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SUPPLEMENTARY MATERIAL TO

Process optimization and economic calculation of photocatalytic degradation of methylene blue over sulfur doped g-C_3N_4

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EXPERIMENTAL

Characterization techniques

The crystal phase composition of the product was determined by X-ray diffraction (XRD), conducted on a Rigaku D/max-3B X-ray diffractometer (Japan). The functional groups of the sample were analyzed by Fourier transform infrared spectroscopy (FTIR), operated on a Nicolet Nexus infrared spectrometer (United States). The microscopic morphology of the sample was observed by field emission scanning electron microscopy (FESEM), realized on a FEISirion 200 scanning electron microscope (Netherlands). The microstructure of the sample was observed by transmission electron microscopy (TEM), obtained on a JEOL JEM-2010 transmission electron microscope (Netherlands). The optical absorption edge and band gap of S-doped g-C_3N_4 were analyzed by UV-vis diffuse reflectance spectroscopy (UV-vis DRS), recorded on an Ocean Optics USB4000 UV-visible diffuse reflectance spectrometer with integrating sphere, using a South African optical standard template was used as the reference. The content of total organic carbon (TOC) was measured by a XPERT-TOC/TNb TOC analyzer (Netherlands).

Photocatalytic experiments

The photocatalytic performance of S-doped g-C_3N_4 was evaluated under a 300W xenon lamp (100 mW/m^2), using MB dye as the target pollutant. The experimental procedures are as follows: 10 mg L^{-1} MB dye solution was prepared, and the absorbance of the standard solution was measured by a 722-type spectrophotometer, marked as A_0. 100 mL MB working solution was put into a 250 mL glass breaker. Then, a certain amount of S-doped g-C_3N_4 sample was added to this solution. After being stirred for 60 min, the adsorption equilibrium of the dye was obtained, and then the lamp was turned on. The schematic diagram of photocatalytic reactor is displayed in Fig. S1. During the photocatalytic reaction, about 5 mL of suspension was extracted at a specific reaction time. The supernatant was centrifuged and separated. The absorbance of the supernatant was measured and marked as A_i. The MB degradation rate was calculated by the following equation: $Y(\%)=(A_0-A_i)/A_0\times100\%$. Meanwhile, under identical experimental

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conditions, random experiments were carried out to verify the repeatability of the experimental results.

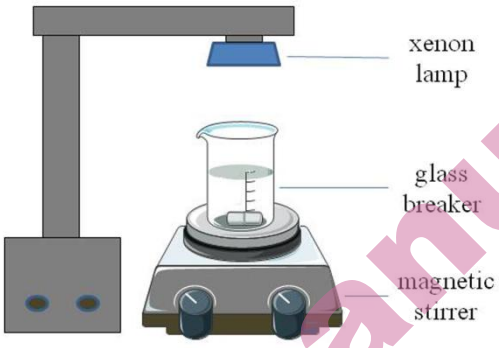

Fig. S1. Schematic diagram of the photocatalytic reactor.

RSM optimization method

In this work, four parameters were selected as variables, namely initial MB concentration (mg L^{-1}), catalyst dosage (g L^{-1}), solution pH, and reaction time (min), which were labeled as X_1, X_2, X_3, and X_4, respectively. At the same time, the degradation rate of MB dye was used as the output response (Y). The experimental design, mathematical modeling and response optimization were completed by Design Expert 8.0.7.1 software (Stat-Ease, Inc.). For statistical calculation, the variable X_i was encoded as x_i according to the equation (S1):

$$x_i = \frac{X_i - X_0}{\delta X} \quad \text{(S1)}$$

Where, x_i is the coded value, X_i is the uncoded value, X_0 is the center point value of X_i, and δX represents the step size. In addition, a second-order regression model was used to determine and analyze the response of independent variables. The formula is shown in Equation (S2):

$$Y = \beta_0 + \sum_{i=1}^{k} \beta_i X_i + \sum_{i=1}^{k} \beta_{ii} X_i^2 + \sum_i \sum_j \beta_{ij} X_i X_j \quad \text{(S2)}$$

Where, Y is the response value (MB degradation rate), X_i and X_j are the variables that affect the response value, β_i is the first-order regression coefficient, β_{ii} is the second-order regression coefficient, and β_{ij} is the interaction coefficient of two independent variables. Finally, the significance and correlation coefficient of the mathematical model were determined by analysis of variance (ANOVA). The quality and predictive reliability of the polynomial were determined by the correlation coefficient (R^2). The range and level of independent variables for MB photodegradation over S-doped g-C_3N_4 are shown in Table SI.

TABLE SI. Variables and their codes with corresponding real experimental values

Variables	Coded levels				
	-2	-1	0	1	2
X_1 (mg L^{-1})	3	9	15	21	27
X_2 (g L^{-1})	1	2	3	4	5
X_3	3	5	7	9	11
X_4 (min)	30	60	90	120	150

Economic calculation method

(1) Cost calculation of raw materials

The cost of raw materials mainly included the preparation cost of S-doped g-C_3N_4 and the consumption cost of acid-alkaline regulating reagents, which were the core component of the fixed cost of the photocatalytic process over S-doped g-C_3N_4.

The unit preparation cost of S-doped g-C_3N_4 included raw material procurement, energy consumption, and equipment depreciation, and was determined to be 80 CNY kg^{-1}. The preparation cost for treating 1 m^3 of MB dye wastewater was calculated as follows: Catalyst cost = catalyst mass (kg)×80 CNY kg^{-1}.

The pH adjustment required sodium hydroxide (or hydrochloric acid), with an industrial cost of approximately 2.5 CNY kg^{-1}. The acid/alkali reagent cost for treating 1 m^3 of MB dye wastewater was calculated as follows: acid/alkali reagent cost=acid/alkali reagent dosage (kg)×2.5 CNY kg^{-1}.

(2) Cost calculation of operation

The operating costs mainly included energy consumption (irradiation and stirring) and labor costs. As the main variable-cost component, operating cost depended directly on the reaction time and treatment scale.

Energy consumption in this photocatalytic process primarily arose from the light source and the stirrer. A 300 W xenon lamp was used for irradiation, with an electricity tariff of 0.6 CNY kWh^{-1}, and stirring was provided by a 50 W mixer. As the energy consumption increased with reaction time, the energy-consumption cost for treating 1 m^3 of methylene blue wastewater was calculated as: energy cost=[light source power (kW)+stirrer power (kW)]×reaction time (h)×0.6 CNY kWh^{-1}.

The labor cost mainly included wastewater monitoring, parameter adjustment, equipment maintenance, and other labor costs. The per capita wage of industrial production was set as 6,000 CNY $month^{-1}$, equivalent to 30 CNY $hour^{-1}$. Assuming that the operation time was positively correlated with the reaction time, the labor cost for treating 1 m^3 MB dye wastewater was calculated as follows: labor cost=reaction time (h)×30 CNY h^{-1}.

(3) Integrated cost calculation

Combined with raw material cost and operation cost, the integrated cost for treating 1 m^3 MB dye wastewater could be calculated as follows: integrated cost=(raw material cost + operation cost)=(catalyst cost + acid/alkali reagent cost + energy cost + labor cost).

RESULTS AND DISCUSSION

TABLE SII. Experimental matrix designed by CDD and experimental and predicted values of Y response

runs	X_1	X_2	X_3	X_4	Y (%)	
					experimental	predicted
1	0.000	0.000	0.000	0.000	66.78	66.39
2	-1.000	-1.000	1.000	1.000	62.91	61.26
3	0.000	0.000	0.000	0.000	66.24	66.39
4	2.000	0.000	0.000	0.000	63.4	60.13
5	-1.000	1.000	-1.000	-1.000	11.02	5.64
6	0.000	2.000	0.000	0.000	16.78	17.38
7	-1.000	1.000	-1.000	1.000	31.93	31.90
8	-2.000	0.000	0.000	0.000	40.84	42.36
9	-1.000	1.000	1.000	1.000	60.29	60.22
10	1.000	1.000	-1.000	1.000	34.64	38.95
11	1.000	-1.000	1.000	1.000	98.72	95.11
12	0.000	0.000	0.000	-2.000	21.47	23.43
13	0.000	0.000	0.000	2.000	81.74	79.24
14	1.000	-1.000	-1.000	1.000	73.5	69.18
15	-1.000	-1.000	-1.000	1.000	58.38	59.48
16	0.000	-2.000	0.000	0.000	76.11	75.89
17	0.000	0.000	0.000	0.000	66.27	63.18
18	0.000	0.000	-2.000	0.000	25.59	25.78
19	0.000	0.000	2.000	0.000	16.76	16.49
20	0.000	0.000	0.000	0.000	66.17	66.36
21	0.000	0.000	0.000	0.000	66.87	66.36
22	1.000	1.000	-1.000	-1.000	16.53	16.59
23	-1.000	1.000	1.000	-1.000	31.56	32.13
24	0.000	0.000	0.000	0.000	66.43	66.36
25	-1.000	-1.000	1.000	-1.000	62.88	61.86
26	-1.000	-1.000	-1.000	-1.000	29.54	29.13
27	1.000	-1.000	1.000	-1.000	70.79	71.00
28	1.000	-1.000	-1.000	-1.000	39.89	40.16
29	1.000	1.000	1.000	1.000	67.48	67.16
30	1.000	1.000	1.000	-1.000	41.42	41.10

Table SIII. ANOVA analysis for second-order polynomial regression.

Source	Sum of squares	Degree of freedom	Mean square	F value	p value (Prob > F)	
model	13659.70	14	975.69	8.09	0.0001	significant
X_1	811.77	1	811.77	6.73	0.0204	
X_2	4277.34	1	4277.34	35.45	< 0.0001	
X_3	1394.77	1	1394.77	11.56	0.0040	
X_4	3869.94	1	3869.94	32.07	< 0.0001	
X_1X_2	120.56	1	120.56	1.00	0.3334	
X_1X_3	45.83	1	45.83	0.38	0.5469	
X_1X_4	46.24	1	46.24	0.38	0.5452	
X_2X_3	9.99	1	9.99	0.083	0.7775	
X_2X_4	0.72	1	0.72	0.006	0.9393	
X_3X_4	21.90	1	21.90	0.18	0.6761	
X_1^2	168.67	1	168.67	1.40	0.2555	
X_2^2	416.88	1	416.88	3.45	0.0828	
X_3^2	2862.65	1	2862.65	23.72	0.0002	
X_4^2	186.64	1	186.64	1.55	0.2327	
resudiul	1810.03	15	120.67			
R^2	0.9588					
ajusted R^2	0.9189					

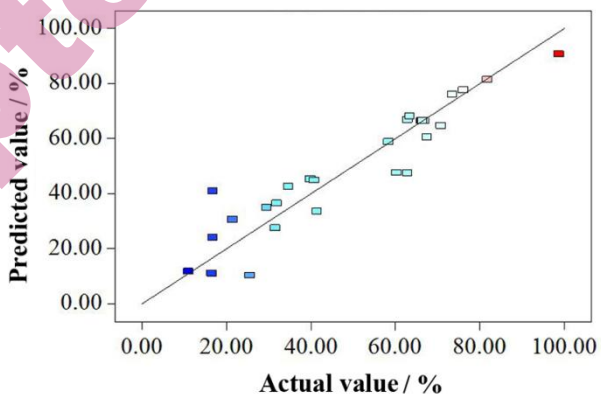

Fig. S2. The plots of predicted values versus actual values.

Table SIV. Comparative analysis data of raw material cost for treating 1 m^3 MB wastewater before and after optimization.

	catalyst cost data		acid-alkaline cost data		net saving (CNY)
	dosage (kg)	cost (CNY)	dosage (kg)	cost (CNY)	
before optimization	5	400	0	0	
after optimization	4.1	328	0.12	0.3	71.7
saving cost	—	72	—	-0.3	

Table SV. Comparative analysis data of operation cost for treating 1 m^3 MB wastewater before and after optimization.

	energy cost data		labor cost data		net saving (CNY)
	energy consumption (kWh)	cost (CNY)	operation time (h)	cost (CNY)	
before optimization	1.050	0.630	3.5	105	
after optimization	0.742	0.445	2.5	75	30.185
saving cost	—	0.185	—	30	