PCCC-8

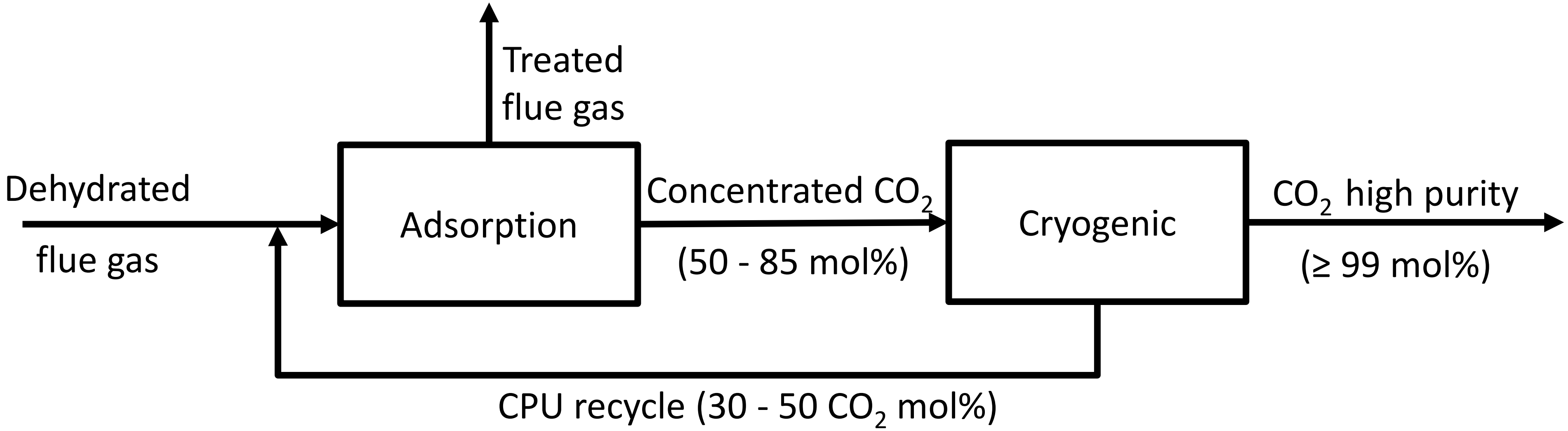
Optimization of a hybrid CO_2 capture process combining a vacuum pressure swing adsorption with MOFs and a carbon purification unit

Arnaud Henrotin[a], Alexis Costa[a], Nicolas Heymans[a], Lionel Dubois[b], Diane Thomas[b], Guy De Weireld[a]

[a] Thermodynamics and Mathematical Physics Unit, University of Mons (UMONS), Place du parc 20, 7000 Mons, Belgium
[b] Chemical and Biochemical Process Engineering Unit, University of Mons (UMONS), Place du parc 20, 7000 Mons, Belgium

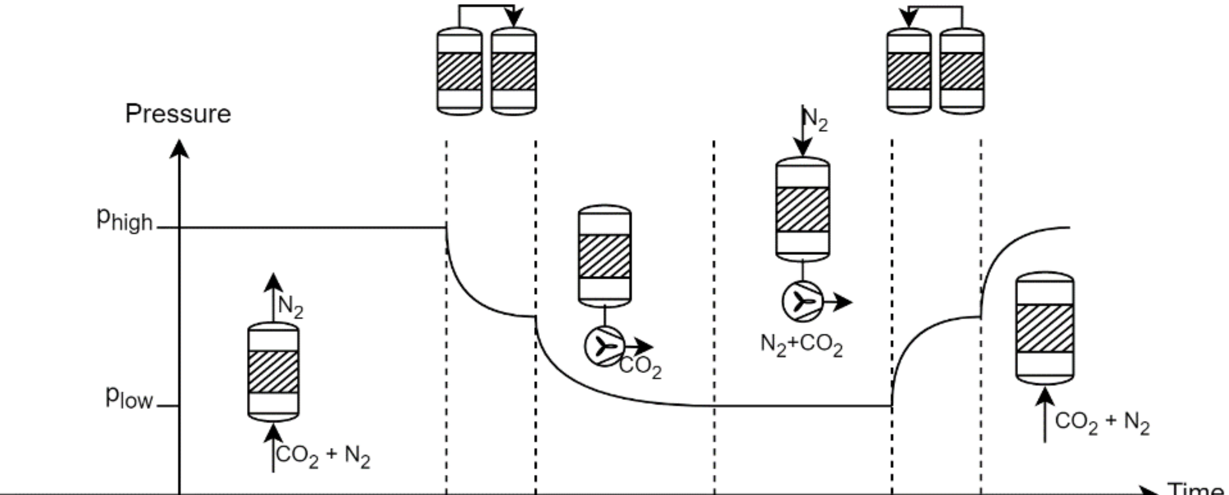
VPSA + CPU objectives

- Transportation of CO_2 and storage required a high purity of CO_2 (ex: 99.81% for Northern Light)
- Such purity cannot by obtained by adsorption process alone while maintaining a high recovery (> 90%)
- Cryogenic processes can reach high purity but need pre-concentrated CO_2 to be efficient
- By coupling both adsorption and cryogenic, high recovery and purity can be obtained



Adsorption process (VPSA)

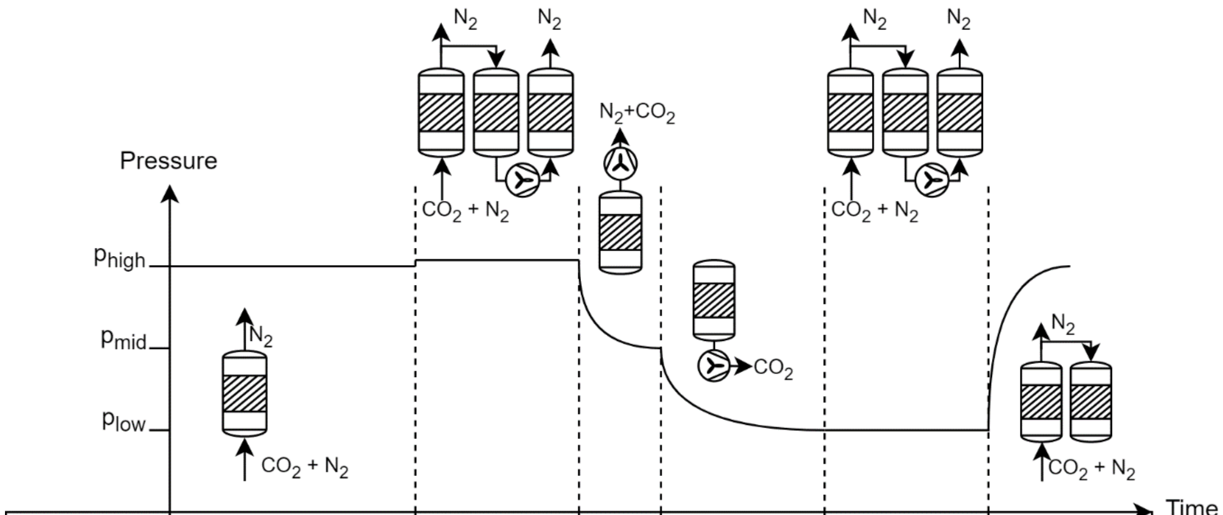
2-bed 5-step cycle (Skarstrom)



Bed 1	Adsorption		Pressure Equalization	Blowdown		Purge	Pressure Equalization	Pressu-rization
Bed 2	Blow-down	Purge	Pressure Equalization	Pressu-rization	Adsorption		Pressure Equalization	Blow-down

+ Process well known in adsorption (3 parameters)
+ 2 Adsorption beds ; 1 compressor ; 1 vacuum pump
- Purity obtained is low for high recovery

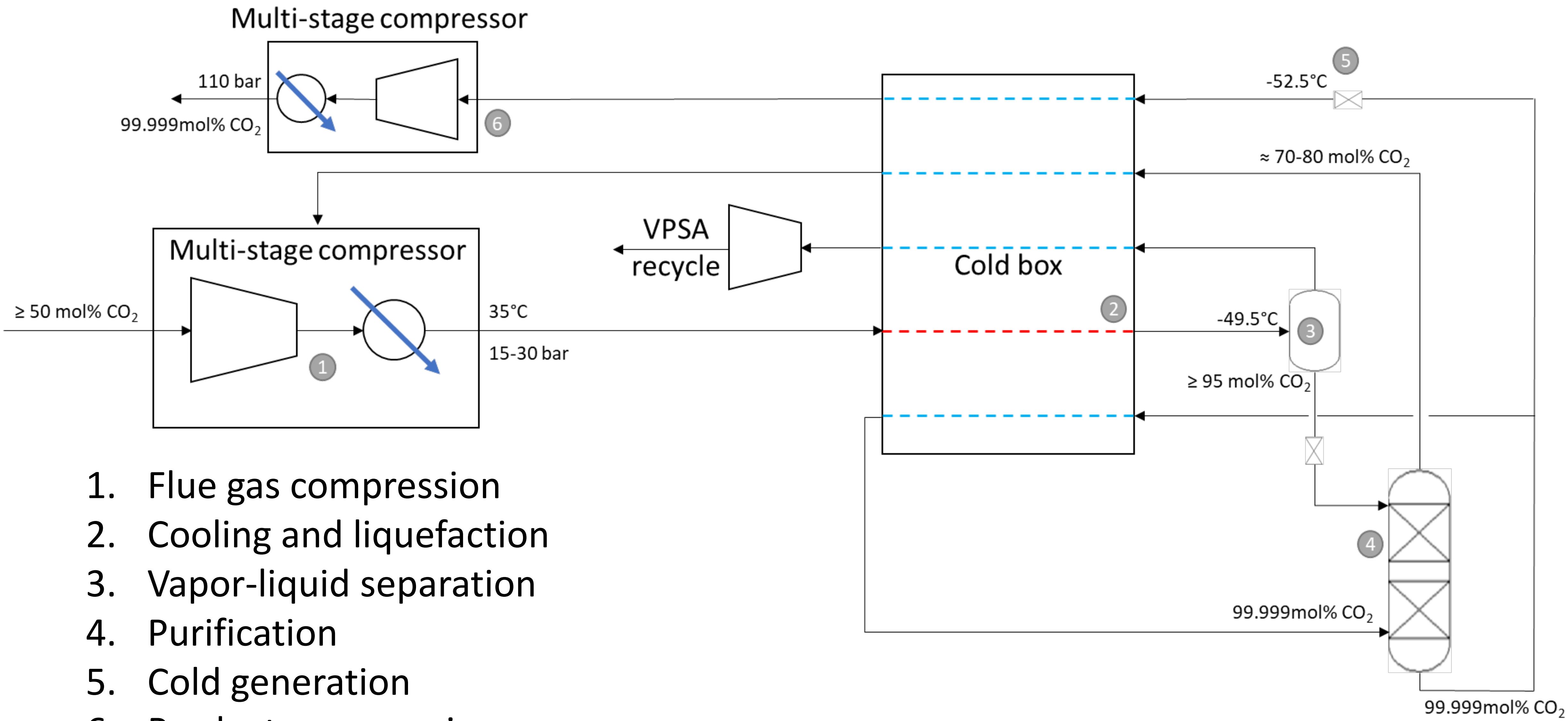
3-bed 6-step cycle



Bed 1	Adsorption			HR	co-evac	cn-evac	LR	LPP	
Bed 2	LR	LPP		Adsorption			HR	co-evac	cn-evac
Bed 3	HR	co-evac	cn-evac	LR	LPP		Adsorption		

+ High purity and high recovery can be both obtained
- More complex cycle (5 parameters)
- 3 Adsorption beds ; 2 compressors ; 2 vacuum pumps

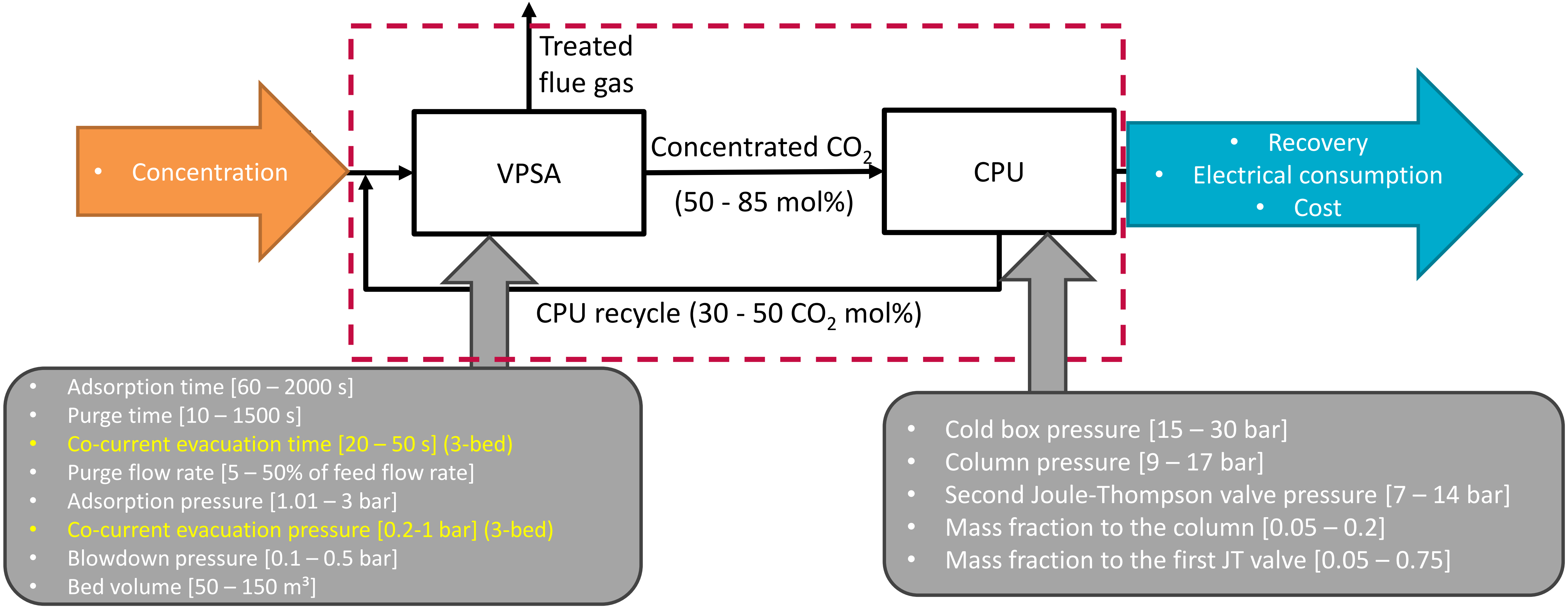
Carbon Purification Unit (CPU)



1. Flue gas compression
2. Cooling and liquefaction
3. Vapor-liquid separation
4. Purification
5. Cold generation
6. Product compression

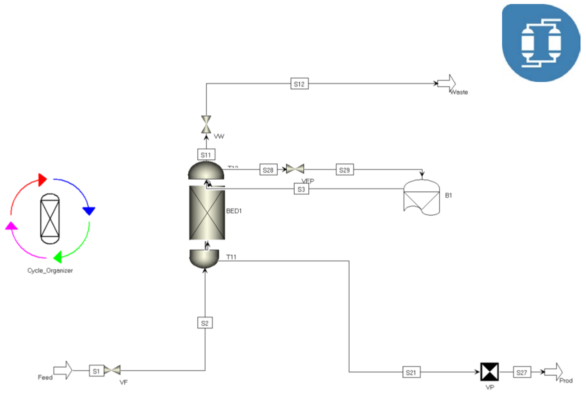
VPSA + CPU inputs & outputs

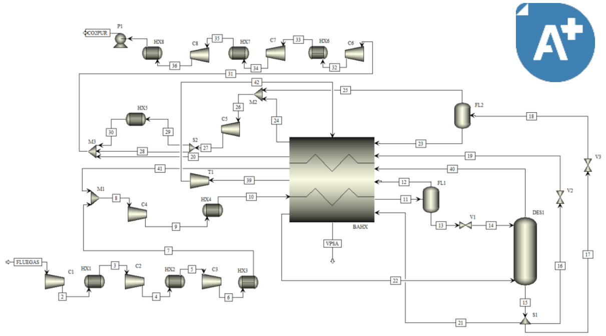
- Total flow rate of 70 000 Nm^3/h is considered with 5 to 20% CO_2 concentration
- 5 parallel VPSA units are considered to divide the flow



VPSA + CPU proceeding

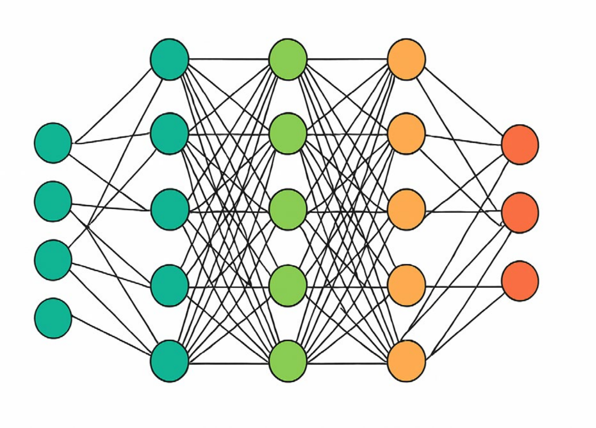
Aspen modeling





Data treatment

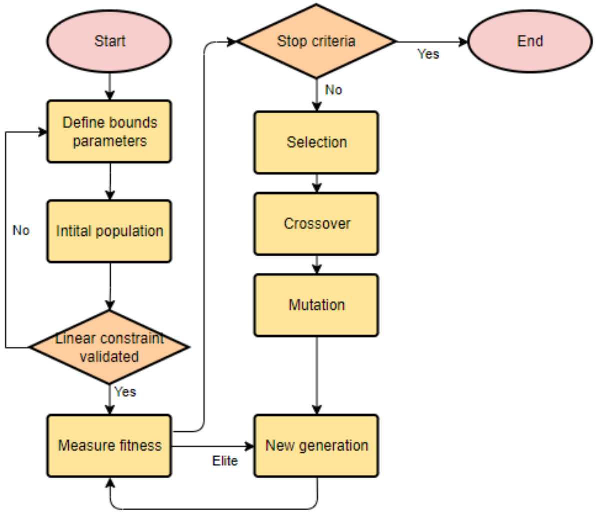
Surrogate building



- ANN model with 3 layers of neurons
- 2500 simulations per adsorbent
- 20% of simulations are used as a test set
- $R^2 > 99\%$

VPSA + CPU coupling

Optimization



NSGA III algorithm is used for optimization of the complete unit

A. Costa et Al., *Chem. Eng. J.*, vol. 493, p. 152345, Aug. 2024, doi: 10.1016/J.CEJ.2024.152345.

Adsorbents tested

Zeolite 13X was tested as a benchmark material and two MOFs were investigated: MIL-160(Al) and MIL-120(Al)

- Literature data was used for zeolite [1], own experimental data were used for MOFs
- Adsorbents are considered spherical with 3 mm diameter

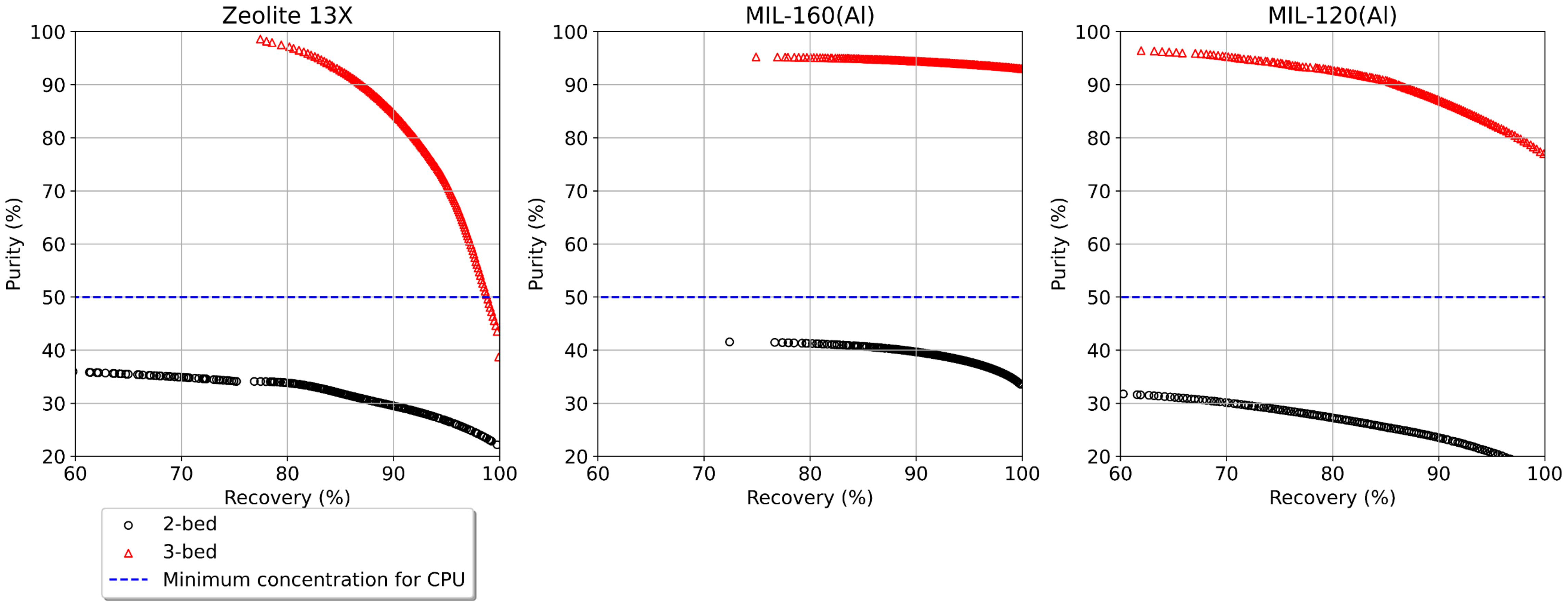
	Zeolite 13X	MIL-160(Al)	MIL-120(Al)
Packing density [kg/m³]	689	419	684
Price [€/kg]	1.5	26 [2]	13 [3]
Heat of adsorption [kJ/mol]	40	33	39
Working capacity (0.1 to 1 bar) [mmol/g]	1.83	0.95	1.46
Selectivity (1 bar,25°C,y_{CO2} = 0.15)	248	40	105

[1] A. H. Farmahini et Al., *Ind. Eng. Chem. Res.*, vol. 57, no. 45, pp. 15491–15511, 2018, doi: 10.1021/acs.iecr.8b03065.
[2] M. I. Severino et Al., *Faraday Discuss.*, vol. 231, no. 0, pp. 326–341, 2021, doi: 10.1039/D1FD00018G.
[3] B. Chen *et al.*, *Adv. Sci.*, vol. 11, no. 21, p. 2401070, Jun. 2024, doi: https://doi.org/10.1002/advs.202401070.

VPSA performance

Optimization of the VPSA unit alone to obtain the pareto of purity and recovery

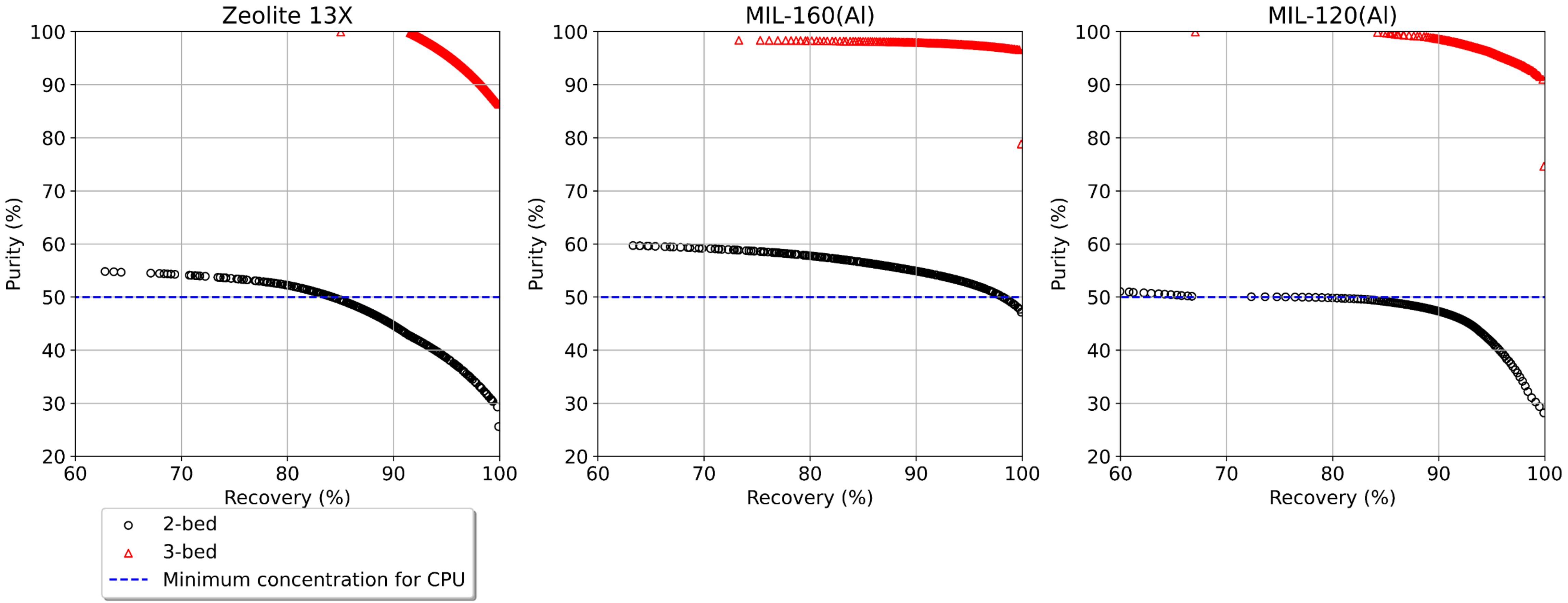
- A minimal concentration of 50% is required for the CPU unit → **<u>5% case</u>** cannot be treated by 2-bed 5-step configuration



VPSA performance

Optimization of the VPSA unit alone to obtain the pareto of purity and recovery

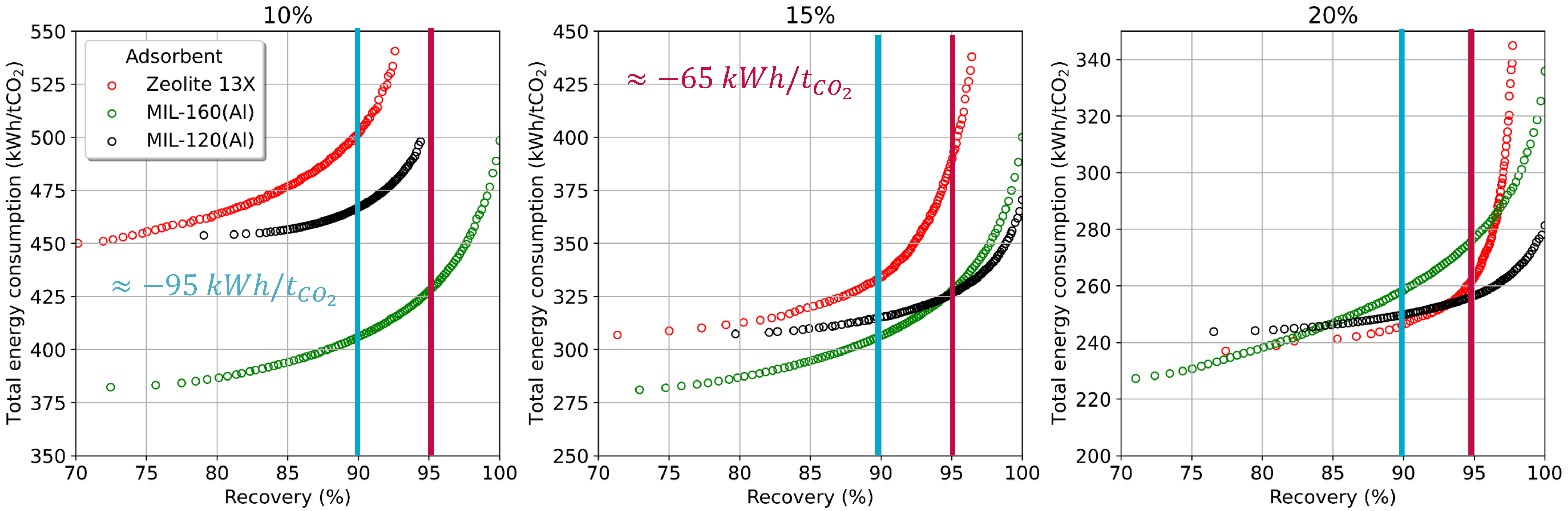
- A minimal concentration of 50% is required for the CPU unit → for **10% case** and higher both configurations are working



VPSA + CPU – Energy consumption for 2-bed 5-step

Energy consumption and recovery were optimized with NSGA-III for the three materials and three CO_2 concentrations:

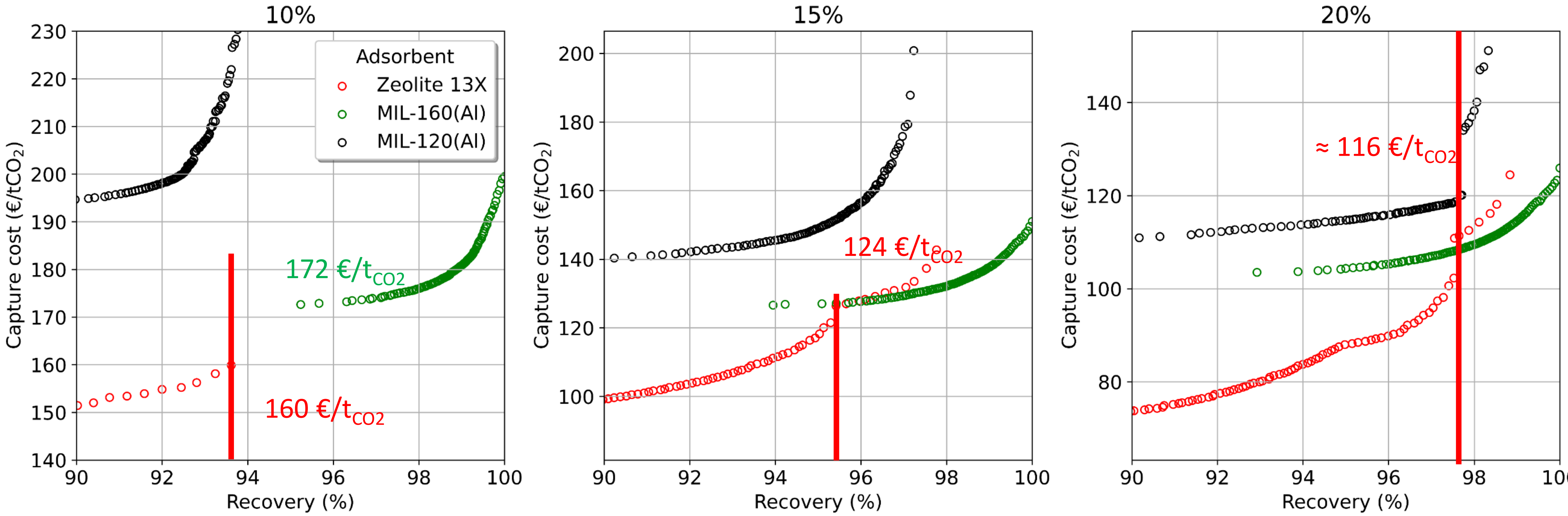
- MIL-160(Al) outperforms zeolite 13X and MIL-120(Al) for a CO_2 concentration of 10%
- Both MOFs are slightly better than zeolite 13X for 15%
- Energy consumption is quite similar for the three adsorbents at 20%



VPSA + CPU – Capture cost for 2-bed 5-step

Capture cost and recovery were optimized with NSGA-III:

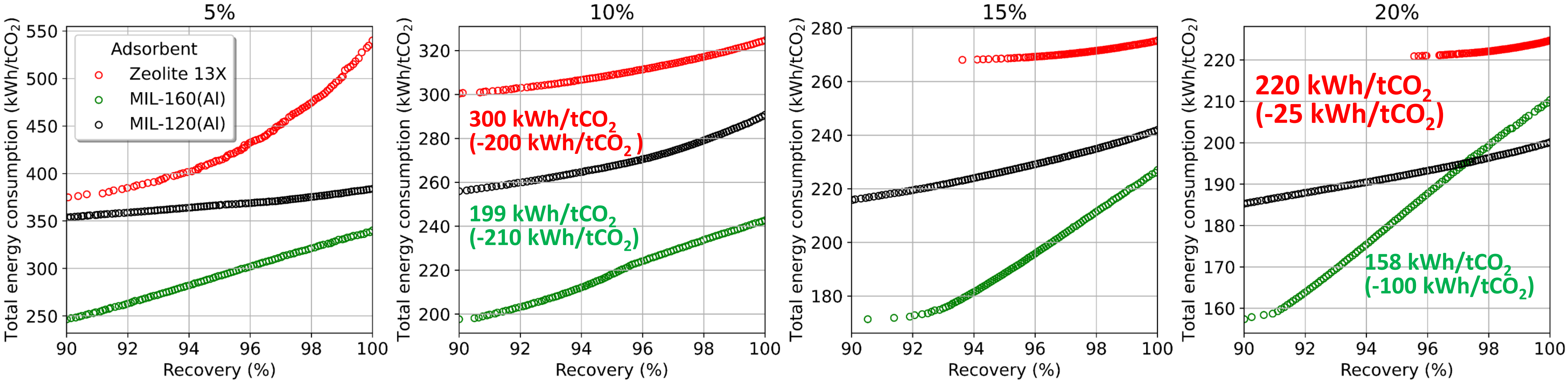
- Cost include OPEX (energy consumption) and CAPEX (price of materials) Electricity price is 0.1 €/kWh (mean price in EU)
- Zeolite 13X is more interesting for recovery lower than 95%
- MIL-160(Al) is competitive to reach higher recovery for the 10 and 15% case



VPSA + CPU – Energy consumption for 3-bed 6-step

Energy consumption and recovery were optimized with the same methodology as 2-bed 5-step:

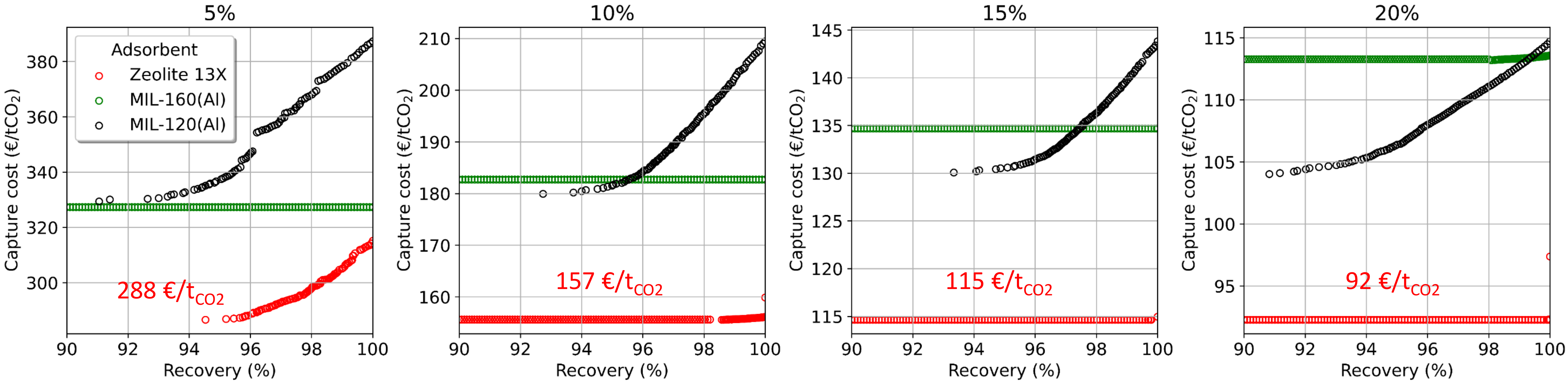
- Flue gas with 5% CO_2 can be treated with reasonable energy consumption
- MIL-160(Al) is the best material for almost all the cases followed by MIL-120(Al) and zeolite 13X
- Lower energy consumption compared to 2-bed 5-step cycle



VPSA + CPU – Capture cost for 3-bed 6-step

Capture cost and recovery were optimized with NSGA-III:

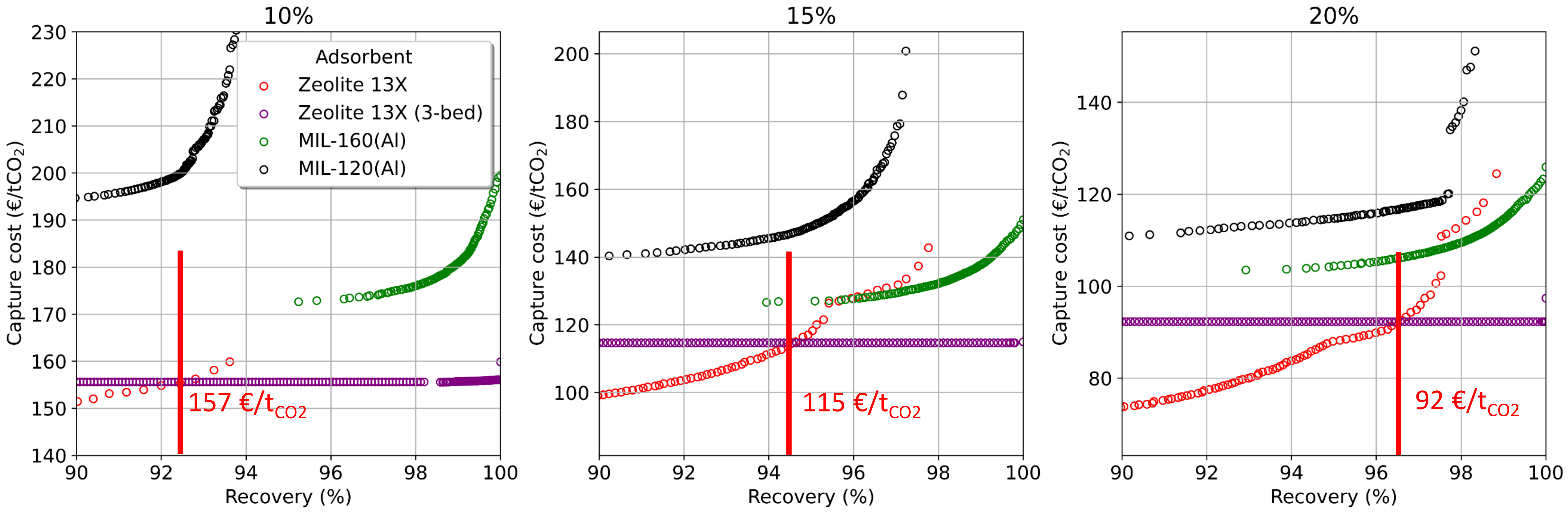
- Cost include OPEX (energy consumption) and CAPEX (price of materials)
- Electricity price is 0.1 €/kWh (mean price in EU)
- Zeolite 13X is always the lowest
- Price of the MOFs make them uneconomically for this configuration



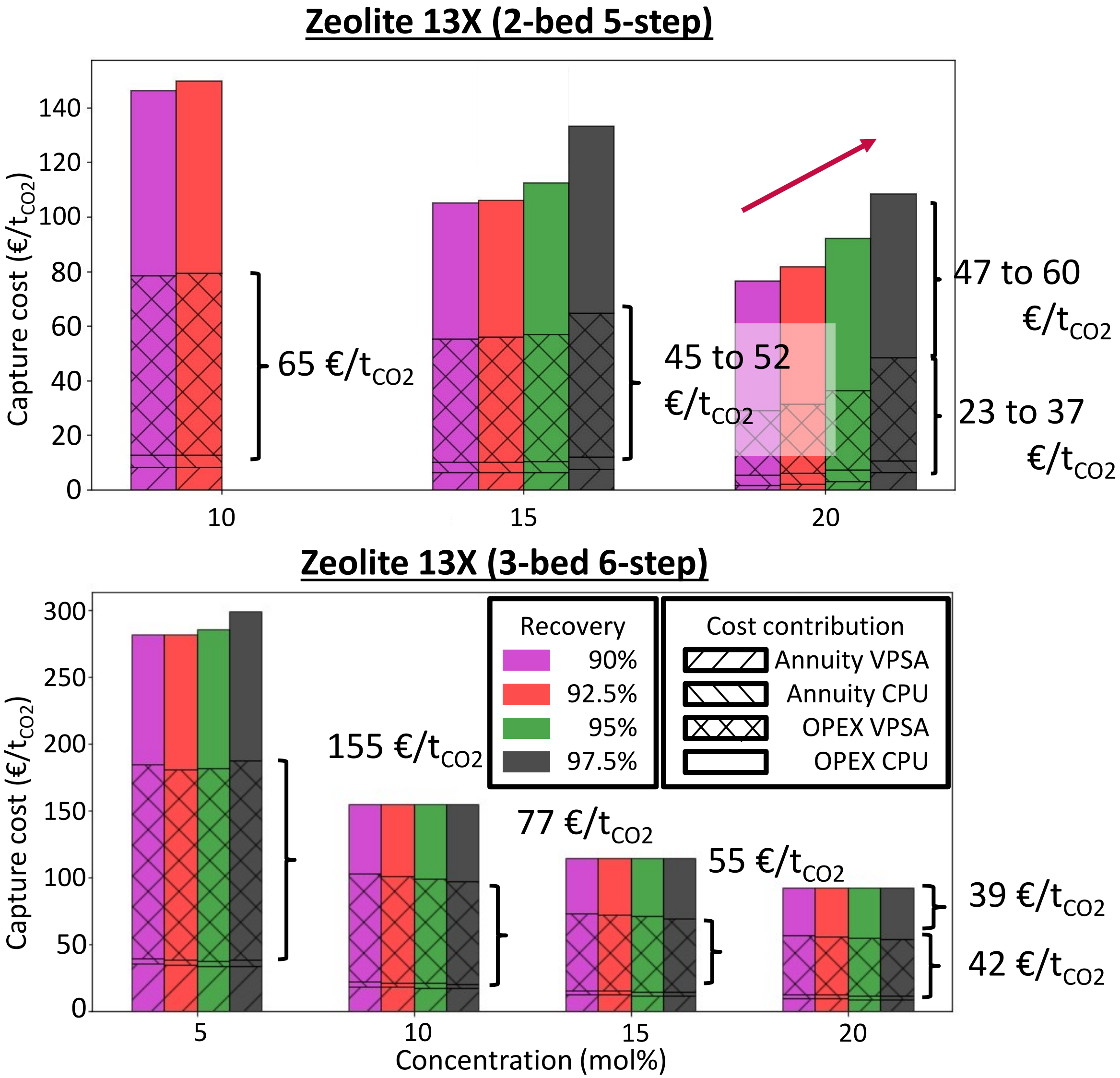
VPSA + CPU – Capture cost comparison

Trade-off between 2-bed or 3-bed configuration with zeolite 13X is recovery dependent

- For highest recovery, 3-bed 6-step configuration is cheaper
- The switching recovery between 2-bed and 3-bed increases with the flue gas concentration



VPSA + CPU – OPEX & CAPEX



- For both configurations OPEX is more important than CAPEX.
- OPEX also include maintenance of equipment which is higher for 3-bed 6-step cycle.
- For 2-bed 5-step VPSA and CPU have the same cost for low recovery and low concentration. When both increase the CPU OPEX become larger
- For 3-bed 6-step VPSA OPEX are always larger than CPU. The higher purity at the outlet of this configuration decreases the energy consumption of the CPU.

Conclusion

- VPSA and CPU units were optimized for three different materials and two configurations
- The 3-bed 6-step cycle offers a reduced energy consumption compared to the 2-bed 5-step thanks to the higher purity of this cycle. This cycle also allows to treat flue gas with only 5% CO_2
- While the total energy consumption can be drastically reduced with MOFs for both configuration, the high cost of these materials make the use uneconomical compared to zeolite 13X
- 3-bed 6-step is more expensive due to equipment cost. This cycle could be used when high recovery is needed
- Reduction of MOFs price can globally reduce the price of CO_2 capture with this technology
- LCA should be conducted in addition to techno-economical analysis for adsorbent and cycle selection

Acknowledgments

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- R.V. Pinto

MOF's shaping

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- Su Kyong Lee

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