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Experimental and computational investigation of adsorption performance of TC-5A and PSA-5A for manned spacecraft

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Abstract Two kinds of molecular sieve materials, TC-5A and PSA-5A, were produced to satisfy with special requirement of manned space flight. Their CO_2 adsorption performances were investigated and compared through two experiments, the thermo gravimetric analysis (TGA) experiment and packed bed column experiment. Besides, some kinetic equations were compared according to the TGA experimental data, and their errors were analyzed. Finally, the classic linear driving force (LDF) model is improved to the new Avrami's model, and two models are analyzed based on the packed bed data. The TGA data shows that the CO_2 loading has an approximately linear relationship with the CO_2 concentration, and the best fit adsorption temperature range is from 283 to 303 K. The packed bed column results show that water vapor in air can affect the CO_2 adsorption performance badly. The new Avrami's model is proved more suitable to reflect the complex adsorption mechanism for two molecular sieves. The materials are proved having much better adsorption capacity than the other adsorbents with room temperature and low CO_2 concentration ($\leqslant$1.0% in volume), and they can meet the aerospace requirements. This work will benefit the optimal design and simulation of the air revitalization (AR) system for Chinese manned spacecraft.

1. Introduction

CO_2 adsorption and separation technology, such as the solution absorption, membrane separation technique, cryogenic techniques and adsorption over solid sorbents,[1,2] have been explored and widely employed in industrial field. Some mature technologies are even applied to the manned spacecraft, like the Apollo, Skylab and International Space Station (ISS).

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Short-duration manned spacecraft, such as Mercury, Apollo and Space Shuttle of America, "Shenzhou" series of China, generally adopts hydroxide adsorbent in non-regenerative way.[3] But a regenerative environmental control system (ECS) needs to be developed in order to keep cabin's atmospheric quality control for its complex long-term space exploration missions.[4,5] At present, the integrated air revitalization (AR) subsystem has low adsorption efficiency in regenerative process,[6] and the high-efficiency adsorbent needs to be developed for the closed-loop AR subsystem to satisfy the requirement of long-duration manned spacecraft.[5,7–9] As the adsorption performance of adsorbents determines the system's character, such as volume, mass, cost of power, cycle duration, service life and the possible pollution,[3,6,10,11] the adsorption performance of adsorbent should be investigated in great detail.

In the past few years, various adsorbents have been developed and applied in separation processes in industry. The materials include Zeolite 3A and 4A, carbon molecular sieves (CMS), natural clinoptilolite membrane, molecular basket sorbent (MBS), hollow polymeric fibers, oxide octahedral molecular sieve (OMS-2) catalysts, etc.[12–19] Some of them even considered the influencing factors, such as initial concentrations, temperatures, and particle sizes. According to the four consecutive elementary steps of adsorption process mechanism, different equations for particles and the fixed bed have been proposed, including the Pseudo-first order equation, Elovich's equation, Pseudo-second order rate equation, Avrami's kinetic equation and Fractional order kinetic equation.[20–28] Besides, the mass transfer mechanism in a fixed bed column can be described by modeling and simulation so as to predict the adsorbent performance under any condition.[1,6,29–34]

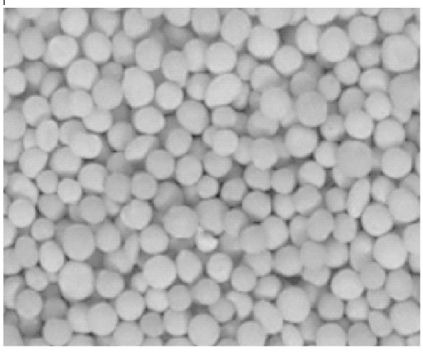
In this paper, two molecular sieves materials, TC-5A and PSA-5A, are investigated regarding their adsorption performance for the future manned space application in China. The CO_2 adsorption performance experiments for particles were tested by the TGA experiment, and the best fit kinetic equation is proposed based on the experimental results. In addition, the influences of some factors, such as initial concentration, temperature and relative humidity (RH), on the CO_2 adsorption are also studied in the packed column experiments. Finally, the improved mathematical model for two adsorption materials in the fixed bed is established by using an Avrami's equation.

2. TC-5A and PSA-5A molecular sieve for manned spacecraft

The CO_2 adsorption performance of molecular sieve determines the efficiency of AR subsystem,[6] hence the development of materials is one of the critical factors for the manned technologies. For this purpose, two kinds of molecular sieves products, PSA-5A and TC-5A, were made for the future manned space application in China. The producing process has been adjusted a lot to come up with the requirement of the manned environment. Fig. 1 shows the formation images of TC-5A and PSA-5A, two molecular sieves used basically identical raw materials, but shaped different average particle sizes. The physical parameters are shown in Table 1.

The standard tests show that their rigidity, thermal stability and mean diameter can satisfy special requirements of AR subsystem. Their thermal vacuum desorption and revitalization in packed bed column are easy to carry out under the condition of 423–573 K and low pressure vacuum (< 100 Pa).

(a) TC-5A molecular sieve



(b) PSA-5A molecular sieve

Fig. 1 Two molecular sieve materials.

Table 1 Physical parameters of molecular sieves.

Parameter	TC-5A	PSA-5A
Porosity ε_b (%)	0.500	0.454
Density ρ_p (kg/m^3)	1223	1223
Specific surface area A_s (m^2/g)	552	647
Mean diameter D_p (mm)	2.00	0.75
Pore volume V (10^{-6} m^3/g)	0.27	0.40

3. TGA experiments and adsorption kinetic equations

In order to investigate the CO_2 adsorption performance of two molecular sieves and to build the corresponding kinetic equations, the TGA experiments were carried out at different concentration and temperature conditions.

The CO_2 adsorption of molecular sieve is a physical process and its equilibrium adsorption capacity is greatly influenced by the adsorption temperature and the CO_2 concentration. In the following experiments, the isothermal adsorption process would be used to obtain the CO_2 adsorption performance. In the experiments, the temperature range was 293–323 K and the CO_2 concentration was less than 1.0% in volume.

3.1. Experiments setup and procedure

Schematic diagram and apparatus photo of TGA experiment are shown in Figs. 2 and 3, respectively. The experimental design steps are as follows: