Supporting Information for

Optimizing the process parameters for preparation of powdered activated coke (PAC) to achieve maximum SO_2 adsorption capacity using response surface methodology (RSM)

Binxuan Zhou [a], Tao Wang [a, *], Tianming Xu [a], Cheng Li [a], Yuan Zhao [a], Jiapeng Fu [a], Zhen Zhang [b], Zhanlong Song [a], Chunyuan Ma [a, *]

[a] National Engineering Laboratory for Reducing Emissions from Coal Combustion, Engineering Research Center of Environmental Thermal Technology of Ministry of Education, Shandong Key Laboratory of Energy Carbon Reduction and Resource Utilization, School of Energy and Power Engineering, Shandong University, Jinan 250061, China

[b] School of Electric Power, North China University of Water Resources and Electric Power, Zhengzhou 450045, China

E-mail: wtao@sdu.edu.cn; chym@sdu.edu.cn; Tel: 0531-88395877-612.

Fixed-bed SO_2 adsorption system and the adsorption condition:

The SO_2 adsorption capacity of the PAC was evaluated at 75℃ using a fixed bed experimental system, as shown in Fig. S1. This system mainly consists of a fixed-bed glass reactor (inner diameter is 17 mm, wall thickness is 1.5 mm), an electric heater, a hot water bath, a portable Fourier transform infrared (FTIR) instrument from Finland Gasmet Company, valves and mass flow meters. Specifically, 1g of sample was loaded into the glass reactor, when the temperature of the reaction zone reached the required value and maintained a stable state, the total flow rate (0.5 L/min) was introduced into the reactor by simulating flue gas (1500 ppm of SO_2, with 6% O_2, with 8% H_2O, N_2 balance). The H_2O stream was introduced by a hot water bath and controlled by bubbling a certain amount of N_2. We continuously monitored the concentrations of SO_2/H_2O in the inlet and outlet of the fixed-bed reactor using the FTIR. Then we used the following formula to calculate the SO_2 adsorption capacity (S) of the experimental samples.

$$S=28.6\times\int_0^t\frac{(C_{\mathrm{in}}\text{-}C_{\mathrm{out}})V}{M}\mathrm{dt}, \text{ (S1)}$$

where, C_{in} and C_{out} are the concentrations of SO_2 (ppm) of the reactor inlet and outlet; V is the total flow rate (L/min) of simulated flue gas; M is the weight (g) of the sample packed into the glass reactor.

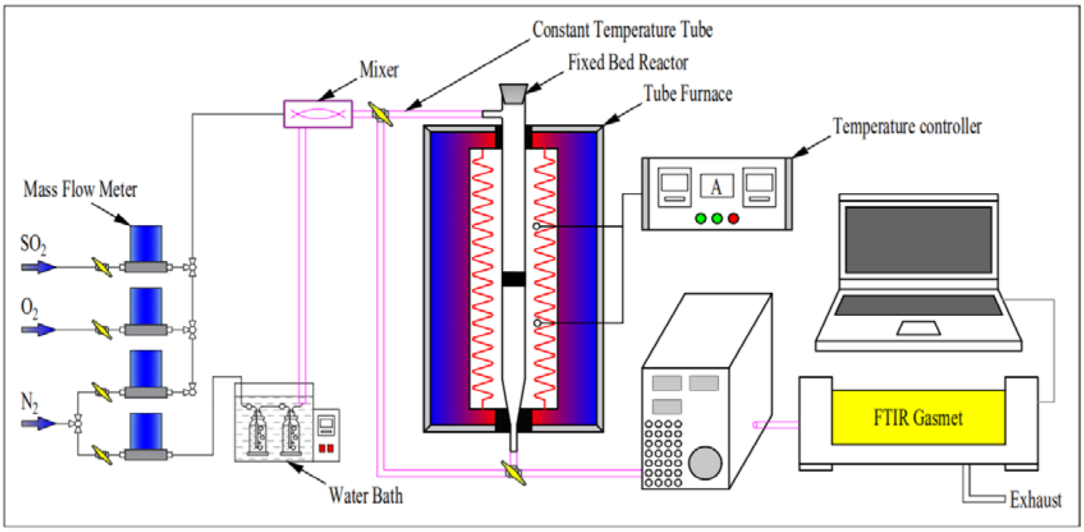

Fig. S1. Fixed-bed SO_2 adsorption system.

Pore structural characterization:

N_2 adsorption-desorption isotherm of PAC-OP, Commercia AC1 and Commercial AC2 were obtained at 77 K by a Micromeritics ASAP 2020 analyzer. The surface area (S_{BET}) was estimated using the Brunauer-Emmett-Teller (BET) multi-points method. The micropore surface (S_{mic}) was calculated by the t-plot method. The micropore volume (V_{mic}) was obtained by the DR method. The total pore volume (V_{tot}) was calculated by the analysis software at relative pressure larger than 0.97 [S1, S2]. The pore size distributions of each sample were analyzed with the QSDFT method, and through which the ultra-micropore volume ($V_{\mathrm{mic} < 1\ \mathrm{nm}}$) could be obtained [S3].

FTIR data:

The FTIR spectrum of PAC-OP was similar to the two commercial ACs. The spectrum exhibited strong absorption band in the waveband of 3700–3200 cm^{-1}, 1800–1300 cm^{-1} and 1300–900 cm^{-1}. The weak absorption peaks were seen at 2930, 2854, 2371, 2340, and 800 cm^{-1}. Among them, the absorption band in the 3700–3200 cm^{-1} can be ascribed to O–H stretching vibrations in hydroxyl, carboxylic, and phenolic groups due to the existence of surface hydroxyl groups and chemisorbed water. The absorption band in the 2850–2950 and 1460–1350 cm^{-1} can be assigned to stretching vibrations of aliphatic C–H groups. The absorption band in the 2400–2300 cm^{-1} can be attributed to CO_2 structure. The presence of bands at 1800–1300 cm^{-1} can be attributed to the stretching vibrations of C=O in carboxylic acids, anhydrides, lactones, esters, carboxylic salts, carboxylo-carbonates, quinones, hydroxyquinones, C=C in carboxylic or pyridine-like structure. The presence of bands at 1300–900 cm^{-1} range can be attributed to the stretching vibrations of C–O, C–O–C, OH in carboxylic acids, anhydrides, lactones, esters, ethers, phenols, epoxides and carboxyl-carbonates, which were also overlapped. The absorption band in the 900–700 cm^{-1} can be attributed to the aromatic hydrocarbon groups, also, there is the C=N group located at 800 cm^{-1} [S4-S7].

PAC regeneration system and condition:

Regeneration experiments of the samples after SO_2 adsorption were completed in a thermal regeneration system, as shown in Fig. S2. This system is similar to the SO_2 adsorption system, except that the regeneration gas is N_2, and the regeneration temperature is also different. The detailed regeneration process is as follows: PAC was heated in a flow of N_2 (0.5 L/min), at a heating rate of 10 ℃/min, and maintained at 450℃ for 1 hour and then cooled to room temperature while the N_2 purge was continued.

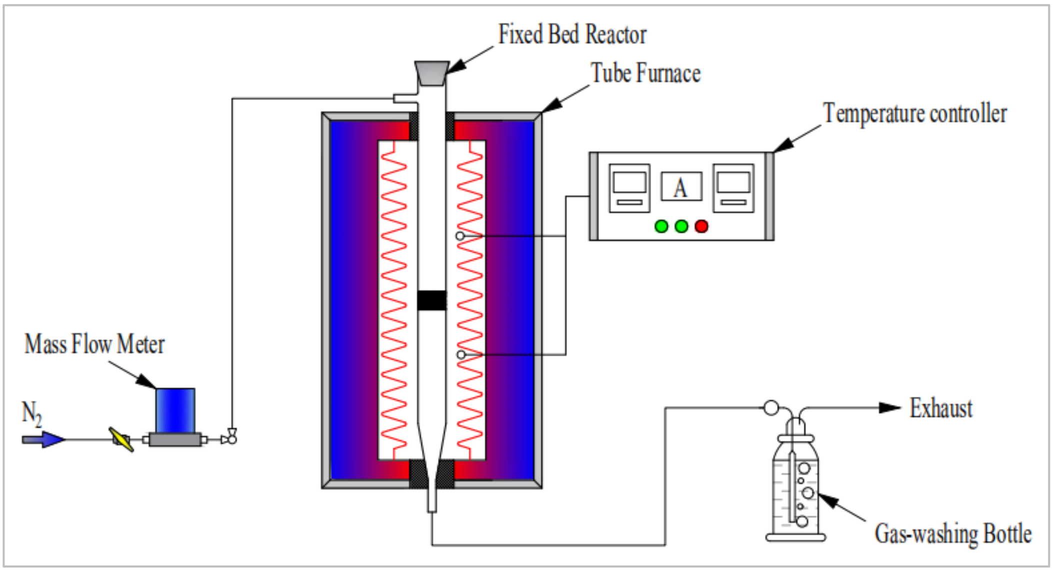

Fig. S2. PAC regeneration system.

References:

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