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## Investigation of Hydrogen Sulfide Adsorption in Metallic Scaffold MOF-5 Nanocomposite Based on Activated Carbon for the Use of Respiratory Mask Cartridge

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### Abstract

**Introduction:** Hydrogen sulfide is one of the most important impurities in natural gas. Since this gas is hazardous, toxic, corrosive and volatile, therefore, the removal of hydrogen sulfide has been studied using several methods. In the present study, activated carbon and activated carbon-based composite scaffolds (MOF-5) were used as a cartridge mask to remove hydrogen sulfide from respiratory air.

**Material and Methods:** Activated carbon (AC) was converted to powder form by ball mill, and AC / MOF-5 composite with 10%, 25%, and 40% MOF-5 / AC was synthesized from the MOF-5 metal-organic scaffold. The rates of adsorption and breakthrough time were then tested using a designed setup. The Aeroqual S500 Direct-reading sensor with 0.01 ppm accuracy was applied to measure the exact amount of hydrogen sulfide gas.

**Results:** The AC/MOF-5 composite showed higher adsorption and breakthrough time compare to the other adsorbents. The maximum adsorption (mg/gS) and breakthrough time (min) were related to AC/MOF-5<sub>(40 Wt. %)</sub> adsorbent with 60.41 mg/gS and 56.26 min. By adding more than 25% MOF-5 metal-metal scaffold to activated carbon, the amount of adsorption, breakthrough time, and pressure drop were increased.

**Conclusion:** AC / MOF-5 composite adsorbent due to its porous structure, high specific surface area, and most importantly, having Zn-O-C groups increased the adsorption rate as well as the pollutant breakthrough time. However, it showed a relatively higher pressure drop than commercial activated carbon (AC).

**Keywords:** Composite, MOF-5, Breakthrough time, adsorption, Zn-BDC, H<sub>2</sub>S

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## 1. Introduction

Hydrogen sulfide (H<sub>2</sub>S) is one of the major air pollutants, widely found in industrial processes including drilling, oil refining, natural gas, and wastewater treatment and is detrimental to human and environmental health due to its high toxicity [1-4].

Studies have been carried out to remove hydrogen sulfide. Various methods and several types of adsorbents such as metal oxides, activated carbon, and zeolites were used. Pure MOFs as a sorbent alone are not economical, and on the other hand, they have less mechanical resistance in the powdered state and are more sensitive to moisture. Hence, attempts have been made to combine them with other porous materials and to form various composites such as MOF / silica, MOF / Organic polymers and MOF / carbon [5-7].

## 2. Material and Methods

The activated carbon / organic-metal scaffold composite was synthesized and the human respiratory system simulator was then designed and fabricated. Finally, the adsorbents were tested in a practical condition.

Activated carbon (AC) was converted to powder form by ball mill, and AC / MOF-5 composite with 10%, 25%, and 40% MOF-5 / AC was synthesized from the MOF-5 metal-organic scaffold. Then, the rates of adsorption and breakthrough time were tested using a designed setup in two ranges of temperature, humidity, and concentration. To survey the adsorbents, a system consisting of a rotameter, heater chamber, air mixing chamber, cartridge, suction pump, humidifier (ALP X), moisture meter (TAIPO H 992-TK), thermometer, timer, and a U-shaped manometer were designed (Figure 1) [8]. We applied XRD, SEM and BET to determine the properties of composite adsorbents. The Aeroqual S500 Direct-reading sensor with 0.01 ppm accuracy was used to measure the exact amount of hydrogen sulfide gas.

## 3. Results and Discussion

Totally, we analyzed 96 samples of four commercial

activated carbon adsorbents and AC / MOF-5 composites at 10, 25 and 40 wt% of MOF-5. The concentration of hydrogen sulfide inlet to the adsorbents was 10 ppm and 20 ppm with a flow rate of 6-7 lit/min and pressure of 1 atm.

The SEM figure (2) showed well that commercially activated carbon is broken down to particle less than 5 microns. The AC/MOF-5 composite showed higher adsorption and breakthrough time compare to the other adsorbents (Diagram 1). The Specific surface area (BET), average pore diameter, and total pore volume of the adsorbent were 814 m<sup>2</sup> /g, 1.6795 nm, and 0.342 cm<sup>3</sup> /g, respectively. The isotherm diagram showed that, according to IUPAC, most of the pore size of this adsorbent was classified in the micro-porous group.

According to the results of the X-ray diffraction pattern, the presence of two major peaks ( $2\theta = 6.8^\circ$  and  $2\theta = 9.6^\circ$ ) indicated the successful synthesis of the activated carbon-based MOF-5 structure for the AC / MOF-5 composite. Also, the  $2\theta = 24.7^\circ$  peak is another indicator peak for the MOF-5 crystal structure. SEM analysis showed that carbon had an amorphous structure. The crystal structure of the XRD pattern also indicated that the corresponding MOF-5 structures were homogeneously distributed within the activated carbon.

The maximum adsorption (mg/gS) and breakthrough time (min) were related to AC/MOF-5(40 Wt. %) adsorbent with 60.41 mg/gS (SD = 1.08) and 56.26 min (SD = 2.38) at a temperature of 15 ° C, a concentration of 9.88 ppm (SD = 0.70), a moisture content of 51.06% (SD = 0.15) and a pressure drop of 51.34 mm water. By adding more than 25% MOF-5 metal-metal scaffold to activated carbon, the amount of adsorption, breakthrough time and pressure drop were increased.

Among the studied adsorbents, the lowest and highest pressure drop (mm H<sub>2</sub>O) was related to commercially activated carbon and AC / MOF-5 adsorbents, respectively. With increasing moisture content as well as the percentage of organic-metal scaffolds this pressure decrease was more pronounced; because these two factors and their

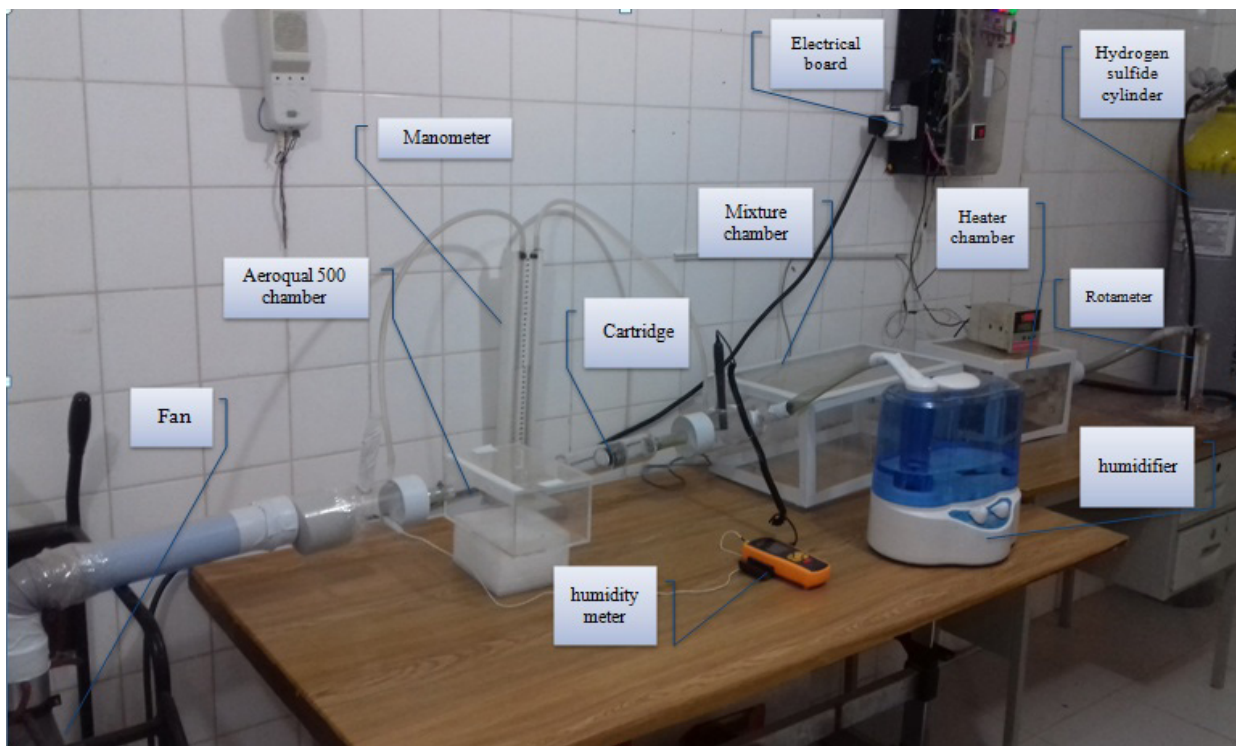


Fig. 1. Simulation system of the human respiratory system and its various components

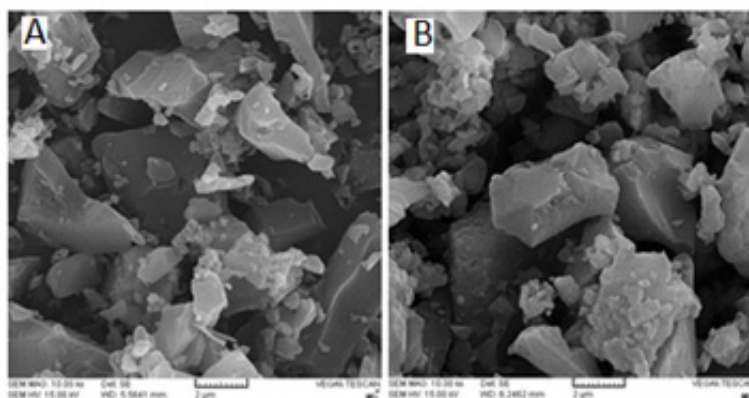


Fig. 2. SEM Figure A: Pure Activated Carbon B: AC / MOF-5 composite

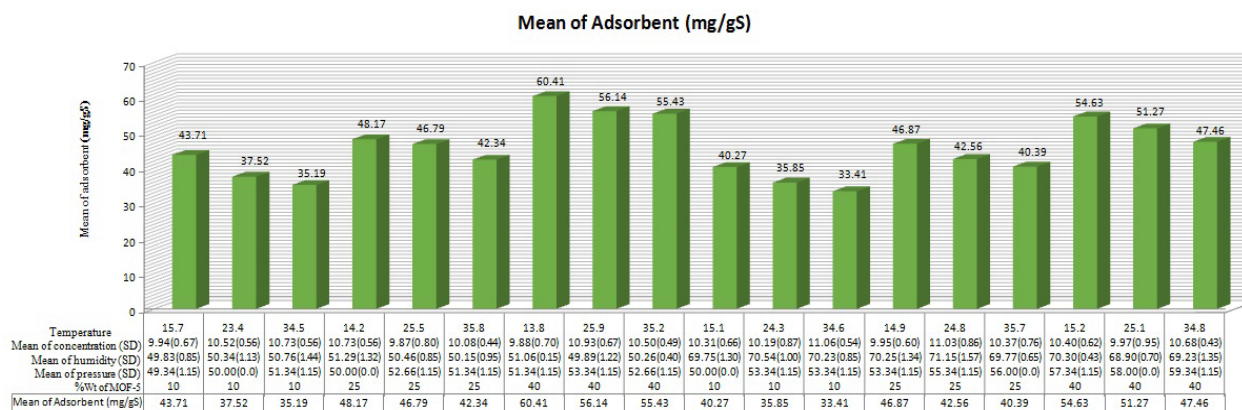


Diagram 1. Average H2S adsorption rate at 10 ppm concentration of AC / MOF-5 adsorbent in different weight percentages and influence of temperature, humidity and pressure factors

effects on absorption increased positive pressure on the pump side for suction and consequently increased pressure drop.

As the results showed, by adding organic-metal MOF-5 scaffold to the activated carbon, the amount of adsorption and breakthrough time was increased; however, its pressure drop also increased. The standard deviations (SD), amount of adsorption, and Breakthrough time in the adsorbents were lower and more stable, which could be due to the high equilibrium constant of zinc compared to other metals.

#### 4. Conclusion

Due to the porous structure, high specific surface area, and most importantly, having Zn-O-C groups, AC /MOF-5 composite adsorbent increased the adsorption rate as well as the pollutant breakthrough time. However, it showed a relatively higher pressure drop than commercial activated carbon (AC). This study aimed to optimize a carbon adsorbent that could be used as a cartridge for the respiratory masks. Generally, our results showed that these adsorbents can be used for low humidity and 50 ppm concentration of hydrogen sulfide gas.

#### 5. Acknowledgements

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