A Comparative Study of Different Sorbents in the Context of Direct Air Capture (DAC): Evaluation of Key Performance Indicators and Comparisons

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Supporting Information

Table S1 Dimensionless number values of the mathematical model

	MOF-177	MOF-5	MIL-101	APDES-NFC-FD	SI-AEATPMS
			Adsorption stage		
Re	$1.30 \cdot 10^{4}$	$1.87 \cdot 10^{4}$	$1.87 \cdot 10^{4}$	$2.20 \cdot 10^{3}$	$2.08 \cdot 10^{4}$
Sc	$2.62 \cdot 10^{-3}$	$1.81 \cdot 10^{-3}$	$1.81 \cdot 10^{-3}$	$2.03 \cdot 10^{-2}$	$8.57 \cdot 10^{-4}$
Sh	$4.74 \cdot 10^{1}$	$5.21 \cdot 10^{1}$	$5.21 \cdot 10^{1}$	$3.28 \cdot 10^{1}$	$4.37 \cdot 10^{1}$
			Desorption stage		
Re	$1.30 \cdot 10^{4}$	$1.87 \cdot 10^{4}$	$1.87 \cdot 10^{4}$	$2.20 \cdot 10^{3}$	$2.08 \cdot 10^{4}$
Sc	$1.74 \cdot 10^{-3}$	$1.21 \cdot 10^{-3}$	$1.21 \cdot 10^{-3}$	$1.35 \cdot 10^{-2}$	$5.72 \cdot 10^{-4}$
Sh	$4.17 \cdot 10^{1}$	$4.58 \cdot 10^{1}$	$4.58 \cdot 10^{1}$	$2.89 \cdot 10^{1}$	$3.85 \cdot 10^{1}$

Table S2 Inputs used in Matches calculator for cost analysis

Adsorbent bed	
Vessel type	column, no internal, medium
Vessel weight	1200 kg
Material	carbon steel

Fan	
Fan type	axial, small
Fan diameter	14.8 in
Material	carbon steel

Table S3 CAPEX of different adsorbent beds

Sorbent	APDES-NFC-FD	SI-AEATPMS	MIL-101	MOF-177	MOF-5
Fan					
Air flow rate (m^3/h)	$1.03 \cdot 10^4$	$1.03 \cdot 10^4$	$1.03 \cdot 10^4$	$1.03 \cdot 10^4$	$1.03 \cdot 10^4$
Power (kW)	2	2	5	5	5
Diameter (m)	$3.8 \cdot 10^{-1}$	$3.8 \cdot 10^{-1}$	$3.8 \cdot 10^{-1}$	$3.8 \cdot 10^{-1}$	$3.8 \cdot 10^{-1}$
Cost ($)	$2.05 \cdot 10^3$	$2.05 \cdot 10^3$	$2.05 \cdot 10^3$	$2.05 \cdot 10^3$	$2.05 \cdot 10^3$
Adsorber					
Weight shell (kg)	$1.2 \cdot 10^3$	$1.2 \cdot 10^3$	$1.2 \cdot 10^3$	$1.2 \cdot 10^3$	$1.2 \cdot 10^3$
Cost ($)	$3.23 \cdot 10^4$	$3.23 \cdot 10^4$	$3.23 \cdot 10^4$	$3.23 \cdot 10^4$	$3.23 \cdot 10^4$
Equipment cost ($)	$3.44 \cdot 10^4$	$3.44 \cdot 10^4$	$3.44 \cdot 10^4$	$3.44 \cdot 10^4$	$3.44 \cdot 10^4$
Installation ($)	$1.34 \cdot 10^4$	$1.34 \cdot 10^4$	$1.34 \cdot 10^4$	$1.34 \cdot 10^4$	$1.34 \cdot 10^4$
Instrumentation and control ($)	$4.47 \cdot 10^3$	$4.47 \cdot 10^3$	$4.47 \cdot 10^3$	$4.47 \cdot 10^3$	$4.47 \cdot 10^3$
Piping ($)	$1.07 \cdot 10^4$	$1.07 \cdot 10^4$	$1.07 \cdot 10^4$	$1.07 \cdot 10^4$	$1.07 \cdot 10^4$
Electrical ($)	$3.44 \cdot 10^3$	$3.44 \cdot 10^3$	$3.44 \cdot 10^3$	$3.44 \cdot 10^3$	$3.44 \cdot 10^3$
Buildings ($)	$9.97 \cdot 10^3$	$9.97 \cdot 10^3$	$9.97 \cdot 10^3$	$9.97 \cdot 10^3$	$9.97 \cdot 10^3$
Yard improvements ($)	$3.44 \cdot 10^3$	$3.44 \cdot 10^3$	$3.44 \cdot 10^3$	$3.44 \cdot 10^3$	$3.44 \cdot 10^3$
Service facilities ($)	$1.89 \cdot 10^4$	$1.89 \cdot 10^4$	$1.89 \cdot 10^4$	$1.89 \cdot 10^4$	$1.89 \cdot 10^4$
Land ($)	$2.06 \cdot 10^3$	$2.06 \cdot 10^3$	$2.06 \cdot 10^3$	$2.06 \cdot 10^3$	$2.06 \cdot 10^3$
Total direct FCI ($)	$1.01 \cdot 10^5$	$1.01 \cdot 10^5$	$1.01 \cdot 10^5$	$1.01 \cdot 10^5$	$1.01 \cdot 10^5$
Engineering and supervision ($)	$1.1 \cdot 10^4$	$1.1 \cdot 10^4$	$1.1 \cdot 10^4$	$1.1 \cdot 10^4$	$1.1 \cdot 10^4$
Construction expenses ($)	$1.17 \cdot 10^4$	$1.17 \cdot 10^4$	$1.17 \cdot 10^4$	$1.17 \cdot 10^4$	$1.17 \cdot 10^4$
Total indirect FCI ($)	$2.27 \cdot 10^4$	$2.27 \cdot 10^4$	$2.27 \cdot 10^4$	$2.27 \cdot 10^4$	$2.27 \cdot 10^4$
Direct+Indirect cost ($)	$1.23 \cdot 10^5$	$1.23 \cdot 10^5$	$1.23 \cdot 10^5$	$1.23 \cdot 10^5$	$1.23 \cdot 10^5$
Contractor's fee ($)	$6.17 \cdot 10^3$	$6.17 \cdot 10^3$	$6.17 \cdot 10^3$	$6.17 \cdot 10^3$	$6.17 \cdot 10^3$
Contingency ($)	$1.23 \cdot 10^4$	$1.23 \cdot 10^4$	$1.23 \cdot 10^4$	$1.23 \cdot 10^4$	$1.23 \cdot 10^4$
Fixed capital investment ($)	$1.42 \cdot 10^5$	$1.42 \cdot 10^5$	$1.42 \cdot 10^5$	$1.42 \cdot 10^5$	$1.42 \cdot 10^5$
Working capital ($)	$2.51 \cdot 10^4$	$2.51 \cdot 10^4$	$2.51 \cdot 10^4$	$2.51 \cdot 10^4$	$2.51 \cdot 10^4$
CAPEX ($) (USA)	$1.67 \cdot 10^5$	$1.67 \cdot 10^5$	$1.67 \cdot 10^5$	$1.67 \cdot 10^5$	$1.67 \cdot 10^5$
Location factor, 2021	$5.8 \cdot 10^{-1}$	$5.8 \cdot 10^{-1}$	$5.8 \cdot 10^{-1}$	$5.8 \cdot 10^{-1}$	$5.8 \cdot 10^{-1}$
CAPEX ($) (Switzerland)	$9.77 \cdot 10^4$	$9.77 \cdot 10^4$	$9.77 \cdot 10^4$	$9.77 \cdot 10^4$	$9.77 \cdot 10^4$
i	$1 \cdot 10^{-1}$	$1 \cdot 10^{-1}$	$1 \cdot 10^{-1}$	$1 \cdot 10^{-1}$	$1 \cdot 10^{-1}$
lifetime (years)	20	20	20	20	20
CRF	$1.17 \cdot 10^{-1}$	$1.17 \cdot 10^{-1}$	$1.17 \cdot 10^{-1}$	$1.17 \cdot 10^{-1}$	$1.17 \cdot 10^{-1}$
CAPEX ($/year)	$1.15 \cdot 10^4$	$1.15 \cdot 10^4$	$1.15 \cdot 10^4$	$1.15 \cdot 10^4$	$1.15 \cdot 10^4$
CAPEX ($/tonne$CO_2$)	$2.14 \cdot 10^2$	$2.21 \cdot 10^2$	$4.46 \cdot 10^2$	$4.47 \cdot 10^2$	$4.79 \cdot 10^2$

Table S4 OPEX of different adsorbent beds

Sorbent	APDES-NFC-FD	SI-AEATPMS	MIL-101	MOF-177	MOF-5
Raw materials					
Sorbent ($/year)	$4.13 \cdot 10^2$	$8.74 \cdot 10^3$	$8.66 \cdot 10^3$	$6 \cdot 10^3$	$8.67 \cdot 10^3$
Operating labour ($/year)					
Direct supervisory and clerical labor ($/year)					
Utilities					
Electrical energy ($/year)	$1.61 \cdot 10^3$	$1.85 \cdot 10^3$	$3.96 \cdot 10^3$	$3.47 \cdot 10^3$	$3.65 \cdot 10^3$
Thermal energy ($/year)	$1.84 \cdot 10^3$	$2.35 \cdot 10^3$	$6.59 \cdot 10^5$	$7.98 \cdot 10^5$	$2.84 \cdot 10^5$
Cooling water ($/year)	$2.53 \cdot 10^3$	$3.22 \cdot 10^3$	$9.06 \cdot 10^5$	$1.1 \cdot 10^5$	$3.9 \cdot 10^4$
Maintenance and repairs ($/year)	$2.84 \cdot 10^3$	$2.84 \cdot 10^3$	$2.84 \cdot 10^3$	$2.84 \cdot 10^3$	$2.84 \cdot 10^3$
Operating supplies ($/year)	$2.84 \cdot 10^2$	$2.84 \cdot 10^2$	$2.84 \cdot 10^2$	$2.84 \cdot 10^2$	$2.84 \cdot 10^2$
Patent and royalts ($/year)	$1.42 \cdot 10^3$	$1.42 \cdot 10^3$	$1.42 \cdot 10^3$	$1.42 \cdot 10^3$	$1.42 \cdot 10^3$
Direct production costs ($/year)	$1.09 \cdot 10^4$	$2.07 \cdot 10^4$	$1.58 \cdot 10^6$	$9.22 \cdot 10^5$	$3.4 \cdot 10^5$
Depreciation ($/year)	$1.42 \cdot 10^4$	$1.42 \cdot 10^4$	$1.42 \cdot 10^4$	$1.42 \cdot 10^4$	$1.42 \cdot 10^4$
Local taxes ($/year)	$1.42 \cdot 10^3$	$1.42 \cdot 10^3$	$1.42 \cdot 10^3$	$1.42 \cdot 10^3$	$1.42 \cdot 10^3$
Insurance ($/year)	$5.68 \cdot 10^2$	$5.68 \cdot 10^2$	$5.68 \cdot 10^2$	$5.68 \cdot 10^2$	$5.68 \cdot 10^2$
Fixed charges ($/year)	$1.62 \cdot 10^4$	$1.62 \cdot 10^4$	$1.62 \cdot 10^4$	$1.62 \cdot 10^4$	$1.62 \cdot 10^4$
Administrative costs ($/year)	$5.77 \cdot 10^3$	$7.85 \cdot 10^2$	$3.4 \cdot 10^4$	$2 \cdot 10^4$	$7.58 \cdot 10^3$
Distribution and selling costs ($/year)	$5.77 \cdot 10^3$	$7.85 \cdot 10^2$	$3.4 \cdot 10^4$	$2 \cdot 10^4$	$7.58 \cdot 10^3$
Research and development costs ($/year)	$5.77 \cdot 10^3$	$7.85 \cdot 10^2$	$3.4 \cdot 10^4$	$2 \cdot 10^4$	$7.58 \cdot 10^3$
OPEX ($/year)	$2.88 \cdot 10^4$	$3.92 \cdot 10^4$	$1.7 \cdot 10^6$	$9.98 \cdot 10^5$	$3.79 \cdot 10^5$
OPEX ($/tonne$CO_2$)	$5.37 \cdot 10^2$	$7.56 \cdot 10^2$	$6.61 \cdot 10^4$	$3.89 \cdot 10^4$	$1.58 \cdot 10^4$

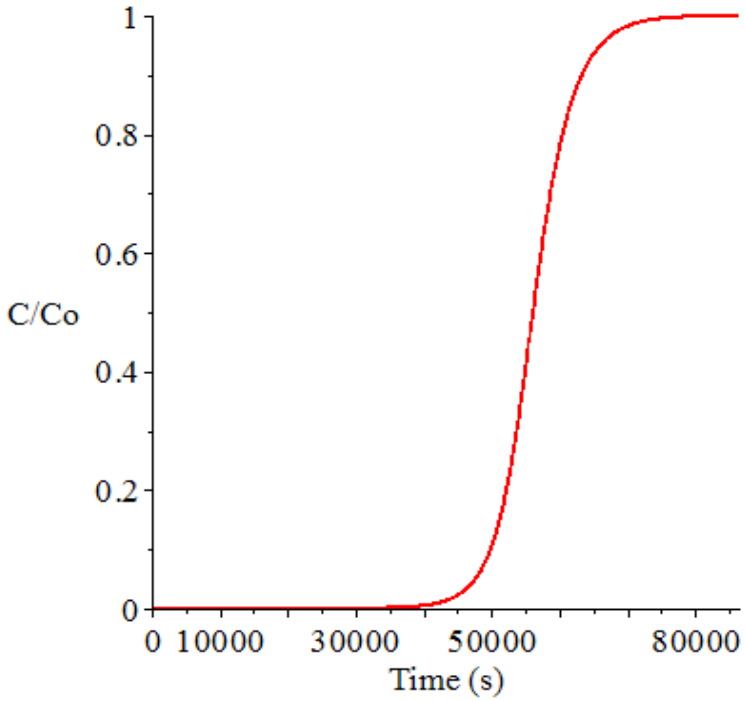

Figure S1 Breakthrough curve (CO_2 concentration at the outlet/CO_2 concentration at the inlet) for the experimental apparatus used in Wurzbacher (2015)

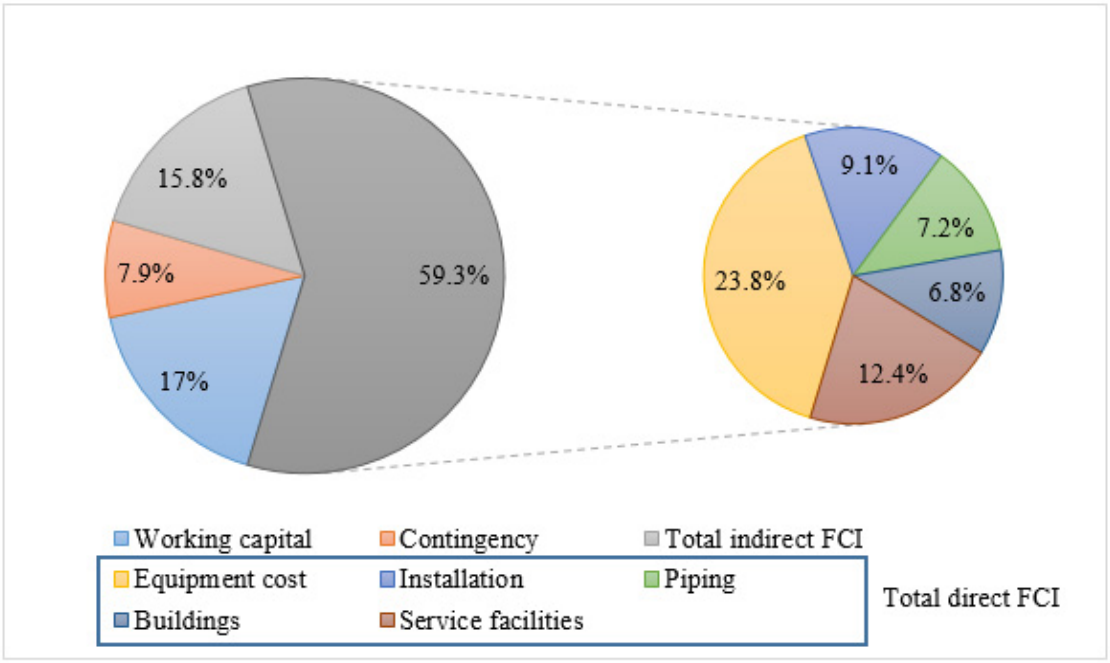

Figure S2 Breakdown of the main contributions (cut-off 5%) to CAPEX for all adsorbent beds

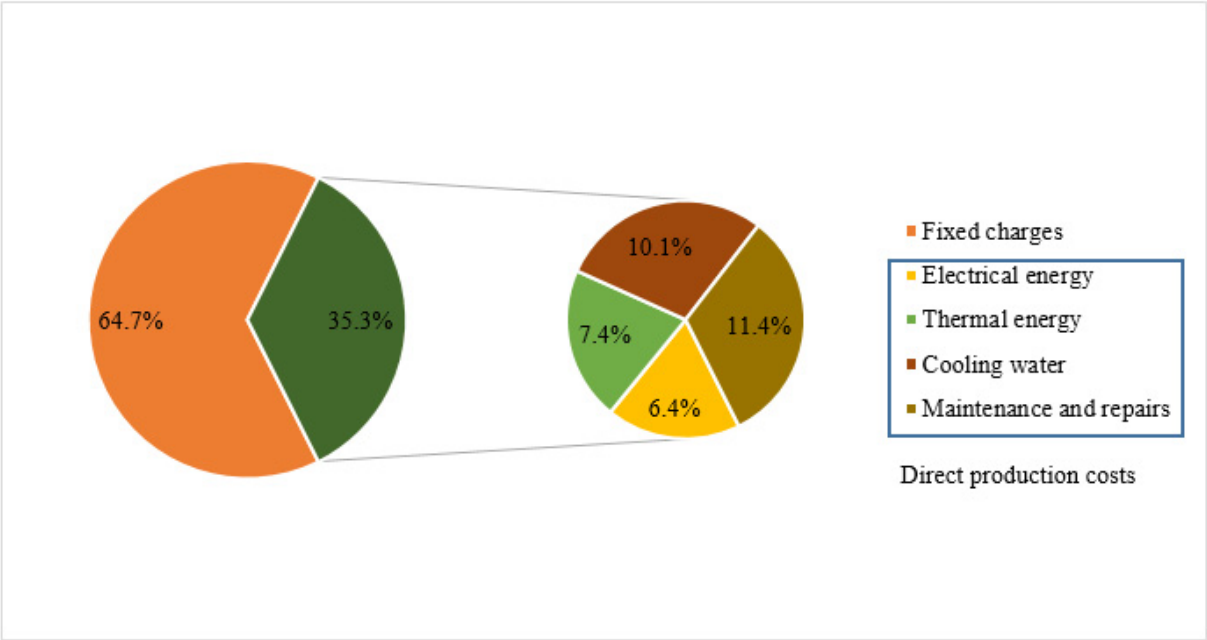

Figure S3 Breakdown of the main contributions (cut-off 5%) to OPEX for the adsorbent bed with APDES-NFC-FD

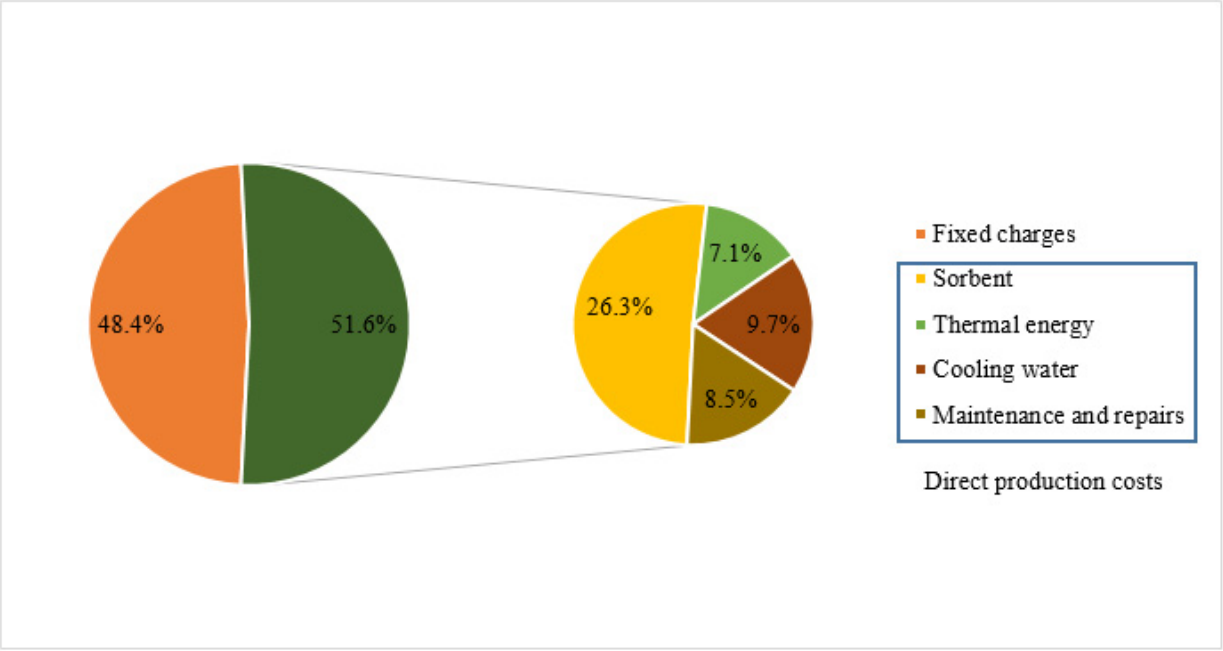

Figure S4 Breakdown of the main contributions (cut-off 5%) to OPEX for the adsorbent bed with SI-AEATPMS

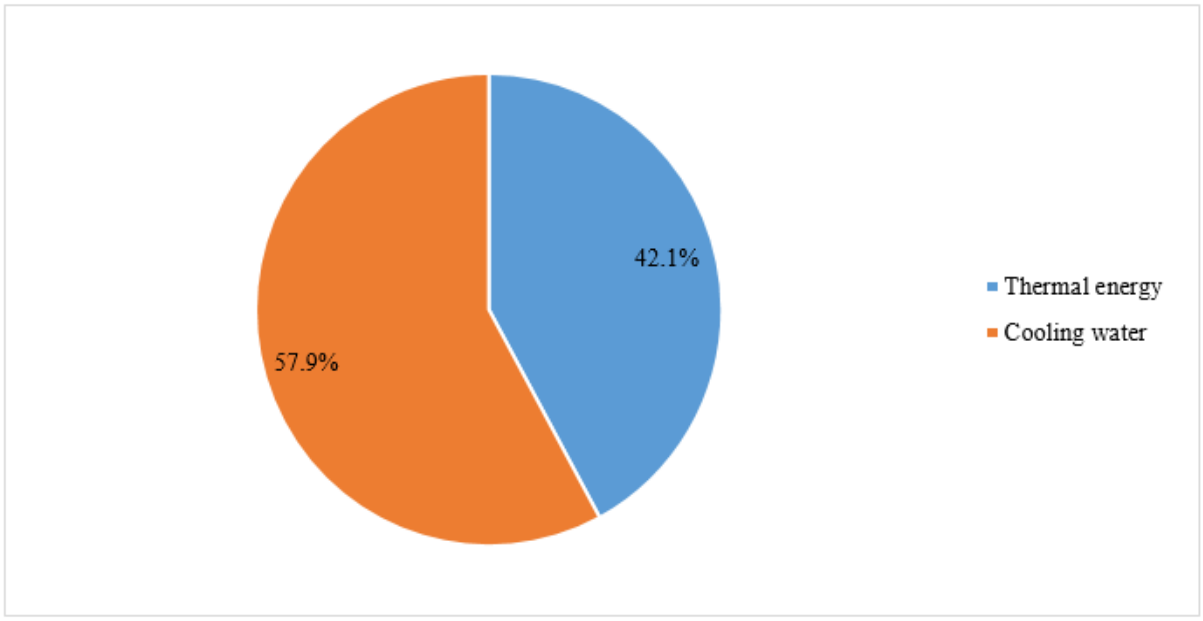

Figure S5 Breakdown of the main contributions (cut-off 5%) to OPEX for the adsorbent bed with MIL-101

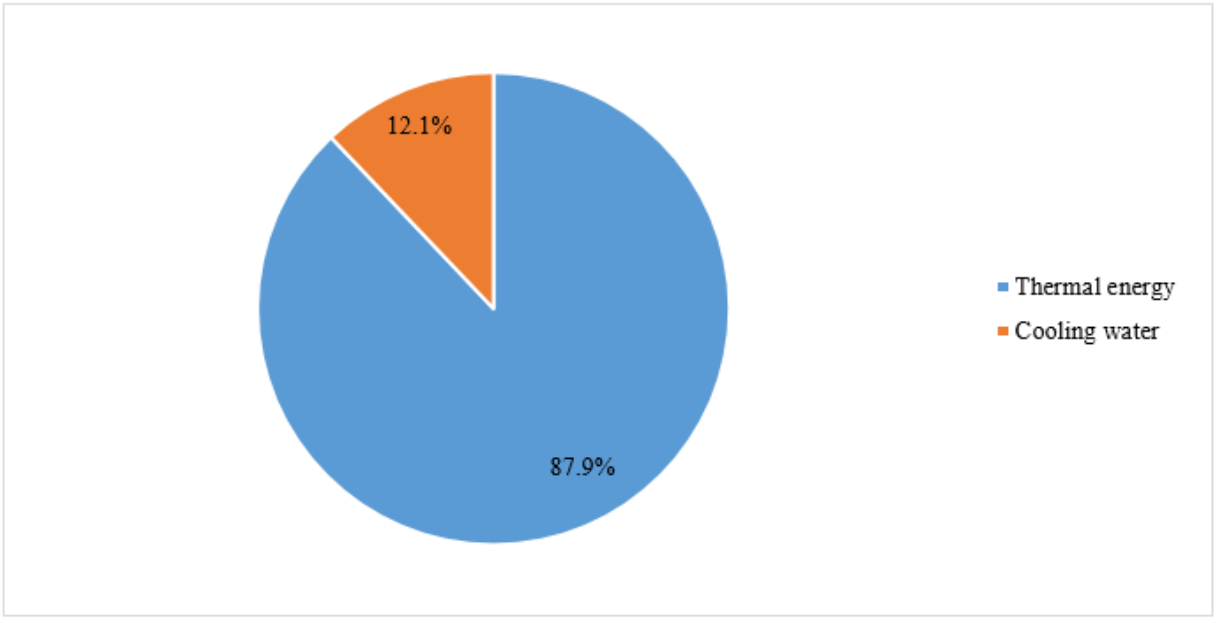

Figure S6 Breakdown of the main contributions (cut-off 5%) to OPEX for the adsorbent bed with MOF-177

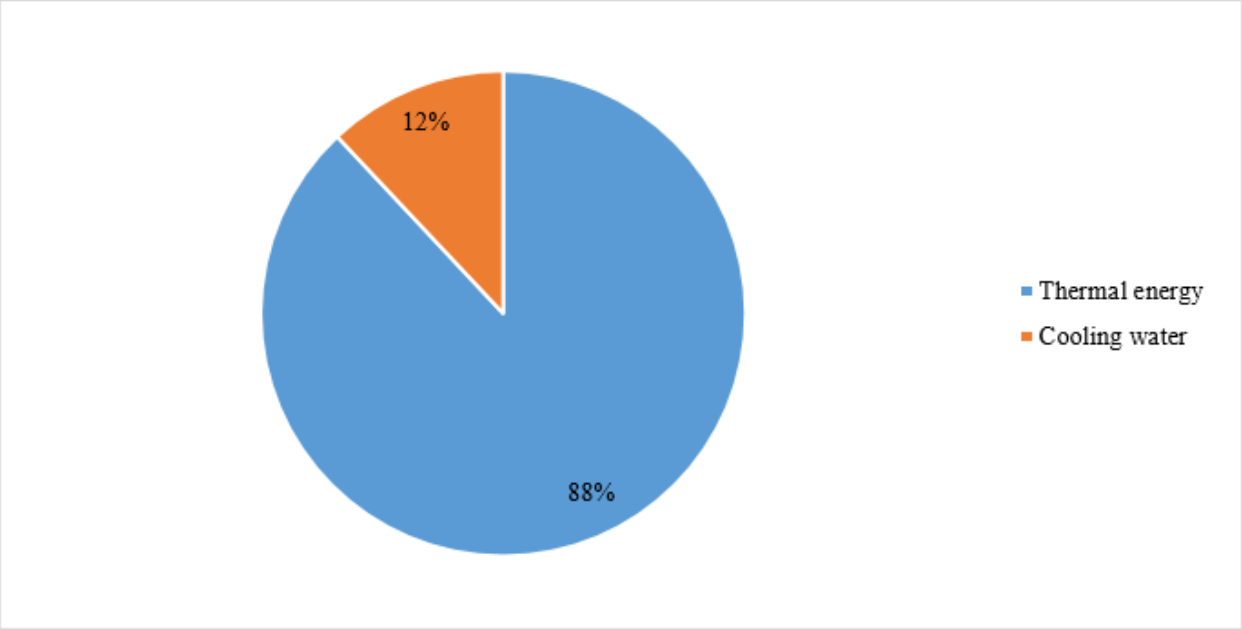

Figure S7 Breakdown of the main contributions (cut-off 5%) to OPEX for the adsorbent bed with MOF-5

Reference

Wurzbacher, J.A. 2015. Development of a temperature-vacuum swing process for CO_2 capture from ambient air, PhD Thesis, ETH Zurich.