Analysis and modelling of CO_2 adsorption from air

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Introduction and Objectives

Global CO_2 emissions are increasing, with the global energy demand, reaching a historical high of 33.1 Gt CO_2 in 2019 [1]. As a consequence, atmospheric CO_2 concentrations have increased with an average rate of 2.4 ppm/year in the past decade, achieving 414 ppm in May 2019 [2]. With the aim to solve this environmental problem, the direct air capture (DAC) has been proposed to capture CO_2 from air as a GHG mitigation and negative emissions technology. Several technologies are developed by different companies as shown in Fig. 1. In this context, the objectives of this research work are:

- Analyze and model adsorption technology using three different metal organic frameworks and two different amine functionalized sorbents
- Compare the results with those from the Climeworks company

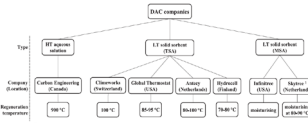

Figure 1. Technologies and companies active in the field of CO_2 DAC [3]

Materials and Methods

Adsorption/Desorption model equations

- Gas phase material balance

$$\frac{dc_{co2}}{dt} = -v_{gas}\frac{dc_{co2}}{dz} + D_z\frac{d^2c_{co2}}{dz^2} - \frac{1-\varepsilon_b}{\varepsilon_b}\rho_p\frac{dq}{dt}$$

- Adsorbed phase material balance

$$\frac{dq}{dt} = k_t(q^* - q)$$

Sorbents and adsorber definition

1) SI-AEATPMS ([N-(2-aminoethyl)-3-aminopropyl]trimethoxysilane (AEATPMS) grafted on silica gel) (Class 2)

2) APDES-NFC-FD (3-aminopropylmethyldiethoxysilane (APDES) onto nanofibrillated cellulose (NFC)) (Class 2)

3) MOFs: MIL-101, MOF-177, MOF-5

Initial and boundary conditions for the adsorption phase model

$$c_{co2} = c_{co2,Inlet} \quad z = 0, t = 0 \qquad c_{co2} = c_{co2,Inlet} \quad z = 0, t > 0$$

$$c_{co2} = 0 \quad 0 < z \leq L, t = 0 \qquad \frac{dc_{co2}}{dz} = 0 \quad z = L, t > 0$$

$$q = 0 \quad t = 0$$

Initial and boundary conditions for the desorption phase model

$$c_{co2} = c_{co2,Inlet} \quad t = 0 \qquad c_{co2} = 0 \quad z = 0, t > 0$$

$$q = q_{inlet} \quad t = 0 \qquad \frac{dc_{co2}}{dz} = 0 \quad z = L, t > 0$$

Area footprint excl. options	20 m^2
Height	3.2 m
CO_2 flow rate, inlet	180 kg/day
Y_{CO2}, inlet	0.0004
Air flow rate, inlet	246800 m^3/day

Table 1. Data of adsorber

Results

	MIL-101	MOF-177	MOF-5	SI-AEATPMS	APDES-NFC-FD	Climeworks (APDES-NFC-FD)
Full cycle (hr)	0.01	0.09	0.29	89.4	9.5	4-6 (*)
Cycle/day	207	271	81	0.27	2.5	6-4
CO_2 captured (kg/day)	73	72	68	147	151	135
Average single pass recovery	0.52	0.59	0.53	0.86	0.89	0.9
Regeneration mode	TSA	TSA	TSA	TSA	TSA	TSVA
Regeneration temperature (K)	373	373	373	383	373	373
Electric consumption (kWh_{el}/tonCO_2)	1388 (fan)	1218 (fan)	1373 (fan)	322 (fan)	270 (fan)	200-450 (fan+control)
Regeneration energy (kWh_{th}/tonCO_2)	1068100	1296600	493900	1884	1427	1500-2000
CAPEX ($/ton$CO_2$)	825	827	885	408	395	600 [4]
OPEX ($/ton$CO_2$)	39000	5910	3320	752	542	

Table 2. Results of adsorption modelling for different sorbents (*After 5 h adsorption time, the CO_2 uptake curves are still considerably increasing, while the corresponding H_2O curves have reached a constant plateau for all RH values [5])

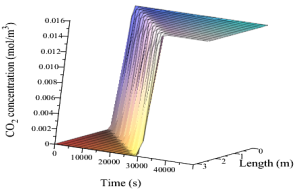

Figure 2. CO_2 concentration for the adsorption phase with APDES-NFC-FD sorbent

Conclusions

- APDES-NFC-FD sorbent has lower energy requirements in terms of fan power and energy for regeneration
- MOFs have an electric consumption comparable to that reported in the literature and greater than those of amine functionalized sorbents [3]
- MOFs have a high value for energy regeneration due to a low value of equilibrium loading, that is a critical parameter
- OPEX and CAPEX are greater than that of Climeworks due to the different economy of scale

References

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