The Calculation of VOCs Diffusion Coefficient for Building Materials

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Abstract. Volatile Organic Compounds (VOCS), as one of the major sources of air contaminations, has an important bearing on one's general health. The adsorption capacity and velocity of the material for VOCs can be described separately using. In this paper, the detailed process and method of VOCs diffusion and partition coefficients by genetic algorithm is introduced, the algorithm is realized easily by computer program and the result by the method is precise and practical.

1. Introduction
In recent years, with the development of economy, the extensive fitting-up craze has appeared in the city and the indoor pollutant problem is outstanding day by day. The report found about hundreds of thousands of people are killed every year from decorate pollution in our country, the experts say the killer is VOCs. Because of the greatest threat to people, many experts are studying the diffusion problem of VOCs in building materials [1-3]. Among them, the Bodalal model was cited by many scholars, which described VOCs diffusion procedure by partial differential equation. Genetic Algorithms (GAs) are search algorithms based on of natural evolution processing including selection, mutation and crossover operations on the genes of individuals or potential solutions. and adopts a natural evolution mechanism to represent complex phenomenon. It searches through the total solution space and can find the optimal solution globally over a domain. In this paper, the calculation of VOCs diffusion and partition coefficients by genetic algorithm is introduced for the Bodalal model.

2. Introduction of The Model
Bodalal segregated a large chamber into two equal volumes of chambers. A certain concentration of VOC is introduced into one of the two equal volumes of chambers. After a period of time, Bodalal measured variation of VOC concentration in two chambers, and then the mathematical model of the diffusion process been established.

The model can be described as follows:
The diffusion equation is:
\[ \frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} \]  

\( D \) 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
\[
\begin{align*}
At & \quad x = 0, C = k_1 C_1 \\
At & \quad x = l, C = k_2 C_2
\end{align*}
\]

Initial condition
\[
At \quad t = 0, C = 0, 0 \leq x \leq l
\]

The concentration in the low and high concentration compartments are expressed by Eqns. (2) and (3), respectively

\[
\begin{align*}
C_1 &= \frac{DA}{V_1} \int_0^t \left( \frac{\partial C}{\partial x} \right)_{x=0} dt \\
C_2 &= C_0 - \frac{DA}{V_2} \int_0^t \left( \frac{\partial C}{\partial x} \right)_{x=d} dt
\end{align*}
\]

Eventually, the equations are derived

\[
\begin{align*}
\ln \left( \frac{C_2 - C_1}{C_0} \right) &= -4\alpha \left( \frac{q^2 D}{l^2} \right) t + \\
\ln \left( \frac{4\alpha}{q^2 + \alpha(2 + \alpha)} \right) &= \tan(q) = \frac{2\alpha q}{q^2 - \alpha^2} \quad (4)
\end{align*}
\]

\[
\alpha = \frac{k_2 Al}{V} \quad (6)
\]

Called

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

Where \( q \) are the positive roots of the characteristic equation:

\[
\tan q = \frac{2\alpha q}{q^2 - \alpha^2}
\]

3. The Calculation of The Diffusion Coefficient

3.1. Graphical method

The Bodalal model used graphical method to calculate the VOCs diffusion and partition coefficients, in reference [4]. Details are as follows:

Firstly, experimentally determined values \( C_0, C_1, C_2, t \). According to the formula, the straight line

\[
\ln \left( \frac{C_2 - C_1}{C_0} \right) vs. t
\]

is drawn, the values of \( r \) and \( u \) are calculated by the least-square regression method.

\[
\tan q = \frac{2\alpha q}{q^2 - \alpha^2}
\]

Secondly, the picture of \( q vs. \alpha \) is drawn with different values of \( u \) as shown in Figure1.
Finally, by observing the intersections of curve 1 and 2, the values of $\alpha$ and $q$ are concluded. The diffusion and partition coefficients are calculated using

$$ r = \frac{-q^2 D}{l^2} \quad \text{and} \quad \alpha = \frac{k_c A l}{V} $$

respectively.

Figure 1. $q$ vs. $\alpha$

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

1. The solution by Drawing is not accurate, so there will be a great error. When $u = -0.32$, the values of $\alpha$ and $q$ as shown in Figure 1 are 1.75 and 1.76. Substituting $\alpha$ and $q$ into the equation

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

After close examination, it is not difficult to draw that the value of the left side of the equation is -5.222, but the value of the right side of the equation is -175.498. The value is not the same on both sides, it is obviously wrong.

2. The range of $u$ is only -0.4 to -0.04 as shown in Figure 1, the values of $u$ are limited which cannot meet the practical demands.

3.2. Genetic Algorithms

In view of the problem of the graphic method, in reference [5], based on the function extremum theory, Extremum-Search Method is designed by the author. The algorithm is effective to solve the problems of the graphical method and can be realized easily by the computer program, but step size of Extremum-Search Method is certain to search, it has low probability of finding the global optimal solution efficiency and tend to be trapped by local optimizations.

In the Bodalal model, the solving process of and with the characteristic equation

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

and the equation

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

which may be transformed into solving the value of $\alpha$ and $q$ to make the equation was established.

\[
\begin{align*}
[\tan(q)(q^2 - \alpha^2) &- 2\alpha q]^2 + \\
\left(e^u[q^2 + \alpha(2 + \alpha)] - 4\alpha\right)^2 & = 0
\end{align*}
\]

The above process is exactly to make the following function getting minimum value by solving the value of $\alpha$ and $q$.
\[ y = f(\alpha, q) \\
= [\tan(q)(q^2 - \alpha^2) - 2\alpha q]^2 + \\
\{e^n[q^2 + \alpha(2 + \alpha)] - 4\alpha\}^2 \]

(7)

It is a typical dualistic function extremum problem, and genetic algorithm (GA) can be designed to solve it. Because of the powerful operation ability of MATLAB, genetic algorithm Toolbox of MATLAB can realize the global optimization of traditional genetic algorithm, and has high accuracy, so, the extremum problem is solved with MATLAB toolbox.

The detailed process of GA is described as follows:

Firstly, the fitness function of genetic algorithm should be created, ga function in genetic algorithm and direct search toolbox is to solve the minimum of objective function, minimizing the problem's objective function, the objective function can be make into fitness function. So, the fitness function of this extremum problem is function (7).

Secondly, open the GUI interface of the genetic algorithm to set parameters. The parameters which include population size, crossover Fraction, Migration Fraction and Generations, adopt the default parameters of the Matlab toolbox, you can adjust these parameters according to the needs of your application. The generation of initial population is random.

Finally, click the Start button. GUI will automatically run the genetic algorithm program, and the run results are indicated.

Mean fitness, best fitness and current best individual can be obtained through the GUI running genetic algorithm As shown in figure 2, 3.

![Figure 2](image1.png)

Mean fitness and best fitness

Figure 2. =0.4040, Mean fitness and best fitness

The parameters of Genetic algorithm are encoded, no apriori knowledge of the system is required, it does not has much mathematical requirements to the optimization of multiple solution problem and can improve the convergence speed and global searching ability. this could cause the search to jump out local optimization. For a given value of, the values of and can be precisely calculated. Here are several sets of data such as table 1.

![Figure 3](image2.png)

Current best individual

Figure 3. =0.4040, current best individual
The values of \( r \), \( \alpha \) and \( q \) are introduced into \( r = -\frac{q^2D}{l^2} \) and \( \alpha = \frac{k_rAl}{V} \), the VOCs diffusion and partition coefficients can be obtained from the above process. Such as table 2.

### Table 2. The final data

| \( u \)     | \( r \)     | \( \alpha \) | \( q \)     | \( D \)     | \( k_r \)   |
|------------|------------|-------------|------------|------------|------------|
| -0.4949    | -0.3173    | 0.012       | 0.139      | 2.364*10^5 | 10         |
| -0.122     | -0.1128    | 0.06        | 0.376      | 1.148*10^6 | 50         |
| -0.0458    | -0.1076    | 0.216       | 0.665      | 3.503*10^7 | 180        |
| -0.0288    | -0.1041    | 0.007       | 0.038      | 1.038*10^4 | 5.8333     |
| -0.2666    | -0.1663    | 0.062       | 0.416      | 1.383*10^6 | 51.667     |
| 0.4484     | -0.264     | 0.089       | 0.216      | 8.148*10^6 | 74.167     |
| 0.2724     | -0.1983    | 0.035       | 0.156      | 1.173*10^5 | 29.167     |
| 0.404      | -0.096     | 0.002       | 0.024      | 2.400*10^4 | 1.6667     |
| 0.1801     | -0.0878    | 0.029       | 0.222      | 2.565*10^6 | 24.167     |
| 0.299      | -0.3011    | 0.033       | 0.167      | 1.554*10^5 | 27.5       |

4. Conclusions

For the partial differential equation model of VOCs physicochemical evaporation process, for building materials by Bodalal. This paper introduces the genetic algorithm of VOCs diffusion and partition coefficients in dry building materials. The experiment proved that it is easy to realize the method by computer programming, the algorithm can avoid trap local optimum and has great flexibility. So it can be extended to other similar problems.

5. References

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