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Coal Chemical Wastewater Treatment Process Based on Computer Simulation Technology

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With a focus on coal chemical wastewater treatment, this study establishes a numerical simulation algorithm based on JAVA language for microwave-assisted coal chemical wastewater treatment, compares the testing results with the numerical simulation results, verifies the validity of the proposed numerical calculation method, and analyzes the effects of different pH values and H_2O_2 amount on coal chemical wastewater treatment by numerical simulation. In addition, the study analyzes the working principle of microwave-assisted coal chemical wastewater processor under multi-coupling action by calculating the electric field distribution, average power density, temperature field and concentration field in the furnace chamber. When pH = 3 and pH = 4, the removal rate of PNP in wastewater is the highest, reaching above 92.6%. When pH = 3, the reaction rate reaches 0.213/min. When H_2O_2 amount increases, both the removal efficiency and reaction rate of PNP increase obviously. The highest removal rate of PNP can amount to 93% and the highest reaction rate is 0.211/min. Therefore, the optimal pH value of wastewater treatment is determined to be 3, and the optimal H_2O_2 amount is 350mg/L.Introduction

1. Introduction

Coal is a major energy source around the world and can be chemically converted into a variety of chemical products (Zhang et al., 2017; Zhang, 2010). Coal chemical enterprises will produce a large number of industrial wastewater in the process of coal conversion. The wastewater contains a variety of organic and inorganic waste difficult to degrade, mainly including phenolic organics, heavy metal elements, ammonia and alkane compounds, toxic suspended particles (Zhang et al., 2015; Tomaszewska, 2007). The coal chemical wastewater has caused serious pollution to the ecological environment (Wang and Yang, 2014; Shang, 2013). At present, the coal chemical wastewater treatment has been mainly divided into pretreatment stage, core treatment stage and subsequent deepening treatment stage (Gai et al., 2008). The pretreatment stage is mainly the primary treatment of industrial wastewater, which is performed by electrolysis, filter and other means to reduce oil content and suspended particles in wastewater (Huang et al., 2012; Qin et al., 2016; Yang et al., 2003). The core treatment stage mainly adopts biochemical technologies, such as A^2-O technology, SBR technology, and immobilized biological technology so as to remove most organic and inorganic substances in wastewater (Zhang et al., 2015; Xu and Han, 2013); The subsequent deepening treatment stage is to further degrade and eliminate residual contaminants in wastewater (Liu et al., 2018).

Microwave enhanced oxidation process is a newly proposed high efficiency technology for coal chemical wastewater treatment in recent years. At present, it is in the stage of pilot operation, but it lacks a lot of data of heat transfer and mass transfer for real industrial application. Mass transfer test data (Yu et al., 2009; Yu et al., 2010; Yin et al. 2008). The computer numerical simulation technology can provide powerful information support for the microwave enhanced oxidation process and the reliable simulation results can show the effect of microwave enhanced oxidation process on coal chemical wastewater treatment (Yin et al., 2007).

This study deals with coal chemical wastewater treatment. It establishes a numerical simulation algorithm based on JAVA language for microwave-assisted coal chemical wastewater treatment, compares the testing results with the numerical simulation results, verifies the validity of the proposed numerical calculation method, and analyzes the effect of different pH and H2O2 amount on coal chemical wastewater treatment by numerical simulation.

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2. Numerical Simulation Design of Microwave-assisted Coal Chemical Wastewater Treatment

MW-Fenton is the core technology of microwave-assisted coal chemical wastewater treatment. The wastewater treatment processor is optimized by JAVA language. The activation energy Ea of degradation of organic pollutants can be expressed in logarithmic form as:

$$\ln k_{\mathrm{ap}} = \ln A_0 - \frac{E_{\mathrm{a}}}{R \cdot T} \tag{1}$$

C_{PNP} is the concentration of organic pollutants; T is temperature; R = 8.31J molK. It can be seen from formula (1) that Ink_{ap} and T are inversely proportional. Five temperatures are taken from 270K to 325K to obtain a one-to-one correspondence and fitting curve between T and I*nk*, as shown in Figure 1.

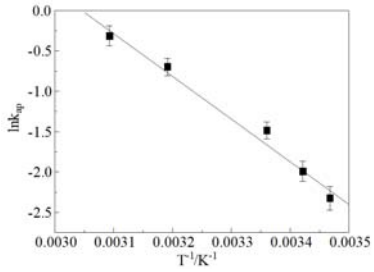

Figure 1: One-to-one correspondence and fitting curve of T and Ink

It can be seen from the figure that T and I*nk* are typically linear with a correlation coefficient of 0.985. According to the linear fitting curve, we can obtain Ea = 45.02Kj/mol. It has been shown that PNP is a typical pollutant in coal chemical wastewater, which be used as the main target of experimental degradation.

The grid division diagram of the numerical model of microwave-assisted coal chemical wastewater treatment is shown in Figure 2. The furnace chamber is set as a cuboid, and the coiler is designed for four circles. The wastewater enters from below the coiler and flows out from above. The maximum size (S_{max}) of grid in the model is obtained according to the following formula:

$$S_{\max} \le \frac{\lambda}{2\sqrt{\varepsilon_r \mu}} \tag{2}$$

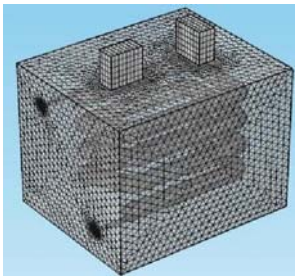

Figure 2: Grid division diagram of the numerical model of wastewater treatment

There are several reaction processes in wastewater treatment by a microwave-assisted reactor, and these reactions are coupling with each other.

Electric field distribution in a microwave oven

$$\nabla \times \mu_{\mathrm{r}}^{-1} \left(\nabla \times \vec{E} \right) \wedge - k_0^2 \left(\varepsilon_{\mathrm{r}} - \frac{j\sigma}{\omega \varepsilon_0} \right) \vec{E} = 0 \tag{3}$$

The average power density Q of wastewater treatment is calculated according to formula (2);

$$Q = 1 \cdot \pi \cdot f \cdot \varepsilon_0 \cdot \varepsilon_{\mathrm{r}} \left| E \right|^2 \tag{4}$$

f and *ρ* are microwave frequency and chemical wastewater density respectively.
The formula for calculating the temperature field of energy distribution is:

$$\rho C_{\mathrm{p}} \frac{\partial T}{\partial t} + \rho C_{\mathrm{p}} \vec{u} \nabla T = \nabla \left(\kappa \cdot \nabla T \right) + Q \tag{5}$$

The velocity field of chemical wastewater is obtained based on energy conservation of fluid;

$$\rho \left(\vec{u} \cdot \nabla \right) \vec{u} = \nabla \cdot \left[-\rho \vec{I} + \mu \left(\nabla \vec{u} + \left(\nabla \vec{u} \right)^{T} \right) \right] + \vec{F} \tag{6}$$

The concentration field of chemical wastewater can be determined based on formulas (4) and (5);

$$\frac{\partial c}{\partial t} + \nabla \left(-D \nabla c \right) + \vec{u} \cdot \nabla c = k_{ap} \tag{7}$$

3. Test Results and Analysis

3.1 Comparative analysis of numerical simulation and laboratory results;

The experimental measurements are compared with the numerical simulation results to verify the validity of numerical simulation method.
Figure 3 shows the hydraulic retention time comparison curves of numerical simulation and experimental measurements. The test and simulation results at 30-60 kg/h are analyzed. It can be seen from Figure 3 that the hydraulic stay curves calculated by the two methods are roughly the same, indicating that the numerical simulation method is relatively good.
The simulation results are further evaluated by the calculation indexes such as standard deviation error and efficiency coefficient.
Standard deviation error

$$RSR = \frac{\left[\sqrt{\sum_{i=1}^{n} \left(Y_{\mathrm{i}}^{\mathrm{obs}} - Y_{\mathrm{i}}^{\mathrm{sim}} \right)^{2}} \right]}{\left[\sqrt{\sum_{i=1}^{n} \left(Y_{\mathrm{i}}^{\mathrm{obs}} - Y^{\mathrm{mean}} \right)^{2}} \right]} \tag{8}$$

Efficiency coefficient

$$NSE = 1 - \frac{\left[\sqrt{\sum_{i=1}^{n} \left(Y_{\mathrm{i}}^{\mathrm{obs}} - Y_{\mathrm{i}}^{\mathrm{sim}} \right)^{2}} \right]}{\left[\sqrt{\sum_{i=1}^{n} \left(Y_{\mathrm{i}}^{\mathrm{obs}} - Y^{\mathrm{mean}} \right)^{2}} \right]} \tag{9}$$

Relative deviation

$$PBIAS = \left[\frac{\sum_{i=1}^{n} \left(Y_{\mathrm{i}}^{\mathrm{obs}} - Y_{\mathrm{i}}^{\mathrm{sim}} \right)}{\sum_{i=1}^{n} Y_{\mathrm{i}}^{\mathrm{obs}}} \right] \times 100\% \tag{10}$$

When 0 < RSR < 0.5, 0.75 < NSE < 1, PBIAS < 10, the matching between test results and simulation results is excellent. When 0.5 < RSR < 0.6, 0.65 < NSE < 0.75, 10 < PBIAS < 15, the matching between test results and simulation results is good; When RSR > 0.7, NSE < 0.5, PBIAS > 25, the matching between test results and simulation results is poor.
The indicators of test and simulation results for four kinds of qualities in Figure 3 are obtained and the results are shown in Table 1. As shown in the table, the matching results of the two methods are in line with an excellent evaluation, and the theoretical calculation results and the actual measurement results are the same.

Table 1: Matching assessment of hydraulic retention time for numerical simulation and experimental measurement

Mass flow(kg·h^{-1})	Evaluation results		
	NSE	*RSR*	*PBIAS*(%)
60	0.98	0.18	8.30
50	0.97	0.20	10.14
40	0.85	0.40	0.81
30	0.95	0.26	11.20

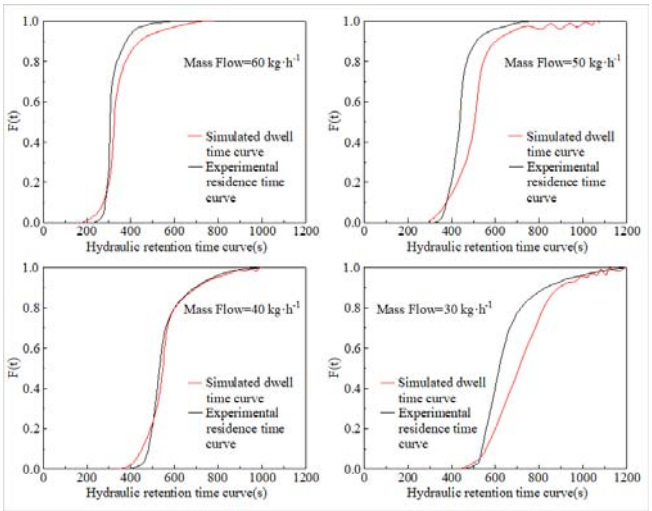

Figure 3: Hydraulic retention time for numerical simulation and experimental measurement

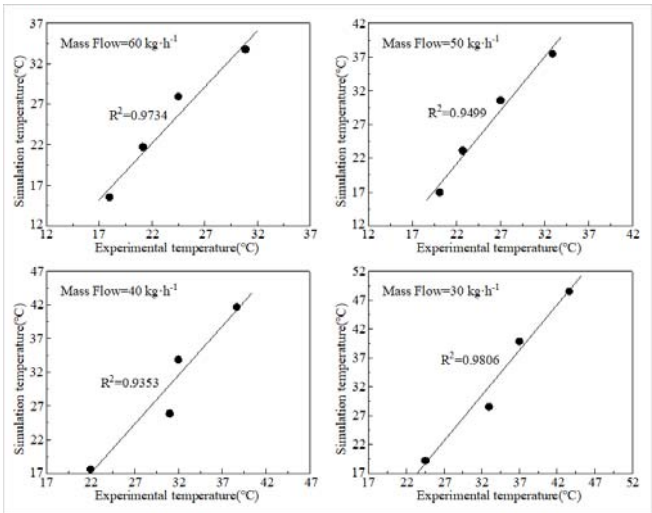

Figure 4: Outlet temperature of numerical simulation and experimental measurement

Figure 4 shows a comparison of the outlet temperature of numerical simulation and experimental measurement. As can be seen from the figure, the matching relationship between the two is good and the correlation coefficient reaches 0.945. The root mean square error is used to evaluate the matching relationship between the two;

$$RMSE = \sqrt{\frac{\sum_{i}^{n} s_i^2}{n}} \tag{11}$$

Table 2: Matching assessment of outlet temperature for numerical simulation and experimental measurement

Mass flow(kg·h^{-1})	60	50	40	30
RMSE(□)	2.81	3.13	3.55	3.22

The root mean square error of the four kinds of wastewater qualities is small, which also proves the validity of the numerical simulation algorithm.

3.2 Effect of different factors on the removal efficiency of PNP from wastewater

The numerical simulation algorithm is used to analyze the effect of different pH and H_2O_2 amount on the removal of PNP from wastewater. Figure 5 (a) shows the removal efficiency of PNP when pH increases from 2 to 5, and Figure 5 (b) shows the effect of different pH values on the reaction rate. As shown in Figure 5 (a), when pH = 3 and pH = 4, the removal rate of PNP in wastewater is the highest, which can reach above 92.6%; When pH = 3, the reaction rate reaches 0.213 min. Therefore, pH = 3 can be selected as the pH value of coal chemical wastewater.

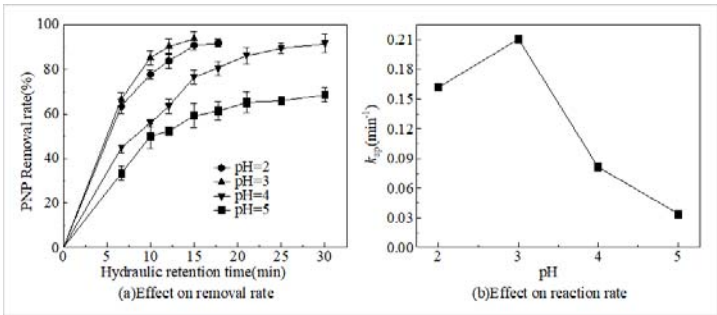

Figure 5: Effect of different pH values on removal efficiency and reaction rate of PNP in wastewater

H_2O_2 is the main oxidant for the degradation of coal chemical wastewater. Figure 6 (a) shows the effect of H_2O_2 amount on the removal efficiency of PNP, and Figure 6 (b) shows the effect of H_2O_2 amount on the reaction rate. It can be seen from the figure that the removal efficiency and reaction rate of PNP increases obviously when H_2O_2 amount increases. The highest removal rate of PNP is 93% and the reaction rate reaches 0.211/min. It can be seen from Figure 6 that the optimal H_2O_2 amount is 350 mg/L.

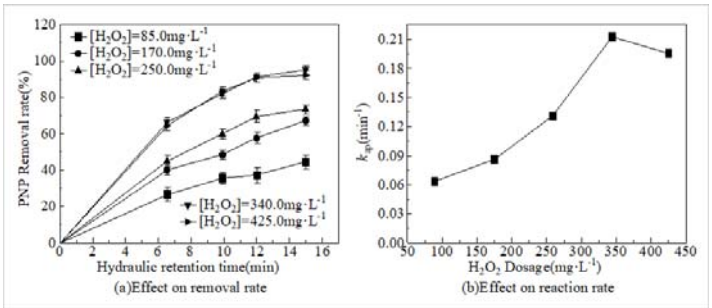

Figure 6: Effect of different H_2O_2 amount on removal efficiency and reaction rate of PNP

4. Conclusions

With a focus on coal chemical wastewater treatment, this study establishes a numerical simulation algorithm based on JAVA language for microwave-assisted coal chemical wastewater treatment, compares the testing results with the numerical simulation results, verifies the validity of the proposed numerical calculation method, and analyzes the effects of different pH values and H_2O_2 amount on coal chemical wastewater treatment by numerical simulation. The conclusions are as follows:

(1) The multi-physical coupling chemical wastewater treatment processor is designed based on JAVA language. The study analyzes the working principle of microwave-assisted coal chemical wastewater processor under multi-coupling action by calculating the electric field distribution, average power density, temperature field and concentration field in the furnace chamber. The comparison of numerical simulation and

experimental measurement of hydraulic retention time and outlet temperature shows that the matching relationship between the two is good. The numerical simulation method can be used for the auxiliary treatment of coal chemical wastewater.

(2) When pH = 3 and pH = 4, the removal rate of PNP in wastewater is the highest, which can reach above 92.6%; When pH = 3, the reaction rate reaches 0.213/min. When H_2O_2 amount increases, both the removal efficiency and reaction rate of PNP increase obviously. The highest removal rate of PNP is 93% and the highest reaction rate is 0.211/min. The optimal pH value of wastewater treatment is determined to be 3 and the optimal H_2O_2 amount is 350mg/L.

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