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Effect of the isotherm shape on water removal from combustion gases using fixed bed adsorption column

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Abstract

This study evaluated the dimensions of a fixed bed adsorption column for water removal from a water-saturated gas stream at low pressures using chabazite, alumina and silica as adsorbents to evaluate the effect of the shape of the different isotherms on the process. Favorable and unfavorable pressure ranges of the isotherms of these materials were evaluated. Fixed bed adsorption was simulated for the three adsorbent samples, indicating that chabazite presented the lowest concentration dispersion among them, due to a wider favorable pressure range. On the other hand, silica presented unfavorable behavior in practically all pressure ranges. The amount of adsorbent and consequently the column length were lower for chabazite and higher for silica. These results demonstrate the influence of the isotherm shape in the process of removal of water saturated streams when using fixed bed adsorption.

Keywords: Adsorption; Fixed bed; Isotherm shape; Water; Simulations

1. Introduction

For decades, energy from combustion has been used in electricity generation and thermal production processes, with CO_2 and steam being the main combustion products [1]. However, anthropogenic CO_2 emissions have significantly increased since the 1950s, becoming the primary contributor to global warming and consequently leading to the rise in sea levels [2]. It is important to note that a significant portion of these emissions originates from the combustion of fossil fuels, for example, in coal-fired power plants, as coal is a cost-effective and relatively abundant resource for power generation [3].

Adsorption processes, using zeolites, are considered an option for CO2 capture. The strong hydrophilic nature of zeolites impairs their ability to effectively adsorb CO2. It is thus necessary to remove the moisture before the CO2 separation process using adsorption. This may be done using fixed bed adsorption columns, in which chabazite, silica, and alumina may be employed as adsorbents, a process also widely used in the drying of natural gas [4]. The selection of an adsorbent depends on the affinity of the material for the adsorbate and its regeneration strategy [5]. Zeolites are extensively used in industrial applications as adsorbents, due to their high affinity for water [4]. Other cheaper adsorbents, such as silica gel and alumina, also have good affinity for water. However, despite its high surface area, silica gel is not as effective as zeolites at low relative pressures [6,7]. Activated alumina adsorbents may also be used, due to their relatively high chemical and mechanical stabilities, as well as their substantial water adsorption capacity (between 20-38 wt%) [8].

This study compares the efficacy of silica, alumina, and chabazite in fixed-bed water adsorption at low water pressures. This is done by model simulations, using mass and energy balances of the fixed-bed adsorption process for water removal from post-combustion gases.

2. Materials and Methods

2.1 Materials

A commercial sample of zeolite of natural occurrence, Chabazite (CHA), shaped as pellets of 1.6 mm of diameter and 5 mm in length, was used [9]. Commercial silica and alumina samples were used as received.

2.2 Water vapor adsorption isotherms

Water vapor isotherms are key parameters for dynamic analysis. They were experimentally measured in an Intelligent Gravimetric Analyzer – IGA 002 (Hiden Isochema Ltd., UK). The device has an ultra-vacuum pump (UHV) and a microbalance (± 1µg resolution) with temperature and pressure control. The temperature inside the measuring cell where adsorption takes place is monitored by a thermocouple located about 5 mm from the sample holder and maintained by a thermostatic bath. The pressure is controlled by three pressure transducers in the ranges of 0 – 10 mbar, 0 – 100 bar, 0 – 1 bar. The water vapor used in the equilibrium test is generated at 55°C in a reservoir containing deionized water that has undergone a degassing stage, where the dissolved air present in the system is removed by steam generation cycles and vacuum application. The pressure range of the tests is therefore limited to the water vapor pressure at 55°C (157.6 mbar). Before each test, the samples were regenerated at 300 °C for 10 h and under a vacuum of less than 10-6 bar. In addition, the data obtained were adjusted according to the proposed model of Aranovich and Dohanue [10].

2.3 Mathematical model

The mathematical model of Morales-Ospino et al. [11] was used for fixed bed adsorption, as well as the associated boundary conditions and equations. The following conditions were used in the model:

- Runoff is axially dispersed for concentration and temperature;
- Local thermal equilibrium between the gas and the adsorbent particles;
- The mass transfer rate of each component from the fluid phase to the particle is represented by a linear driving force (LDF) model;
- The gas phase behaves like an ideal gas mixture;
- There are no gradients of concentration, temperature and pressure in the radial direction.

2.4 Experimental data for simulations

Other parameters required for the simulation, such as particle porosity, solid density, pore volume, specific volume of the solid, mass transfer coefficients, and packing density, were measured in our lab. For the silica simulations, the same physical parameters of alumina were used, due to the lack of specific data for silica. Multicomponent isotherms were not determined, assuming negligible affinity of the other gases with water. The simulations varied the outlet pressure between 1.1 and 1.5 bar and adjusted the bed length to ensure operation for at least 24 hours before regeneration, while keeping other parameters constant. Simulation data include feed of gas at 25°C saturated with water, with flow rate of 2000 NL/min, an internal column diameter of 0.80 m, and a packing density of 660 kg/m^3. Gas and wall properties were estimated from available literature, and energy, momentum, and mass transport parameters were proposed and solved using Gproms ModelBuilder (Process Systems Enterprise Inc., UK).

3. Results and discussion

The isotherms for water adsorption on the three studied adsorbent samples are shown in Figure 1. It may be seen that the silica sample presents a highly unfavorable isotherm shape at all pressures. On the other hand, the chabazite sample presents a highly favorable isotherm shape at low pressures, only becoming slightly unfavorable above 2000 Pa. For the alumina sample, an intermediate behavior may be observed from the data available.

The results of the column simulations are shown in Figure 2, for three different outlet pressures. The concentration profiles of water within the column at the breakthrough time, 10,000 seconds, are shown in Figure 2. From these profiles, it may be noted that the isotherm shape has considerable effect on the concentration profiles inside the adsorption column, with chabazite presenting a very sharp concentration profile.

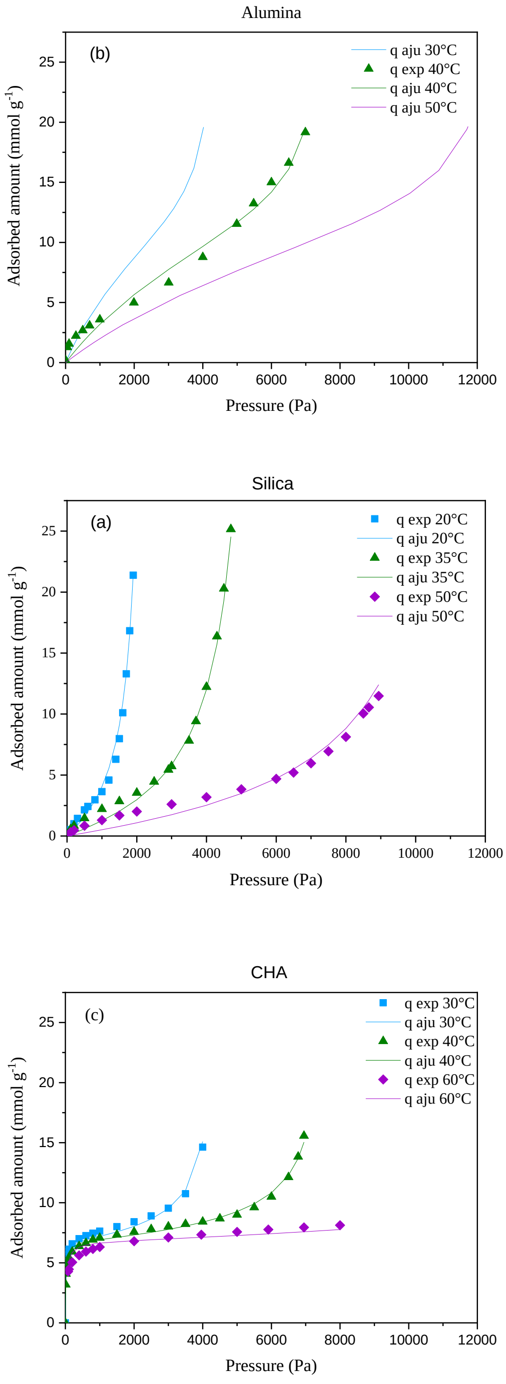

Figure 1. Water vapor adsorption isotherms on sílica (a), alumina (b) and chabazite (c) samples. Experimental data (squares), Aranovich and Dohanue model (lines).

On the other hand, silica and alumina show dispersed profiles, with silica presenting the higher concentration dispersion of the studied samples. In addition, it may be seen that the outlet pressures did not change significantly the breakthrough profiles in the column.

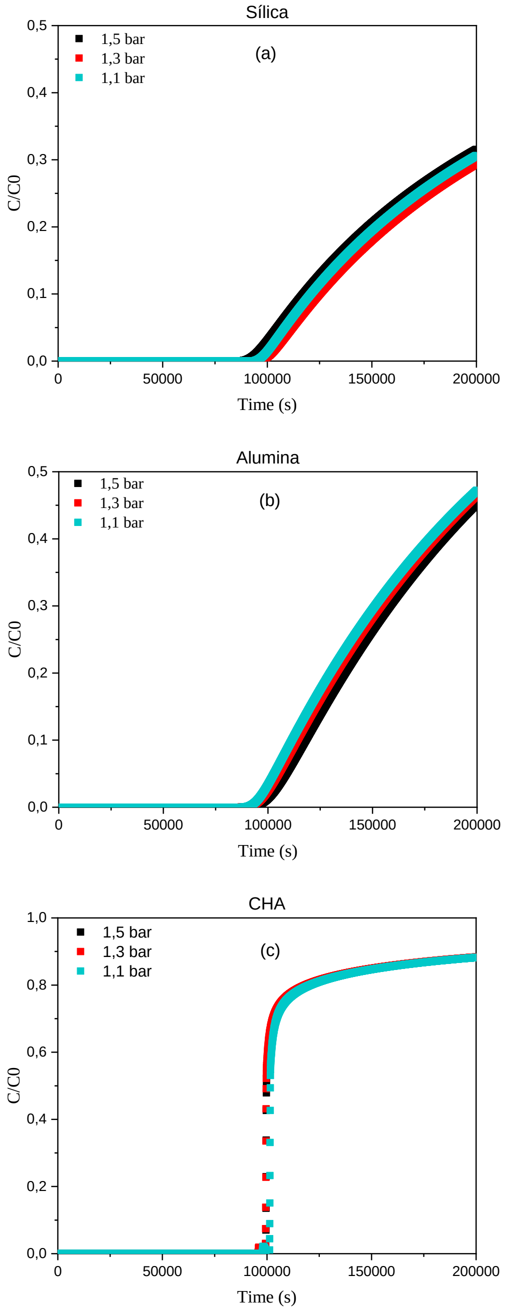

Figure 2. Column concentration profiles for silica (a), alumina (b) and chabazite (c) after 10,000s.

Finally, the estimated column lengths and amounts required for each adsorbent at different outlet pressures, for the required process of water removal from the post-combustion gases, are shown in Table 1. It may be seen that lower lengths and amounts are needed for the chabazite sample, while the silica adsorbent presents the highest needed length and amount among the three studies samples.

Table 1. Column lengths and amounts required for each adsorbent at different outlet pressures.

Outlet pressure (bar)	**Alumina**		**Silica**		**Chabazite**	
	Bed Length (m)	Amount (kg)	Bed Length (m)	Amount (kg)	Bed Length (m)	Amount (kg)
1.1	2.30	763	4.90	1625	1.35	448
1.3	1.91	633	4.18	1386	1.13	376
1.5	1.64	544	3.44	1141	0.955	317

4. Conclusions

This study showed that the amounts of adsorbents needed to remove moisture from the same saturated stream of water in an adsorption column depends strongly on the shape of the isotherms. Favorable isotherms indicate the need of less length and amount of adsorbent inside the column. For materials with similar maximum adsorption capacities, those with a higher pressure range in which the isotherm is favorable are more effective for removing moisture in a fixed bed over a wide pressure range.

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