3D-CFD ANALYSIS OF DIFFUSION AND EMISSION OF VOCs IN A FLEC CAVITY

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ABSTRACT
In this paper, the flow field and the emission field of volatile organic compounds (VOCs) from the surface of indoor building materials in a FLEC (Field and Laboratory Emission Cell) Cavity are examined by 3D CFD analysis. Two types of emission phenomena from building materials are studied here: (1) emission controlled by external diffusion; (2) emission controlled by internal diffusion. The flow field within the FLEC cavity is laminar. With a ventilation rate of 200 ml/min, the air velocity near the test material surface ranges from 0.1cm/s to 1.4cm/s. In the case of the internal diffusion material, with respect to the concentration distribution in the cavity, the local VOC emission rate becomes uniform and the FLEC works well. However, in the case of evaporation type materials, the FLEC is not suitable for emission testing because of the thin FLEC cavity. The diffusion field and emission rate depend on the cavity concentration and on the Loading Factor.

INDEX TERMS
Flow field, VOCs, Emission rate, Mass transfer, Loading Factor

INTRODUCTION
For field measurements, the most popular type of test chamber is the FLEC -Field and Laboratory Emission Cell (P. Wolkoff et al., 1991 and 1995), and a lot of field measurements of VOCs emission rates from building materials using a FLEC have been reported (CHEMATEC, 1997). In this study, the flow field and diffusion field within the FLEC cavity are analyzed by CFD (Computational Fluid Dynamics), and the emission properties of chemical substances from the surface of the building materials are clarified. In this paper, the results of analyzing the emission properties in a FLEC cavity will be reported for external diffusion materials and for internal diffusion materials. Furthermore, the difference in the emission rates of external diffusion materials and internal diffusion materials will be discussed when the (Loading Factor L_t [m^2/m^3])/(air change rate n_t [h^{-1}]) (referred to as L_t/n_t [l/(m/h)]) of the sample building materials is changed. This analysis aims to clarify the characteristics of the emission rate measurement of chemical substances in a FLEC.

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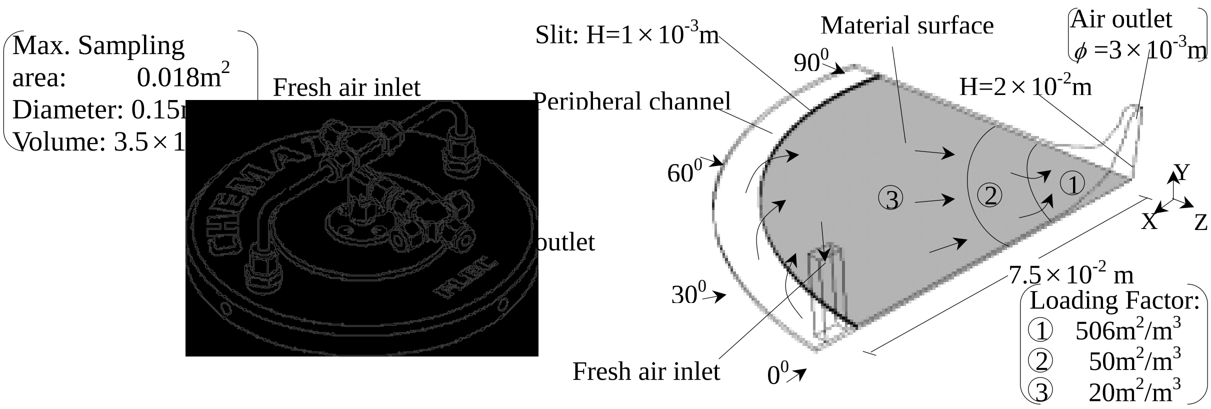
FLEC Cavity and Test Chamber Method

The outline and cross section of the FLEC are shown in Fig.1. In the FLEC, measurement of the emission rates is usually carried out at extremely large air change rates (686 and 343 [h^{-1}] as shown in Table 1. Fresh air at controlled temperature and humidity is supplied to the peripheral channel of the FLEC cavity via a pair of pipes, blown off towards the center from a slit 1 mm in width, converged on the cavity center, and emitted from the upper part. The air supplied from the pipes is not always equally distributed in the peripheral channel of the FLEC. One study has reported that there may be a bias in the airflow inside the chamber (E.Uhde et al., 1998). Since the width of the slit is as narrow as 1 mm, there are still many controversial points in experimentally measuring the air velocity.



(1) Outline (2) Section of FLEC cavity

Figure 1. FLEC & Cavity

The emission test using the test chamber method must be carried out so that the emission is the same as that in an actual room, and so that the repeatability and reliability of the tests can be guaranteed. The gradients of the concentration of chemical substance relating to the emission should be equalized. When the concentrations of the chemical substance within the test chamber and that in the actual room are equal, the following formula (1) holds:

$$w_f A_f / n_f V_f = w_t A_t / n_t V_t \quad (1)$$

where w is the emission rate per unit area, mg/m^2h, A is the area of the building material in m^2, V is the volume in m^3, n is the air change rate in h^{-1}, the subscript f refers to full scale measurements, and the subscript t means a test chamber measurement. L is defined as follows:

$$L = A/V \quad (2)$$

where L is the Loading Factor. From (1) and (2), the Loading Factor and the air change rate have a relationship expressed by the following formula (3), under the condition that w_f should be equalized to w_t.

$$L_f / n_f = L_t / n_t \quad (3)$$

In cases where the building material inside the actual room covers the whole of the floor and the wall, L_t is generally considered to take an approximate value of 0.3 to 1 [m^2/m^3]. n_t for rooms in housing that are general airtight is considered to take an approximate value of 0.1 to

0.5 h^{-1}. Consequently, it is considered reasonable for L_t/n_t for the test chamber to be taken as a value of approx. 0.5 to 10 [1/(m/h)]. If the L_t/n_t value in the test chamber is great, the difference between the concentration inside the chamber and the concentration inside the material (the concentration gradient) becomes small and the measurement values for the emission amounts inside the test chamber tend to be smaller than those inside the actual room, resulting in a tendency to underestimate the measured values for the emission rates. Accordingly, it is safe to take a rather small value for L_t/n_t than otherwise.

Analysis of the Flow field and Diffusion field

Fresh air is unequally supplied from the peripheral channel of the FLEC cavity. The analysis is targeted at only one-fourth of the area, considering the symmetric properties of the cavity. The cases analyzed are shown in Table 1. The conditions of the CFD analysis are shown in Table 2. By sealing the effective emission areas of the building materials, three cases for the Loading Factor L_t [m^2/m^3] are studied. The three cases are 506 m^2/m^3 (effective emission area is a sector of radius 7.5 cm from the center), 56 m^2/m^3 (effective emission area is a sector of radius 2.5 cm from the center) and 20 m^2/m^3 (effective emission area is a sector of radius 1.5 cm from the center). [L_t/n_t] values corresponding to each case are shown in Table 1.

Table 1. Cases analyzed (ambient temperature: 23 ^{o}C)

Case No.	Air Change rate n_t[h^{-1}]	Loading Factor L_t [m^2/m^3]	L_t/n_t [1/(m/h)]	Type of emission process	Boundary condition at the material surface for CFD modeling
1-1	686	506	0.74	External diffusion: water, decane p-xylene, nonane	Giving the concentration of VOCs (saturated vapor phase concentration) at the material surface
1-2		56	0.08		
1-3		20	0.03		
1-4	77	56	0.74		
1-5	27	20			
2-1	343	506	1.48		
2-2		56	0.16		
2-3		20	0.06		
3-1	343	506	1.48	Internal diffusion: (SBR, thickness is 2mm)	Solving the diffusion process within the material to the cavity air field
3-2		56	0.16		
3-3		20	0.06		
3-4	39	56	1.48		
3-5	14	20			

At 23 ^{o}C, the saturated vapor phase concentrations C_o are taken as 19.9 [g/m^3] for water, 0.05[g/m^3] for p-xylene, 0.03[g/m^3] for nonane and 10.0[g/m^3] for decane. The diffusion coefficients in air D_a are taken as 2.27×10^{-5} [m^2/s] for water, 6.63×10^{-6} [m^2/s] for p-xylene, 5.07×10^{-6} [m^2/s] for nonane and 4.75×10^{-6} [m^2/s] for decane (the Chemical Engineering Society, 1968). In the case of internal diffusion, an SBR (styrene-butadiene rubber) plate is used as the emission source. The temperature in the SBR is regarded to be uniform at 23^{o}C and the initial concentration of the VOCs is 192 [g/m^3]. The effective diffusion coefficient D_c

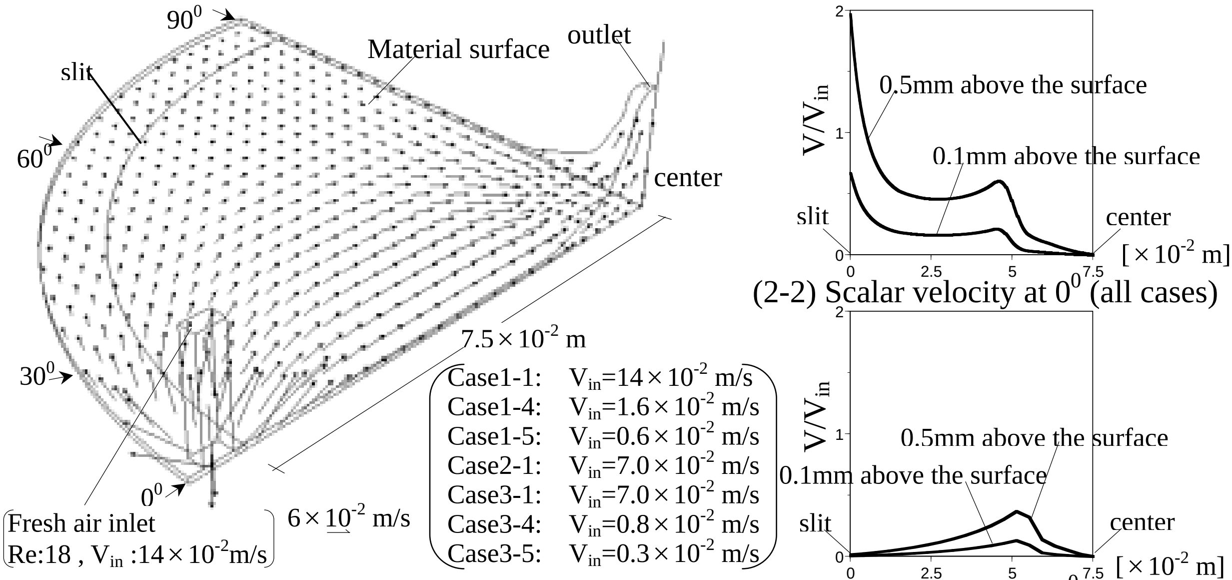
Table 2. Conditions of CFD analysis

Numerical model	: Laminar	Grid points	: 260,000
Space difference		QUICK (convection term)	
Inlet boundary	: $V_{y,in}$=0.14m/s(case1-1,1-2,1-3) $V_{y,in}$=0.07m/s(case2,), $V_{x,z,in}$ =0		
Outlet boundary	: Mass flow	Wall boundary	: no-slip
Symmetry	: $\partial V/\partial x = 0$ $\partial V/\partial y = 0$ $\partial V/\partial z = 0$		

in the SBR is assumed to be 1.1×10^{-14} [m^2/s], and the diffusion coefficients in air D_a is assumed to be 5.94×10^{-6} [m^2/s] at 23 °C(Xudong.Y et al., 1998). The distribution of the VOCs in the SBR is not considered, and the distribution of VOCs is assumed to be uniform at the initial state. The analysis mesh of 300(x)×200(y)×300(z) are prepared in the SBR, and a time-dependent diffusion analysis is carried out under the coupling of all the inside areas of the building material and the FLEC cavity air field.

Results of Predicting the Flow field in the FLEC

Since the Reynolds number for the FLEC cavity is very small (10 to 20 as shown later), the flow field is laminar. The air velocity distribution inside the FLEC cavity by the laminar flow analysis is shown in Fig.2. As shown in Fig.(2-1), in Case 1 (n_t =686 h^{-1}), there is a bias in the velocity inside the cavity. In Case 1, when the air contacts the supply pipe at the peripheral slit of the cavity; that is, at 0°(Fig. 1(2)), the velocity is the fastest at 0.28 m/s. As the air inlet is the furthest from the pipe at 90°, and the velocity is lowered to the lowest value of 0.2×10^{-2} m/s, the blow off velocity to the cavity is not uniform (Fig.(2-2)). Even in the vicinity of the area where the building material (SBR in this case) is placed downstream of the slit, the velocity distribution is uneven, becoming slower in the order from 0° to 90°. Further, the velocity suddenly decreases inside a radius of about 2.5 cm from the center of the cavity (Fig.(2-2), (2-3)). These trends do not correspond quantitatively to the experiment because there are great difficulties with measuring the velocity in the experiment, but correspond well qualitatively to the experiment (E.Uhde et al., 1998). As the Reynolds number defined by the blow off velocity from the slit of the FLEC is 18 in Case 1, and 9 or less in Cases 2 and 3, the flow field inside the cavity is completely laminar, and consequently, it is possible to obtain sufficient reliability for the results of the CFD analysis.



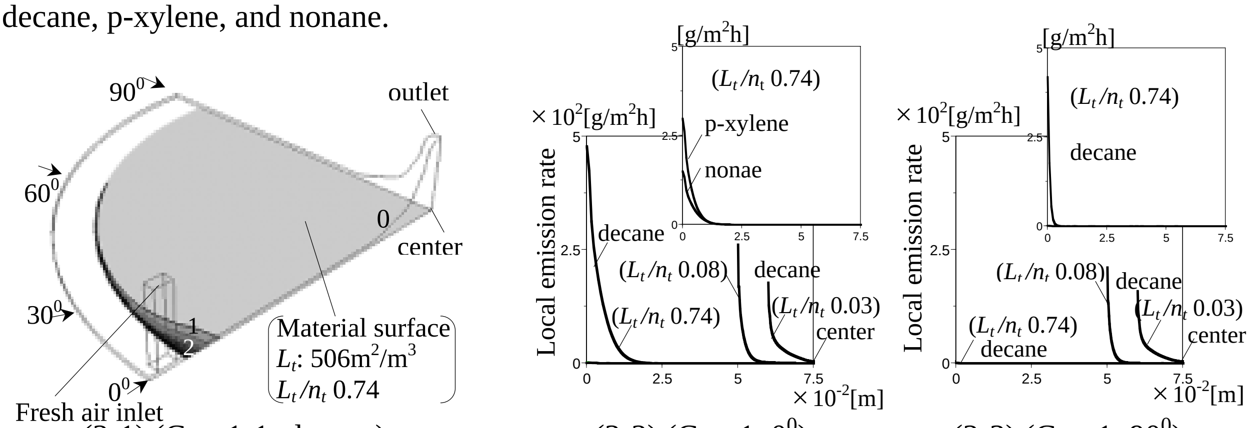
(2-1) Velocity vectors inside the FLEC cavity (Case 1) (2-3) Scalar velocity at 90° (all cases)

Figure 2. Velocity distribution inside the FLEC cavity (for all cases)

Results of Predicting the Diffusion field in the FLEC

Emission controlled by external diffusion

The distribution of the local emission rate of decane at the surface of the building material (here, the liquid decane surface) is shown in Fig.3. When L_t/n_t is 0.74[l/(m/h)] (Fig.(3-2,3-3)), the local emission rate from the surface of the building material shows the greatest value in the vicinity of 0^0 where the pipe is contacted, while the emission rate immediately drops to nearly zero at a distance of only several cm from the slit, and continues to be almost zero in the vicinity of the center. When L_t/n_t is 0.08[l/(m/h)] or 0.03[l/(m/h)] (Fig.(3-2,3-3)), the large distribution of the local emission rate from the surface of building material was eased. The predicted results for the average emission rate and average mass transfer coefficient for decane are shown in Table 4. In all cases except those where L_t/n_t is 0.03 and 0.06 (Case 1-3,2-3), the concentration at the outlet (decane: 9.99[g/m^3]) is equal to those in the vapor-phase on the surface of the building material model in any of the cases for pure water, decane, p-xylene, and nonane.



(3-1) (Case1-1: decane) (3-2) (Case1, 0^0) (3-3) (Case1, 90^0)

Figure 3. Distributions of local emission rate at the surface (Case1, 23 ^{o}C, [g/m^{2}h])

Table 4. The predicted results for the average mass transfer coefficient

		External diffusion type (Decane)								Internal diffusion type (TOVC) (20h)		
Case No.		1-1	1-2	1-3	1-4	1-5	2-1	2-2	2-3	3-1	3-2	3-3
Air change rate n_t [1/h]		686			77	27	343			343		
Loading Factor L_t [m^2/m^3]		506	56	20	56	20	506	56	20	506	56	20
L_t/n_t [1/(m/h)]		0.74	0.08	0.03	0.74		1.48	0.16	0.06	1.48	0.16	0.06
Average emission rate [g/m^{2}h]		13.6	121.7	131.6	13.7	12.9	6.79	59.6	80.5	1.52×10^{-4}	2.06×10^{-4}	2.05×10^{-4}
Surface concentration C_s [g/m^3]		10.0								1.53×10^{-4}	0.47	0.61
Outlet concentration C_o [g/m^3]		9.99	9.98	3.93	9.99	9.69	9.99	9.74	4.65	2.24×10^{-4}	0.68×10^{-4}	0.35×10^{-4}
Average mass transfer coefficient [m/h]	1	∞	∞	21.68	∞	∞	679	229	15.0	-1.46	4.42×10^{-4}	3.36×10^{-4}
	2	1.36	12.2	13.2	1.37	1.29	0.68	5.96	8.05	1.25	4.38×10^{-4}	3.36×10^{-4}

(ambient temperature: 23^{o}C. The average mass transfer coefficients 1 and 2 on the surface of the building material are calculated by setting the concentration at the outlet and at the inlet as reference concentrations. Analysis results for pure water, p-xylene, nonane are not included due to lack of space)

In cases where the L_t/n_t values are the same, the same values were also obtained for the average emission rates. In the measurement of the emission rates for external diffusion material, it is generally a basic assumption that the concentration within the test chamber is lower than the concentration on the surface of the building material. In the case of an FLEC, the assumption is not valid for an evaporation type building material when the area of the sample is relatively large compared with the amount of ventilation; that is, when L_t/n_t is relatively large.

Emission controlled by internal diffusion

As for the results for emission controlled by external diffusion, emission controlled with an internal diffusion material does not give a large distribution for the local emission rate of VOCs from the surface of the material. The rate is hardly affected by the change in (L_t/n_t) and becomes approximately constant in the order of 10^{-4} [g/m^{2}h] at 23^{o}C (Table 4).

CONCLUSIONS

(1) The bias in the airflow distribution within the cavity can be observed by a 3D flow field analysis. The flow field within the FLEC cavity is laminar.

(2) With respect to external diffusion material, in cases where the material surface is relatively larger than the amount of ventilation and (L_t/n_t) is larger than 0.08, the measurement values for the emission rates are tend to be underestimate. In order to solve these problems, it is necessary to make (L_t/n_t) 0.08 or less. In short, it is considered that the average emission rate from the surface of the evaporation type building material can be measured in the FLEC by making the Loading Factor L_t pretty small or by increasing the air change rate n_t.

(3) In the case of internal diffusion material, independently of the concentration distribution inside the FLEC cavity, the local mass emission rate from the surface of the building material becomes uniform on the surface of the material. Concerning internal diffusion materials like SBR, it is considered that the average emission rate from the surface of the building material being tested can be correctly measured in the FLEC.

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REFERENCES.

CHEMATEC. 1997. FLEC- Field and Laboratory Emission Cell.

E.Uhde,et al. 1998. Characterization of the Field and Laboratory Emission Cell-FLEC: Flow Field and Air Velocities, *Atmospheric Environment*, 773-781.

P.Wolkoff, et al. 1991. Field and Laboratory Emission Cell: FLEC, IAQ **91** *Healthy Buildings*.

P.Wolkoff, et al. 1995. Application of the Field and Laboratory Emission Cell: FLEC - Performance Study, Intercomparison Study and Case Study of Damaged Linoleum in an office, *Indoor Air* 196-203.

P.Wolkoff. 1995. Volatile Organic Compounds Sources, Measurements, Emission, and the Impact on Indoor Air Quality, *Indoor Air*, 43-45.

The Chemical Engineering Society, 1968. *The Handbook of the Chemical Engineering Sciences*.

Xudong, Y., Q, Chen., et al, 1998. Prediction of Short-Term and Long-Term VOC Emissions from SBR Bitumen-Backed Carpet Under Different Temperatures, *ASHRAE*.