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# Visual prediction of gas diffusion concentration based on regression analysis and BP neural network

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**Abstract:** In order to realise the prediction of the diffusion trend of chemical gases under toxic, flammable, and explosive conditions, this article used a multiple regression model and a back propagation (BP) neural network model, established two kinds of leakage gas diffusion models based on Fluent simulation data. First, the multivariate function relation between multiple influencing factors and diffusion concentration is established by using linear fitting method, i.e. multivariate regression model. Second, according to the large number and non-linearity of Fluent simulation data of leakage gas, a three-layer BP neural network prediction model for leakage gas, wind speed, *X*-axis diffusion distance, and *Y*-axis diffusion distance was established by using BP neural network algorithm. Under the same data conditions, the prediction error of BP neural network prediction model is smaller than that of multivariate reversion model, and the fitting degree is high, but the stability of multiple linear regression is better.

## 1 Introduction

In recent years, there have been many traffic accidents involving dangerous chemicals transport vehicles, which has aroused widespread concern in society. Therefore, after the accident, how to scientifically guide the rescue personnel to deal with the accident becomes more and more important. The rapid and accurate estimation and evaluation of the diffusion trend of the dangerous substances and the concentration distribution can effectively reduce the loss [1–3].

Ge Wei and Y. Wenjun [4] calculated the diffusion concentration of toxic gases by Gaussian Plume model, and compared the diffusion concentration distribution field and safety division of $NH_3$ and $Cl_2$ under two extreme atmospheric stability conditions. Yao Jian *et al.* [5] applied MATLAB to simulate the process of toxic gas leakage and diffusion, established a correlation function between the diffusion concentration and the diffusion distance of the toxic gas leakage process, and performed parameters such as atmospheric stability, wind speed, and surface roughness that affect the diffusion of toxic gas. Sensitivity analysis. Wu Yaju *et al.* [6] analysed and evaluated the changes and uncertainties of wind speed and leakage rate affecting the diffusion of toxic gas. In order to analyze and evaluate the variation and uncertainty of wind speed and leakage rate affected by gas leakage, Monte Carlo adopt simulation and non-parametric statistical method based on the allowable limit of Wilks formula were used to calculate the risk probability curve and the range influenced by toxic gas that leaks and spreads in different risks.

Based on Fluent simulation data, this paper establishes a regression model of wind speed, diffusion distance, and diffusion concentration, and tests the data to verify the accuracy of the model. BP neural network algorithm is applied to wind speed, diffusion distance, and gas in two directions. The diffusion concentration was established by the diffusion concentration prediction model, and the model was tested. On this basis, this model and the multiple regression model are compared under the same data conditions.

## 2 Regression model of gas diffusion

When establishing the one-way regression model and the multiple regression model, it is assumed that the fluid is a homogeneous flow, and the gas does not undergo a chemical reaction during the diffusion process; the ambient temperature is 300 K, the turbulence intensity is 10, the leakage velocity is constant at 2.5 m/s, and the surface roughness has no effect on gas diffusion [7–9].

### *2.1 One-way regression model of wind speed and diffusion concentration*

The diffusion concentration of the leaking gas under different wind speed conditions is shown in Table 1. The regression analysis of the data in Table 1 by EXCEL gives the fitting formula of wind speed and diffusion concentration as follows:

$$y = -0.0026x^4 + 0.134x^3 - 0.196x^2 - 0.0005x + 1.1762 \tag{1}$$

where $y$ is the leakage gas concentration, $x$ is the wind speed at the place where the accident occurred.

From the fitting graph of wind speed and gas diffusion concentration in Fig. 1, it can be seen that the quadratic regression model of wind speed and concentration can better reflect the relationship between wind speed and diffusion concentration, and the larger the wind speed, the smaller the gas diffusion concentration.

**Table 1** Gas diffusion concentration under different wind speed conditions

| Wind speed, m/s | Diffusion concentration, kg/m$^3$ | Wind speed, m/s | Diffusion concentration, kg/m$^3$ |
|---|---|---|---|
| 0.000000 | 1.176344 | 1.500002 | 1.163207 |
| 0.100000 | 1.175502 | 2.000000 | 1.162125 |
| 0.500010 | 1.173079 | 2.500000 | 1.158409 |
| 1.000000 | 1.166243 | 3.000004 | 1.146456 |

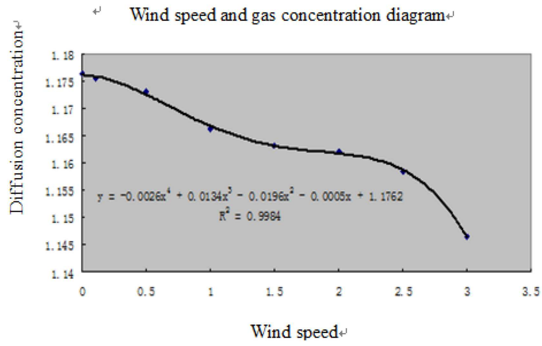


**Fig. 1** *Wind speed and gas concentration diagram*

**Table 2** *X*-axial distance and gas diffusion concentration

| *X*-axial distance, m | Diffusion concentration, kg/m$^3$ | *X*-axial distance, m | Diffusion concentration, kg/m$^3$ |
|---|---|---|---|
| 0.10000 | 1.17663 | 1.90000 | 1.176593 |
| 0.30000 | 1.17662 | 2.00000 | 1.176594 |
| 0.10000 | 1.17663 | 1.90000 | 1.176593 |
| 0.30000 | 1.17662 | 2.00000 | 1.176594 |
| 0.50000 | 1.17662 | 2.09999 | 1.176595 |
| 0.80000 | 1.17661 | 2.20000 | 1.176596 |
| 1.00000 | 1.17660 | 2.40000 | 1.176599 |
| 1.10000 | 1.17659 | 2.50000 | 1.176602 |
| 1.40000 | 1.17659 | 2.80000 | 1.176609 |
| 1.50000 | 1.17659 | 3.00000 | 1.176627 |

**Table 3** *X*-axial distance and gas diffusion concentration

| *Y*-axial distance, m | Diffusion concentration, kg/m$^3$ | *Y*-axial distance, m | Diffusion concentration, kg/m$^3$ |
|---|---|---|---|
| 0.00000 | 1.176638 | 2.90001 | 1.176445 |
| 0.50000 | 1.176619 | 3.00000 | 1.176444 |
| 0.80000 | 1.176602 | 3.20001 | 1.176447 |
| 1.00000 | 1.176589 | 3.40001 | 1.176457 |
| 1.30000 | 1.176567 | 3.90001 | 1.176511 |
| 1.50000 | 1.176550 | 4.30002 | 1.176569 |
| 1.70001 | 1.176532 | 4.50000 | 1.176597 |
| 2.00000 | 1.176504 | 5.00000 | 1.176649 |
| 2.20001 | 1.176486 | 5.69998 | 1.176674 |
| 2.50000 | 1.176463 | 7.00000 | 1.176674 |

### *2.2 One-way regression model of diffusion distance and diffusion concentration*

See Tables 2 and 3 for the diffusion concentration of the leaking gas under different diffusion distance conditions. In order to study its regularity, the data of Tables 2 and 3 were subjected to one-way regression analysis using EXCEL, and the fitting formulas of diffusion distance and diffusion concentration were obtained.

The formula for fitting the *X*-axial distance to the diffusion concentration is as follows:

$$y = 2.2E - 6x^3 + 5.3E - 6x^2 - 4E - 5x + 1.1766 \quad (2)$$

where $y$ is the leakage gas concentration, $x$ is the *X*-axial gas diffusion distance $m$, and $E$ is the science and technology law, which is the number of powers of 10.

The formula for fitting the *Y*-axial distance to the diffusion concentration is as follows:

$$y = (4.3E - 6)x^4 - 0.00005x^3 + 0.0002x^2 - 0.000084x + 1.1766 \quad (3)$$

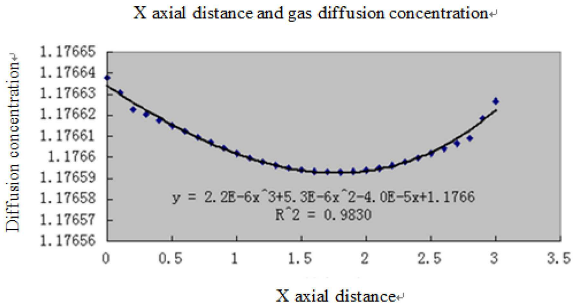


**Fig. 2** *Relationship between X-axial distance and gas diffusion concentration*

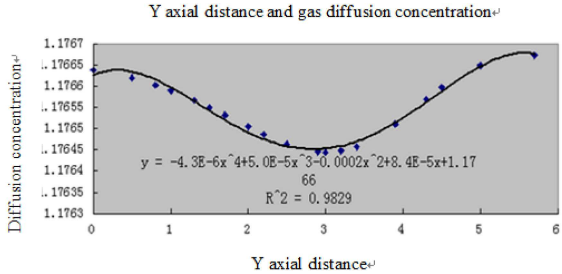


**Fig. 3** *Relationship between Y-axial distance and gas diffusion concentration*

where $y$ is the leakage gas concentration, and $x$ is the *Y*-axis of the gas diffusion distance.

It can be seen from Figs. 2 and 3 that the fitting degree of the one-dimensional cubic regression model of the *X*-axis diffusion distance and the diffusion concentration is 0.98; the fitting degree of the *Y*-axis diffusion distance and the diffusion concentration of the quadratic regression model is also 0.98. A one-way regression model has a good fit to the original data.

### *2.3 Multiple regression model*

Based on the one-way regression function relationship, this paper uses SPSS software to establish multiple regression models of wind speed, diffusion distance, and diffusion concentration, and uses test data to test the accuracy of the model. Due to space limitations, this article does not list the data needed to build a model.

In SPSS, the data of the first, second, and third parties and the output variable (diffusion concentration) of the three input variables (wind speed, *X*, *Y* diffusion distance) are entered in columns, and then the regression operation is performed. The regression coefficient of each order variable to the diffusion concentration is written as a formula as shown in (4):

$$\begin{aligned} y = {} & 1.17223 + 0.00016x_1^3 - 0.00086x_1^2 - 0.00259x_1 \\ & +0.00385x_2^3 - 0.016395x_2^2 + 0.01175x_2 \\ & +0.000493x_3^3 - 0.0052x_3^2 + 0.01344x_3 \end{aligned} \quad (4)$$

where $X_1$ is the wind speed at the place where the accident occurred, $X_2$ is the *X*-axis gas diffusion distance, and $X_3$ is the gas diffusion distance in the *Y*-axis.

Equation (4) is a multiple regression model of established wind speed, *X*-axis diffusion distance, *Y*-axis diffusion distance, and diffusion concentration. The model ignores the influence of the roughness of the ground on the gas diffusion. The gas does not react during the diffusion process, and the leakage velocity, turbulence intensity, and ambient temperature are constant values.

The actual value in Fig. 4 refers to the calculation result of the fluid dynamic model, in which the solid line represents the predicted value of the multiple regression model and the broken line represents the actual value. In the figure, the abscissa indicates the serial number of the test data, and the ordinate indicates the magnitude of the leakage gas diffusion concentration value. It can be seen from Fig. 4 that when the diffusion concentration is larger,

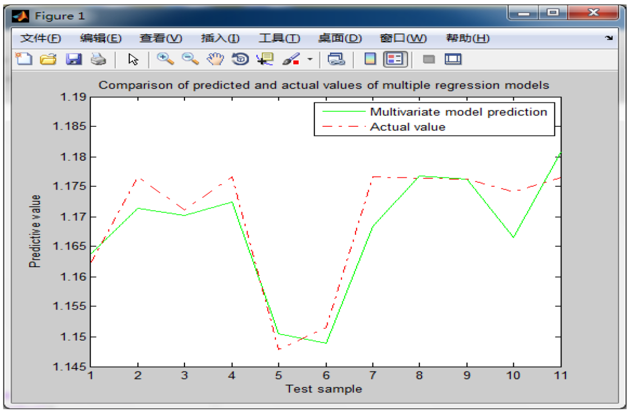


**Fig. 4** *Diffusion concentration actual value and predicted value*

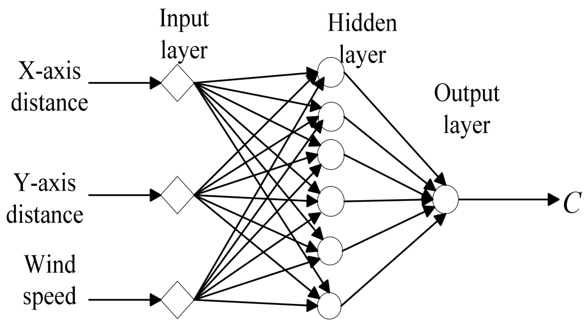


**Fig. 5** *Three-layer BP network structure*

the difference between the predicted value and the actual value of the model is slightly larger, which may be due to the unstable diffusion tendency of the gas diffusion time in the initial stage of the leakage; when the diffusion concentration is in the model of prediction, the value is very close to the actual value, and the model predicts better.

## 3 Design of BP neural network model

### *3.1 Design of BP neural network model*

According to the simulation data of the classical fluid dynamic model, three influence factors are extracted as input vectors, and the actual diffusion concentration $C$ is taken as the target vector. The influence factors are as follows: $X$-axis diffusion distance $x(m)$, $Y$-axis diffusion distance $y(m)$, and wind speed $v(m/s)$. According to the number of input and output factors, it can be determined that the number of input layer nodes of the BP network structure is 3, and the number of output layer nodes is 1.

The number of neurons in the hidden layer is designed to be six. After multiple comparison experiments, it is found that when the number of hidden layer neurons is 6, the error is the smallest and the fitting degree is also high. Therefore, the BP network prediction model of this paper the number of hidden layers is set to 6.

The function is trained by the function traingdx. When the traingdx is selected for training, the convergence rate is slow. After 1000 trainings, the target error is still not met. When using the function traingdx for training, after a short time, set the target error performance that can be achieved. So when building a diffusion model for leaking gas, choose the function traingdx to train the network.

Through the above design of the neural network structure, a three-layer neural network structure diagram for leakage gas diffusion concentration is shown in Fig. 5.

Input vector in the figure is $x = (x, y, v)^{\mathrm{T}}_{p\times 3}$, the output of the hidden layer is $x'$, the output of the output layer is $d = (c)^{\mathrm{T}}_{p\times l}$; the right of the input layer and the hidden layer is $\lfloor w_{ij} \rfloor_{6\times 3}$ and threshold is $[\theta_1]_{6\times 1}$; the right of the hidden layer and the output layer is $\lfloor w_{jk} \rfloor_{1\times 6}$ and threshold is $[\theta_2]_{1\times 1}$; and the expected output of the sample data is $t = (c)^{\mathrm{T}}_{p\times l}$.

### *3.2 BP neural network algorithm flow*

The specific process is as follows:

*Step 1:* Initialisation. Adding randomly generated weights and thresholds $w_{\mathrm{sq}}(0) = Random(\bullet)$ (sq □ $ij$、$jk$) to the hidden layer.

*Step 2:* In the training samples, sequentially input the sample into the network as shown in Fig. 5, first taking an input $n_1 = 1$. The calculation of hidden layer and output layer is as follows:

$$
\begin{aligned}
x' &= f\left(\sum_{i=0}^{2} w_{ij}x - \theta_1\right) \\
d &= f\left(\sum_{j=0}^{2} w_{jk}x' - \theta_2\right)
\end{aligned}
\tag{5}
$$

The function $f$ in the formula is as follows:

$$
f(u) = \frac{1}{1 + e^{-uj}} = \frac{1}{1 + e^{-(\Sigma w_j x_j - \theta_j)}}
$$

*Step 3:* Determine whether the error $e_p = (1/2)\sum_k (t_k - d_k)^2$ meets the requirements; if it is satisfied, the network training ends; otherwise, the error of each layer is calculated layer by layer from the output layer according to formulas (3)–(2), and the calculation is as follows:

$$
\begin{aligned}
\delta_{jk}^{p_1} &= \left(t^{p_1}k - d^{p_1}k\right) d_k^{p_1}\left(1 - d^{p_1}k\right) \\
\delta_{ij}^{p_1} &= \sum_{k=0}^{p_1} \delta_{jk}^{p_1} w_{jk} x'^{p_1}\left(1 - x'^{p_1}\right)
\end{aligned}
\tag{6}
$$

*Step 4:* Adjust the weights of each layer from the back to the front according to (7). The specific calculation is as follows:

$$
\begin{aligned}
w_{jk}(n_0 + 1) &= w_{jk}(n_0) + \eta \sum_{p_1=1}^{p} \delta_{jk}^{p_1} x'^{p_1} \\
w_{ij}(n_0 + 1) &= w_{ij}(n_0) + \eta \sum_{p_1=1}^{p} \delta_{ij}^{p_1} x'^{p_1}
\end{aligned}
\tag{7}
$$

*Step 5:* After the adjustment is completed, continue to input the sample and repeat the calculation process in Step 2 with the new weight. The training is stopped until the error meets the requirements.

*Step 6:* Preserve well-trained neural networks and predict with trained neural networks.

The BP neural network model of the leakage gas diffusion concentration was obtained by simulating the constructed neural network under MATLAB, and the simulation result corresponding to the actually defined weight matrix; the BP neural network model of the leakage gas diffusion concentration can be obtained as follows: (see (8)) .

### *3.3 Performance analysis of BP neural network model*

It can be seen from Fig. 3 and Table 4 that the BP neural network has better follow-up between the predicted output and the actual output, the error at the individual points is slightly larger, the total prediction error is in the range of 2.3%, and the fit of the network model is 0.9. So the BP neural network prediction model is effective (Fig. 6).

## 4 Result analysis

Under the condition of MATLAB, the predicted values of the two models are compared with the calculation results of the fluid dynamic model, and the prediction errors of the two models are

**Table 4** Prediction error statistics

| Serial number | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|---|---|---|---|---|---|---|---|---|---|---|
| Predictive value | 1.1733 | 1.1758 | 1.1733 | 1.1757 | 1.1495 | 1.1505 | 1.1746 | 1.1758 | 1.1753 | 1.1752 |
| Actual value | 1.1624 | 1.1767 | 1.1712 | 1.1767 | 1.1479 | 1.1515 | 1.1767 | 1.1764 | 1.1763 | 1.1742 |
| Absolute error | 0.0110 | 0.0010 | 0.0021 | 0.0010 | 0.0017 | 0.0010 | 0.0020 | 0.0006 | 0.0010 | 0.0010 |

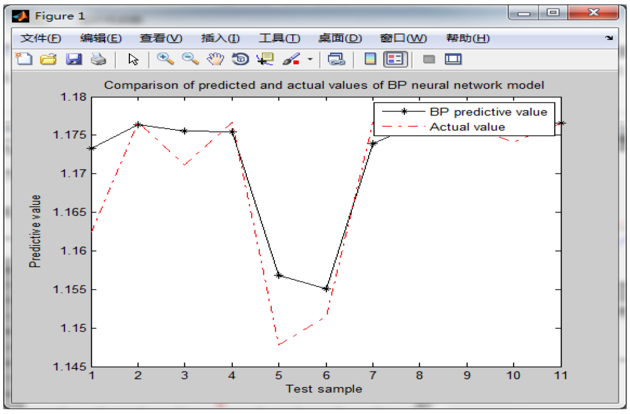


**Fig. 6** *Comparison of predicted and actual values of BP neural network model*

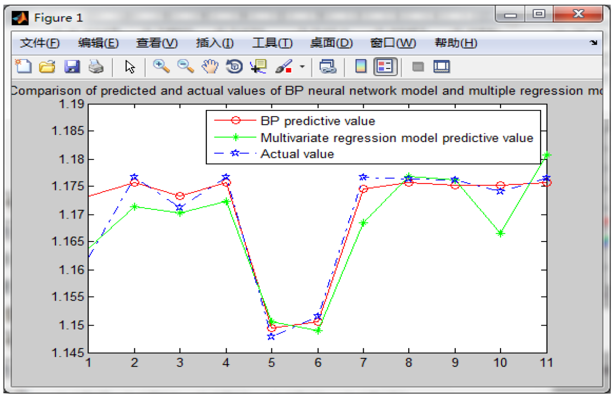


**Fig. 7** *Comparison of predicted and actual values of BP neural network model and multiple regression model*

compared. The comparison results are shown in Figs. 7 and 8. Among them, the blue line in Fig. 7 represents the actual value, that is, the calculated value of the fluid dynamic model, the green line represents the predicted value of the multiple regression model, and the red line represents the predicted value of the BP neural network model. The red line in Fig. 8 represents the prediction error of the BP neural network model, and the blue line represents the prediction error of the multiple regression model.

It can be seen from Fig. 7 that the predicted value of the BP neural network prediction model is closer to the actual value than the predicted value of the multiple regression model; as can be seen from Fig. 8, the error of the BP neural network prediction model is smaller near zero. However, the prediction error of the multiple regression model is relatively higher than that of the oscillation. It can also be concluded that the prediction error of the BP neural network prediction model is smaller than that of the multivariate return model.

To further illustrate the BP neural network prediction model with better accuracy, the average of the prediction errors of the two models is calculated. The results are shown in Table 4.

It can be seen from Table 5 that under the same hypothetical environmental conditions and data conditions, the BP neural network model improves the accuracy of leakage gas diffusion concentration prediction compared with the multiple regression model.

## 5 Conclusion

In this paper, the diffusion behaviour of leaking gas in storage tanks is studied. The diffusion of leakage gas is modelled by linear regression and BP neural network, and the following conclusions are obtained:

(i) The multivariate regression model of gas diffusion is established by linear fitting algorithm, the prediction error of 11 randomly selected test data is about 3.4%, and the goodness of fit $R^2 = 0.86$ can basically carry out the concentration of gas diffusion within the error range prediction.

(ii) The three-layer BP neural network prediction model is established by neural network algorithm, the total prediction error

$$
\begin{aligned}
\theta_1 &= [-2.5436 \quad -1.6781 \quad 0.8255 \quad 1.0153 \quad 3.2708 \quad -5.6983]^{\mathrm{T}} \\
w_{ij} &= \begin{bmatrix} 1.1808 & 2.3756 & -1.0478 & 1.017 & -0.0964 & -0.3012 \\ -1.3067 & 2.224 & 1.444 & 2.2725 & -4.9265 & 502578 \\ 1.4167 & 0.2590 & 0.3421 & -2.0414 & -0.6952 & -0.6588 \end{bmatrix}^{\mathrm{T}} \\
w_{jk} &= [-1.3461 \quad -0.3856 \quad 0.5137 \quad -0.8359 \quad 0.8674 \quad 2.8288] \\
\theta_2 &= [1.8466]
\end{aligned}
\tag{8}
$$

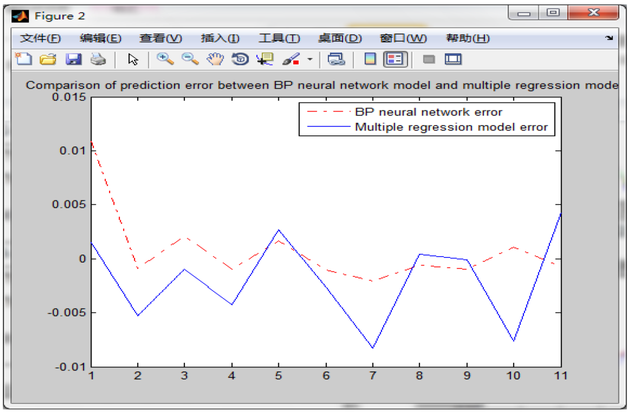


**Fig. 8** *Comparison of prediction error between BP neural network model and multiple regression model*

**Table 5** Data error

| Algorithm | Total error of 11 groups of data | Average error *E* of 11 groups of data |
|---|---|---|
| Multiple regression model | 0.0379 | 0.0034 |
| BP neural network model | 0.0231 | 0.0021 |

of the test data is 0.0231, the fitting degree of the network model is $R^2 = 0.9$. The BP neural network model is more scalable, and it can be easily adapted to the increase of the influence of leakage gas diffusion by adjusting the structure of the network. Therefore, the application range of the model is wider than that of the multiple regression model.

## 6 Acknowledgments

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