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Research Article
Calculation of VOCS Diffusion Coefficient Based on Extremum-search Method

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Abstract

Background: A wide variety of dry materials are used to construct and furnish residential and commercial buildings. It is very important to predict emission characteristics of Volatile Organic Compounds (VOCSs) from building materials. So, Bodalal had provided the mathematical model of VOCS physical emission process, the diffusion and partition coefficients of VOCSs are obtained by the method of drawing, but this method can only obtain fuzzy and imprecise solution. It is necessary to design a new method to solve the model. **Materials and Methods:** In this study, on the basis of the data of the experiment and the function extreme value theory, diffusion and partition coefficients function is constructed, the function extreme value is calculated by the Extremum-Search Method. **Results:** So that, a new method for calculation of the internal diffusion coefficient (D) and partition coefficient (k_e) of VOCSs is given for dry building materials. **Conclusion:** The method to calculate the diffusion and partition coefficients of VOCSs is very accurate and practical and the algorithm can be realized easily by the computer program. The VOCS diffusion process can be known accurately, it is significant to reduce indoor pollution.

Key words: Diffusion coefficient, partition coefficient, graphical method, equation method, extremum-search method

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INTRODUCTION

At present, with the propulsion of industrial process, many pollutants especially Volatile Organic Compounds (VOCS) in living atmosphere pollute seriously living condition and do harm to people's health. So, the study of formaldehyde and VOCS diffusivity has attracted many scholars' attention[1-3], including Bodalal who provided VOCS adsorption diffusion modes from several kinds of building materials by creating the mathematical model of VOCS physical emission process[4]. The method uses the diffusion coefficient and the distribution coefficient to describe the ability and speed which the building materials adsorb VOCS[5]. The model is reasonable, but the method of the calculation of the diffusion and partition coefficients is not perfect.

In this study, for the mathematical model which had been provided by Bodalal etc., several methods of the calculation of the diffusion and partition coefficients are given and comparison of these methods is also given.

MATERIALS AND METHODS

Introduction of the model: Bodalal segregated a large chamber into two equal volumes of chambers. A certain concentration of VOCS is introduced into one of the two equal volumes of chambers. After a period of time, Bodalal measured variation of VOCS concentration in two chambers and then the mathematical model of the diffusion process been established. The model can be described as follows:

The diffusion Eq. 1 is:

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} \quad (1)$$

where, D is diffusion coefficient of the compound within the specimen, C is concentration of the compound within the specimen, x is linear distance, t is time.

Boundary conditions:

$$\text{At } x = 0,\ C = k_e C_1$$

$$\text{At } x = l,\ C = k_e C_2$$

Initial condition:

$$\text{At } t = 0,\ C = 0,\ 0 \le x \le l$$

The concentration in the low and high concentration compartments are expressed by Eq. 2 and 3, respectively:

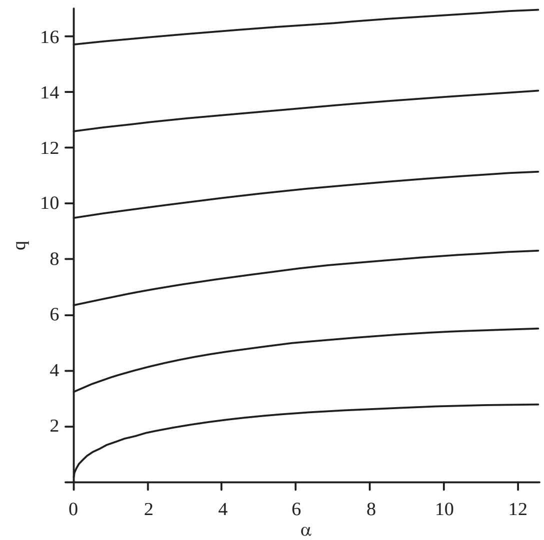

Fig. 1: Graphic of $\tan(q) = \frac{2\alpha q}{(q^2 - \alpha^2)}$

$$C_1 = \frac{DA}{V_1}\int_0^t \left(\frac{\partial C}{\partial x}\right)_{x=0} dt \quad (2)$$

$$C_2 = C_0 - \frac{DA}{V_2}\int_0^t \left(\frac{\partial C}{\partial x}\right)_{x=1} dt \quad (3)$$

Eventually, the Eq. 4-6 are derived:

$$\ln\frac{(C_2 - C_1)}{C_0} = \ln\left(\frac{4\alpha}{q^2 + \alpha(2+\alpha)}\right) - \left(\frac{q^2 D}{l^2}\right)t \quad (4)$$

$$\tan(q) = \frac{2\alpha q}{(q^2 - \alpha^2)} \quad (5)$$

$$\alpha = \frac{k_e A l}{V} \quad (6)$$

Called:

$$r = \frac{-q^2 D}{l^2},\ u = \ln\left(\frac{4\alpha}{q^2 + \alpha(2+\alpha)}\right)$$

where, q_1 are the positive roots of the characteristic equation:

$$\tan(q) = \frac{2\alpha q}{(q^2 - \alpha^2)}$$

The graphic of $\tan(q) = \frac{2\alpha q}{(q^2 - \alpha^2)}$ as shown in Fig. 1.

RESULTS

There are several methods to calculate the diffusion and partition coefficients.

Method 1

Graphical method: According to the calculation method of the diffusion and partition coefficients[4], which is summarized below.

Experimentally determined values C_0, C_1, C_2, t, According to the formula, the straight line of the plot C_2-C_1/C_0 vs t is drawn, the values of r and u are calculated by the least-square regression method, where:

$$r = \frac{-q^2 D}{l^2},\ u = \ln\left(\frac{4\alpha}{q^2 + \alpha(2+\alpha)}\right)$$

The picture of:

$$\tan(q) = \frac{2\alpha q}{(q^2 - \alpha^2)}$$

is drawn, where the range of α is 0-3. Under the same coordinate system, the curve of q vs α is drawn with different values of u as shown in Fig. 2.

By observing the intersections of curve 1 and 2, the values of α and q are concluded. Finally, the diffusion and partition coefficients are calculated using $r = \frac{-q^2 D}{l^2}$ and $\alpha = \frac{k_e A l}{V}$, respectively.

It is not difficult to find that the drawing method has the following disadvantages:

- If the drawing is not accurate, the solution can make a big error. For example, when u = 0.32, the values of α and q as shown in Fig. 2 are 1. 75 and 1. 76. Substituting α and q into the equation $\tan(q) = \frac{2\alpha q}{(q^2 - \alpha^2)}$, the value of $\frac{2\alpha q}{(q^2 - \alpha^2)}$ is 175. 498 and the value of tan (q) is -5. 222, values are not equal on both sides of the equation, this is obviously wrong
- The range of u is only -0. 4 to -0. 04 as shown in Fig. 2, the values of u are limited which cannot meet the practical demands

Method 2

Method of solving equation: The key of the model is that the values of α and q are calculated through solving equations:

$$u = \ln\left(\frac{4\alpha}{q^2 + \alpha(2+\alpha)}\right)$$

and:

$$\tan(q) = \frac{2\alpha q}{(q^2 - \alpha^2)}$$

then, the diffusion and partition coefficients are calculated using $r = \frac{-q^2 D}{l^2}$ and $\alpha = \frac{k_e A l}{V}$, respectively. Getting the values

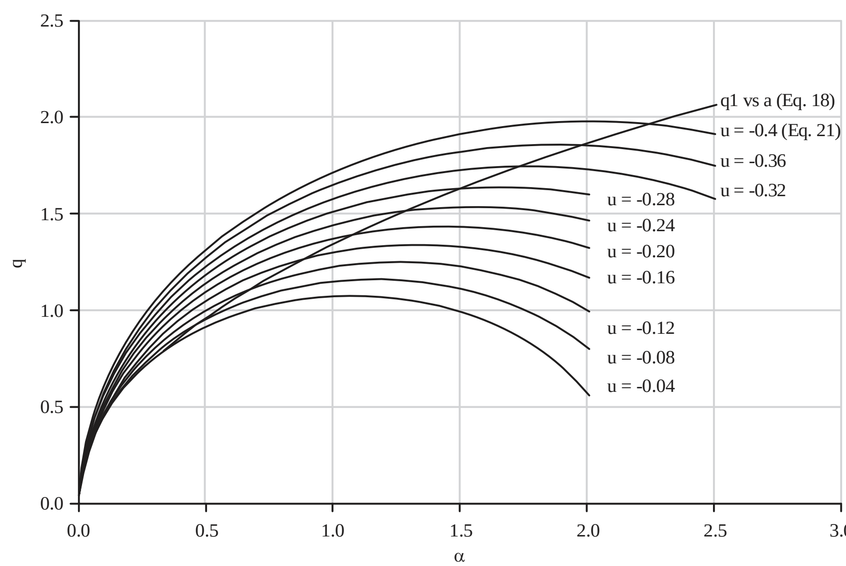

Fig. 2: q vs α

of r and u is the same as earlier. The following command can be used in maple to solve the equation (for example, u = -0.36):

$$g:=u\rightarrow \text{fsolve}(\{\tan(q)=\frac{2\alpha q}{(q^2-\alpha^2)},\frac{4\alpha}{q^2+\alpha(2+\alpha)}=$$
$$e^u,\{\alpha=0..3,q=0..3\})$$
$$g(-0.36)$$
$$\{\alpha=2.313329184,q=1.812429524\}$$

The solution is accurate based on the method and this method solves the problem that the value of u is limited in the graphic method. But this method is not so good, such as, when the value of u is smaller, the solution of this method is not a goal, but is zero. For example, when u = -0.04, according to the above command, the values of α and q are close to zero and this obviously fails to fit the facts.

Method 3

Extremum-search method: Based on the problems of the method 1 and 2, the extremum-search method[6-8] can be used to solve the model.

How to get the solution of the equation:

$$\tan(q)=\frac{2\alpha q}{(q^2-\alpha^2)}$$

and:

$$u=\ln\left(\frac{4\alpha}{q^2+\alpha(2+\alpha)}\right)$$

Among which, u is known. It is obviously that the equation:

$$\tan(q)=\frac{2\alpha q}{(q^2-\alpha^2)}$$

and:

$$u=\ln\left(\frac{4\alpha}{q^2+\alpha(2+\alpha)}\right)$$

is also true, when α and q satisfy the equation:

$$\tan(q)\,(q^2-\alpha^2)-2\alpha q]^2+\{e^u[q^2+\alpha(2+\alpha)]-4\alpha\}^2=0$$

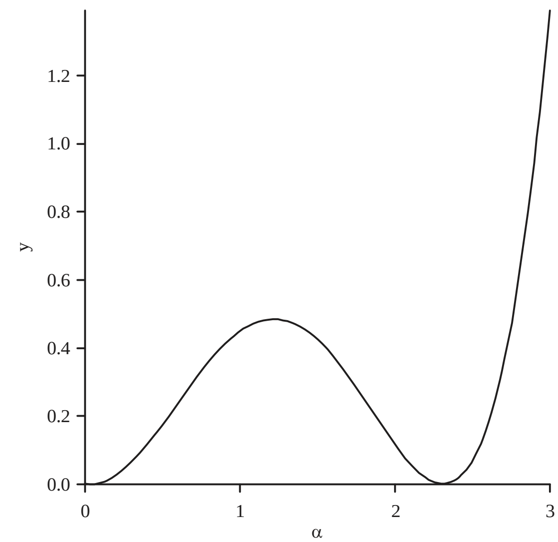

Fig. 3: q is determined, y vs α

So that, the following function is established:

$$Y=f(\alpha,q)=[\tan(q)\,(q^2-\alpha^2)-2\alpha q]^2+\{e^u[q^2+\alpha(2+\alpha)]-4\alpha\}^2$$

By determining the ranges of α and q to make the above function getting the minimum value. It is obviously that the equation $\tan(q)\,(q^2-\alpha^2)-2\alpha q=0$ and $e^u\,[q^2+\alpha(2+\alpha)]-4\alpha=0]$ are simultaneously true, when the minimum value of function is close to zero, namely the equation:

$$\tan(q)=\frac{2\alpha q}{(q^2-\alpha^2)}$$

and:

$$u=\ln\left(\frac{4\alpha}{q^2+\alpha(2+\alpha)}\right)$$

are true. So, the α and q which make the above function to obtain the minimum value corresponds with the model.

In order to determine the minimum value of f (α, q), firstly the minimum value of f (α, q) is determined, when q ranges from 0-2. 5, as shown in Fig. 3. Then the minimum value of min $([\tan(q)\,(q^2-\alpha^2)-2\alpha q]^2+\{e^u\,[q^2+\alpha(2+\alpha)]-4\alpha\}^2)$ is determined, when α ranges from 0-3, as shown in Fig. 4.

Thus, it can be seen that the basic principle of extremum-search method is that the function extremum theory is adopted to find two points of the curve of $[\tan(q)\,(q^2-\alpha^2)-2\alpha q]^2$ and $\{e^u\,[q^2+\alpha(2+\alpha)]-4\alpha\}^2$ and the distance between the two points is minimum. Therefore, a flow chart is drawn as in Fig. 5.

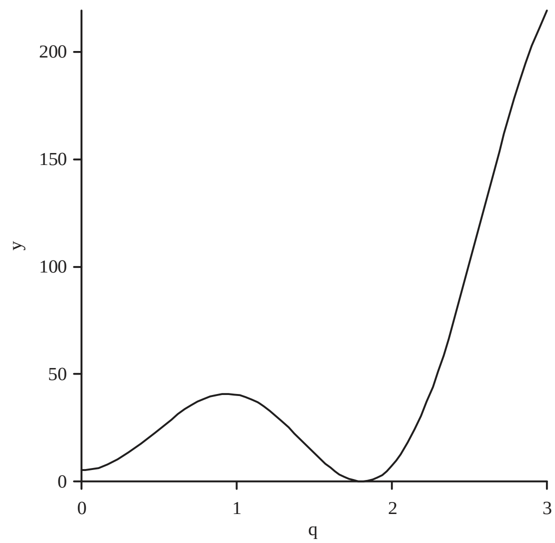

Fig. 4: α is determined, y vs q

According to the experimental data of r and u, much more accurate result of α and q can be get through the method and determine the diffusion and partition coefficients of VOCS from building materials. several sets of data are given here, as shown in Table 1.

Table 1: Data are obtained by extremum-search method

u	r	α	q	D	k_e
-0.0643	-0.0034	1.597	1.581	1.95×10^{-9}	1330.8
-0.4573	-0.0027	2.998	1.976	9.95×10^{-10}	2498.3
-0.7953	-0.0021	0.004	0.157	1.22×10^{-7}	3.3333
-0.4364	-0.0092	2.867	1.948	3.49×10^{-9}	2389.2
-0.6605	-0.0075	3.00	1.978	2.76×10^{-9}	2500.0
-0.1966	-0.0217	1.634	1.595	1.22×10^{-8}	1361.7
-0.1952	-0.0328	1.634	1.595	1.85×10^{-8}	1361.7
-0.0195	-0.0036	1.592	1.579	2.07×10^{-9}	1326.7
-0.1016	-0.0042	1.605	1.584	2.41×10^{-9}	1337.5
-0.4176	-0.0052	2.725	1.916	2.03×10^{-9}	2270.8

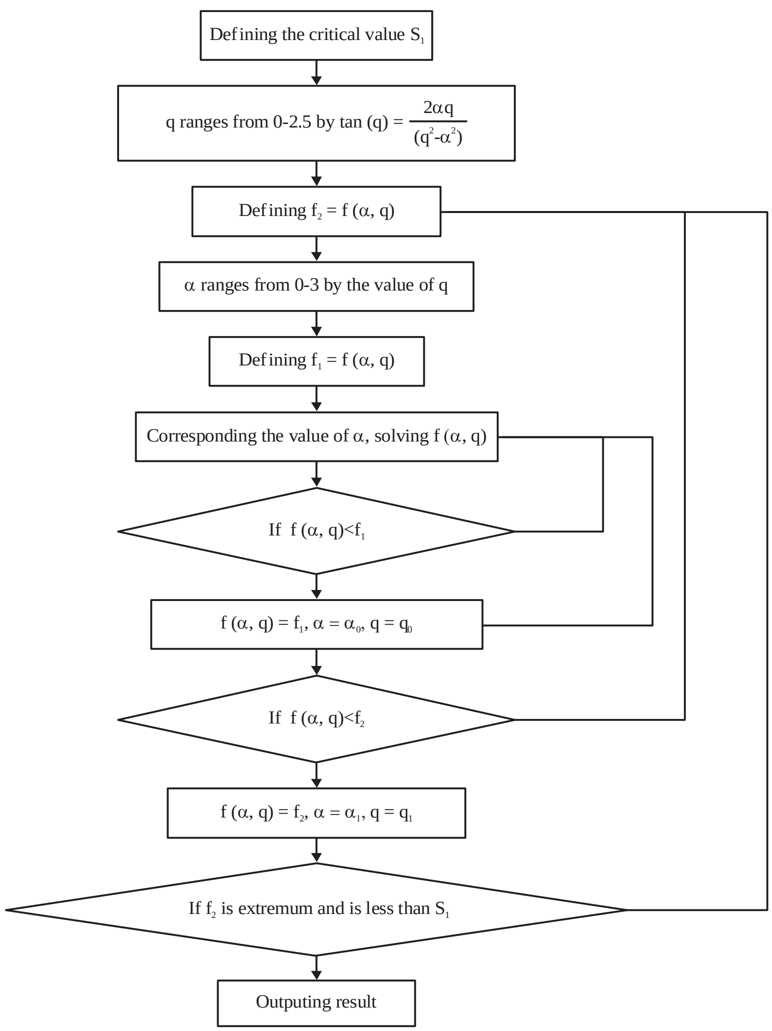

Fig. 5: A flow chart of algorithm

DISCUSSION

Extremum-search method is an adaptive control method, which was proposed by professor Tsien in 1954. In recent years, people pay more and more attention to study of extremum search method. In theory, minimum searching method is put forward by analyzing the calculating formulas of digital speckles' correlation[9] and in order to overcome the problem of step by step searching method in the fractional fourier domain extremum seeking of fractional fourier is given[10]. In practice, a systematic procedure for synthesis of neural network adaptive synergetic control is proposed for a class of affine multivariable extremum seeking system[6] and among all MPPT schemes Extremum Seeking Control (ESC) is attractive because it does not rely on the mathematical model[11]. In this study, the diffusion and partition coefficients of VOCS are calculated by the extremum-search method which based on the theory of the function extreme value, this method is easy and the result is very precise.

CONCLUSION

A new method for the solution of the mathematical model which had been provided by Bodalal is developed. Using the new method developed, the diffusion and partition coefficients of VOCS are calculated precisely. The key of solving process is to use extremum-search method to find the values of α and q when the minimum value of function is close to zero. This method is practical and accurate and it can be applied to other analogy problems.

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