect of temperature on the viscosity of air, Sutherland's equation was applied: it has an error less than 2% for a temperature range of 170–1900 K (White, 1992). D_a was estimated using the Wilke and Lee method (Perry *et al.*, 1973), which has 4.3% of the absolute average error for about 150 compounds and less than 8% of the average errors for all classes of compounds except acids.

The thickness and the length of the material, and the air velocity are constant as 0.008 m, 4.5 m and 0.1 m/s, respectively. The Reynolds number is independent of VOC and only depends on ρ and μ: Re_L was 31 692, 29 352 and 27 363 at the temperature of 10.5, 23 and 35°C, respectively. The other parameters that vary with the temperature and VOC are presented in Table 1. D_a, ρ and μ affect the convective mass transfer coefficient h_D. The changes in h_D relative to that of 23°C are less than 5% for all VOCs considered; hence, the influence of temperature is minor on convective transfer. The temperature significantly affects D_a/D_s and $(\varepsilon + K)$, but the effects vary with VOC. The general tendency is that both D_a/D_s and $(\varepsilon + K)$ decrease with increasing temperature. This may give synergic effects to the influence of temperature on the source and sink behaviour of porous building materials. Table 1 also presents the simulated results of the dimensional total transfer time t_{total}. The temperature may significantly affect t_{total}: for the case of dodecane, t_{total} is almost 1 year at 10.5°C but it reduces to a little more than 1 month at 35°C. The effects of temperature vary with VOCs, but generally more differences are observed between 10.5 and 23°C.

Table 1 Effect of temperature

VOC	Temperature	D_a (m^2/s)	*Sc*	h_D (m/s)	D_a/D_s	($\varepsilon + K$)	t_{inf} (day)
Ethyl benzene	10.5°C	6.88×10^{-6}	2.06	2.30×10^{-4}	398.8	278.4	21.7
	23°C	7.48×10^{-6}	2.05	2.40×10^{-4}	151.0	204.0	5.7
	35°C	8.08×10^{-6}	2.04	2.50×10^{-4}	106.5	108.8	2.1
Benzaldehyde	10.5°C	7.23×10^{-6}	1.96	2.38×10^{-4}	128.4	3413.9	85.3
	23°C	7.87×10^{-6}	1.95	2.48×10^{-4}	82.0	865.0	13.2
	35°C	8.49×10^{-6}	1.94	2.58×10^{-4}	25.0	782.5	4.2
1,4-Dichlorobenzene	10.5°C	6.73×10^{-6}	2.11	2.27×10^{-4}	73.1	2718.4	43.4
	23°C	7.32×10^{-6}	2.09	2.38×10^{-4}	32.8	1643.3	12.3
	35°C	7.91×10^{-6}	2.08	2.46×10^{-4}	17.4	871.4	3.9
Undecane	10.5°C	5.01×10^{-6}	2.83	1.86×10^{-4}	170.2	4976.4	232.8
	23°C	5.46×10^{-6}	2.81	1.95×10^{-4}	–	–	–
	35°C	5.89×10^{-6}	2.79	2.03×10^{-4}	29.2	2112.0	17.8
Dodecane	10.5°C	4.75×10^{-6}	2.99	1.80×10^{-4}	69.7	16800.4	359.8
	23°C	5.17×10^{-6}	2.97	1.88×10^{-4}	28.5	15344.6	142.9
	35°C	5.59×10^{-6}	2.94	1.95×10^{-4}	16.6	5995.1	33.0

Figure 3 shows the normalized wall concentration C_w, which is equivalent to the ratio of the emission/sink rate R at time t, to the initial emission/sink rate R_0, versus time normalized by t_{total}. R is larger at higher temperature level throughout the whole emission/sink period. At lower temperature, R decreases abruptly at the early stage of emission. After this period, R is logarithmically linear. Also, R is more sensitive to temperature in the range 10.5–23°C, than it is in the range 23–35°C.

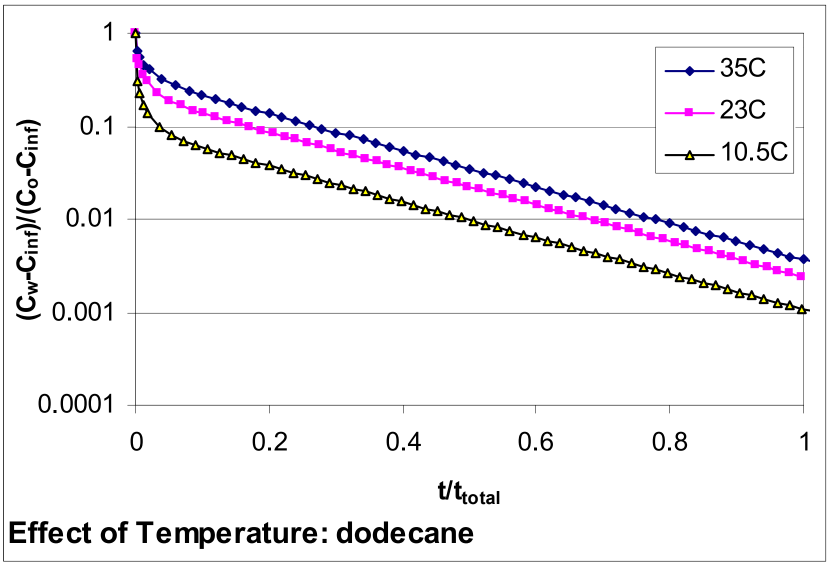

Figure 3 Effect of temperature on dodecane emission/sink rate of carpet.

CONCLUSION

The effects of Reynolds number (air velocity) and temperature on the VOC source and sink behaviour of porous building materials were investigated theoretically. The parametric study on the impact of Reynolds number was carried out for a wide range of material properties, expressed as ratio of diffusion coefficient in the air to effective diffusion coefficient of material D_a/D_s, thickness to length ratio b/L and combined porosity and sorption partition coefficient factor ($\varepsilon + K$). The study indicated that $(D_a/D_s) \times (b/L)$ is a good measure to determine the effect of Reynolds number. As $(D_a/D_s) \times (b/L)$ increases, the effect of Reynolds number decreases. For $(D_a/D_s) \times (b/L)$ larger than 1.0, Reynolds number has little impact on the emission and sink behaviour.

The effect of temperature on source/sink behaviour was investigated at 10.5, 23 and 35°C of isothermal condition considering the changes in the temperature dependent parameters. The convective transfer properties like D_a, density and viscosity of air were obtained using the existing validated prediction methods. Material properties of carpet reported by Zhang *et al.* (2001) were applied. The effects of temperature were significant for all five VOCs considered, but the impact varies with the compound. Since the change in the convective mass transfer is minor in the temperature range considered the effect of temperature is mainly caused by the temperature dependence of material properties. Hence, more detailed investigation is required for the effects of temperature on the material properties like D_s and K.

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