Establishment and Simulation of Mathematical Model System for Air Quality in Chemical Plant Area Based on Matlab

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1. Introduction
Due to the complicated conditions of the pollution sources in the chemical plant areas, the amount of calculation of the data management and regional atmospheric concentration is large, and the processing of the initial data, as well as the output, storage and query of the calculation results are complicated and difficult to operate (Manisha et al., 2017; Muradova and Hristopulos, 2016). In order to achieve the accuracy, generalization and automation of atmospheric environmental impact prediction and evaluation, and to facilitate the work of environmental evaluators, this paper uses Matlab to develop a regional environmental air quality model system (Tveit et al., 2015; Wu et al., 2017). The system is written in Matlab and applies Window 2000 (or above) as the operating system. It can be applied to regional atmospheric environmental impact assessment, atmospheric total amount control, and atmospheric environment planning. In this paper, To facilitate the prediction of regional environmental air quality, a set of regional environmental air quality model system software was developed using Matlab. Based on Matlab, a mathematical model system of the chemical plant area is built and simulated.

2. Air quality assessment system
Air quality is a complex issue involving health medicine, building environmental science and architectural design. There are many mathematical models for evaluating the air quality, but these models cannot conduct quantitative description of the impact degree of various factors in the air quality assessment system (Trautt et al., 2012). Therefore, it is necessary to improve the existing model and establish a new dynamic assessment model and give corresponding assessment methods, so that it can be suitable for different places or act as the main basis for regulating and improving air quality (Elhoseny and Hassanien, 2019; Strocchi et al, 2017).

Table 1 is the physical indicator standard for air quality, and Table 2 is the chemical indicator standard for air quality.

DOI: 10.3303/CET1871123

Please cite this article as: Gao R., 2018, Establishment and simulation of mathematical model system for air quality in chemical plant area based on matlab, Chemical Engineering Transactions, 71, 733-738  DOI:10.3303/CET1871123
Table 1: Standards for physical quality of air quality

<table>
<thead>
<tr>
<th>Serial number</th>
<th>Parameter</th>
<th>Standard value</th>
<th>Remarks</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Temperature/℃</td>
<td>22~28</td>
<td>Summer</td>
</tr>
<tr>
<td></td>
<td></td>
<td>16~24</td>
<td>Winter</td>
</tr>
<tr>
<td>2</td>
<td>Relative humidity/%</td>
<td>40~80</td>
<td>Summer</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Winter</td>
</tr>
<tr>
<td>3</td>
<td>Air velocity/m·s⁻¹</td>
<td>0.3</td>
<td>Summer</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.2</td>
<td>Winter</td>
</tr>
<tr>
<td>4</td>
<td>Fresh air rate/m³.(h·people)-¹</td>
<td>30</td>
<td></td>
</tr>
</tbody>
</table>

Table 2: Air quality chemical index standard

<table>
<thead>
<tr>
<th>Serial number</th>
<th>Parameter</th>
<th>Standard value</th>
<th>Remarks</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>SO2/mg·m⁻³</td>
<td>0.5</td>
<td>1h mean value</td>
</tr>
<tr>
<td>2</td>
<td>NO2/mg·m⁻³</td>
<td>0.24</td>
<td>1h mean value</td>
</tr>
<tr>
<td>3</td>
<td>CO/mg·m⁻³</td>
<td>10</td>
<td>1h mean value</td>
</tr>
<tr>
<td>4</td>
<td>CO2%</td>
<td>0.1</td>
<td>24h mean value</td>
</tr>
<tr>
<td>5</td>
<td>NH3/mg·m⁻³</td>
<td>0.2</td>
<td>1h mean value</td>
</tr>
<tr>
<td>6</td>
<td>O3/mg·m⁻³</td>
<td>0.16</td>
<td>1h mean value</td>
</tr>
<tr>
<td>7</td>
<td>HCHO/mg·m⁻³</td>
<td>0.1</td>
<td>1h mean value</td>
</tr>
<tr>
<td>8</td>
<td>C6H6/mg·m⁻³</td>
<td>0.11</td>
<td>1h mean value</td>
</tr>
<tr>
<td>9</td>
<td>C7H8/mg·m⁻³</td>
<td>0.2</td>
<td>1h mean value</td>
</tr>
<tr>
<td>10</td>
<td>C8H10/mg·m⁻³</td>
<td>0.2</td>
<td>1h mean value</td>
</tr>
<tr>
<td>11</td>
<td>B(a)P/ng·m⁻³</td>
<td>1</td>
<td>24h mean value</td>
</tr>
<tr>
<td>12</td>
<td>PM10/mg·m⁻³</td>
<td>0.15</td>
<td>24h mean value</td>
</tr>
<tr>
<td>13</td>
<td>TVOC/mg·m⁻³</td>
<td>0.6</td>
<td>8h mean value</td>
</tr>
</tbody>
</table>

3. Calculation formula for the mathematical model

3.1 Point source diffusion mode under the windy condition (U₁₀≥1.5)

\[
c = \left(\frac{Q}{2\pi U \sigma_y \sigma_z}\right) \exp\left(-\frac{y}{2\sigma_y^2}\right) F
\]

\[
F = \sum_{n=-k}^{+k} \left\{ \exp\left(-\frac{(2nh-H_e)^2}{2\sigma_z^2}\right) + \exp\left(-\frac{(2nh+H_e)^2}{2\sigma_z^2}\right) \right\}
\]

\[
U(H) = U_{10}\left(\frac{H}{10}\right)^\nu, \quad H \leq 200
\]

\[
U(H) = U_{10}\left(\frac{200}{10}\right)^\nu, \quad H \leq 200
\]

\[
H_e = H + \Delta H
\]

\[
\sigma_y = \gamma_1 x^{\delta_1}, \quad \sigma_z = \gamma_2 x^{\delta_2}
\]

Where: c-ground concentration of the pollutant, mg/m³; U-average wind speed at the outlet of the exhaust pipe, m/s; \( \sigma_y \)-diffusion parameter in the horizontal direction, m; \( \sigma_z \)-diffusion parameter in the vertical direction, m; y-vertical distance between the calculation point and the average wind direction axis through the exhaust pipe on the horizontal plane, m; h-height of the mixed layer, m; H-geometric height of the exhaust pipe from
the ground, m; \( H \) - effective height of the exhaust pipe, m; \( \Delta H \) - rising height of the gas, m; \( P \) - wind speed height index, \( \alpha_1, \alpha_2 \) - regression indices of horizontal and vertical diffusion parameters; \( \gamma_1, \gamma_2 \) - regression coefficients for lateral and vertical diffusion parameters; \( x \) - horizontal distance from the downwind direction of the exhaust pipe, m.

3.2 Small wind (1.5 > \( U_{10} \) ≥ 0.5) and static wind (\( U_{10} < 0.5 \)) point source diffusion modes

\[
c(x, y) = \frac{2Q}{2\pi x^2} G
\]

\[
\eta^2 = \left( x^2 + y^2 + \frac{\gamma_{01}^2}{\gamma_{02}^2} H^2 \right)
\]

\[
G = e^{-U_{10}^2} \left\{ 1 + \sqrt{2\pi} \frac{x^2}{s} \varphi(s) \right\}
\]

\[
\varphi(s) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{s} e^{-t^2} dt
\]

\[
s = \frac{U_{10}}{\gamma_{01}\eta}
\]

\( \gamma_{01}, \gamma_{02} \) - Regression coefficients of lateral and vertical diffusion parameters.

3.3 Long-term average concentration mode

\[
c(X, Y) = \sum_i \sum_j \sum_k \left( \sum_r ^{-} c_{ijk} f_{ijk} + \sum_r ^{-} c_{Lijk} f_{ijk} \right)
\]

Where: \( c_{ijk} \) - concentration of the i wind direction with j stability in the k wind speed segment under the windy condition; \( c_{Lijk} \) - concentration of the i wind direction with j stability in the k wind speed segment under the small wind condition and the static wind condition.

3.4 Daily average concentration mode

Statistically calculate the joint frequency of wind direction, wind speed and stability of the daily meteorological data, and then calculate the long-term average concentration mode.

4. Fuzzy comprehensive assessment model based on cloud model

4.1 Determine the factor set

The n factors related to the assessment object are selected to constitute a factor set \( U \), that is, \( U = \{ u_1 ,..., u_n \} \), where \( u_i \) represents the i-th assessment factor.

4.2 Determine the comment set

According to the relevant criteria or standards, the assessment objects are divided into m levels to determine the comment set \( V = \{ v_1 ,..., v_m \} \).

4.3 Determine the evaluation factor cloud model weight set

The weight of each assessment factor is determined by AHP, which constitutes a weight set \( A = \{ a_1 ,..., a_n \} \); the weight of each assessment factor is taken as the expectation of its weight cloud model, that is, for the i-th assessment factor \( u_i \), its weight \( a_i \) is taken as the expectation of its weight cloud model: \( Ex_{a_i} = a_i \), then according
to the fuzziness and randomness of the expert judgment, the appropriate entropy $E_{n_i}$ and super entropy $H_{e_i}$ are selected to form the weight cloud model $C_i(\text{Ex}_{n_i}, E_{n_i}, H_{e_i})$ of the assessment factors. The weight cloud model of each assessment factor constitutes the cloud model weight set:

$$A = \left[ \begin{array}{c}
\text{Ex}_{n_1}, E_{n_1}, H_{e_1} \\
\vdots \\
\text{Ex}_{n_m}, E_{n_m}, H_{e_m}
\end{array} \right]^T$$

(12)

here, we take:

$$A = \left[ \begin{array}{c}
(0.2015, 0.1, 0.01) \\
(0.6025, 0.1, 0.01) \\
(0.1217, 0.1, 0.01) \\
(0.0743, 0.1, 0.01)
\end{array} \right]^T$$

(13)

4.4 **Determine the cloud model of the comment set**

The standard for each assessment factor specified in each comment are set as the expectation of the assessment factor in the comment. For example, if the Class-I standard of formaldehyde is 0.5 mg/m$^{-3}$ in the indoor air quality assessment, the expectation of Class-I is $\text{Ex} = 0.5$. Then, select a proper entropy $E_{n_i}$ and a super entropy $H_{e_i}$ to construct the cloud model of the assessment factor in the comment, and use the fuzzy composition operator to combine the weight cloud model with the cloud model of the assessment factors of each level to construct the comment cloud model (Zhang, et al., 2014) $C_i(\text{Ex}_{n_i}, E_{n_i}, H_{e_i}), i=1,...,m$, thus forming a comment cloud model:

$$A = \left[ \begin{array}{c}
(0.2015, 0.1, 0.01) \\
(0.6025, 0.1, 0.01) \\
(0.1217, 0.1, 0.01) \\
(0.0743, 0.1, 0.01)
\end{array} \right]^T$$

(14)

Comment cloud models of each level: $C_1=(0.6379,0.1586,0.0158)$, $C_2=(1.2758,0.3165,0.0316)$, $C_3=(2.5516,0.6326,0.0632)$, $C_4=(3.8274,0.9488,0.949)$, $C_5=(7.6548,1.8974,0.1897)$

![Figure 1: Cloud model of air quality grade](image)

The above five cloud models respectively represent the levels of indoor air quality. Figure 1 shows the above five cloud models, which represent Level-I, Level-II, Level-III, Level-IV, and Level-V from left to right, of which
4.5 Determine the membership cloud model

Determine the cloud model of each assessment factor of the assessment objects \( C_j(\text{Ex}_j, \text{En}_j, \text{He}_j) \), \( j=1,\ldots,m \), and construct the membership cloud model:

\[
R = \begin{pmatrix}
\text{Ex}_{y1}, \text{En}_{y1}, \text{He}_{y1} \\
\vdots \\
\text{Ex}_{yn}, \text{En}_{yn}, \text{He}_{yn}
\end{pmatrix}
\]  

\[(15)\]

5. Result analysis

It can be seen intuitively from Figure 2(a) that the red cloud is located between Level-III and Level-IV, the fit to Level-IV is tighter, and \( \text{En}=0.5581, \text{He}=0.0558 \), both of which are smaller, as a result, the distribution of cloud is denser, indicating that the indoor air quality at monitoring point 1 trends towards Level-IV, and in a very small range, it trends towards Level-III; it can be seen from Figure 2(b) that the red cloud is located between Level-IV and Level-V, \( \text{Ex}=5.5679 \), Level-IV’s \( \text{Ex}=3.8274 \), Level-V’s \( \text{Ex}=7.6548 \), the expectation of the red cloud slightly trends towards Level-IV, but for this cloud, \( \text{En}=1.5868, \text{He}=0.1587 \), these two values are slightly larger, resulting in a more dispersed cloud, indicating that monitoring point 2 trends towards Level-IV or Level-V within a certain range; as shown in Figure 2(c), the red cloud almost overlaps with Level-II, and for this red cloud, \( \text{En}=0.2478, \text{He}=0.0248 \), both values are smaller, so that the assessment results cloud distribution is more concentrated, therefore, the indoor air quality of monitoring point 3 can be considered as Level-II; from Figure 2 (d) we can know that, the red cloud better coincides with Level-III, \( \text{En}=0.4978 \),
He=0.0498, these two values are slightly larger, resulting in a slightly scattered cloud distribution, indicating that the monitoring point 4 is more likely to be Level-III, and in a small range, it trends towards Level-IV.

6. Conclusion

Based on the cloud model, this paper established a new assessment model for the fuzzy comprehensive assessment model of air quality in chemical plant areas, and applied it to the air quality assessment of chemical plant areas. For the problems of the traditional model, such as it's difficult to describe the randomness and fuzziness in the assessment process using the traditional model, and its description of the assessment results is inaccurate and not detailed, this paper combined the cloud model with the fuzzy comprehensive assessment model to construct a fuzzy comprehensive evaluation model based on cloud model, determined the comment set, weight set and assessment matrix of the cloud model, and quantitatively described the randomness and fuzziness in the assessment process using the entropy and super entropy, which not only extended the representation method of the assessment results from point to intervals, but also make the assessment results more accurate and detailed, and then the simulation verification was performed. In summary, this paper systematically organized the methods of air quality assessment in chemical plant area, and proposed a method to establish a mathematical model of air quality assessment and carried out an example simulation. The verification results showed that the air quality assessment method of the chemical plant area established in this paper was effective and universal, which laid a good foundation for further research on how to improve the air quality of the chemical plant area.

Reference


Laura C., Massimiliano I.G., Gianluca I., Selena S., 2018, Comparison of Field Inspections and Dispersion Modelling as a Tool to Estimate Odour Emission Rates from Landfill Surfaces, Chemical Engineering Transactions, 68, 187-192, DOI: 10.3303/CET1868032


