SUPPORTING INFORMATION

Separation of CO_2 from Air by Temperature-Vacuum Swing Adsorption Using Diamine-Functionalized Silica Gel

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N_2 Adsorption/Desorption Isotherms

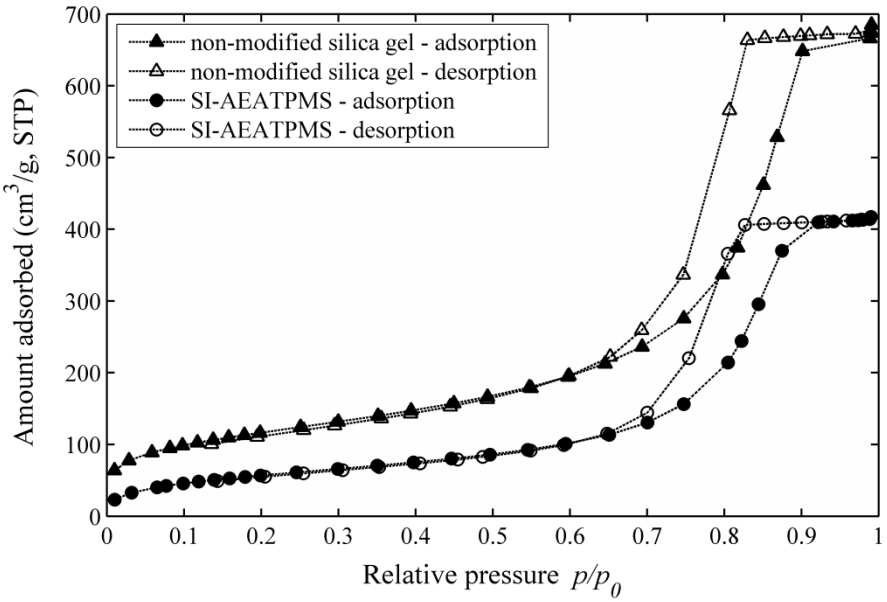

Figure S1. N_2 adsorption (closed symbols) and desorption (open symbols) isotherms for non-modified silica gel support (ZEObeads™ B2, triangles) and SI-AEATPMS sorbent material (circles).

Energy Requirements

The energy requirements for sorbent regeneration in the TVS process were estimated using the assumptions summarized in Table S1. The work W_{comp} required for compression of the CO_2 from desorption pressure to ambient pressure was calculated according to Eq. (S**1**. The heat (low-temperature heat at below 95 °C) required for heating up the sorbent material to the desorption temperature Q_{sens} and for desorption of CO_2 and co-adsorbed H_2O Q_{des} was calculated according to Eq. (S**2** and Eq. (S**3**, respectively. The total required heat Q is the sum of Q_{sens} and Q_{des} (Eq. (S**4**). A ratio of co-adsorbed water and adsorbed CO_2 of approximately 1 was assumed.[1]

$$W_{comp} = \frac{1}{\eta_{pump}} \cdot R \cdot T \cdot ln\left(\frac{p_{amb}}{p_{des}}\right) \quad \text{(S1)}$$

$$Q_{sens} = \frac{1}{\Delta q_{\mathrm{TVS}}} \cdot c_p \cdot \Delta T \quad \text{(S2)}$$

$$Q_{des} = Q_{des,CO2} + Q_{des,H2O} \quad \text{(S3)}$$

$$Q = Q_{sens} + Q_{des} \quad \text{(S4)}$$

Assumption	Symbol	Value	Source
Cyclic CO_2 capacity of sorbent (SI-AEAPTMS material used in this work)	Δq_{TVS}	0.2 mmol/g	this work
Cyclic CO_2 capacity of sorbent (advanced sorbent material with higher cyclic capacity)	Δq_{TVS}	2 mmol/g	[2]
Heat capacity of the sorbent material (silica)	c_p	$0.9\ \frac{\mathrm{kJ}}{\mathrm{kg \cdot K}}$	[3]
Temperature difference between adsorption and desorption	ΔT	65 K	this work
Heat of desorption, CO_2	$Q_{des,CO2}$	$\approx 90\ \frac{\mathrm{kJ}}{\mathrm{mol}}$	[4, 5]
Heat of desorption, co-adsorbed H_2O	$Q_{des,H2O}$	$\approx 47\ \frac{\mathrm{kJ}}{\mathrm{mol}}$	[4]
Amount of co-adsorbed H_2O	n_{H2O}/n_{CO2}	1	[1]
Desorption pressure	p_{des}	100 mbar	this work
Vacuum pump efficiency (with respect to isothermal compression at T = 350 K)	η_{pump}	0.7	estimation

Table S1. Assumptions for energy requirement estimation.

References

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