Prediction of mass transfer rate on the surface of tested building material using CFD analysis

Janghoo SEO[1]

[1] Chosun University, School of Architecture, Gwangju, Korea 501-759

Abstract

We developed an airflow control unit for small chambers for uniformly controlling airflow on the surface of tested building material in the small chambers. We will present the mass transfer rate on the surface of tested building materials corresponding to an actual building in order to exactly evaluate the performance of the reduced amount and concentration of released chemical materials with the small chambers. We measured the airflow velocity on the surface of building materials in the small chamber with the developed airflow control unit and the fan speed for airflow control. We reviewed the distribution of water vapor concentration in the small chamber by means of CFD (Computational Fluid Dynamics) and estimated the mass transfer rate on the surface of building material to confirm test reliability.

Keywords: small chamber, mass transfer rate, CFD analysis

Introduction

For measuring the amount of chemical materials released from building materials and the like, many countries including Korea have instituted laws or specifications for measurement methods applicable to their own country. For measuring the amount of chemical materials released from building materials, small chambers are generally used, considering the advantages of easy experiments, expenses, etc. Meanwhile, in Korea, KS M ISO 16000-9 was instituted and publicized as a criterion for the small chamber law to specify small 20-liter chambers (ADvanced Pollution and Air Quality Chamber: ADPAC) for measuring the amount of released chemical materials. In Japan, the small 20-liter chambers are generally used for measuring the amount of released chemical materials (JIS A 1901) and for evaluating the performance of reduced concentration of materials for reducing the concentration of chemical materials (JIS A 1905-1, 2) as well.

The aforementioned small chambers keep the mass transfer rate for water vapor diffusion on the surface of tested building material uniform at approximately 2 to 3m/h, which is far below the mass transfer rate of 9 to 18m/h (12 to 18m/h in the method of evaluating performance of reduced chemical material concentration) recommended in JIS A 1901, JIS A 1905-1,2, etc. This means that actual material transfer in the small chamber is different from the inside of an actual architectural space.

In order to settle the aforementioned problems in this study, we developed an airflow control unit for small chambers for uniformly controlling airflow on the surface of tested building material in the small chambers. We will present the mass transfer rate on the surface of tested building materials corresponding to an actual building in order to exactly evaluate the performance of the reduced amount and concentration of released chemical materials with the small chambers. We measured the airflow velocity on the surface of building materials in the small chamber with the developed airflow control unit and the fan speed for airflow control. We reviewed the distribution of water vapor concentration in the small chamber by means of CFD (Computational Fluid Dynamics) and estimated the mass transfer rate on the surface of building material to confirm test reliability.

Configuration of the airflow control unit and the small chamber

The airflow control unit consists of a case made of SUS 304 and a Teflon fan to avoid chemical materials to be adsorbed and decomposed and is shown in Figure 1.

The fan for generating uniform airflow in the airflow control unit was installed on the bottom of the chamber in order to minimize the influence of air flow formed by air supply and exhaust of the chamber as shown in Figure 2. In the chamber, 3 types of mechanical ventilation are performed and can be controlled to keep wind velocity uniform on the surface of the tested building material according to fan rotation. To avoid pollutants to be generated by the fan in the chamber, the fan rotates by means of magnetic force in connection with the driving unit out of the chamber. The area for installing the tested building material in the airflow control unit is 0.043m^2, which corresponds to the product loading factor of 2.2 m^2/m^3.

Method

The example of analyzing the airflow field on the basis of average wind velocity (U_{center}) in the center of the airflow control unit and the wind velocity (U_{fan}) of the fan is shown in Table 1. The temperature and the number of ventilations in the small chamber was set to 28°C and 0.5 times/h, respectively. With respect to the average wind velocity U_{center} in the airflow control unit, the airflow field was analyzed for 5 cases from 8.27×10^{-4}m/s(U_{fan} =0.01m/s) to 3.57×10^{-1}m/s(U_{fan} =4m/s). For each case, the Reynold's number ($=U_0L_0/\nu$: U_0 is an average wind velocity in the airflow control unit[m/s]. L0 is a half of the internal height of airflow control unit (Line X×1/2, shown in Figure 3)[m]) was 1, 10, 160, 350 and 600, respectively.

The airflow field was subject to 3 dimensional analysis with the low Reynold's number type k-ε model (Abe–Nagano model). The wall coordinate (y^+) of the first mesh on the surface of the building material in the airflow control unit is at most 1. Numerical analysis was carried out only for the 1/2 of the space as shown in Figure 2(a), considering symmetry of the analyzed object. The boundary condition of CFD analysis is shown in Table 2.

After analyzing the airflow field, the boundary condition of evaporation dominating building materials was given on the side where the building material was provided, as a model of releasing chemical materials. The surface of the evaporation dominating building material was modeled with liquid of a simply single component. The model of building material was water (distilled water) and water evaporation from the liquid surface to the air, that is, the mass transfer rate was reviewed on the surface of the building material. Diffusion field analysis was carried out, assuming the isothermal state (28°C) without considering latent heat on the surface of building material in the surface model of the building material for this analysis. The surface concentration of the building material was set to being uniform (C_s=constant) to use the water saturation concentration as a boundary condition. In this study, it was assumed that water is a passive contaminant to calculate the distribution of water concentration, and water (vapor) diffusion in the air is expressed as a diffusion equation (1). The water (vapor) diffusion coefficient in the air was calculable by means of the equations (2) to (4).

$$\frac{\partial \overline{C}_1}{\partial t} + \frac{\partial \overline{U}_j \overline{C}_1}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\left(D_a + \frac{\nu_t}{\sigma_t}\right)\frac{\partial \overline{C}_1}{\partial x_j}\right) \quad \text{(Eq. 1)}$$

$$\log_{10} P_w = \frac{A-B}{(C+T)} - 3 \quad \text{(Eq. 2)}$$

$$C_0 = \rho_a \frac{M_1}{M_2} \frac{P_w}{P-P_w} \quad \text{(Eq. 3)}$$

$$D_a = \frac{6.7\times10^{-8}\times T^{1.83}}{P} \times \left[\left(\frac{T_{c1}}{P_{c1}}\right)^{\frac{1}{3}} + \left(\frac{T_{c2}}{P_{c2}}\right)^{\frac{1}{3}}\right]^{-3} \sqrt{\frac{1}{M_1}+\frac{1}{M_2}} \quad \text{(Eq. 4)}$$

where,

C_1 : pollutant concentration at a spatial point (μg/m^3)

D_a : molecular pollutant diffusion coefficient (m^2/s)

U_j : wind velocity (m/s)

v_t : eddy viscosity (m^2/s)

σ_t : turbulent Schmidt's number (-)

P_w : water vapor pressure (Pa)

A, B, C : empirical constant (A:7.7423, B:1554.16, C:219)

T : temperature (˚C)

C_0 : saturation concentration (g/m^3)

ρ_a : air density (g/m^3)

M_1, M_2 : molecular weight

P : atmospheric pressure in the chamber (Pa)

T_{c1}, T_{c2} : critical temperature (˚C)

P_{c1}, P_{c2} : critical pressure (Pa)

The water (vapor) diffusivity D_a in the air calculated by means of equations (2) to (4) is $2.30\times10^{-5}m^2/s$ and the water concentration at the small chamber supply is zero (0).

Results and Discussion

Figure 4 shows the average velocity vector (case 3) of airflow in the airflow control unit and the small chamber. The air supplied from the small chamber supply is mixed with the air in the small chamber just before reaching the airflow control unit. It is seen that the mixed air flows uniformly from the upper part to the lower part of the airflow control unit.

Table 3 shows the velocity of released water on the surface of building material and the mass transfer rate. Figure 5 shows correlation among the airflow velocity, the velocity of released water in the airflow control unit and the mass transfer rate in the airflow control unit.

For the case 1 where the Reynold's number is 1, the average velocity of released water is $3.29g/m^2\cdot h$. As the Reynold's number increases to 10 and 160, the velocity of released water increased to $4.07g/m^2\cdot h$ (case 2) and $4.49g/m^2\cdot h$ (case 3). It is considered that the increased Reynold's number depending on the increased central wind velocity in the airflow control unit contributes to smooth diffusion of the material in the airflow control unit, thus to make the difference (gradient) between the water surface and the water concentration in the air larger. Meanwhile, in cases 4 and 5, although the Reynold's number increased as in Figure 5, the average velocity of released water did not increase and was kept almost at a constant number. It is considered that, although airflow due to fan rotation occurs, the materials in the airflow control unit are completely mixed when the airflow in the airflow control unit reaches at a given velocity and a water concentration difference between on the water surface and in the air is not caused any more. The result of average mass transfer rate exhibits similarity to the result of average release velocity. The mass transfer rate of case 3 where the Reynold's number is 160 and case 4 where the Reynold's number is 350 was 14.43m/h and 18.07m/h, respectively, and it is estimated to be similar to the material transfer phenomenon in an actual architectural space. In particular, case 3 analyzed with the same condition as that of the experiment did not exhibit significant difference from the mass transfer rate measured in the experiment. For case 5 where the Reynold's number is 600, the mass transfer rate was predicted to be 21.55m/h which is slightly above the specification of JIS and the like.

Table 3 and Figure 6 show the result (the average concentration (C_s) on the surface of building material released side is 1) of non-dimensionalizing the chamber exhaust concentration and the concentration distribution in the chamber on the basis of the surface concentration of the building material.

In case 3, the concentration at the chamber exhaust for the surface concentration of the building material became 0.98, so that it is seen that the water concentration in the chamber reached almost saturation and it was almost the same as the measurement result checked in the experiment. In cases 1 and 2, the water concentration in the airflow control unit exhibited uniform distribution, but a slight concentration difference from the concentration distribution in chamber outside of the airflow control unit was observed. A small concentration boundary layer was formed by means of airflow caused by the fan around the surface of the building material. Meanwhile, in case 3 where the mass transfer rate is 14.43m/h, a concentration boundary layer was observed, e.g. a certain concentration gradient was formed around the surface of the building material.

If the wind velocity is not strong on the surface of the building material as in cases 1 and 2, non-uniform concentration distributions (35 to 90% of the surface concentration of the building material) were exhibited in the small chamber. Since the small chamber method of installing the building material as an experiment sample in a small chamber to test release or evaluate performance of reduced concentration assumes complete mixture, it is considered that it is desirable to control airflow in the chamber to form uniform concentration distribution higher than a certain level.

Conclusions

In this study, we developed an airflow control unit for small chambers for controlling the mass transfer rate to be constant on the surface of tested building material in a small chamber. We presented the mass transfer rate on the surface of tested building material corresponding to an actual architectural space for which the amount of released chemical material and performance of reduced concentration can be exactly evaluated. The conclusion derived on the basis of such results is described in the following.

When installing an airflow control unit in a small chamber to control fan speed (U_{fan}) at 1m/s (U_{center}=9.31×10^{-2}m/s, Reynold's number of 160), the mass transfer rate of water vapor diffusion was shown approximately 12m/h for the experiment number, and 14.43m/h for the numerical analysis. Therefore, it is considered that the numbers are the most similar to the mass transfer rate in an actual architectural space. Therefore, it is expected that application of the airflow control unit and the airflow velocity proposed in this study will contribute to achieving an even higher level of measuring the amount of released chemical materials and evaluating performance of reduced chemical material concentration of reduced pollutant concentration materials. When using the airflow control unit in the small chamber, it was seen that the velocity of released materials and the mass transfer rate highly depended on the airflow velocity by the fan, that is the Reynold's number. Increasing the Reynold's number depending on the increased airflow velocity of the fan resulted in smaller concentration difference (gradient) of the materials on the surface of building material and in the air thus to enable smooth material diffusion in the chamber. However, it is necessary to be careful because the amount of release from tested samples might be overestimated when measuring the amount of released chemical materials.

Acknowledgments

This work was supported by the Biohousing Research Center and the Grant of the Korean Ministry of Education, Science and Technology. (The Regional Core Research Program / Biohousing Research Institute)

References

1. K. Kim et al., "A Study on Prediction of an Indoor Volatile Organic Compound and Formaldehyde Considering the Emission Characteristics of Interior Finishing Materials", *Journal of AIJ, Planning & Design*, 21(12), 2005, pp.255-260.

2. D. Kim et al., "An Analysis of Convective Mass Transfer Coefficient of Material surface in Small Chamber Simulation Method", *Proceedings of Annual conference of AIK*, 23(1), 2005, pp.243~246.

3. J. Seo et al., "Study on Measurement of Mass Transfer Coefficient and Compounds Emitted from Electrical Appliances and Furniture Using Large Test Chamber Method", *Journal of AIJ, Planning & Design*, 23(7), 2007, pp.287-294

4. H. Yu et al., “A Study on the Emission Characteristic of Formaldehyde and TVOC from Indoor Finishing Materials”, *Journal of AIJ, Planning & Design*, 21(7), 2005, pp.141-148

5. K.Han et al., “A Study on the Improvement of Emission Test Method for Paints”, *Proceedings of Annual conference of AIK*, 27(1), 2007, pp.833~836.

6. Handbook of chemistry (1999), *The society of chemical engineers*, Japan.

7. J Seo, S Kato (2007). A new way to reduce pollutant? Adsorptive materials and VOCs, *AHSRAE IAQ APPLICATION*, 8(3), pp.9-12.

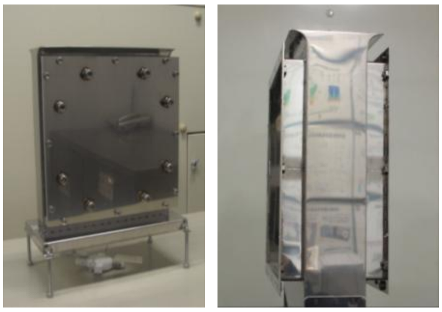
8. J Seo, S Kato, Y Ataka and S Nagao (2006). Measurement and CFD analysis on decreasing effect of toluene concentration with activated carbon and adsorptive building material, *Proceedings of Healthy building* 2006, 5, pp.101-106.

9. K Abe, T Kondoh and Y Nagano (1994). A new turbulence model for predicting fluid flow and heat transfer in separating and reattaching flows. Flow field calculations, *Int. J. Heat Mass Transfer*, 37(1), pp.139-151.

10. R Funaki, S Tanabe and H Tanaka (2003). The performance test of a small chamber for the measurement of aldehydes and VOCs emission rates from building materials and the comparison of formaldehyde emissions between two different chambers, *Journal of environmental engineering*, AIJ, 572, pp.47-54.

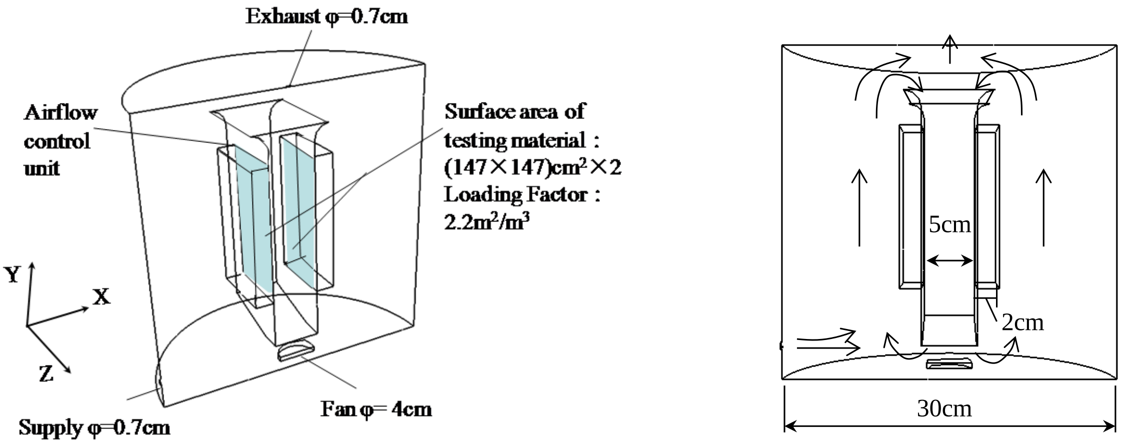
11. S Murakami, S Kato, Q Zhu, S Tanabe and K Ito (2001). Physical modeling and numerical analysis of VOCs emission from building materials (Part 27) CFD analysis of VOCs emission within ADPAC, *Summaries of tech. paper of annual meeting AIJ*, D-2, pp.811-812. (In japanese)

12. Z Qingyu, S Kato, Y Ataka (2004), Examination of influence of mass transfer coefficient on emission rate in medium density fiberboard by test chamber experiment and CFD analysis : Study on test chamber method for measuring emission rate of formaldehyde, *Journal of environmental engineering*, No.582, pp.67-74. (In japanese)



(a) Front view (b) Side view

Fig. 1 Airflow control unit



(a) Airflow control unit and small chamber (b) Airflow in small chamber

Fig. 2 Simplified view of airflow control unit and small chamber

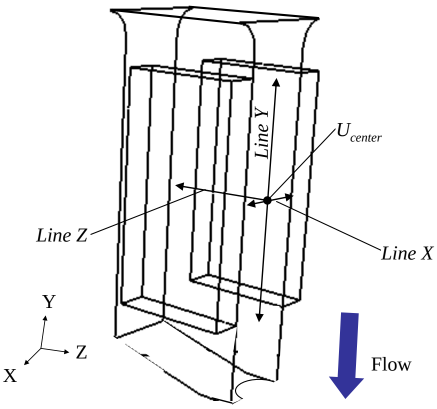


Fig. 3 Point for measuring wind velocity in airflow control unit

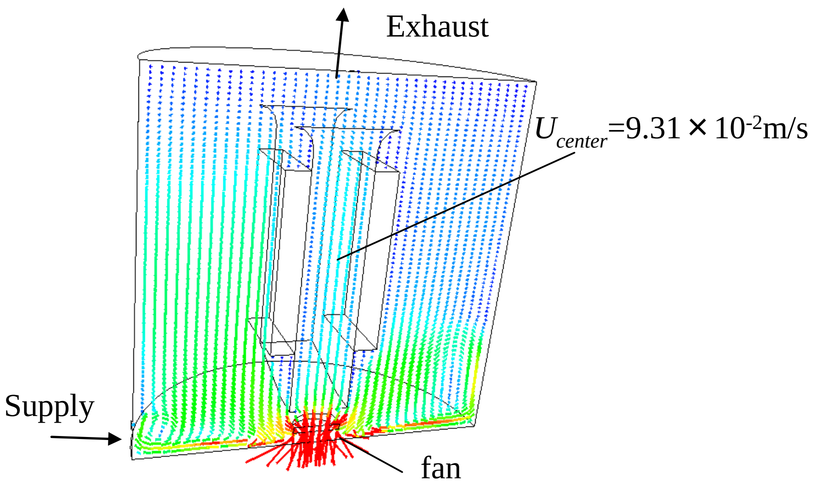


Fig. 4 Velocity vector (cross section X-Y) : case 3

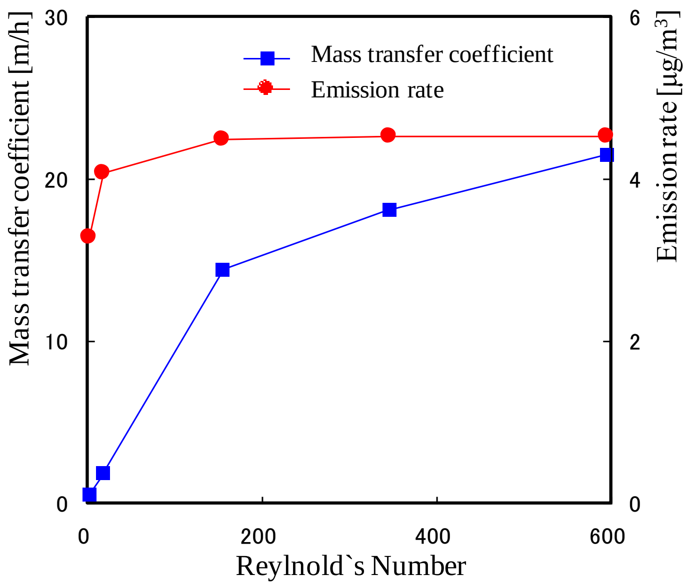
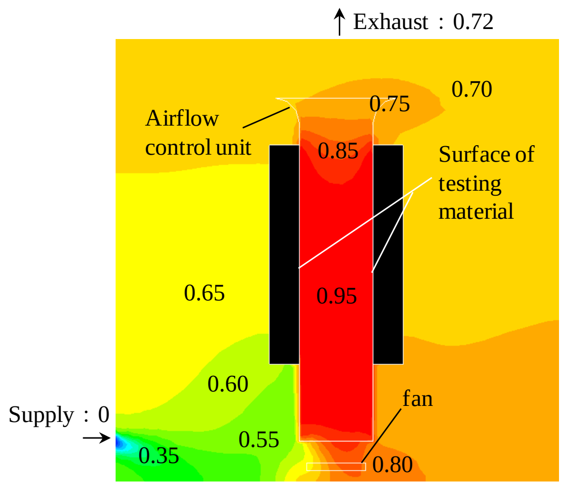
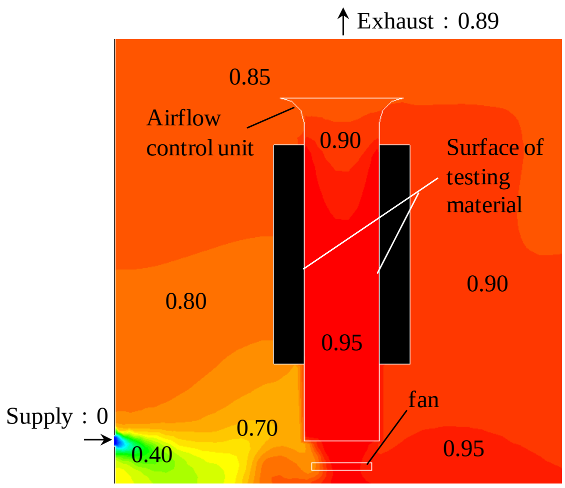


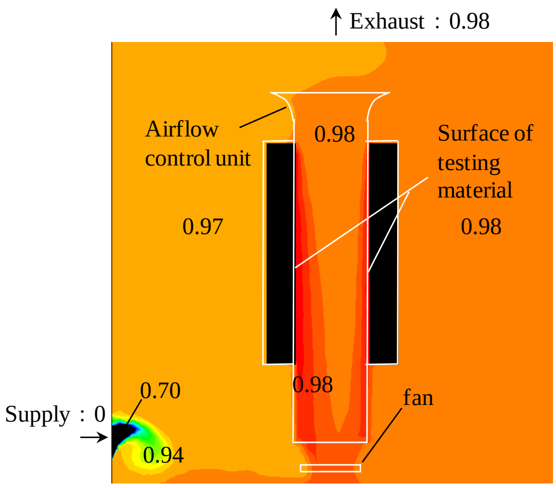
Fig. 5 Correlation between airflow velocity and mass transfer rate/released velocity in the airflow control unit



(a) Case 1 (Reynold's number: 1)



(b) Case 2 (Reynold's number: 10),



(c) Case 3 (Reynold's number: 160)

Fig. 6 Distribution of water (distilled water) concentration in the small chamber (C/C_S), cross section X-Y

Table 1 Cases of numerical analysis (Temp: 28°C)

Case	U_{center} (U_{fan}) [m/s]	Reynold's [U_0L_0/v]	Ventilation rates[h^{-1}]	Release model
1	8.27×10^{-4} (0.01)	1	0.5	Evaporation dominating building material (distilled water)
2	3.86×10^{-3} (0.05)	10		
3	9.31×10^{-2} (1)	160		
4	2.07×10^{-1} (2)	350		
5	3.57×10^{-1} (4)	600		

Table 2 Conditions of numerical analysis

Turbulent flow model	Low Reynold's number type k-ε model (Abe-Nagano model)
Number of meshes	270,690
Scheme	Space difference : Second order upwind
Inflow boundary	$U_{x,in}$=7.2×10^{-2}m/s, $U_{y,in}$=0, $U_{z,in}$=0 $k_{in}=3/2\cdot(U_{in}\times0.05)^2$, $\varepsilon_{in}=C_\mu\cdot k_{in}^{3/2}/L_{in}$ $L_{in}=1/7L_o$, $L_o=7.0\times10^{-4}$m
Outflow boundary	U_{out}=Mass flow, k_{out}, ε_{out}=free slip
Fan boundary	U_{fan}=0.01, 0.05, 1, 2, 4 (m/s)
Wall boundary	No-slip
Analysis of diffusion field	Considering 3-dimensional symmetry, only the 1/2 of the chamber area was analyzed. After airflow field analysis, the water (distilled water) saturation concentration on the surface of building material was set to the condition of C_s=constant to analyze pollutant diffusion in the chamber.

Table 3 Result of predicting average release velocity and average mass transfer rate

Case	U_{center} [m/s]	Reynold's number [U_0L_0/v]	C_{out}/C_s	C_s	Average release velocity [$g/m^2\cdot h$]	Average mass transfer rate [m/h]
1	8.27×10^{-4}	1	0.72	1 (constant)	3.29	0.61
2	3.86×10^{-3}	10	0.89		4.07	1.89
3	9.31×10^{-2}	160	0.98		4.49	14.43
4	2.07×10^{-1}	350	0.99		4.52	18.07
5	3.57×10^{-1}	600	0.99		4.53	21.55