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RSM, ANN-GA and ANN-PSO modeling of SDBS removal from greywater in rural areas via Fe_2O_3-coated volcanic rocks

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Supplementary text

Text S1 List of chemical reagents

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Supplementary text

Text S1 List of chemical reagents

SDBS (AR grade, mixture), ferric chloride ($FeCl_3 \cdot 6H_2O$), cetyltrimethylammonium bromide (CTAB) and sodium salts (NaCl, Na_2SO_4, $NaHCO_3$, $NaNO_3$) were all supplied by Aladdin (Shanghai, China). H_2SO_4 (98 wt%), trichloromethane, NaOH (96 wt%), HCl (37 wt%), methylene blue and humic acid were purchased from Beijing Yili Fine Chemicals Co., Ltd. (Beijing, China). The SDBS stock was prepared by mixing 1.0g into 1000 mL of DI water that had been stored at 4℃.

Text S2 Preparation of Fe_2O_3-coated volcanic rocks (Fe_2O_3-VR)

Modified filter materials were prepared by heating evaporation method. Before coating the VR surface with iron, VR was cleaned a few times with DI water and soaked in 1 N HCl for 12h to remove its surface impurities. Then, it was rinsed a few times by deionized water until its effluent acidity reached neutral. VR was then dried at 100°C for 12h to remove the remaining water. Different concentrations of $FeCl_3$ solution (0.05-0.3mol/L) were prepared and added into the pretreated modified filter material according to the solid-liquid ratio of 1:3. The modified filter materials were dried at 110°C and coated repeatedly for three times with stirring every half an hour during the process. Then put the dried filter materials into a tubular furnace and calcine it for two hours in air atmosphere. The obtained materials were cooled to room temperature and washed by DI water for several times to remove extra iron coated surface that adhered loosely. Finally, the material was dried at 110°C and Fe_2O_3-coated volcanic rocks (Fe_2O_3-VR) were obtained.

Text S3 Characterization of Fe_2O_3-coated volcanic rocks (Fe_2O_3-VR)

For observation of volcanic rock morphology and identification of atomic elements and relative concentrations of elements in volcanic rock samples the characterizations of pumice were analyzed using field emission scanning electron microscopy (FE-SEM), together with Energy Dispersive X-Ray Spectroscopy (EDX) analysis (SEM-EDX, SU8020, Japan). The specific surface area of natural and modified adsorbent was measured using a nitrogen adsorption technique based on the Brunauer–Emmet–Teller isotherm model (Autosorb iQ/Quantachrome). Transmission Fourier Transform Infrared (FTIR) spectra were registered on a Perkin Elmer FTIR spectrometer model Frontier in the range 400-4000 cm^{-1}, using KBr pellets. KBr was ground with a small amount of the solid to be analyzed, and the spectra were collected with a resolution of 4 cm^{-1} and accumulation of 32 scans. The crystalline structures of the used adsorbents were determined using an X ray diffractometer (XRD) which are collected by means of a D8 Advance with Cu Kα as radiation (1.54056 Å) generated at 40 kV and 40 mA instrument. The diffractograms were obtained with a step width of 0.02° (2θ) and a scan rate of 8°/min. The surface area, total pore volume and average pore diameter (at $P/P_0 = 0.988$) were determined using N_2 adsorption–desorption isotherm measurements by the standard Brunauer–Emmett–Teller (BET) method.

Supplementary figures

Fig. S1 SEM images of VR (a, b) and Fe_2O_3-VR (c, d)

Fig. S2 EDS images of VR (a) and Fe_2O_3-VR (b)

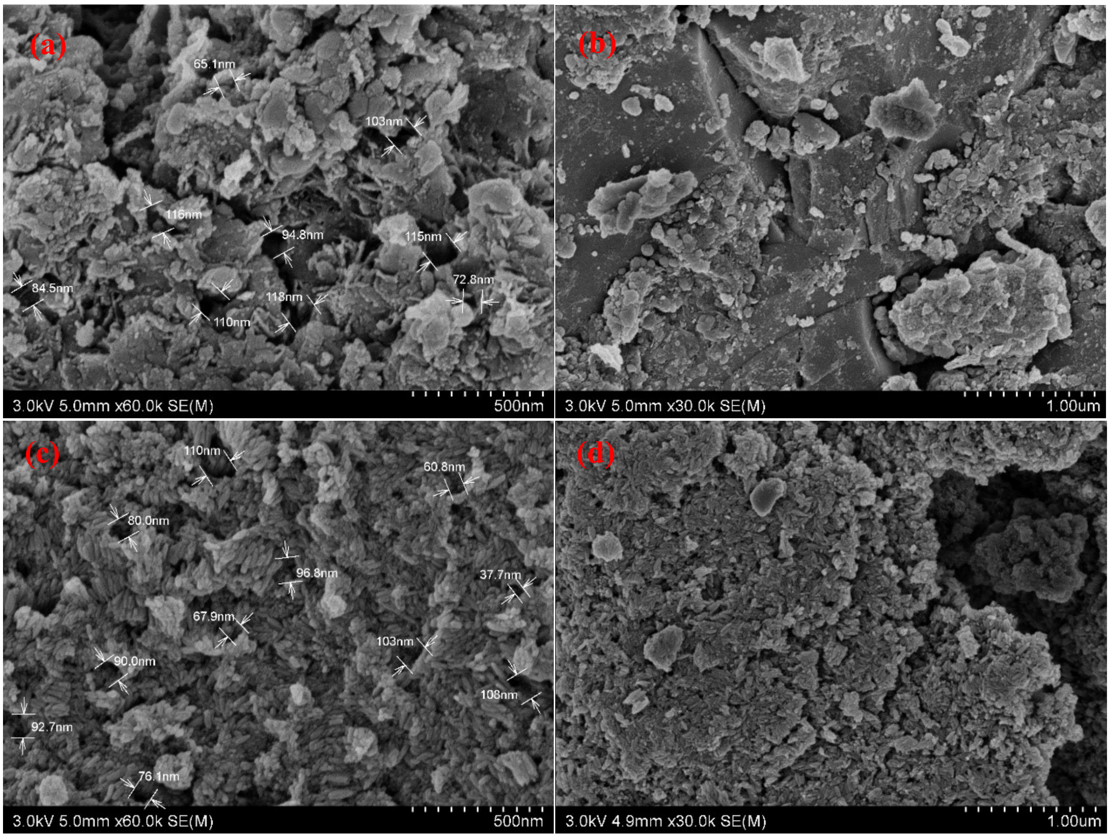

Fig. S1 SEM images of VR (a, b) and Fe_2O_3-VR (c, d)

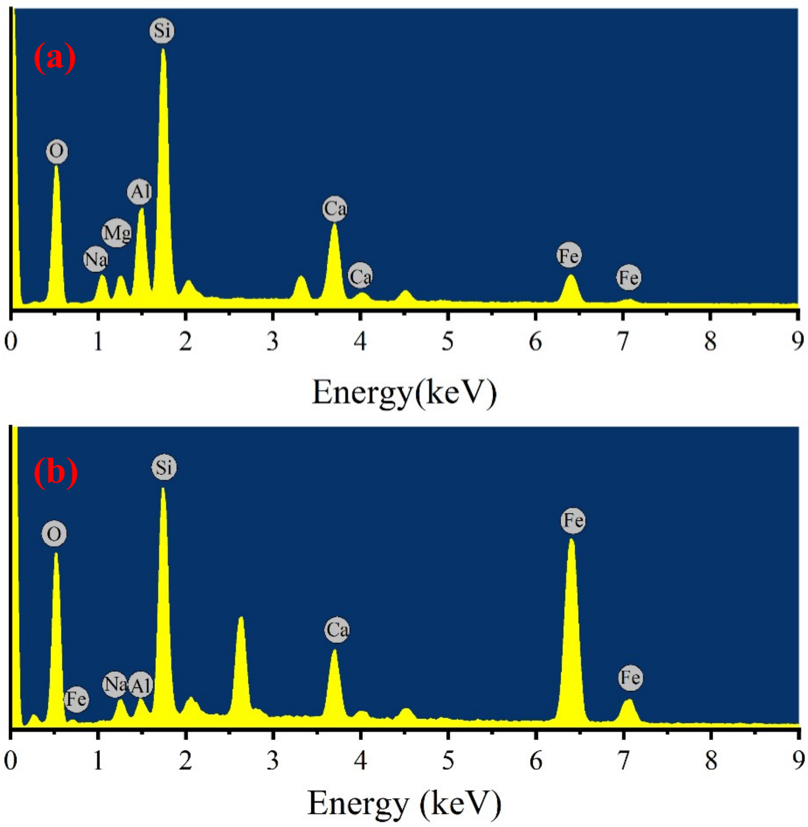

Fig. S2 EDS images of VR (a) and Fe_2O_3-VR (b)

Supplementary tables

Table S1 Experimental ranges and levels of variables

Table S2 RSM and ANN predicted results and errors, along with experimental values of the response

Table S1

Experimental ranges and levels of variables

Factors	Variables	Unit	Levels		
			Low（-1）	Middle（0）	High（+1）
A	Contact time	min	5	92.5	180
B	pH	/	2	6	10
C	SDBS initial concentration	mg/L	10	50	90
D	$FeCl_3$ solution concentration	mol/L	0.05	0.175	0.3
E	Adsorbent dosage	g/L	10	60	110
F	Calcination temperature		200	400	600

Table S2

RSM and ANN predicted results and errors, along with experimental values of the response

Run	Variables						SDBS removal efficiency				
	A	B	C	D	E	F	Experi-ment	RSM	Error	ANN	Error
1	92.5	10	90	0.175	110	400	85.67	80.373	-5.297	85.670	0.000
2	5	2	50	0.05	60	400	32.96	34.421	1.461	32.960	0.000
3	180	2	50	0.3	60	400	75.45	77.493	2.043	75.450	0.000
4	92.5	2	10	0.175	10	400	48.34	52.407	4.067	43.991	-4.349
5	5	6	50	0.3	10	400	37.32	32.882	-4.438	37.320	0.000
6	92.5	10	10	0.175	10	400	58.39	62.187	3.797	58.390	0.000
7	5	6	50	0.05	10	400	27.08	23.190	-3.890	27.080	0.000
8	5	6	50	0.05	110	400	45.66	46.189	0.529	45.660	0.000
9	92.5	10	90	0.175	10	400	45.37	46.109	0.739	45.370	0.000
10	92.5	6	50	0.175	60	400	88.34	87.333	1.953	86.776	1.396
11	5	6	90	0.175	60	600	47.26	50.599	3.339	47.260	0.000
12	92.5	10	50	0.175	10	200	57.32	57.749	0.429	57.320	0.000
13	92.5	10	50	0.175	110	600	90.12	90.936	0.816	90.120	0.000
14	92.5	2	10	0.175	110	400	73.48	73.971	0.491	73.480	0.000
15	92.5	6	90	0.3	60	200	82.59	83.064	0.474	82.590	0.000
16	92.5	6	90	0.05	60	200	71.51	72.321	0.811	71.510	0.000
17	92.5	2	50	0.175	110	600	80.29	78.631	-1.659	75.552	-4.738
18	92.5	6	50	0.175	60	400	88.34	87.333	0.763	86.776	0.206
19	92.5	6	50	0.175	60	400	88.34	87.333	-1.317	86.776	-1.874
20	92.5	2	50	0.175	10	600	52.79	52.997	0.207	52.790	0.000
21	92.5	2	90	0.175	10	400	42.47	39.794	-2.676	42.470	0.000
22	92.5	10	10	0.175	110	400	84.97	86.416	1.446	84.970	0.000
23	92.5	6	10	0.05	60	200	82.65	82.308	-0.342	83.039	0.389
24	5	10	50	0.05	60	400	45.04	42.676	-2.364	45.040	0.000
25	180	6	90	0.175	60	600	83.73	82.573	-1.157	83.730	0.000
26	5	2	50	0.3	60	400	42.23	43.380	1.150	42.230	0.000
27	5	6	90	0.175	60	200	45.02	48.594	3.574	45.020	0.000

28	180	2	50	0.05	60	400	62.63	62.796	0.166	62.630	0.000
29	92.5	6	90	0.3	60	600	85.77	86.431	0.661	85.770	0.000
30	92.5	6	50	0.175	60	400	88.34	87.333	-2.787	86.776	-3.344
31	180	6	50	0.05	10	400	47.35	47.043	-0.307	49.169	1.819
32	92.5	6	10	0.3	60	200	94.21	93.086	-1.124	94.210	0.000
33	92.5	6	50	0.175	60	400	88.34	87.333	0.013	86.776	-0.544
34	92.5	10	50	0.175	110	200	86.92	87.943	1.023	86.920	0.000
35	92.5	6	10	0.05	60	600	84.43	83.637	-0.793	90.091	5.661
36	92.5	2	90	0.175	110	400	73.96	71.393	-2.567	73.960	0.000
37	180	6	50	0.3	110	400	91.09	95.301	4.211	91.090	0.000
38	180	10	50	0.3	60	400	89.78	87.998	-1.782	89.780	0.000
39	92.5	6	90	0.05	60	600	73.56	75.003	1.443	77.072	3.512
40	92.5	2	50	0.175	10	200	50.88	51.294	0.414	50.880	0.000
41	180	6	50	0.05	110	400	78.67	82.787	4.117	80.569	1.899
42	180	6	10	0.175	60	200	94.33	90.673	-3.657	94.330	0.000
43	5	6	10	0.175	60	200	55.62	56.459	0.839	55.620	0.000
44	180	6	90	0.175	60	200	77.87	78.528	0.658	77.870	0.000
45	180	10	50	0.05	60	400	75.58	74.751	-0.829	75.580	0.000
46	92.5	6	50	0.175	60	400	88.34	87.333	1.373	86.776	0.816
47	92.5	2	50	0.175	110	200	81.92	78.823	-3.097	81.920	0.000
48	5	6	50	0.3	110	400	52.98	52.966	-0.014	52.980	0.000
49	180	6	50	0.3	10	400	62.68	62.472	-0.208	62.680	0.000
50	92.5	10	50	0.175	10	600	60.77	62.637	1.867	60.770	0.000
51	92.5	6	10	0.3	60	600	96.23	95.101	-1.129	96.230	0.000
52	5	10	50	0.3	60	400	50.03	50.185	0.155	51.252	1.222
53	5	6	10	0.175	60	600	57.45	57.111	-0.339	57.450	0.000
54	180	6	10	0.175	60	600	96.62	93.365	-3.255	94.852	-1.768