Modelling and optimisation of materials and processes for post-combustion CO_2 capture from flue gas by Pressure Swing Adsorption (PSA) and Vacuum Swing Adsorption (VSA)

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Outline

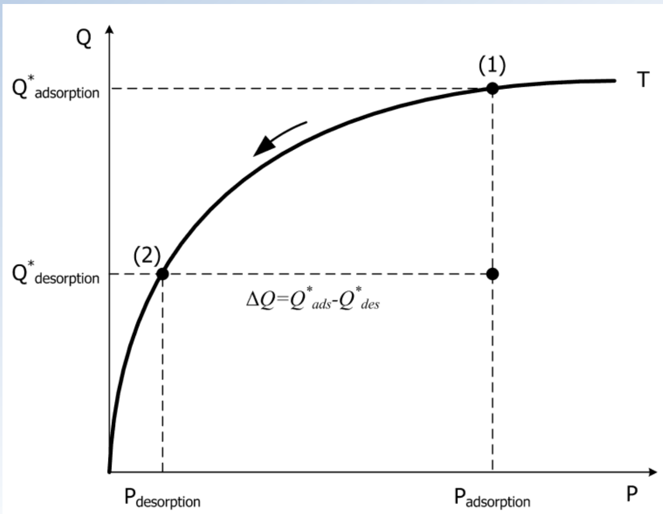
- Introduction
- Modelling challenges and framework
- Implementation aspects
- Application studies and results
- Concluding remarks

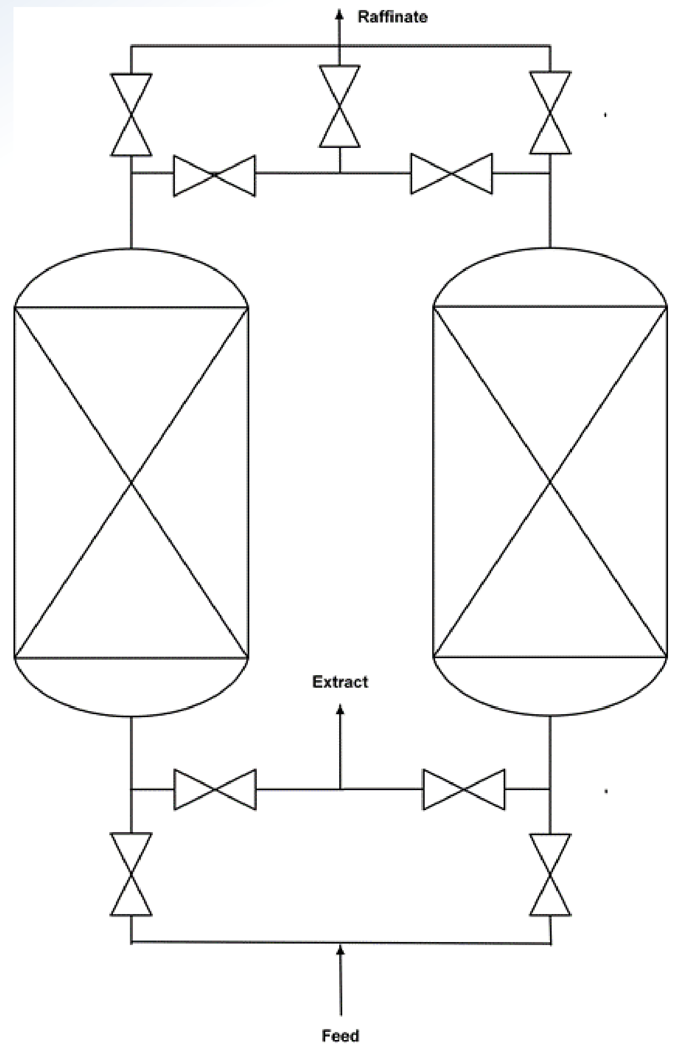
Introduction

- Pressure Swing Adsorption (PSA)
  - A relatively new gas separation process
  - Less energy demanding compared to traditional ones
- Major industrial applications:
  - Air separation (N_2/O_2)
  - Gas drying
  - H_2 production from Coke oven gas or Steam methane reforming off gas (SMROG)
  - CO_2 capture from flue gas (CO_2/N_2)
  - Biogas upgrading
- PSA was originally employed in a 4-step 2-bed configuration (Skarstrom cycle)
- Current industrial practice imposes:
  - Multi-bed configurations
  - More complex cycles

Principle of Operation

Equilibrium Adsorption Isotherm



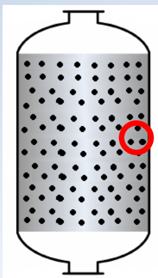


- At least 2 basic steps:
  - High pressure adsorption
  - Regeneration (by reducing pressure)
- A dynamic process operating under transient conditions (in a cyclic manner)

Multi-scale Modelling and Simulation

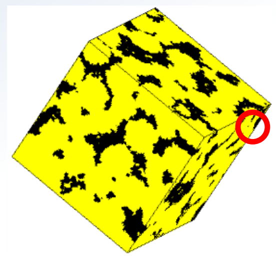
Fixed bed Adsorber

o(m)



Adsorbent

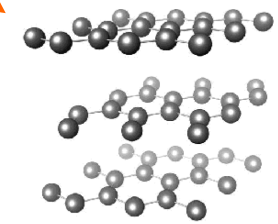
o(mm)



Simulation of pore structure

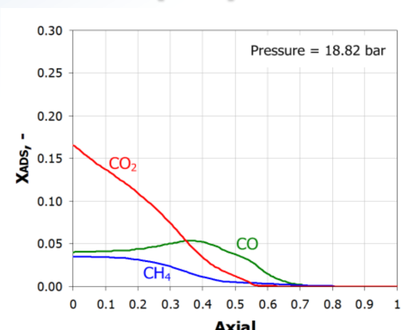
Internal Structure

o(nm)



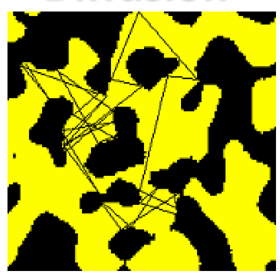
Simulation of microscopic phenomena

Macroscopic phenomena



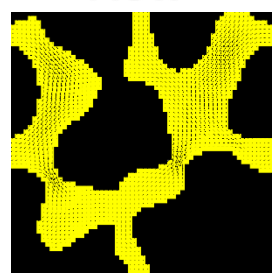
2 m

Diffusion



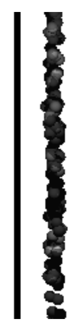
20 μm

Flow

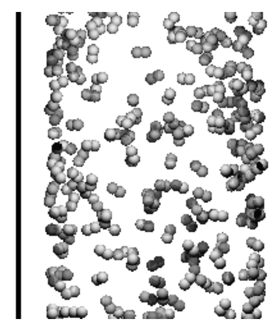


10 μm

Adsorption

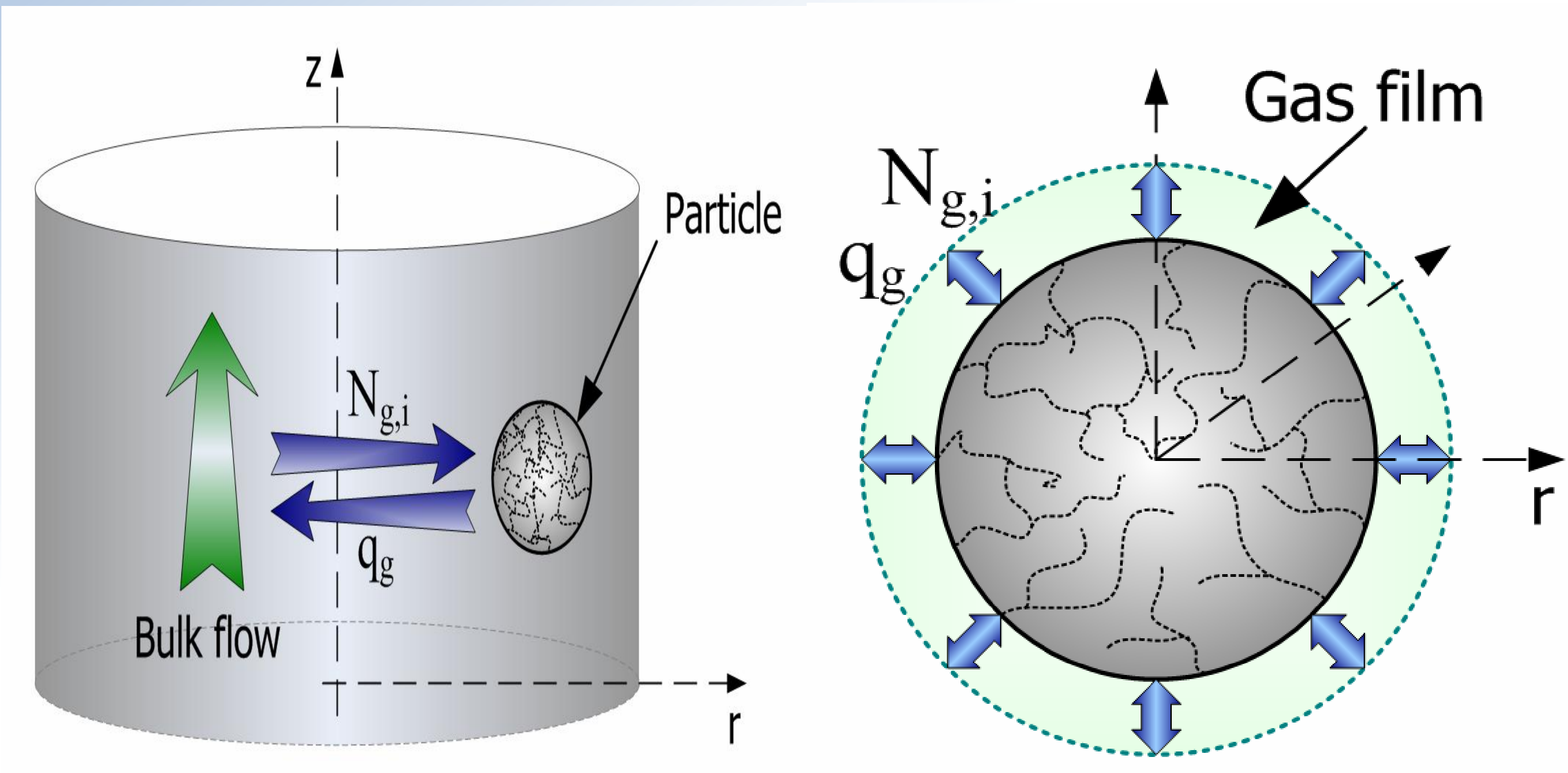


0.6 nm



2.4 nm

Adsorbent layer-Adsorbent particle



PSA model equations[1,2]

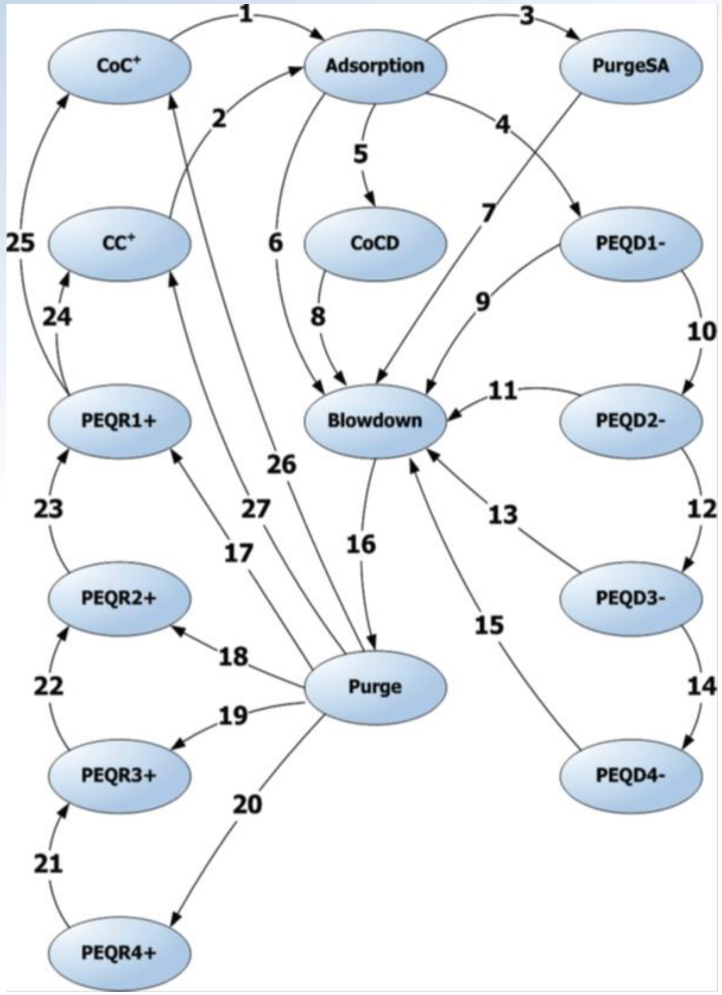
- Mass balance equations
- Heat balance equations
- Momentum balance equations
- Equilibrium isotherm equations
- Transport and thermo-physical properties of the gas mixture
- Boundary conditions according to the operating steps
- Gas valve equations
- Automatic generation of operating procedures through a State Transition Network (STN) approach

Implementation in gPROMS™

1. Nikolic D., Giovanoglou A., Georgiadis M.C., Kikkinides E.S. (2008). Generic modeling framework for gas separations using multibed pressure swing adsorption processes. *Industrial and Engineering Chemistry Research*. 47, 3156-3169.

2. Nikolic D., Kikkinides E.S., Georgiadis M.C. (2009). Optimization of multibed pressure swing adsorption processes. *Industrial and Engineering Chemistry Research*. 48, 5388-5398.

State transition network (STN) with all possible state transitions[1]

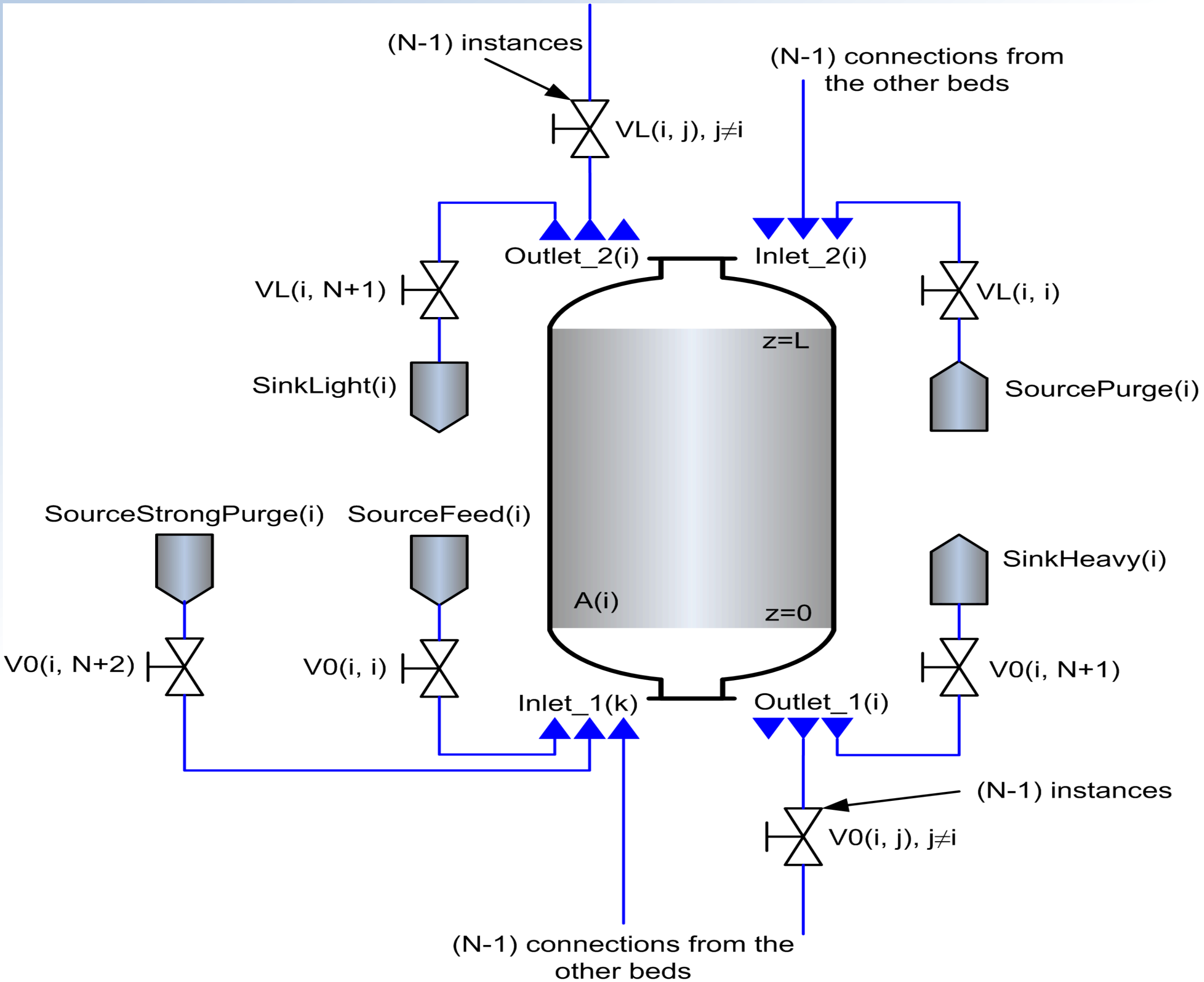


1. Nikolic D., Kikkinides E.S., Georgiadis M.C. (2009) : Optimization of multibed pressure swing adsorption processes . *Industrial and Engineering Chemistry Research*. 48, 5388-5398.

Modelling challenges and implementations

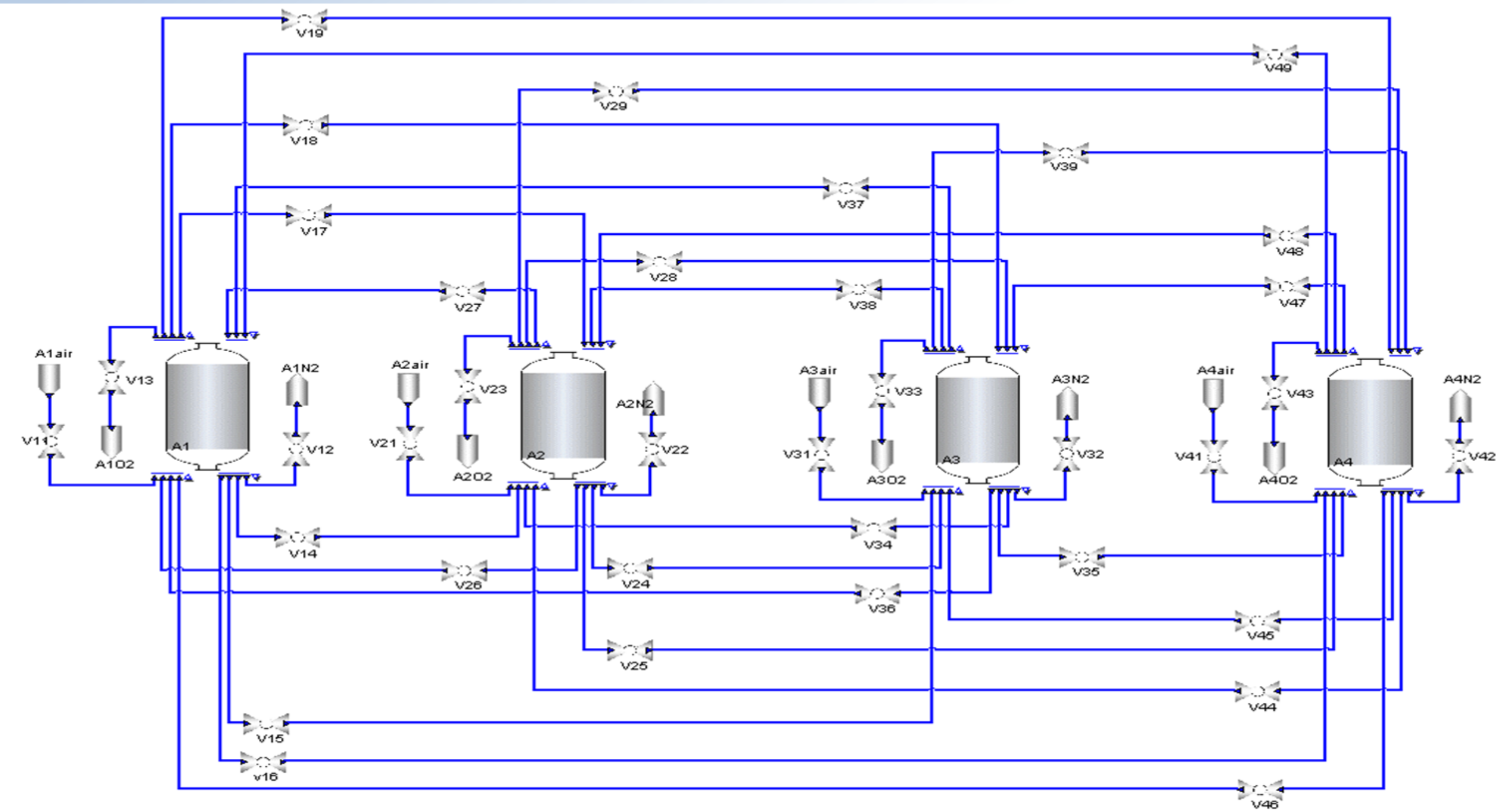
- A gPROMS™-based modelling framework for multi-bed PSA/VSA flowsheets.
- Formulation of detailed mathematical model in the adsorbent bed.
- Complex gas-valves control bed interactions.
- Suitable for an arbitrary number of beds.
- Implementation of complex operating procedures.
- Incorporation of all feasible bed interconnections.
- Automatic generation of operating procedures through a new State Transition Network (STN) approach
- Systematic study of different types of adsorbents for CO_2 capture.
- Exploitation of synergistic benefits between adsorbent materials and processes.

Single adsorbent bed in a typical multibed PSA plant[1]



1. Nikolic D., Giovanoglou A., Georgiadis M.C., Kikkinides E.S. (2008): Generic modeling framework for gas separations using multibed pressure swing adsorption processes. *Industrial and Engineering Chemistry Research*. 47, 3156-3169.

A four-bed PSA flowsheet with all possible bed interconnections[1]



1. Nikolic D., Giovanoglou A., Georgiadis M.C., Kikkinides E.S. (2009). Generic modeling framework for gas separations using multibed pressure swing adsorption processes. *Industrial and Engineering Chemistry Research*. 47, 3156-3169.

Multibed PSA flowsheet

- Several unit arrays
  - Adsorbent beds
  - Gas valves
  - Gas sources and sinks
- Model sufficiently general to support:
  - Arbitrary number of beds
  - All feasible bed configurations
  - All operating steps
  - All feasible bed interconnections

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Case study I
Model validation

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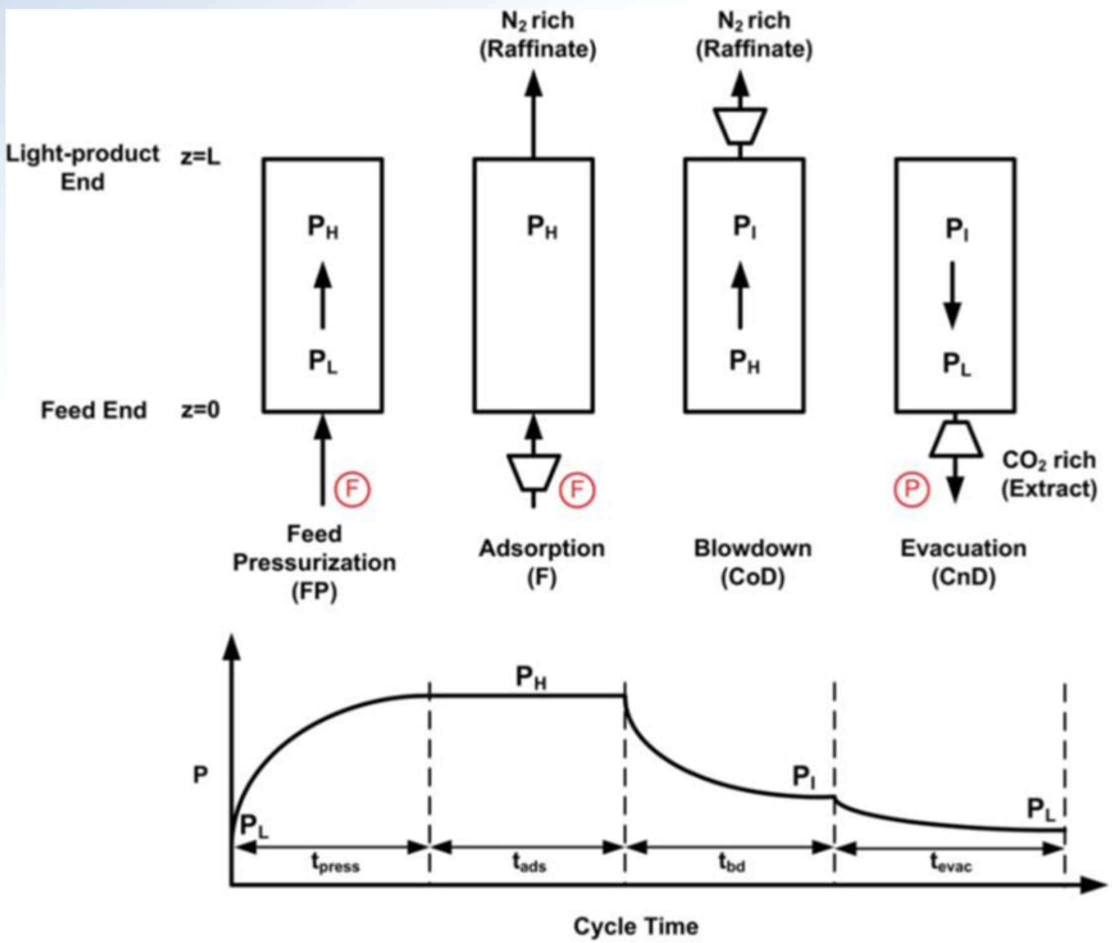
Pressure Swing Adsorption (PSA) for CO_2 capture from dry flue gas using zeolite 13X as adsorbent



Case study I
Model validation - Results

Table 1. Process performance indicators simulation results with absolute deviations from the results of Ko et al. (2005)[1]

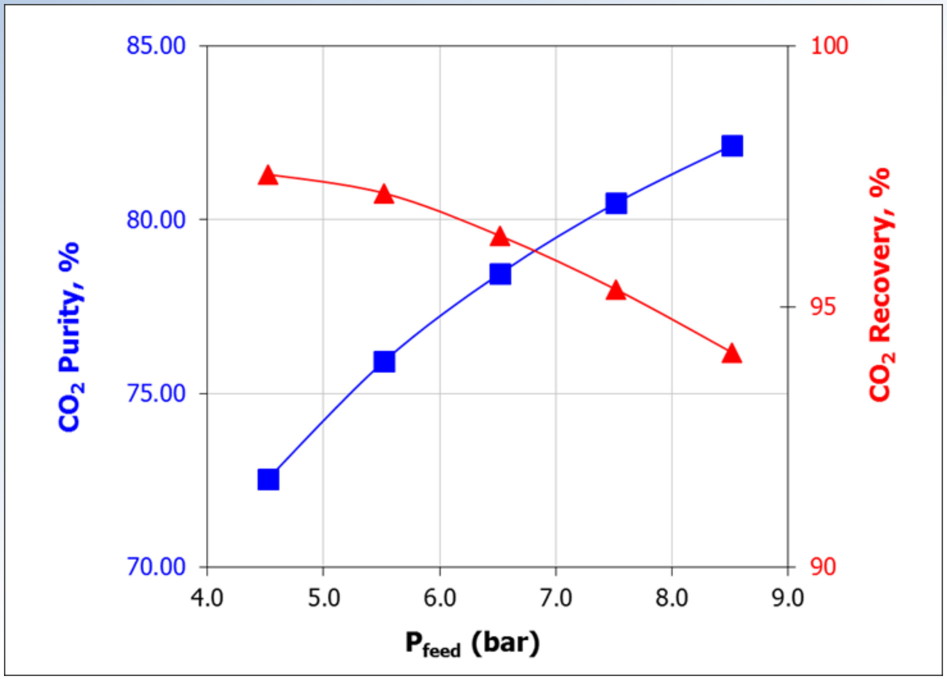
Reference	Pfeed (bar)	Tfeed (K)	L/D	Number of cycles (CSS)	Discretization method	Ko et al Purity CO_2	Ko et al Recovery CO_2	this work Purity CO_2	this work Recovery CO_2	Deviation Purity CO_2	Deviation Recovery CO_2
Ko et al. (2005)	6.52	370.00	11.36	300	CFDM,2,50	88.94	96.90	84.82	97.93	-4.63	1.06
Ko et al. (2005)	6.94	365.32	11.36	300	CFDM,2,50	95.46	15.00	92.12	14.35	-3.50	-4.33
Ko et al. (2005)	8.69	364.42	17.64	300	CFDM,2,50	92.29	80.00	97.19	79.20	5.31	-1.00

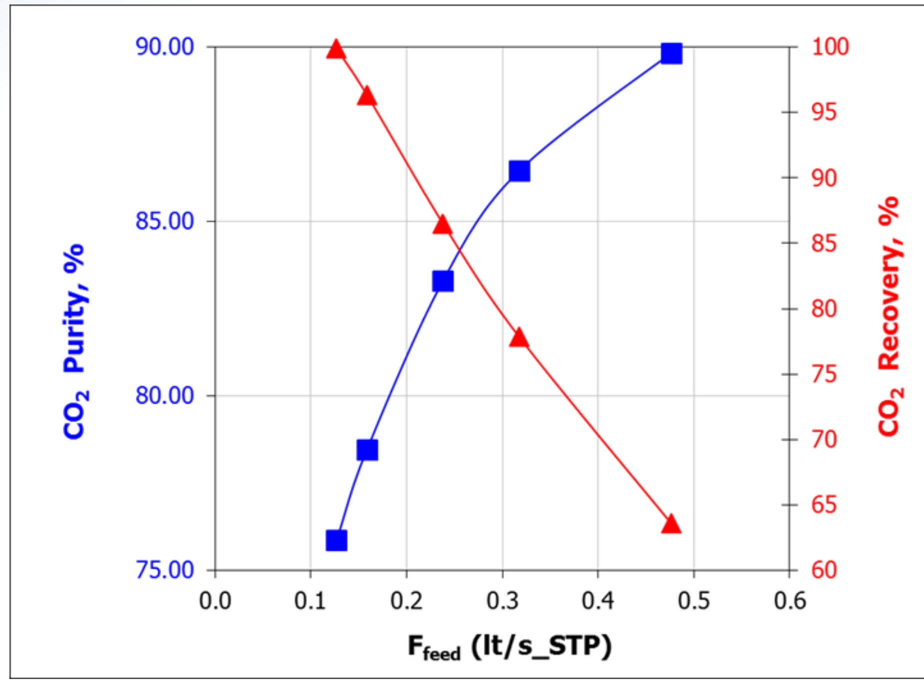
Deviations due to potentially different pressure history profile during the pressure-change steps affected by gas valve equation

Simulation results in good agreement with literature results

1. Ko D., Siriwardane R., Biegler L.T. (2005). Optimization of pressure swing adsorption and fractionated vacuum pressure swing adsorption processes for CO_2 capture. *Industrial and Engineering Chemistry Research*. 44, 8084-8094.

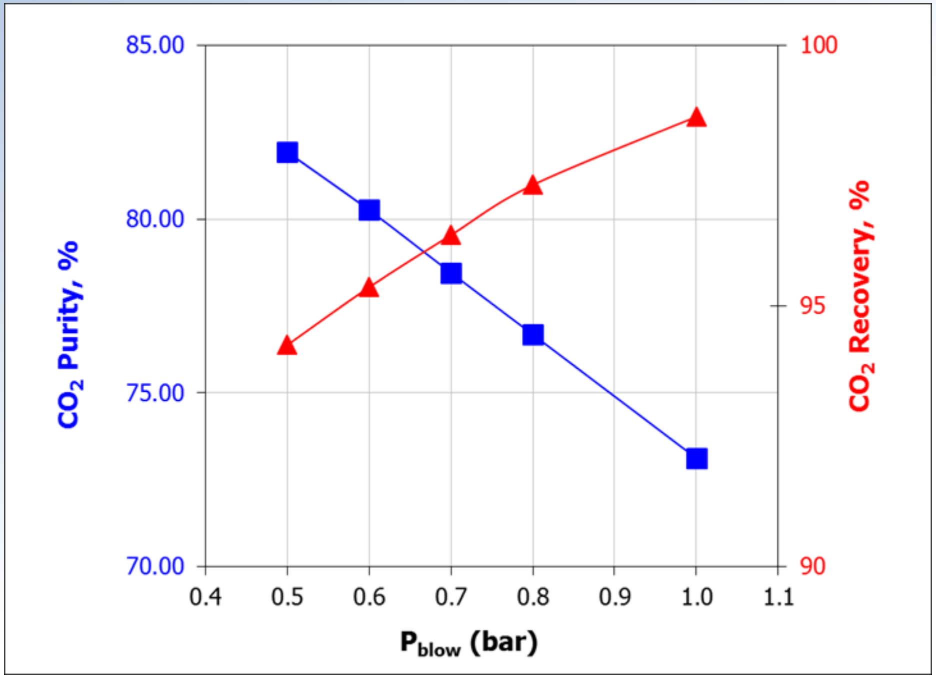
Case study I
Sensitivity analysis

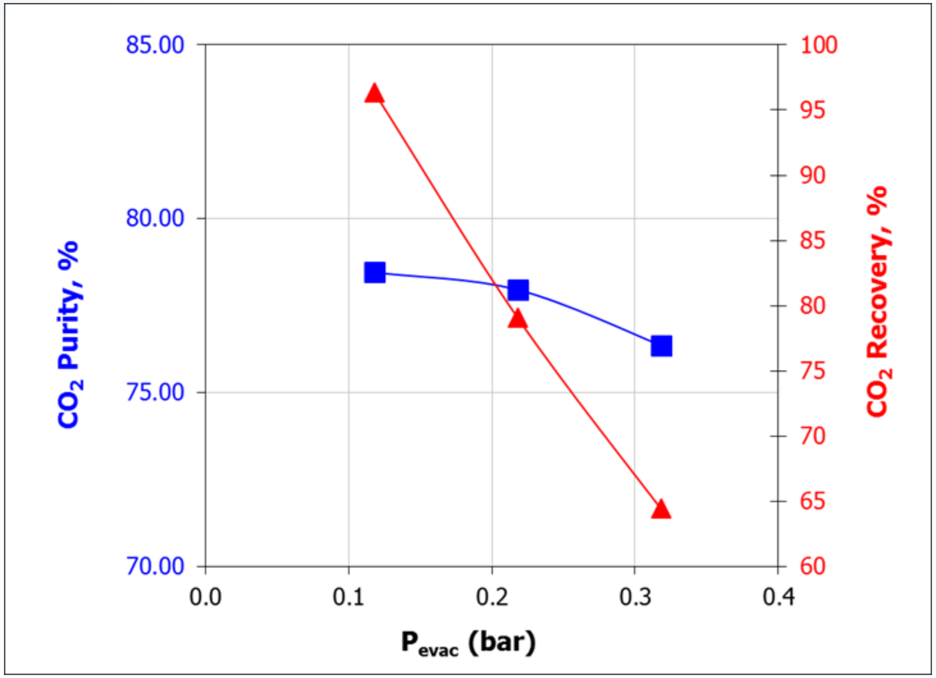




Trade-offs between process performance indicators

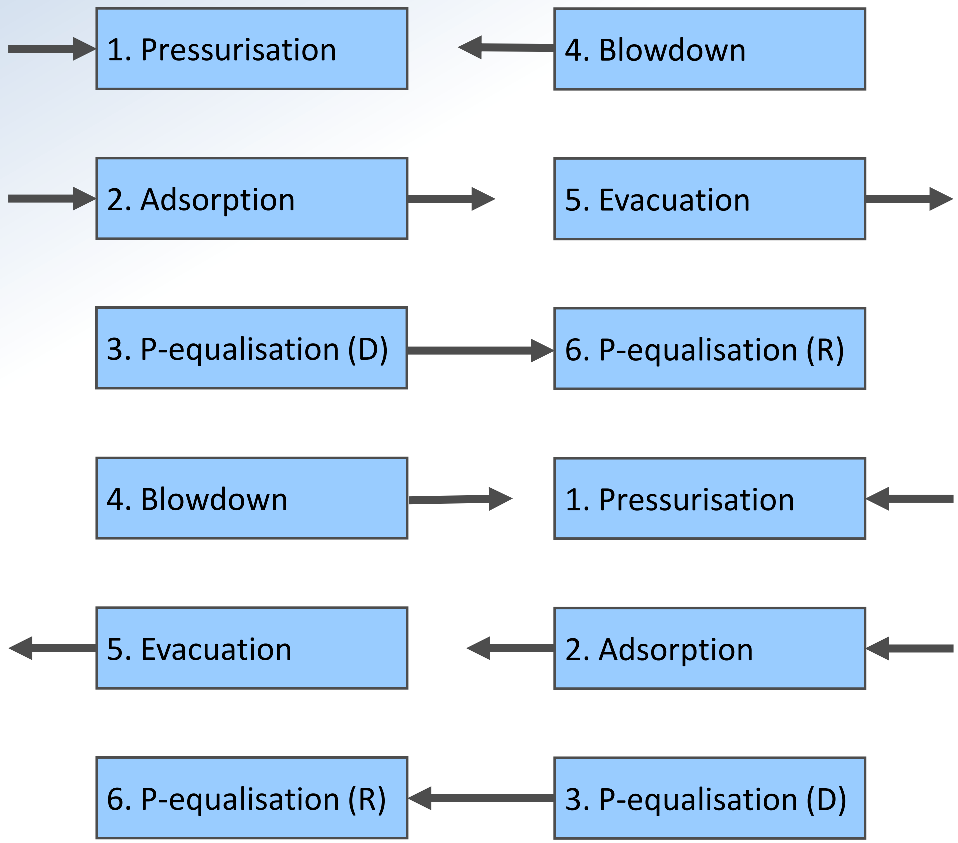
Case study I
Sensitivity analysis





Trade-offs between process performance indicators

Case study I
Two beds operating steps



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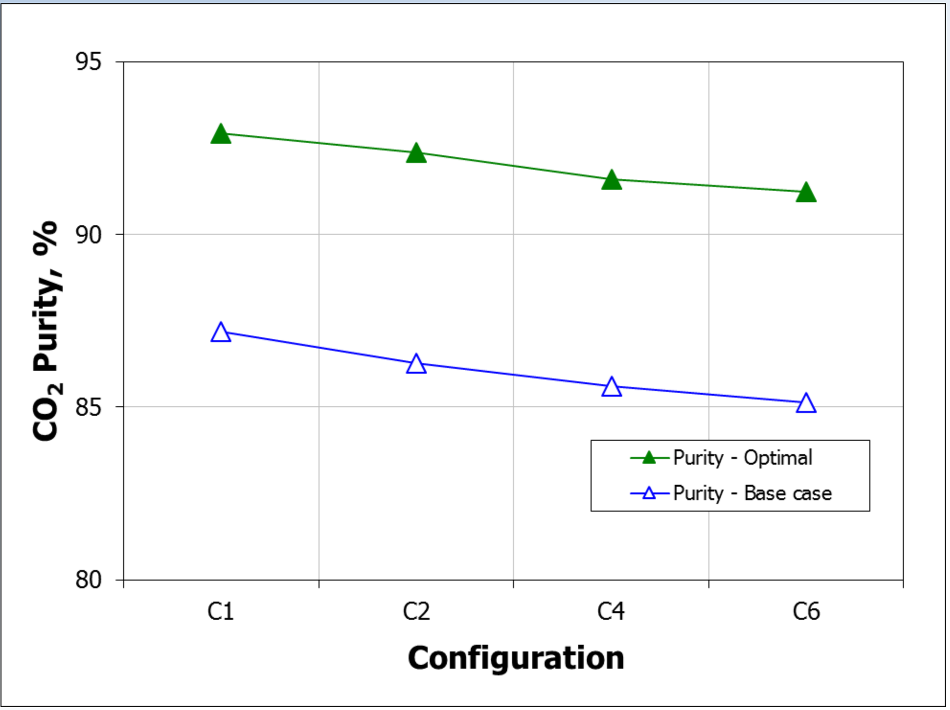
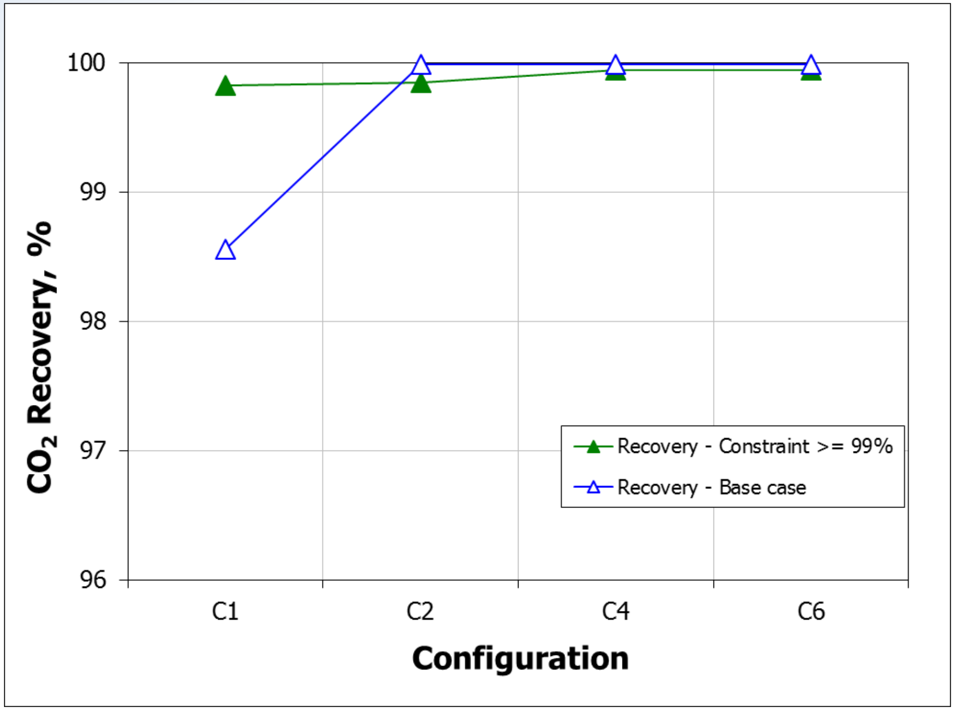
Case study I - Optimisation
Maximize CO_2 purity

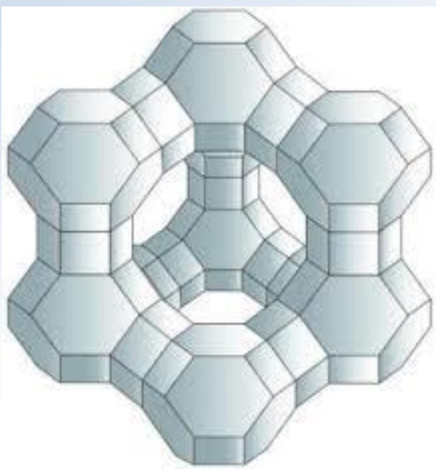




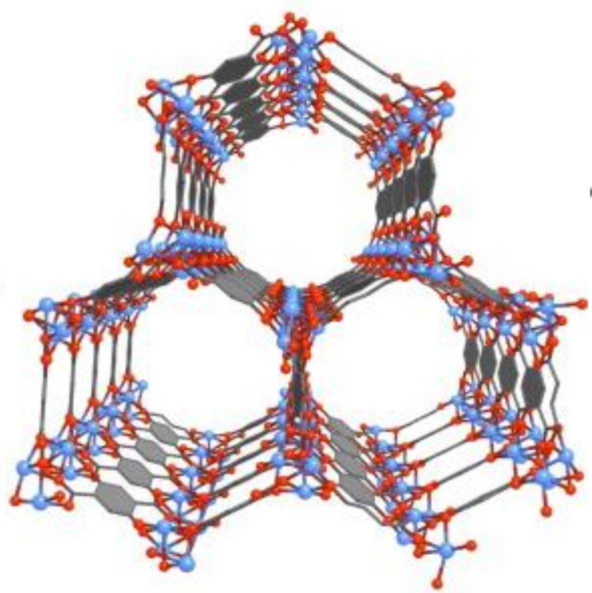
7% improvement in CO_2 purity

Case study II
Comparison of adsorbents

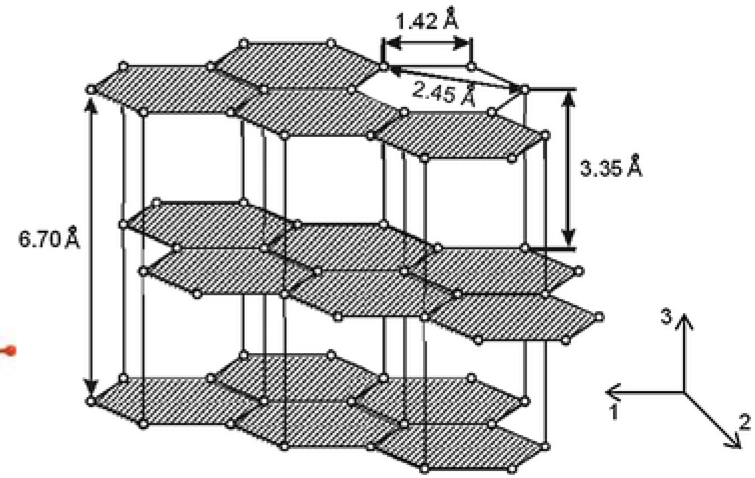
Comparison of Zeolite 13X, Mg-MOF-74 and Activated Cardon for carbon dioxide (CO_2) capture from dry flue gas using PSA/VSA processes.



Zeolite 13X

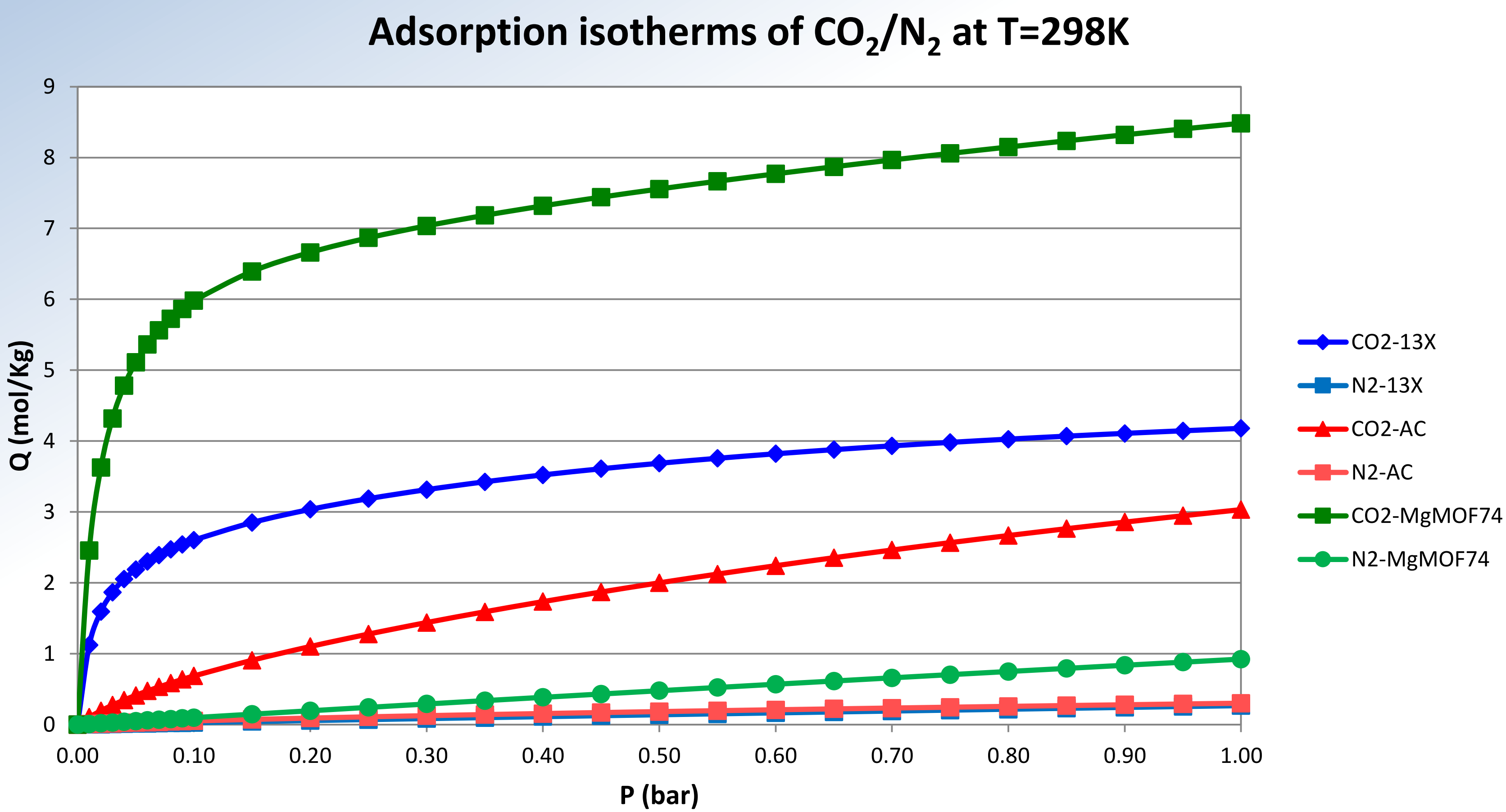


M-MOF-74
(M: Zn, Co, Ni, Mg)



Activated Carbon

Case study II
Adsorption isotherms



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Case study II
Adsorption isotherms

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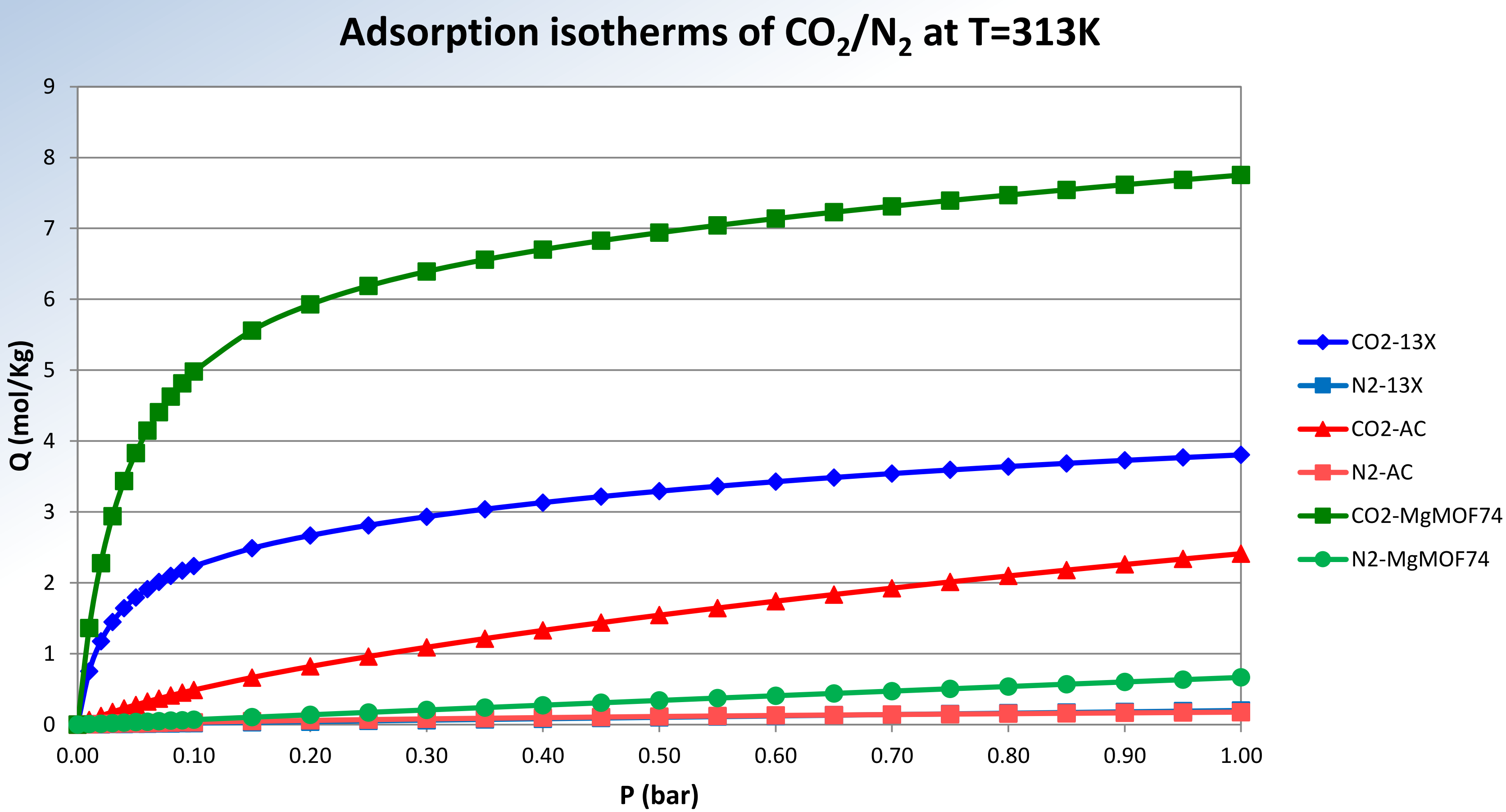

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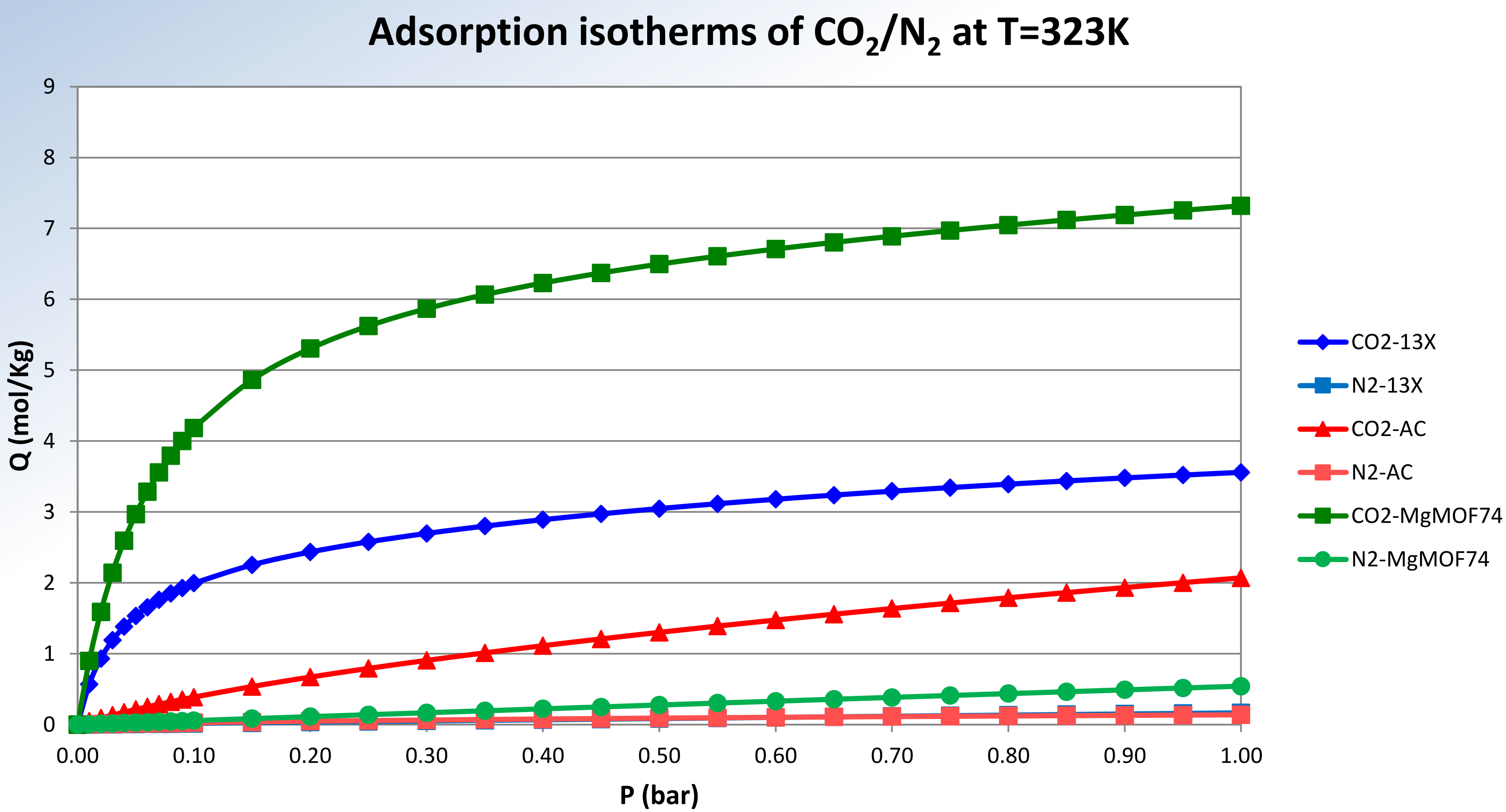
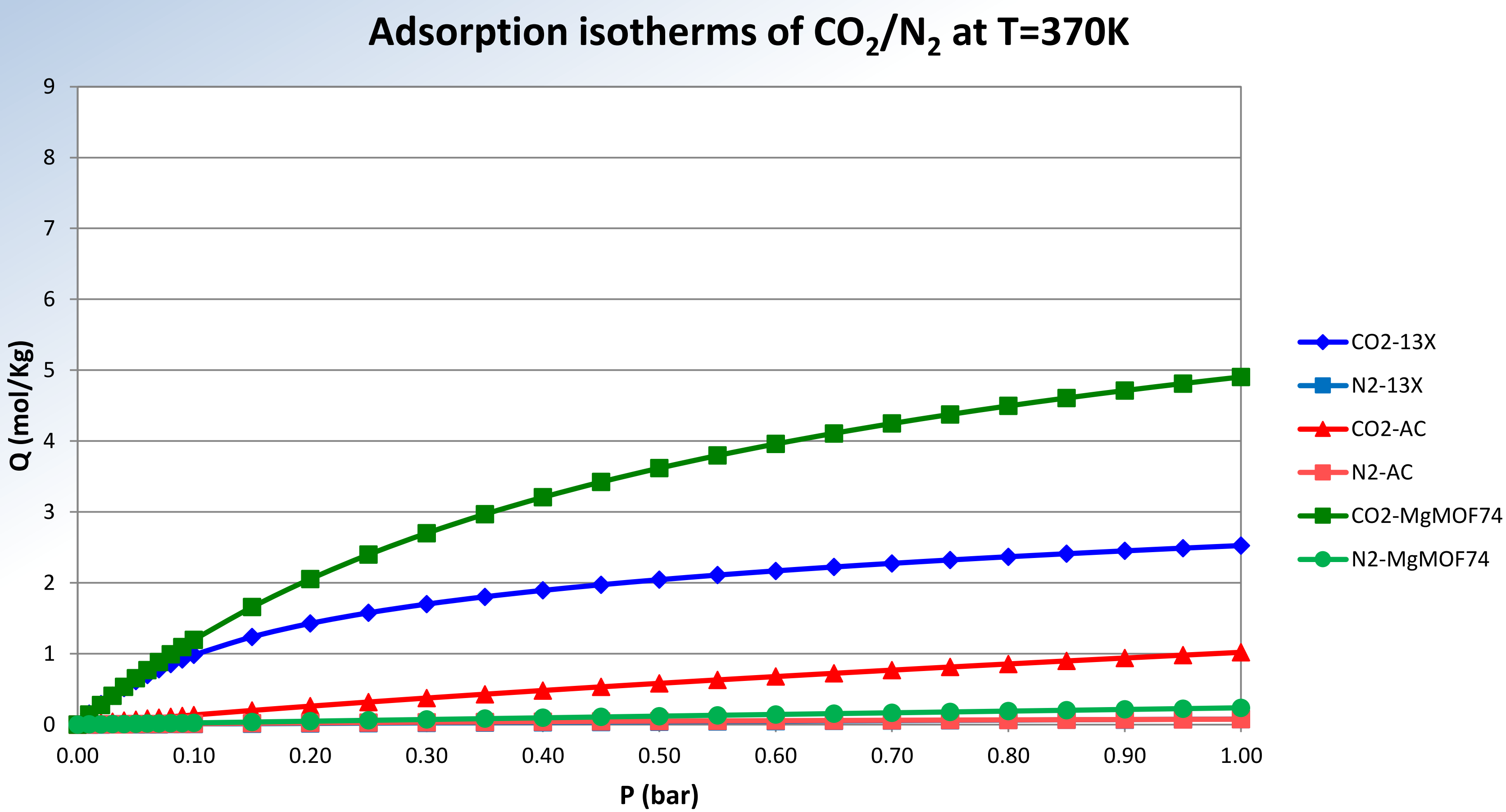
Adsorption isotherms



Case study II
Adsorption isotherms



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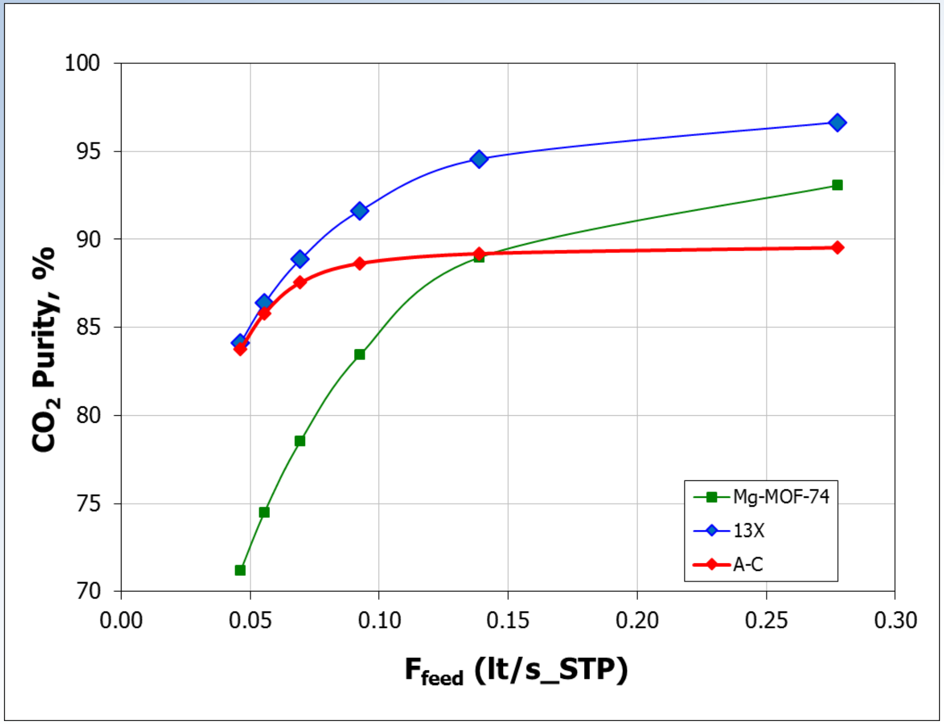
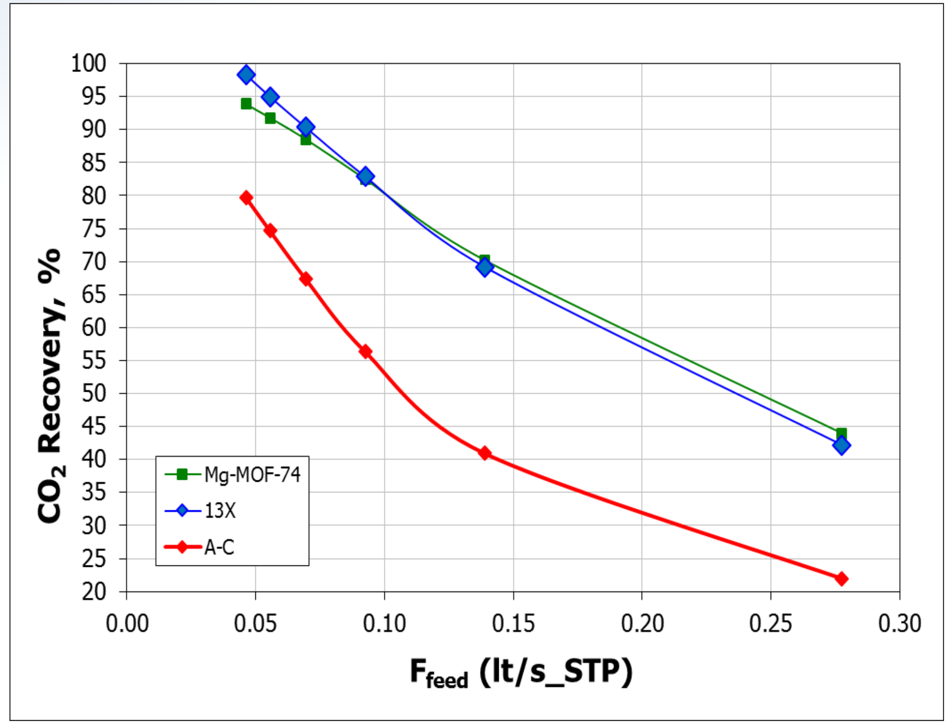
Case study II
PSA/VSA parametric studies

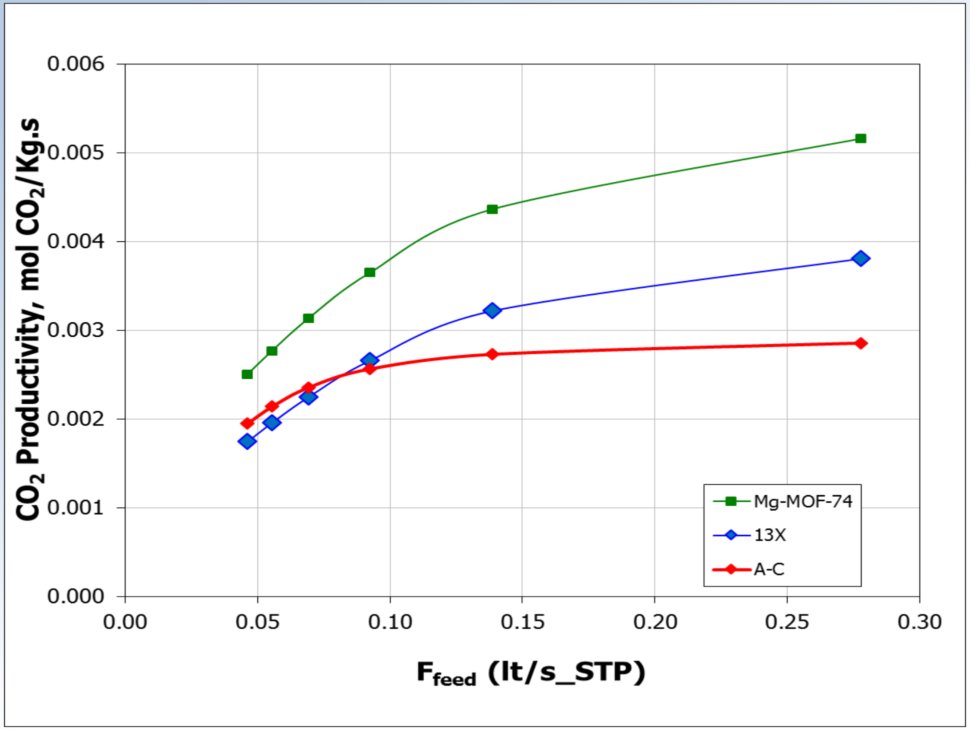


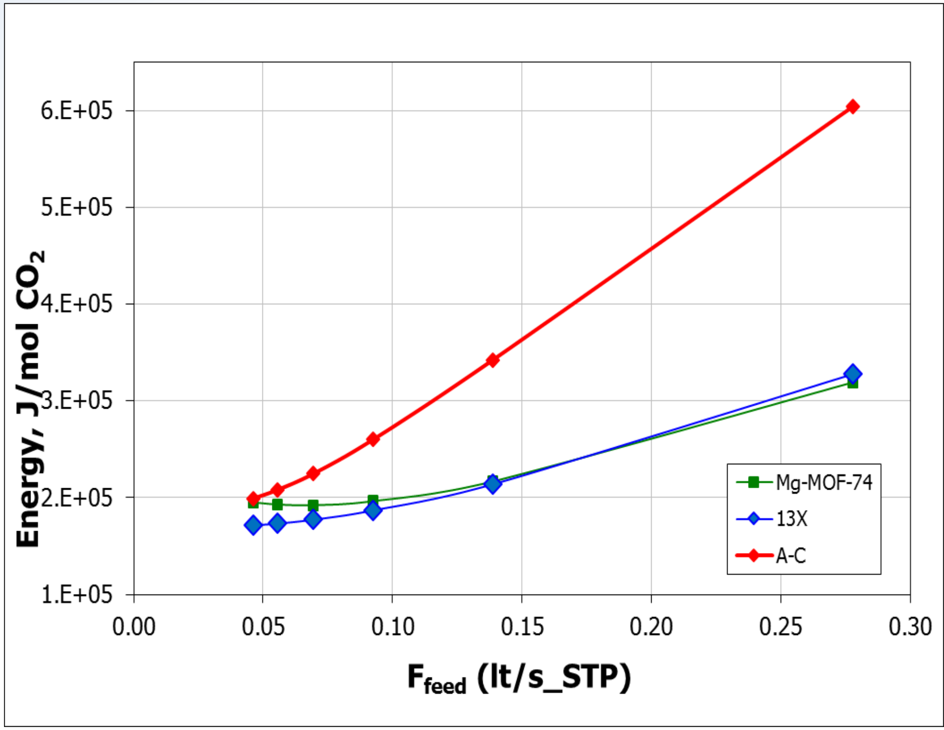


T_{feed}=323K
P_{feed}=1.10bar
P_{blow}=0.20bar
P_{evac}=0.02bar

Krishnamurthy S., Rao V.R., Guntuka S., Sharratt P., Haghpanah R., Rajendran A., Amanullah M., Karimi I.A., Farooq S. (2014). CO_2 capture from dry flue gas by vacuum swing adsorption: a pilot plant study. *AIChE Journal,* 60, 1830–1842.

Case study II
PSA/VSA parametric studies





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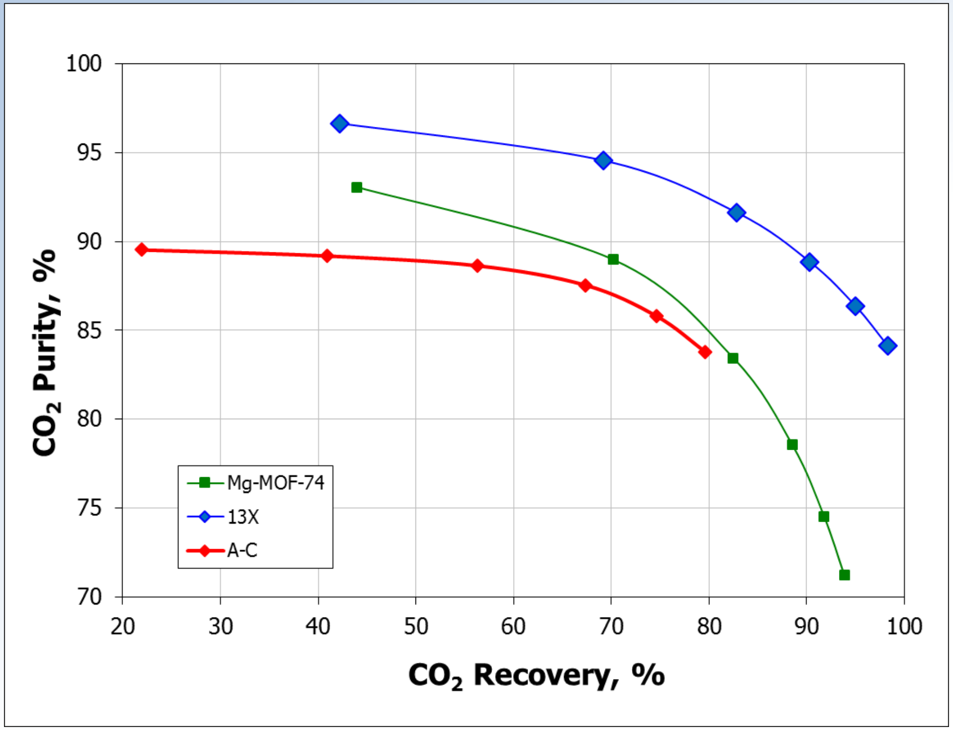
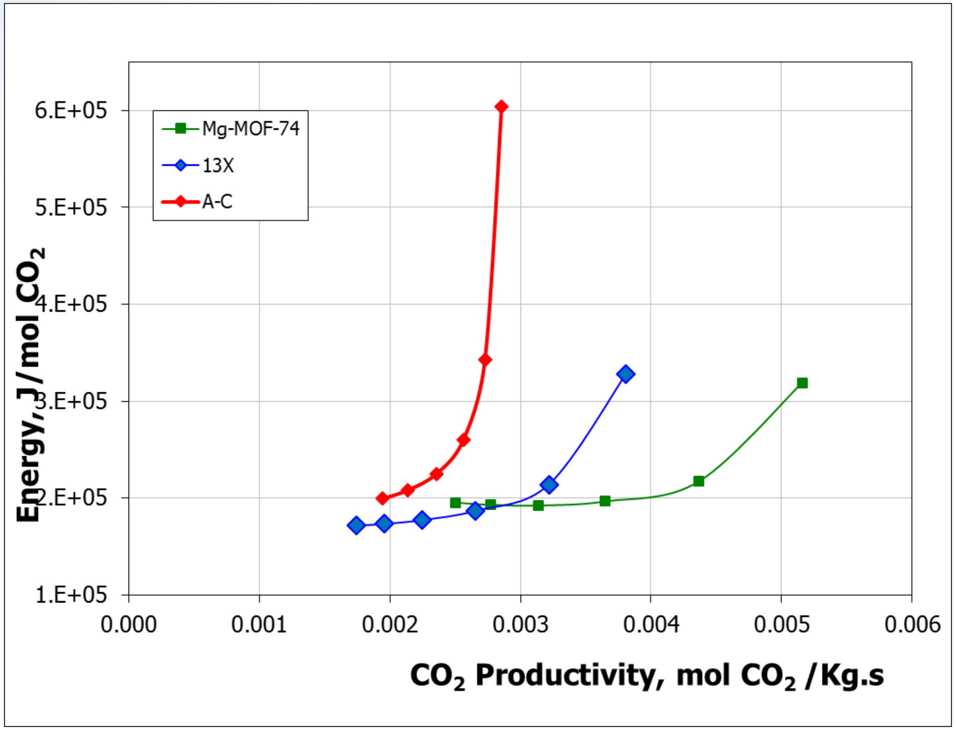
Case study II
PSA/VSA parametric studies





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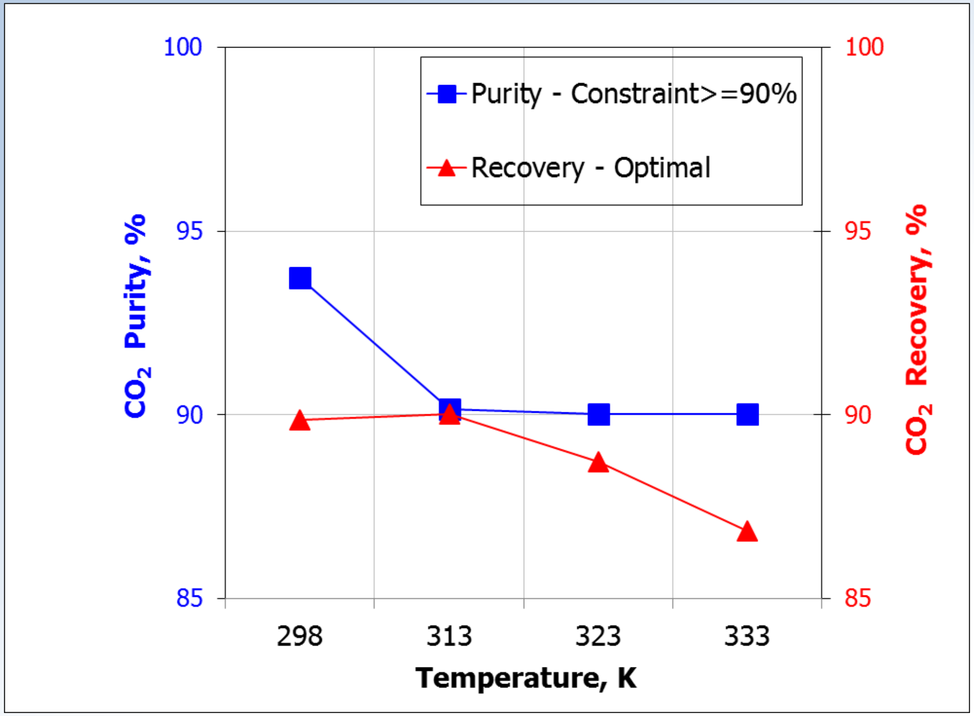
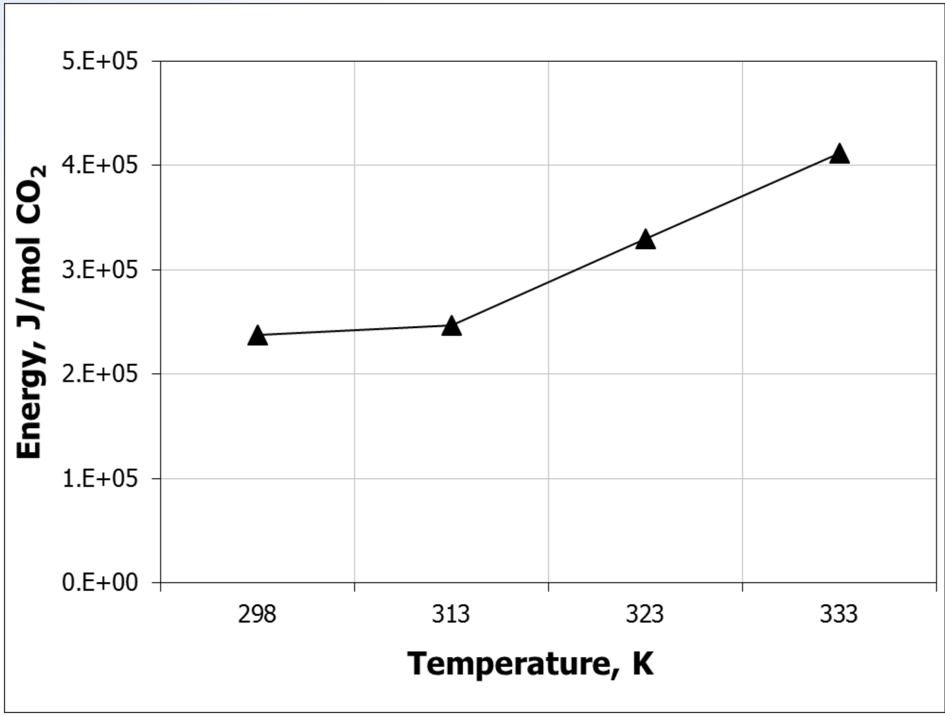
Case study II - Optimisation
Maximize CO_2 recovery (Pfeed=6.1 bar)





Tfeed, K	Pblow, bar	Pevac, bar	Pfeed, bar	spAds, lt/s
298	0.6000	0.0300	6.10	0.1900
313	0.6257	0.0312	6.10	0.1900
323	0.5428	0.0162	6.10	0.1900
333	0.4897	0.0100	6.10	0.1900

Case study II - Optimisation
Maximize CO_2 recovery (Pfeed=1.5 bar)

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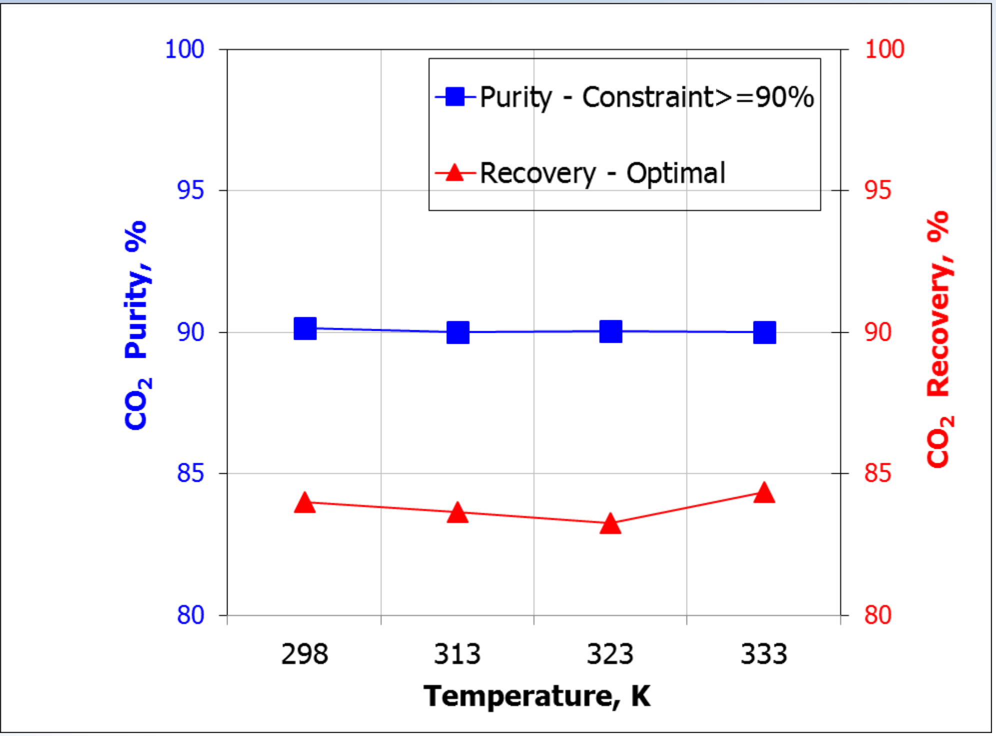

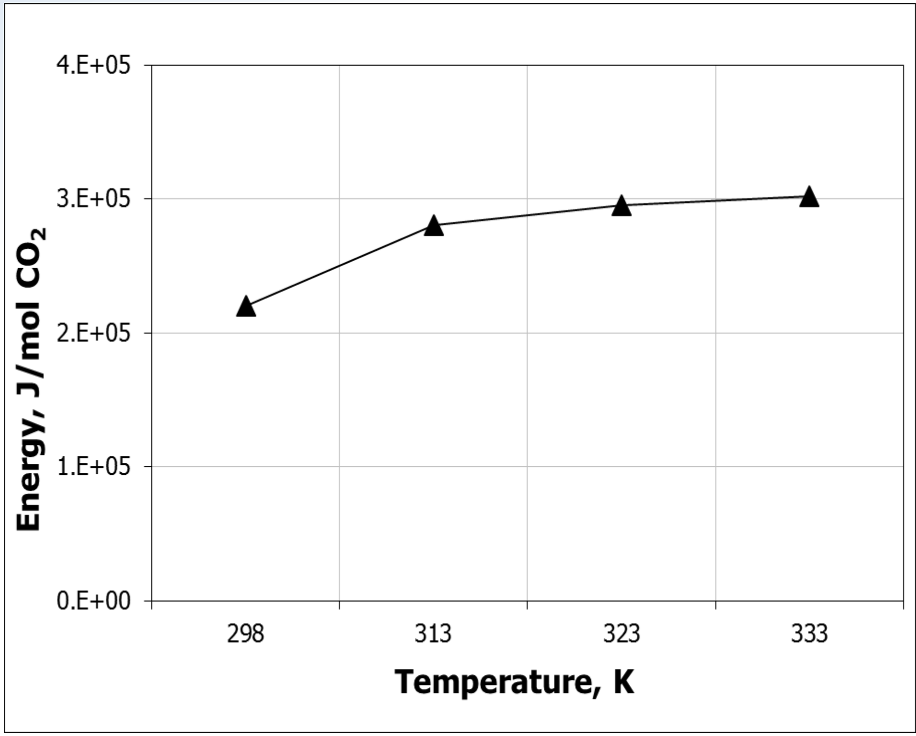

Tfeed, K	Pblow, bar	Pevac, bar	Pfeed, bar	spAds, lt/s
298	0.1100	0.0180	1.50	0.0778
313	0.1100	0.0105	1.50	0.0837
323	0.1100	0.0152	1.50	0.0846
333	0.1100	0.0100	1.50	0.0801

Conclusions

- A gPROMS™-based detailed modelling framework for multi-bed PSA/VSA flowsheets.
- Complex gas-valves control bed interactions.
- Implementation of complex operating procedures.
- Incorporation of all feasible bed interconnections.
- Systematic study of different types of adsorbents for CO_2 capture.
- Optimisation of complex multibed PSA flowsheets.

Current Work

- Optimisation studies of the PSA/VSA process.
- Hybrid PSA/VSA and membrane processes.
- Exploitation of synergistic benefits between different types of adsorbents and processes.
- Multilayer adsorbent processes.

THANK YOU FOR YOUR ATTENTION

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Advanced Process Modelling Forum 2015

Supplementary data

Single bed adsorbent model

- **Mass balance equations**

$$\frac{\partial(uC_i)}{\partial z}+\frac{\partial C_i}{\partial t}+\frac{1-\varepsilon_{bed}}{\varepsilon_{bed}}N_i=D_{z,i}\frac{\partial^2 C_i}{\partial z^2},\ \forall z\in(0,\ L),\ i=1,\ N_{comp}$$

- Local Equilibrium (LEQ): $N_i=\rho_p\frac{\partial \bar{Q}_i}{\partial t}=\rho_p\frac{\partial Q_i^*}{\partial t}$
- Linear Driving Force (LDF): $N_i=\rho_p\frac{\partial \bar{Q}_i}{\partial t}$ $\quad \frac{\partial \bar{Q}_i}{\partial t}=\frac{15D_{e,i}}{R_p^2}\left(Q_i^*-\bar{Q}_i\right)$
- Solid Diffusion (SD): $N_i=\rho_p\frac{\partial \bar{Q}_i}{\partial t}$ (Volume averaged value)

$$\frac{\partial Q_i^p}{\partial t}=D_{s,i}\left(\frac{\partial^2 Q_i^p}{\partial r^2}+\frac{2}{R_p}\frac{\partial Q_i^p}{\partial r}\right),\ \forall r\in(0,\ R_p),\ \forall z\in[0,\ L],\ i=1,\ N_{comp}$$

- Pore Diffusion (PD): $N_i=k_f a\Delta C=\frac{3k_f}{R_p}\left(C_i-C_i^p\big|_{r=R_p}\right)$

$$\frac{\partial C_i^p}{\partial t}+\frac{1-\varepsilon_p}{\varepsilon_p}\rho_p\frac{\partial Q_i^p}{\partial t}=D_{e,i}\left(\frac{\partial^2 C_i^p}{\partial r^2}+\frac{2}{R_p}\frac{\partial C_i^p}{\partial r}\right),\ \forall r\in(0,\ R_p),\ \forall z\in[0,\ L],\ i=1,\ N_{comp}$$

Single bed adsorbent model

- **Heat balance equations**
  - Isothermal (T=const)
  - Nonisothermal:

$$\varepsilon_{bed}\rho_{bc}c_{p,bc}\frac{\partial(uT)}{\partial z}+\left(\varepsilon_{bed}\rho_{bc}c_{p,bc}+(1-\varepsilon_{bed})\rho^{p}c_{p}^{p}\right)\frac{\partial T}{\partial t}+(1-\varepsilon_{bed})\dot{q}+\frac{3k_{h,wall}}{R_{bed}}(T-T_{wall})=\varepsilon_{bed}\lambda_{z}\frac{\partial^{2}T}{\partial z^{2}}$$

$$\forall z\in(0,\ L),\ i=1,\ N_{comp}$$

  - Adiabatic:

$$\varepsilon_{bed}\rho_{bc}c_{p,bc}\frac{\partial(uT)}{\partial z}+\left(\varepsilon_{bed}\rho_{bc}c_{p,bc}+(1-\varepsilon_{bed})\rho^{p}c_{p}^{p}\right)\frac{\partial T}{\partial t}+(1-\varepsilon_{bed})\dot{q}=\varepsilon_{bed}\lambda_{z}\frac{\partial^{2}T}{\partial z^{2}}$$

$$\forall z\in(0,\ L),\ i=1,\ N_{comp}$$

  - Generation term
    - Local Equilibrium (LEQ) & Linear Driving Force (LDF): $\dot{q}=\sum_{i=1}^{N_{comp}}H_{ads,i}\,N_i,\ \forall z\in(0,L)$
    - Solid Diffusion (SD) & Pore Diffusion (PD): $\dot{q}=\sum_{i=1}^{N_{comp}}H_{ads,i}\,N_i,\ \forall z\in(0,L)$

Single bed adsorbent model

- **Momentum balance equations**
  - Darcy's law (Blake Kozeny equation)

$$-\frac{\partial P}{\partial z} = 180\left(\frac{1-\varepsilon_{bed}}{\varepsilon_{bed}}\right)^2 \frac{\mu u}{\left(2R_p\right)^2}, \qquad \forall z \in (0, L)$$

  - Ergun equation

$$-\frac{\partial P}{\partial z} = 150\left(\frac{1-\varepsilon_{bed}}{\varepsilon_{bed}}\right)^2 \frac{\mu u}{\left(2R_p\right)^2} + 1.75\left(\frac{1-\varepsilon_{bed}}{\varepsilon_{bed}}\right)\frac{\rho u|u|}{2R_p}, \qquad \forall z \in (0, L)$$

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Process performance indicators

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$$\text{Product purity} = \frac{\text{Amount of component in the product stream}}{\text{Total amount of product stream}}$$

$$\text{Product recovery} = \frac{\text{Amount of component in the product stream}}{\text{Amount of component in the feed stream}}$$

$$\text{Adsorbent productivity} = \frac{\text{Amount of component in the product stream}}{(\text{Amount of adsorbent used}) \cdot (\text{PSA cycle time})}$$

$$\text{Energy consumption} = \text{Sum of all compression and vacuum sources used}$$

Parameters & Physical properties

Table 1. Parameters of adsorption column model.

parameter	value
bed radius (R_{bed})	1.1×10^{-2} m
bed length (L_{bed})	25×10^{-2} m
pore radius (R_{pore})	0.5×10^{-9} m
particle radius (R_p)	1.0×10^{-3} m
particle tortuosity (τ_p)	4.5
particle porosity (ε_p)	0.38
bed void (ε_{bed})	0.348
universal gas constant (R)	8.314 J/(mol·K)
heat transfer coefficient of the wall ($k_{h,wall}$)	60 J/(m2·K·s)

Table 2. Physical properties of different adsorbents.

Physical property	13X	AC	MgMOF74	units
particle density (ρ_p)	1159.4	800	909	kg/m3
heat capacity of particles (C_p^p)	504	1050	800	J/(kg·K)

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Parameters of the dual-site Langmuir adsorption isotherm

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Table 3. Parameters of the dual-site Langmuir adsorption isotherm.

13X	CO_2 (i = 1)	N_2 (i = 2)	units
k1,i(1)	2.817269	1.889581045	mol/Kg
k2,i(1)	-3.5×10-4	-2.2462×10-4	1/K
k3,i(1)	2.83×10-9	1.163388×10-9	1/Pa
k4,i(1)	2598.203	1944.605788	K
k1,i(2)	3.970888	1.889581045	mol/Kg
k2,i(2)	-4.95×10-3	-2.2462×10-4	1/K
k3,i(2)	4.411×10-9	1.163388×10-9	1/Pa
k4,i(2)	3594.071	1944.605788	K

AC	CO_2 (i = 1)	N_2 (i = 2)	units
k1,i(1)	0,5914	0,1553	mol/Kg
k2,i(1)	0	0	1/K
k3,i(1)	4,05E-10	8,34E-08	1/Pa
k4,i(1)	3776,7621	1719,9904	K
k1,i(2)	7,5055	41,3000	mol/Kg
k2,i(2)	0	0	1/K
k3,i(2)	1,68E-09	7,98E-17	1/Pa
k4,i(2)	2381,5251	6013,9524	K

Mg-MOF-74	CO_2 (i = 1)	N_2 (i = 2)	units
k1,i(1)	6,8	14	mol/Kg
k2,i(1)	0	0	1/K
k3,i(1)	2,44E-11	4,96E-10	1/Pa
k4,i(1)	5051,7200	2165,0229	K
k1,i(2)	9,9	0	mol/Kg
k2,i(2)	0,00E+00	0	1/K
k3,i(2)	1,39E-10	0	1/Pa
k4,i(2)	2886,6971	0	K

Mg_2(dobdc) (dobdc=1,4-dioxido-2,5-benzenedicarboxylate) Mg-MOF-74, CPO-27-Mg, $(Mg(C_4HO_3)(H_2O).4H_2O)$

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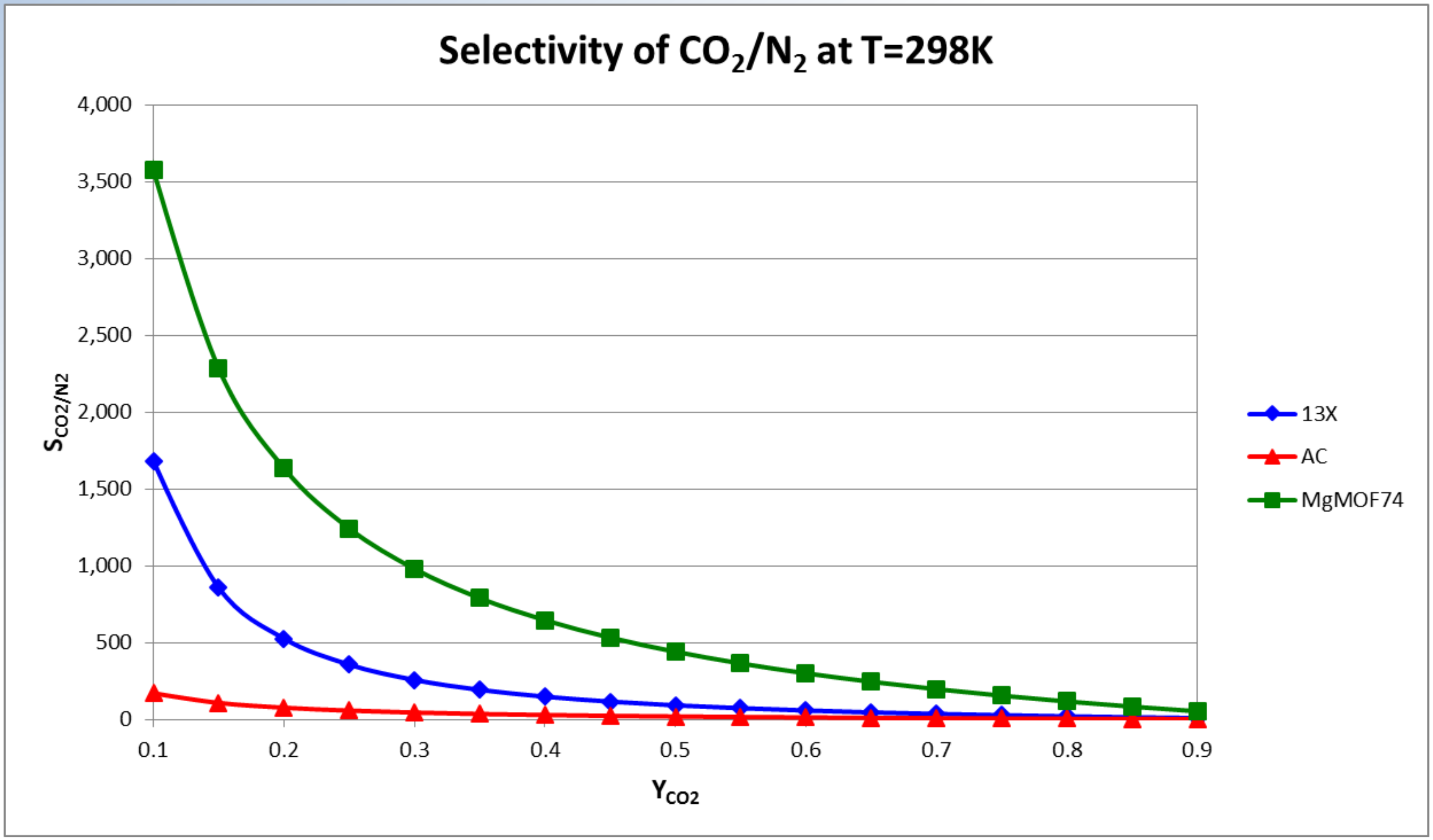
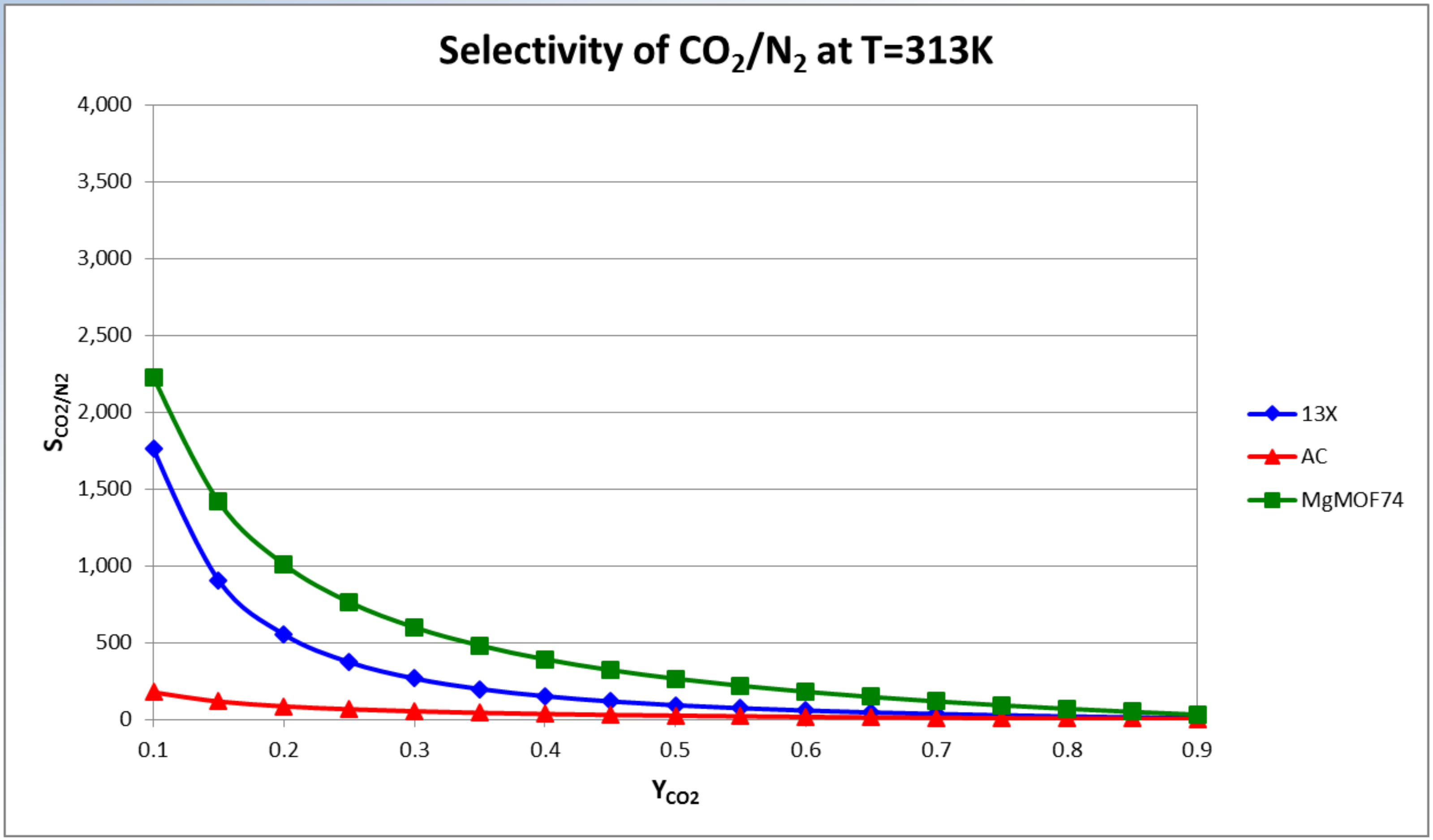
Selectivity of CO_2/N_2 mixture



Selectivity of CO_2/N_2 mixture



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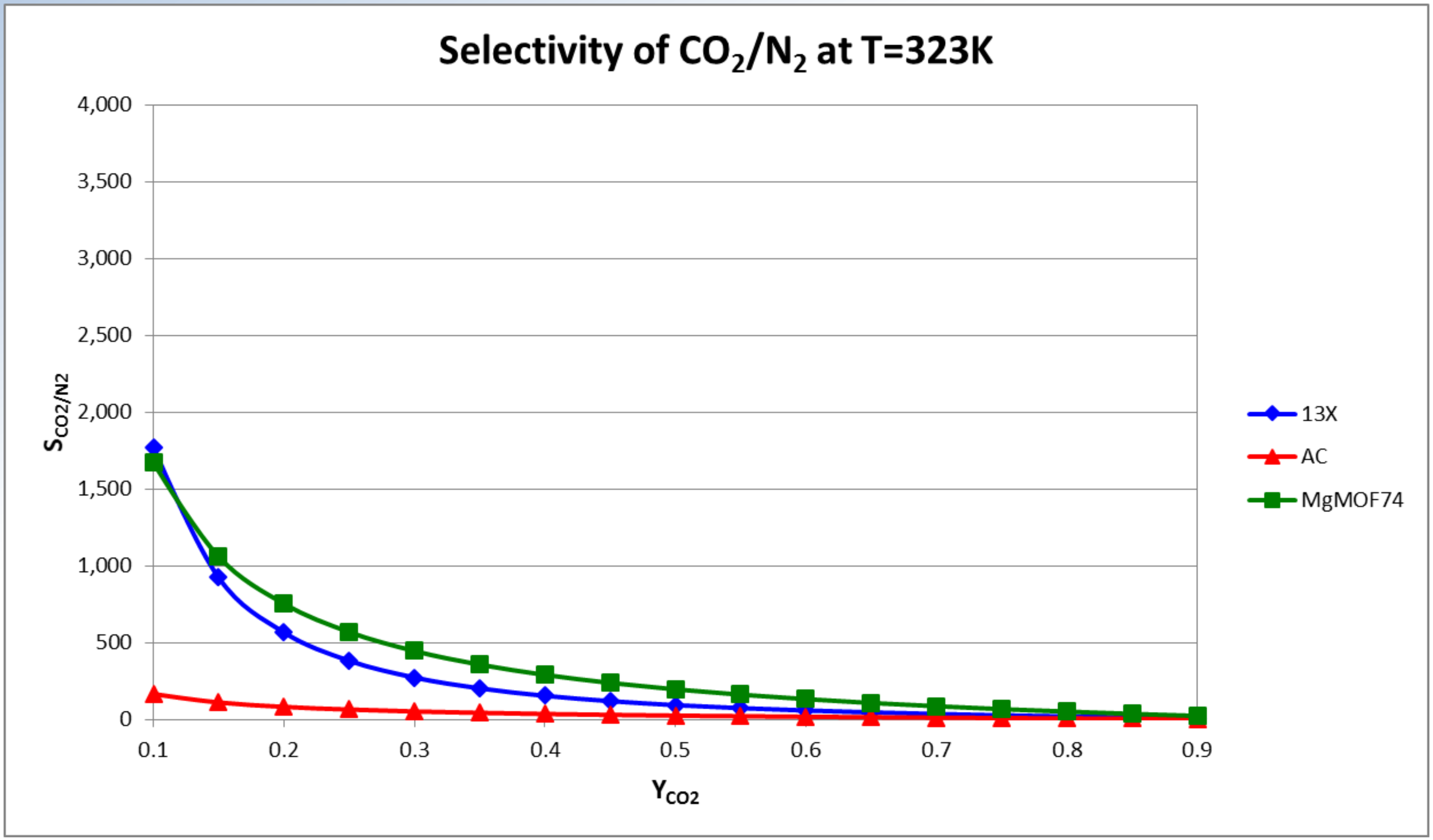

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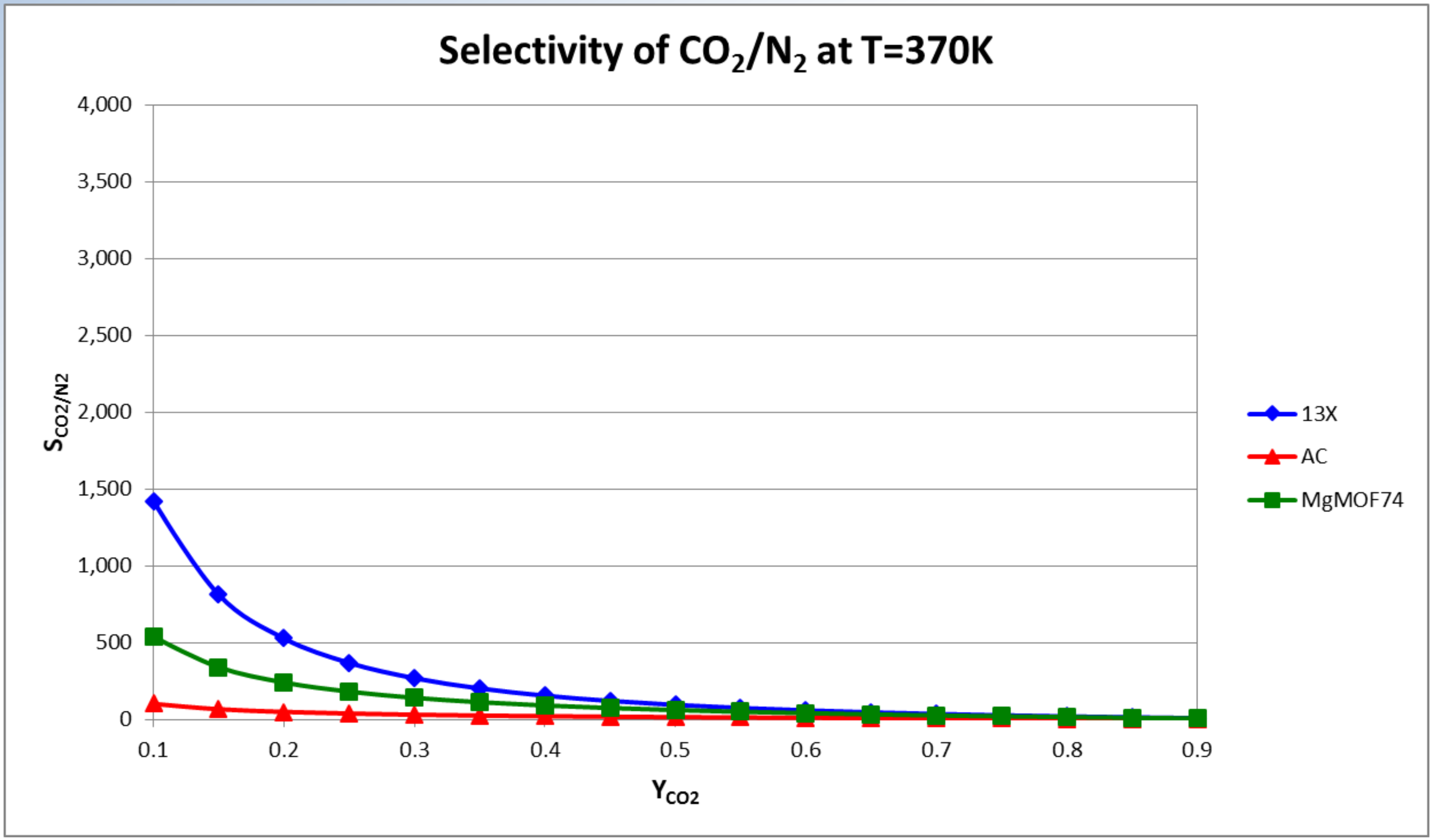

Model validation - Results

Table 4. Process performance indicators simulation results with absolute deviations from the results of Ko et al. (2005)

						Ko et al	Ko et al	this work	this work		
Reference	Pfeed (bar)	Tfeed (K)	L/D	Number of cycles (CSS)	Discretization method	Purity CO_2	Recovery CO_2	Purity CO_2	Recovery CO_2	Deviation Purity CO_2	Deviation Recovery CO_2
Ko et al. (2005)	6.52	370.00	11.36	300	CFDM,2,50	88.94	96.90	84.82	97.93	-4.63	1.06
Ko et al. (2005)	6.94	365.32	11.36	300	CFDM,2,50	95.46	15.00	92.12	14.35	-3.50	-4.33
Ko et al. (2005)	8.69	364.42	17.64	300	CFDM,2,50	92.29	80.00	97.19	79.20	5.31	-1.00

Deviations are due to potentially different pressure history profile during the pressure-change steps affected by gas valve equation

Good predictive power (simulation results are in good agreement with literature results)

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Case study II
Comparison of adsorbents

13X

F_{feed} (lt/s_stp)	CO_2 Purity	CO_2 Recovery	CO_2 Productivity (mol CO_2/Kg.s)	Energy (J/mol CO_2)
0.04627	84.14	98.30	0.001744	1.71E+05
0.05552	86.38	95.00	0.001956	1.73E+05
0.06940	88.86	90.34	0.002248	1.77E+05
0.09254	91.63	82.88	0.002657	1.87E+05
0.13881	94.57	69.22	0.003217	2.14E+05
0.27761	96.66	42.22	0.003805	3.28E+05

Mg-MOF-74

F_{feed} (lt/s_stp)	CO_2 Purity	CO_2 Recovery	CO_2 Productivity (mol CO_2/Kg.s)	Energy (J/mol CO_2)
0.04627	71.20	93.87	0.002505	1.95E+05
0.05552	74.52	91.79	0.002769	1.93E+05
0.06940	78.54	88.55	0.003137	1.92E+05
0.09254	83.45	82.50	0.003649	1.96E+05
0.13881	88.98	70.24	0.004364	2.17E+05
0.27761	93.07	43.99	0.005157	3.19E+05

A-C

F_{feed} (lt/s_stp)	CO_2 Purity	CO_2 Recovery	CO_2 Productivity (mol CO_2/Kg.s)	Energy (J/mol CO_2)
0.04627	83.78	79.66	0.001946	1.99E+05
0.05552	85.80	74.65	0.002138	2.08E+05
0.06940	87.55	67.35	0.002355	2.25E+05
0.09254	88.64	56.32	0.002563	2.60E+05
0.13881	89.19	40.94	0.002728	3.42E+05
0.27761	89.53	21.96	0.002855	6.04E+05

T_{feed}=323K
P_{feed}=1.10bar
P_{blow}=0.20bar
P_{evac}=0.02bar

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An overview of operating steps employed in different configurations

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	1	2a	2b	3	4b	4a
B-1	CoC	Ads	Ads	CoCD	Evac	Evac

	1	2	3a	3b	4	5	6a	6b
B-1	PER1	CoC	Ads	Ads	PED1	CoCD	Evac	Evac
B-2	PED1	CoCD	Evac	Evac	PER1	CoC	Ads	Ads

	1	2	3	4a	4b	5	6	7	8a	8b
B-1	PER2	PER1	CoC	Ads	Ads	PED1	PED2	CoCD	Evac	Evac
B-2	Evac	Evac	PER2	PER1	CoC	Ads	Ads	PED1	PED2	CoCD
B-3	PED2	CoCD	Evac	Evac	PER2	PER1	CoC	Ads	Ads	PED1
B-4	Ads	PED1	PED2	CoCD	Evac	Evac	PER2	PER1	CoC	Ads

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	1	2	3	4	5a	5b	6	7	8	9	10a	10b
B-1	PER3	PER2	PER1	CoC	Ads	Ads	PED1	PED2	PED3	CoCD	Evac	Evac
B-2	Evac	Evac	PER3	PER2	PER1	CoC	Ads	Ads	PED1	PED2	PED3	CoCD
B-3	PED3	CoCD	Evac	Evac	PER3	PER2	PER1	CoC	Ads	Ads	PED1	PED2
B-4	PED1	PED2	PED3	CoCD	Evac	Evac	PER3	PER2	PER1	CoC	Ads	Ads
B-5	Ads	Ads	PED1	PED2	PED3	CoCD	Evac	Evac	PER3	PER2	PER1	CoC
B-6	PER1	CoC	Ads	Ads	PED1	PED2	PED3	CoCD	Evac	Evac	PER3	PER2

Optimization I
Maximize CO_2 purity

CASE STUDY I (MAX CO2 PURITY) **13X**

Base case

Configuration	Pfeed, bar	Rp, mm	L/D	Qfeed, Lstp/s	CO_2 Purity	CO_2 Recovery
C1	6.52	1.00	11.36	0.0694	87.19	98.56
C2	6.52	1.00	11.36	0.0925	86.28	99.99
C4	6.52	1.00	11.36	0.1157	85.61	99.99
C6	6.52	1.00	11.36	0.1388	85.14	99.99

Optimal

Configuration	Pfeed, bar	Rp, mm	L/D	Qfeed, Lstp/s	CO_2 Purity	CO_2 Recovery
C1	8.00	0.70	5.00	0.10	92.95	99.82
C2	8.00	1.00	5.22	0.14	92.37	99.85
C4	8.00	0.86	6.95	0.17	91.61	99.95
C6	8.00	0.74	7.82	0.20	91.25	99.94

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Optimization II
Maximize CO_2 recovery

CASE STUDY II (MAX CO2 RECOVERY - PURITY>90%)

MOF-74

Optimal

Tfeed, K	Pblow, bar	Pevac, bar	Pfeed, bar	spAds, lt/s	CO_2 Purity	CO_2 Recovery	Energy
298	0.1100	0.0180	1.50	0.0778	90.13	83.99	220425.20
313	0.1100	0.0105	1.50	0.0837	90.00	83.63	280049.03
323	0.1100	0.0152	1.50	0.0846	90.04	83.27	295456.36
333	0.1100	0.0100	1.50	0.0801	90.02	84.35	301857.31

Optimal

Tfeed, K	Pblow, bar	Pevac, bar	Pfeed, bar	spAds, lt/s	CO_2 Purity	CO_2 Recovery	Energy
298	0.6000	0.0300	6.10	0.1900	93.74	89.87	237653.09
313	0.6257	0.0312	6.10	0.1900	90.15	90.03	246857.53
323	0.5428	0.0162	6.10	0.1900	90.03	88.72	329767.63
333	0.4897	0.0100	6.10	0.1900	90.02	86.85	411799.41