

# KSCT Fall Meeting

Theoretical Separation  
Feasibility of Zeolites for  
Gas Sweetening Process

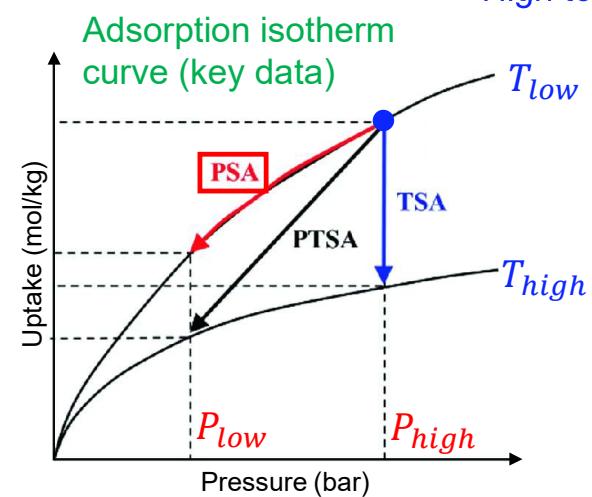
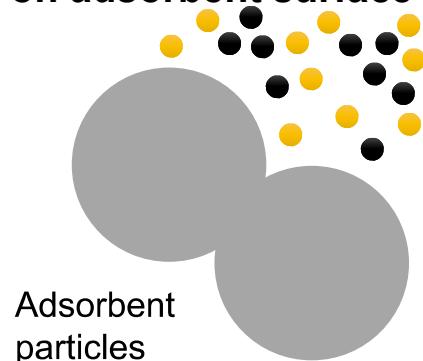
Sep 9<sup>th</sup>  
2021

Seongbin Ga  
Pusan National University



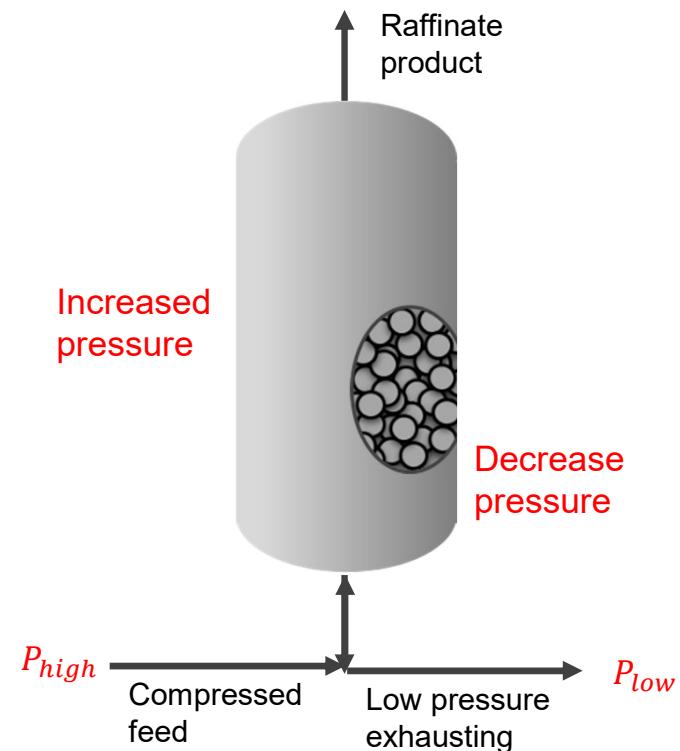
# How Adsorption Processes Work

Adsorption phenomena  
on adsorbent surface

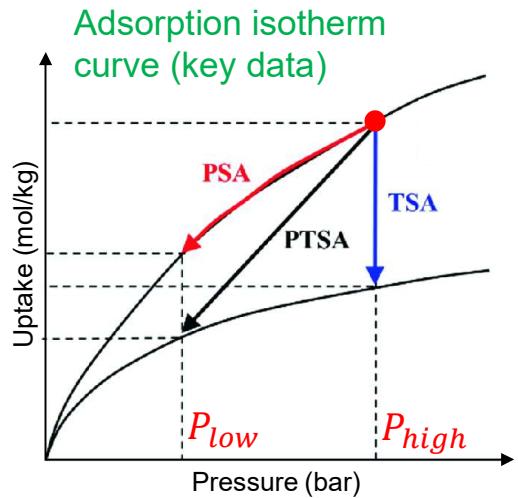


Adsorption at condition 1:  
High pressure ( $P_{high}$ ),  
Low temperature ( $T_{low}$ )

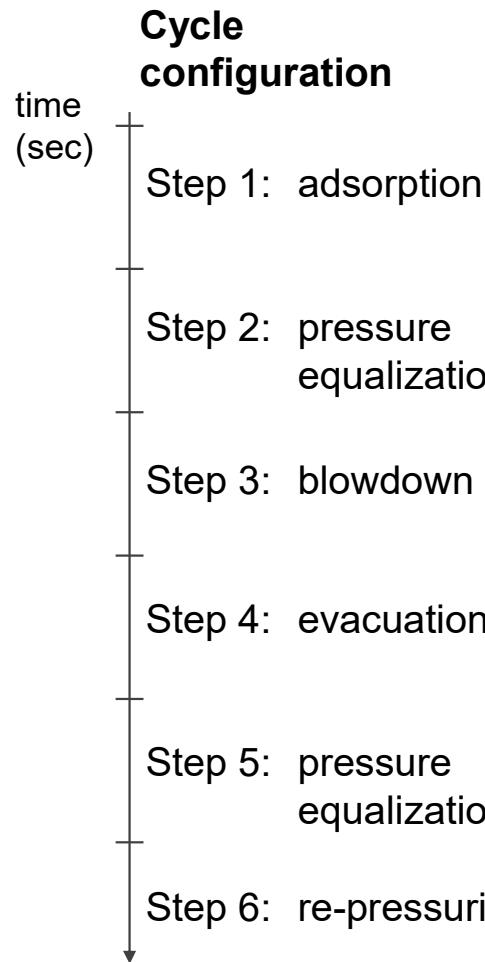
Desorption at condition 2:  
Low pressure ( $P_{low}$ ),  
High temperature ( $T_{high}$ )



# Cyclic Operation of Adsorption Process

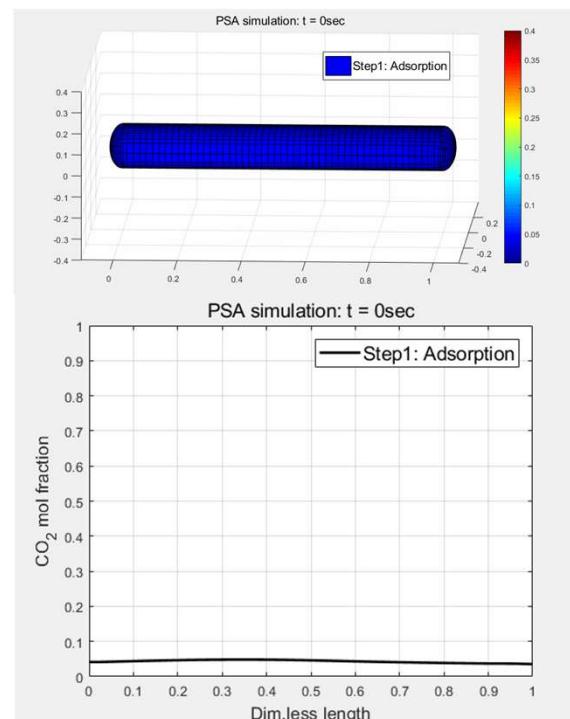


# Cyclic Operation of Adsorption Process



## Simulation results

e.g.  $\text{CO}_2/\text{N}_2$  separation  
(gas phase concentration)



## Process-level performance

Efficiency ( $\text{CO}_2$  ton/ GJ)

$$\eta = \frac{M_{\text{CO}_2}}{E_{\text{comp}}}$$

$\text{CO}_2$  purity (mol/mol)

$$x = \frac{F_{\text{CO}_2,\text{ex}}}{F_{\text{CO}_2,\text{ex}} + F_{\text{N}_2,\text{ex}}}$$

# Problem 1: CPU time

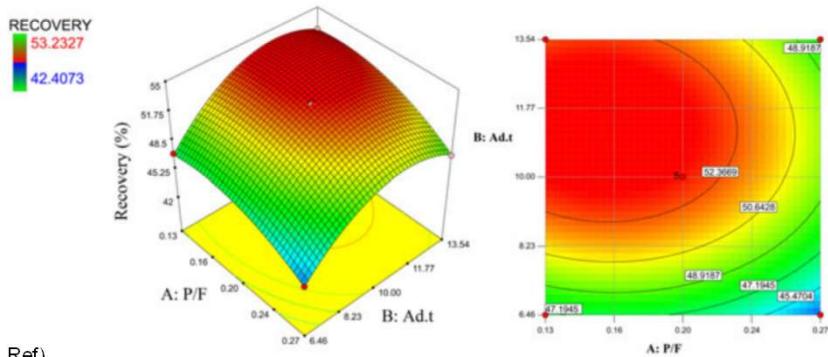
Suppose we have  
**many adsorbents** to evaluate.

For each adsorbent, we need

- 1) Dynamic simulations (min-level)
- 2) Cyclic steady state search (hr-level)
- 3) Design & operation optimization (day-level)

## Operation optimization example

Adsorbent 1       $\neq$       Adsorbent 2  
 → optimal operation set 1      → optimal operation set 2



## Mass, momentum, and energy balance equations

$$\text{Energy balance} \quad \frac{\partial T}{\partial t} = \frac{1}{\epsilon \rho_g c_g + (1-\epsilon) \rho_s c_s} \left( (1-\epsilon) \rho_s \sum_i^2 (-\Delta H_i) \frac{\partial q_i}{\partial t} + \lambda_{ax} \frac{\partial^2 T}{\partial z^2} - \rho_g c_g u \frac{\partial T}{\partial z} - \rho_g c_g T \frac{\partial u}{\partial z} - \frac{2h_i}{r_{b,i}} (T - T_w) \right)$$

Overall mass balance

$$\epsilon \frac{\partial C}{\partial t} + (1-\epsilon) \rho_s \sum_i^2 \frac{\partial q_i}{\partial t} + \epsilon u \frac{\partial C}{\partial z} + \epsilon C \frac{\partial u}{\partial z} = 0$$

$$\text{Component mass balance} \quad \frac{\partial y_1}{\partial t} = -\frac{1-\epsilon}{C\epsilon} \rho_s \frac{\partial q_1}{\partial t} + \frac{D_{ax}}{C} \left( C \frac{\partial^2 y}{\partial z^2} + 2 \frac{\partial C}{\partial z} \frac{\partial y_1}{\partial z} + y_1 \frac{\partial^2 C}{\partial z^2} \right) - u \frac{\partial y_1}{\partial z} + \frac{y_1 (1-\epsilon)}{C \epsilon} \rho_s \sum_i^2 \frac{\partial q_i}{\partial t}$$

Momentum balance

$$-\frac{\partial P}{\partial z} = \frac{150.0 (1-\epsilon)^2}{\epsilon^3} \frac{\mu}{d_p^2} u + 1.75 \times \frac{10^{-4} (1-\epsilon) \rho_g}{\epsilon^3 d_p} u |u|$$

Other assumed equations

$$\text{LDF model: } \frac{\partial q_i}{\partial t} = k_i (q_i^* - q_i) \text{ for } i = 1, 2$$

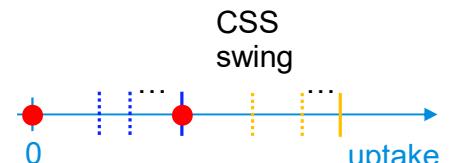
$$\text{Ideal gas equation: } PV = nRT$$

## Cyclic steady state (CSS) conditions

for all  $i$

for all  $\theta$ : all state variables

$$\frac{(\theta_{z_i}|_{t=t_0})_{(n)\text{th cycle}} - (\theta_{z_i}|_{t=t_f})_{(n)\text{th cycle}}}{(\theta_{z_i}|_{t=t_0})_{(n)\text{th cycle}}} < \text{tolerance}$$



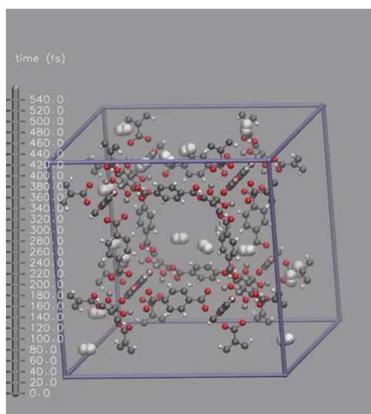
# Problem 2: Limited information

For the dynamic simulation for the PSA process,  
**a variety of adsorbent properties** are essential:

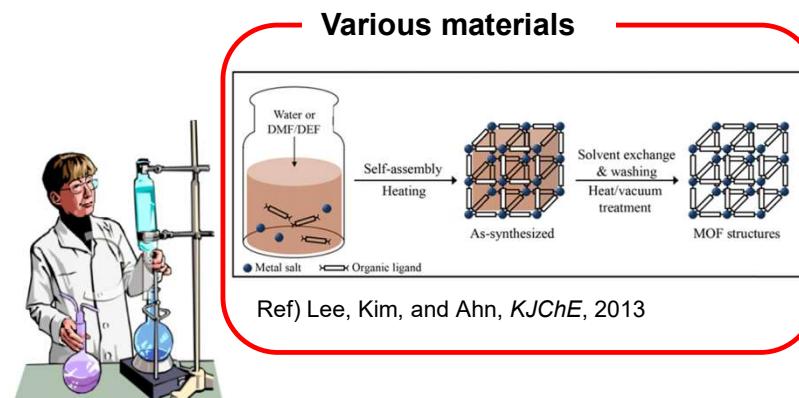
Adsorption isotherm data, heat of adsorption,  
mass/heat transfer coefficients, heat capacity, density ....

Most of them are rarely available,  
especially when they are:  
newly discovered or  
newly developed or  
newly synthesized

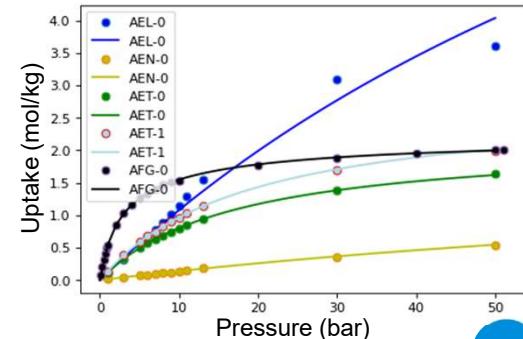
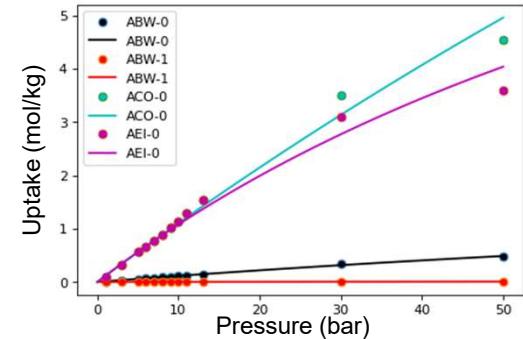
## Molecular simulations



## Synthesis of adsorbents



**Adsorption isotherm curves**  
= The first property they can obtain.

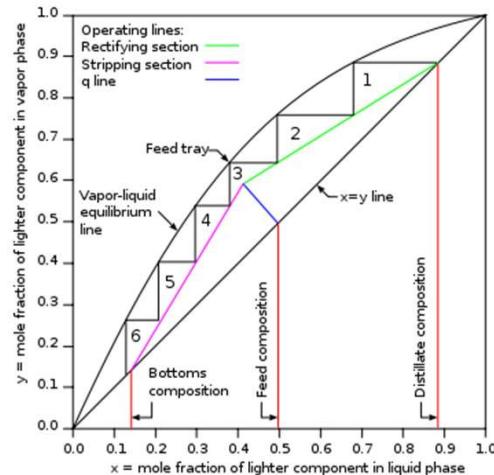
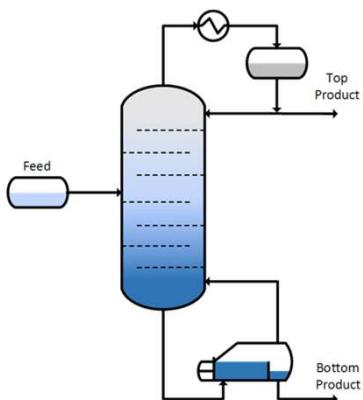


# Idea: Ideal PSA Process

Inspired by McCabe Thiele method  
or Fenske equation

For distillation column

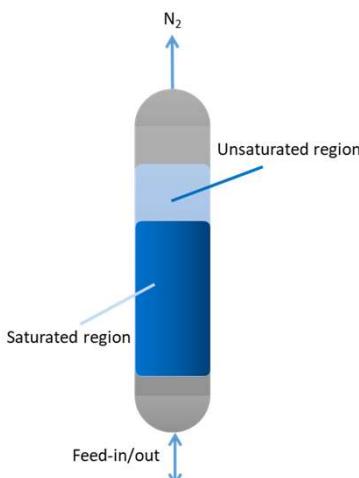
Equilibrium info.  
Feed conditions  
Target purity



[Shortcut method: ideal PSA process]

For pressure swing adsorption (PSA) column

Isotherm info.  
(Usually measured first)  
Feed conditions  
Target purity



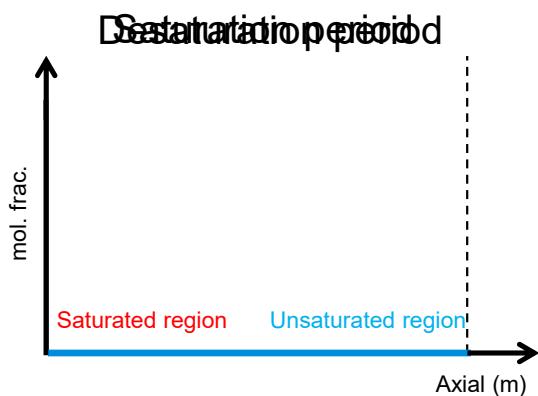
?  
(Available for  
material developers)

# Idea: Ideal PSA Process

[Shortcut method: ideal PSA process]

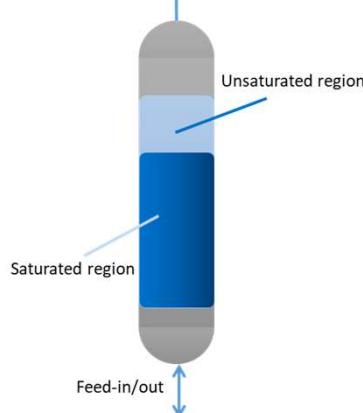
Derivation of the method (formula) starts from a set of assumptions (idealization):

- Two gas components
- No dispersion: clear saturated region boundary
- Two periods: saturation & desaturation
- Full capacity of the adsorbents
- Always in solid/gas equilibrium
- No effect of void volume



For pressure swing adsorption (PSA) column

{ Isotherm info.  
(Usually measured first)  
Feed conditions  
Target purity  
N<sub>2</sub>



{ Required process  
(operation or design)

?  
(Available for material developers)

# Formula: Ideal PSA Process

New shortcut evaluation method

Efficiency

$$\eta = \frac{(\gamma-1)y_{flue}}{\gamma RT \left[ \left( \frac{P_{high}}{P_{flue}} \right)^{\frac{\gamma-1}{\gamma}} - 1 \right]}$$

Purity

$$P_{high} = \frac{P_{low}}{(1 + \bar{b}(x)P_{low})R_q - \bar{b}(y_{flue})P_{low}}$$

where

$$R_q = \frac{q_{m,1}b_1(1-x)y_{flue} - q_{m,2}b_2(1-y_{flue})}{x(1-x)(q_{m,1}b_1 - q_{m,2}b_2)}$$

$$\bar{b}(y_{flue}) = (b_1 - b_2)y_{flue} + b_2$$

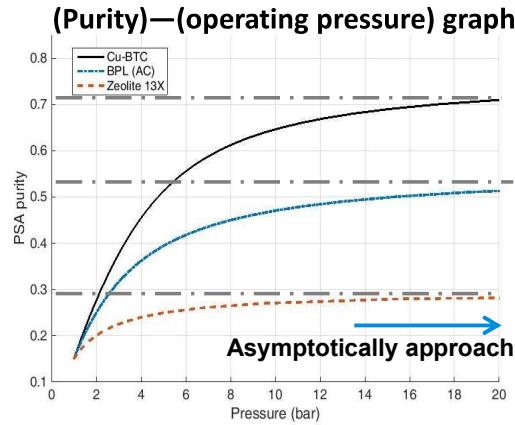
$$\bar{b}(x) = (b_1 - b_2)x + b_2$$

**Advantages of them:**

- ❖ Reflective of the application to the PSA process
- ❖ Easy to use and requiring only isotherm parameters
- ❖ Small computational cost  
(compared to PSA simulation time:  
~2000 sec for testing a single condition)

Proposed in

S. Ga et al., *Comput. Chem. Eng.*, 2017



$$\lim_{P \rightarrow \infty} x = ?$$

[Converges to a certain value]

Find  $x$

such that  $P_{high} \rightarrow \infty$   
(denominator)  $\rightarrow +0$

**Upper limit of purity (purity cannot exceed this)**

$$x_{upper} = \frac{-B - \sqrt{B^2 - 4AC}}{2A}$$

where

$$A = (q_{m,1} - q_{m,2})b_1b_2P_{low}$$

$$B = q_{m,1}(\beta_1 - b_1y_{flue}) + q_{m,2}\{\beta_2 - b_2(1-y_{flue})\}$$

$$C = (1 + b_2P_{low})q_{m,1}b_1y_{flue}$$

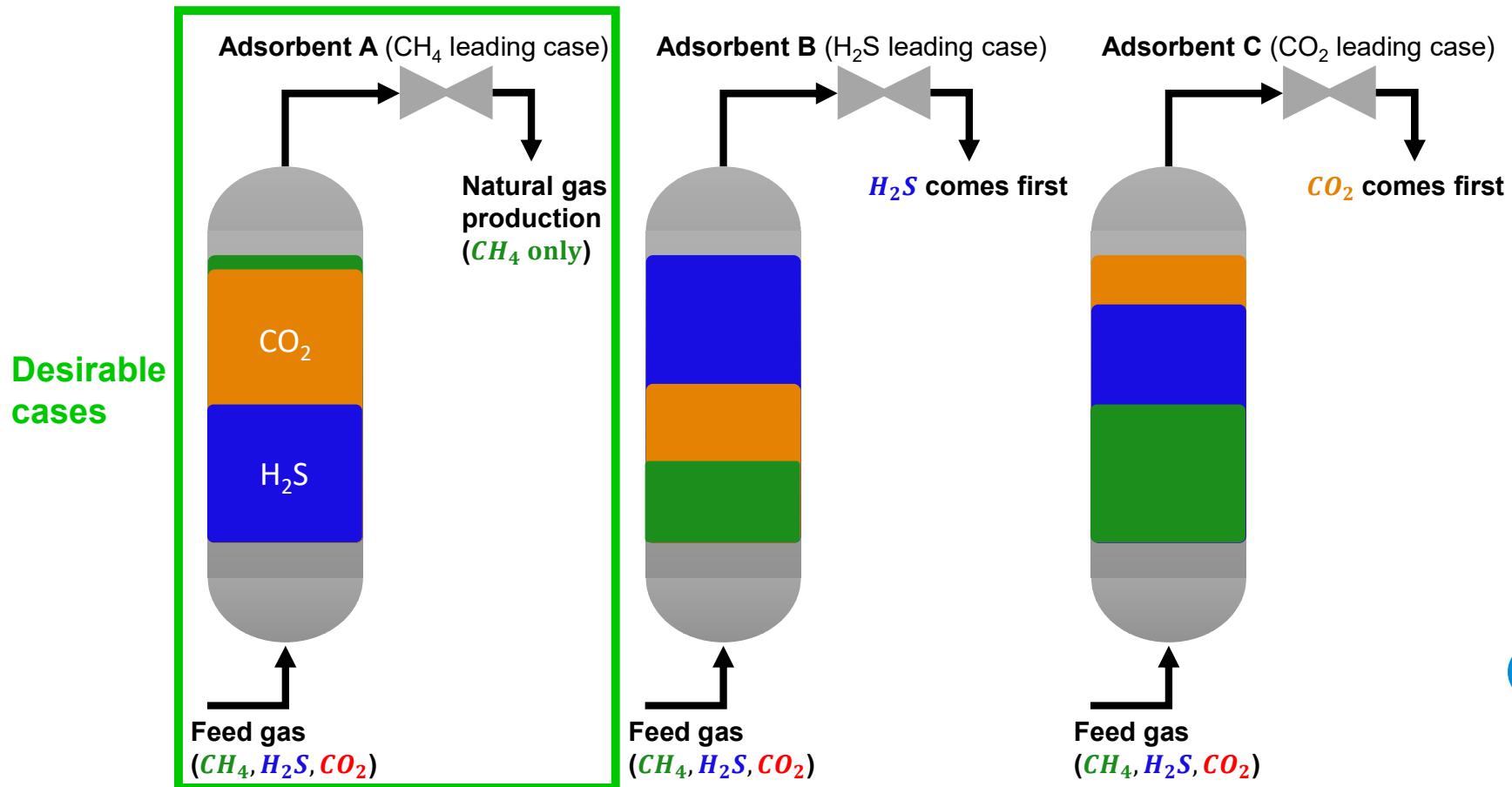
$$\beta_1 = \{b_1(b_1 - b_2) + b_1\bar{b}(y_{flue}) - b_1b_2y_{flue}\}P_{low}$$

$$\beta_2 = -\{b_2^2 + b_2\bar{b}(y_{flue})\}P_{low}$$

# Multi-component Case: $\text{CH}_4/\text{H}_2\text{S}/\text{CO}_2$

Natural gas sweetening process (feed gas contains  $\text{CH}_4/\text{H}_2\text{S}/\text{CO}_2$ ):

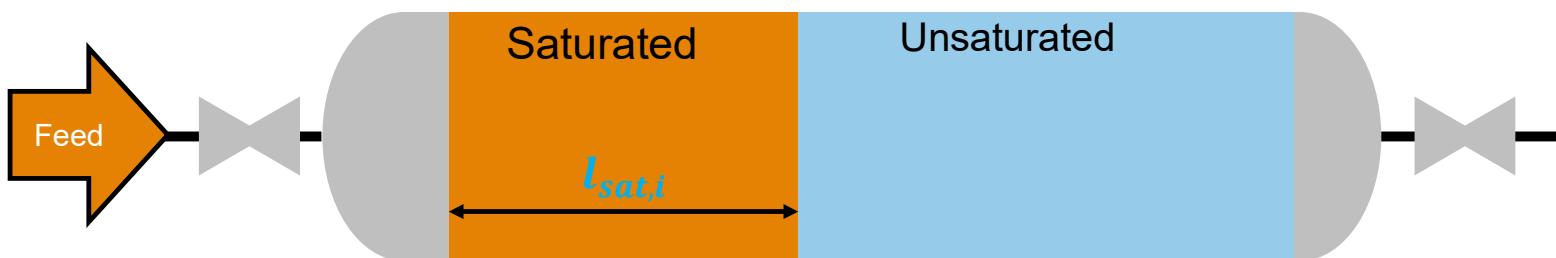
Different adsorbents can be classified into three cases.



# Expansion Set of The Ideal PSA Method

## Leading component concept

- During the adsorption step, the saturated region is propagated by the feed gas.
- The rate of saturation differs for each gas component.
- From the ideal PSA concept, we can calculate the rate of saturation as:



Rate of the saturation  
for component  $i$  ( $r_i$ )

$$r_i = \frac{l_{sat,i}}{\Delta t}$$

[Definition]

From the mass balance,

$$y_{in,i} F_{in} \Delta t = \rho_s (1 - \varepsilon) A l_{sat,i} \Delta q_i$$

$$l_{sat,i} = \frac{y_{in,i} F_{in} \Delta t}{\rho_s (1 - \varepsilon) A \Delta q_i}$$

[Length of  
saturation region]

Therefore,

$$\begin{aligned} r_{CH_4} : r_{H_2S} : r_{CO_2} \\ = \frac{y_{in,CH_4}}{\Delta q_{CH_4}} : \frac{y_{in,H_2S}}{\Delta q_{H_2S}} : \frac{y_{in,CO_2}}{\Delta q_{CO_2}} \end{aligned}$$

[Ratio of the rate]  
= [Ratio of length]

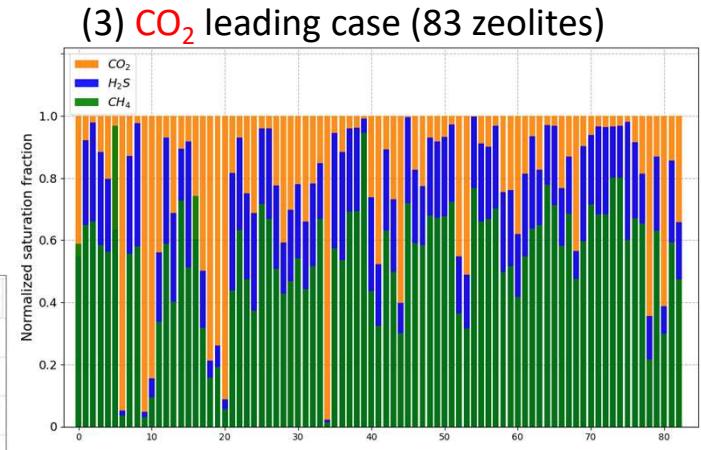
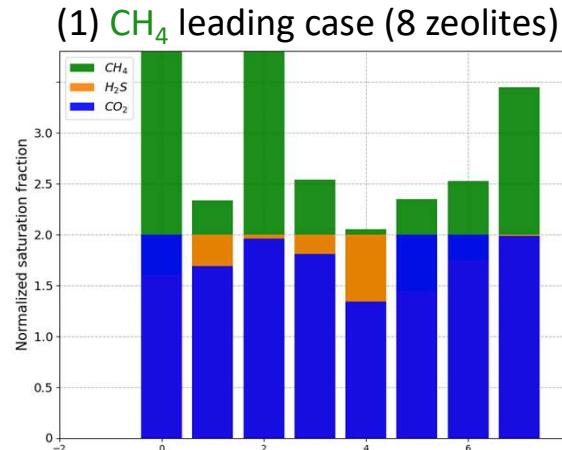
# Application to Zeolite Database

## International Zeolite Association (IZA) database



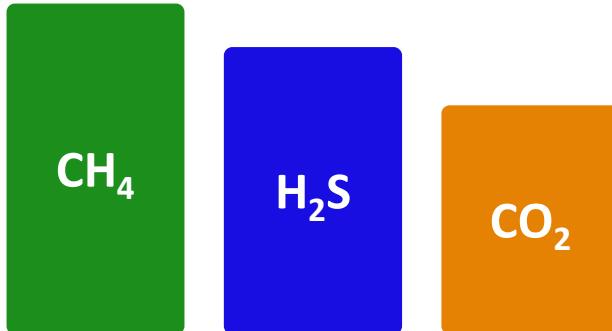
- Database providing structural information of over 300 zeolites
- Data in the crystallographic information framework (\*.cif) file
- Online available database

## Ideal PSA simulation Results: Classifying zeolites of IZA database



# Visualization for Classification

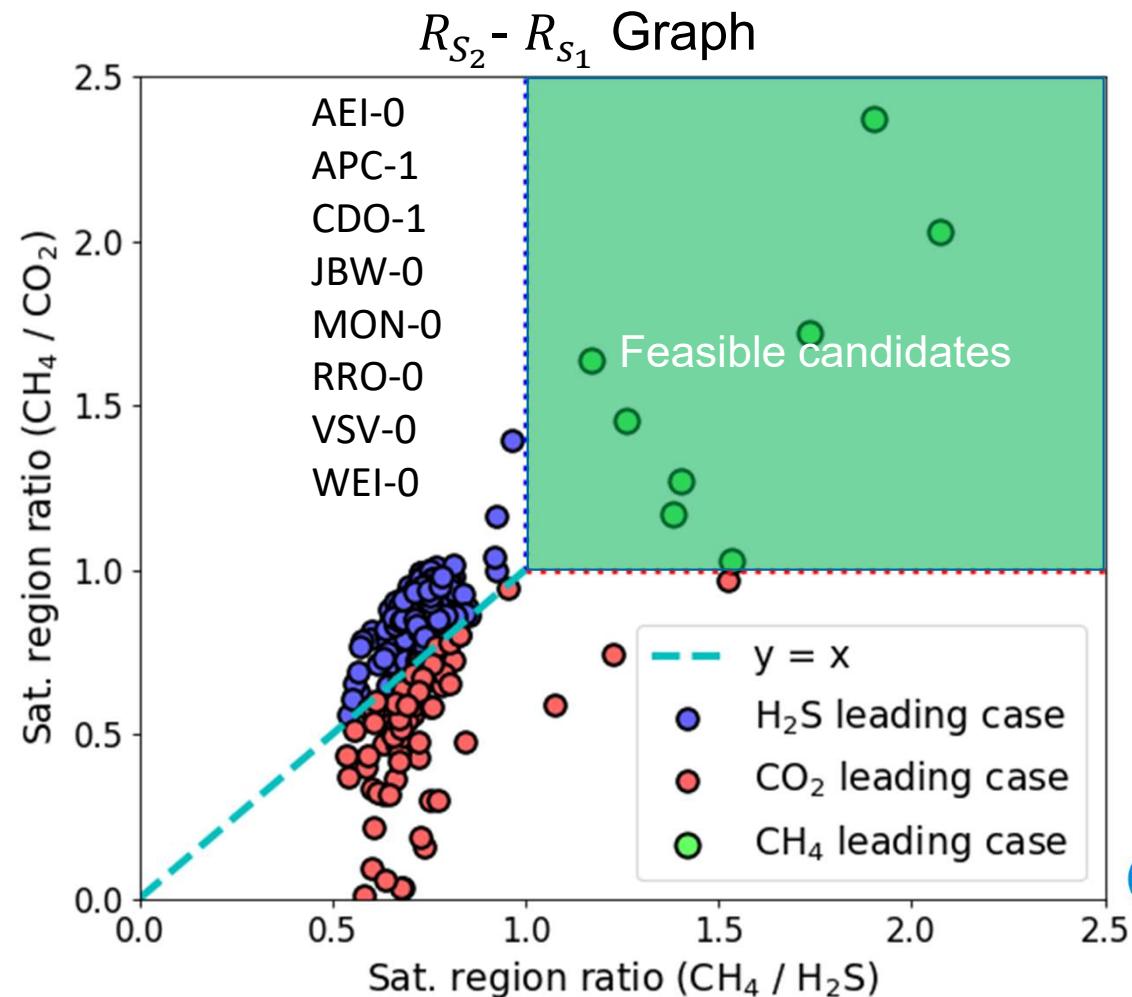
## Different Saturation regions



## Saturation region ratio

$$R_{s1} = \frac{\text{CH}_4}{\text{H}_2\text{S}} > 1$$

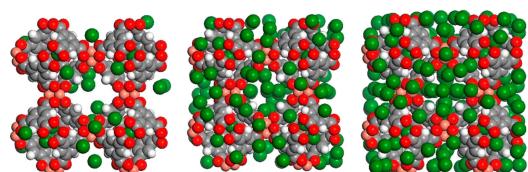
$$R_{s2} = \frac{\text{CH}_4}{\text{CO}_2} > 1$$



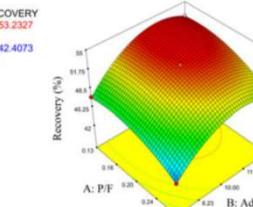
# Advantages of This Method

## Conventional method

Molecular simulations



Process simulations & optimization



For adsorbent #i

ex) design/operation

Condition 1

Condition 2

⋮

Condition N

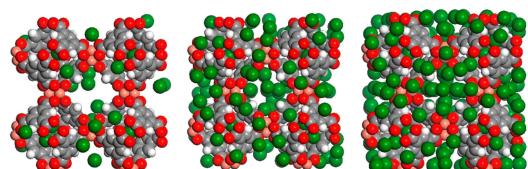
- Feasible
- Infeasible
- Feasible
- Infeasible

- Feasible
- Infeasible

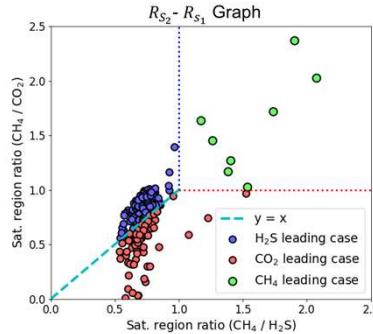
Several CPU weeks  
(to test a single adsorbent)

## New feasibility test method

Molecular simulations



Saturation region ratio



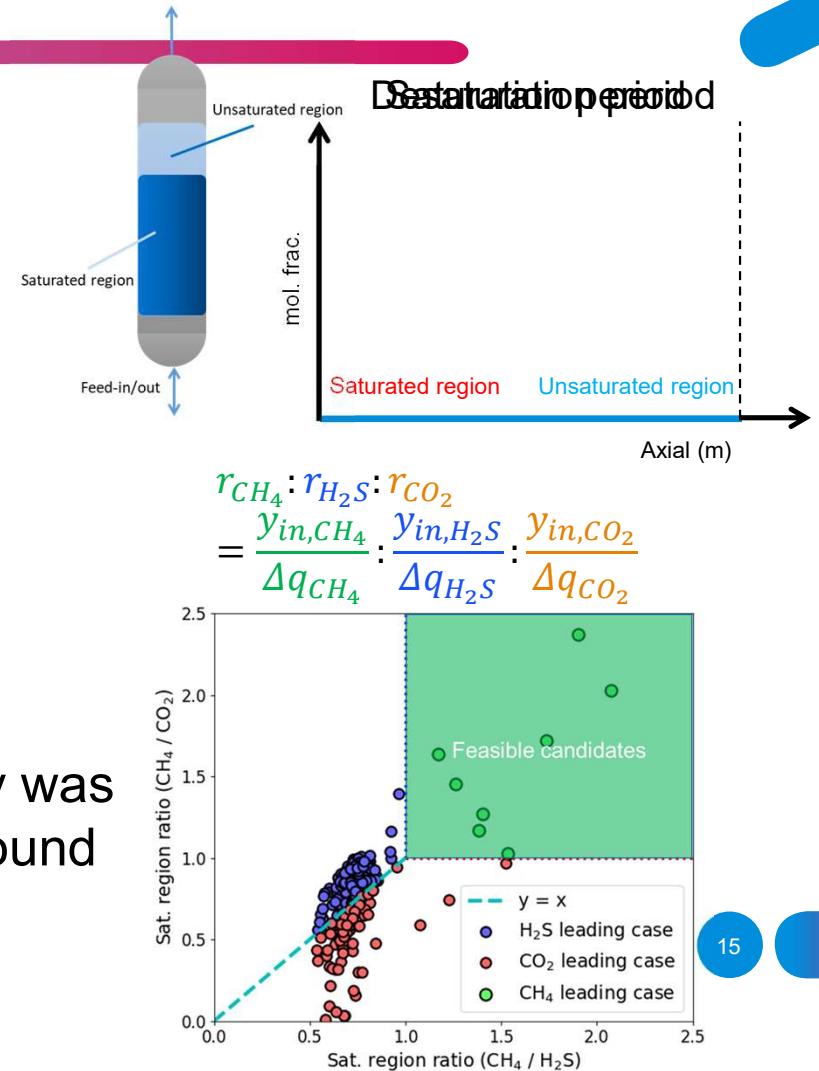
Infeasible

Feasible

Several CPU hours  
(for 346 adsorbents)

# Conclusion

- Shortcut evaluation method:  
Ideal PSA process
- Extension to multicomponent case:  
The shortcut method  
with multiple gas components
- Feasibility test method:  
Feasibility for the separation process
- Using IZA database, the separation feasibility was tested for 346 zeolites, and 8 zeolites were found to be feasible.



*Thank You!*



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# Validation: Ideal PSA Process

In

S. Ga et al., *Comput. Chem. Eng.*, 2017

I theoretically derived the method,  
and roughly validated  
by comparing with the rigorous (dynamic) simulations.

Comparison of the sorbents (if target purity = 0.5)

[Candidates]	$x_{upp}$	<u>PSA dynamic simulation (non-ideal)</u>	Selectivity
Zeolite 13X	0.296	> Λ	0.1992 Λ
BPL (AC)	0.556	> Λ	0.2601 Λ
Cu-BTC	0.76	>	0.333

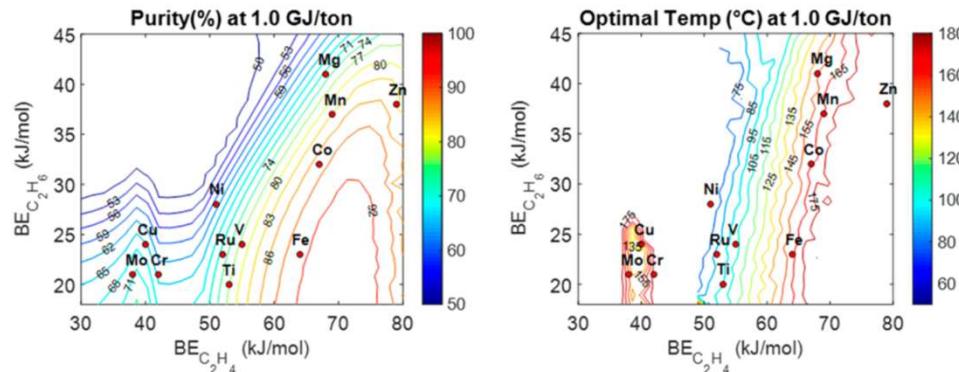
cf) Working capacity (1~15bar)

A: 2.2mol/kg  
B: 0.95mol/kg  
C: 8.1mol/kg

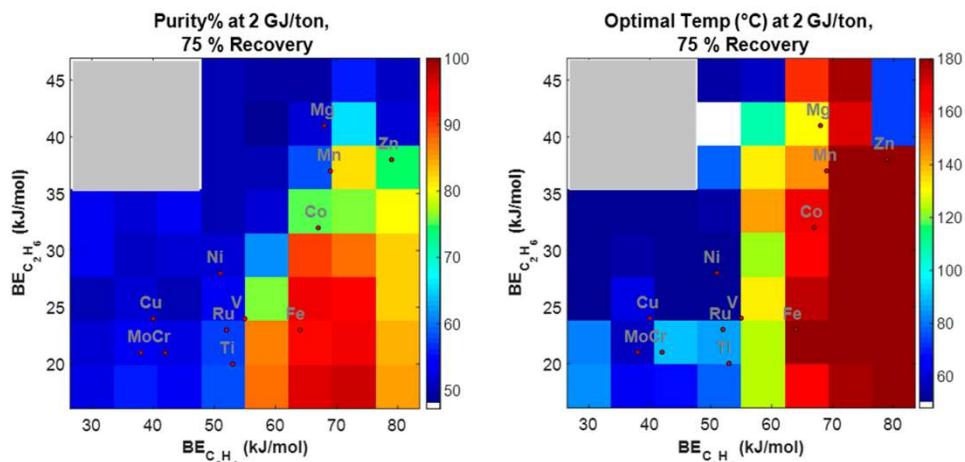
# Validation: Ideal PSA Process

Realff group in Georgia Tech has validated with many adsorbents.

Shortcut method:  
ideal PSA process



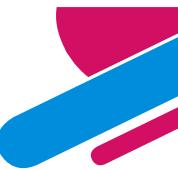
Rigorous simulations:  
dynamic model



You, Sen et al., *Applied Nano Mat.* 2020

# Application of the Method

# Application 1: CO<sub>2</sub> Capture



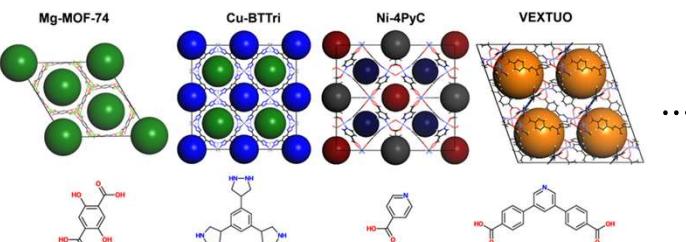
## Use of molecular simulation

(Co-work with Jihan Kim's group in KAIST)

### Sorbent structure information

CoRE MOF Database:

Web available library of MOF structures



Y. Chung, et al., *Science Advances*, 2016

### Property parameters isotherm parameter library database

	b <sub>CO<sub>2</sub></sub>	q <sub>CO<sub>2</sub></sub>	b <sub>N<sub>2</sub></sub>	q <sub>N<sub>2</sub></sub>
2252	62.0802	3.4764	0.0152	1.6397
2253	2.4499	3.1620	0.0844	2.1505
2254	8.6361	2.9557	0.2768	2.1979
2255	4.7177	2.6454	0.0807	2.9359
2256	5.9423	4.7590	0.0881	2.0051
2257	0.8230	3.5430	0.0662	2.4410
2258	8.3305	3.6350	0.2887	2.9215
2259	13.5743	10.2009	0.1669	7.0100
2260	0.3888	6.5473	0.0537	3.6956
2261	1.3008	9.2804	0.0830	6.7860

### Shortcut evaluation method

Ranking of the adsorbents  
for given...

{ Isotherm information  
Feed conditions  
Target purity

#### Ranking of feasible adsorbents

	1	2	3	4	5	A
1	Ranking	ID number	Sorbent candidate ...	CO <sub>2</sub> capture...	Higher press...	
2	1	278 SICDAL_clean		21.0820	2.5894	
3	2	379 CUGLTM_clean		21.0188	2.5974	
4	3	1347 HAOAER_clean		20.9249	2.6093	
5	4	284 KAPGUE_clean		20.8325	2.6211	
6	5	1574 CUGLTM02_clean		20.7924	2.6263	
7	6	1581 CUGLTM01_clean		20.7064	2.6376	
8	7	1976 RENWEM01_clean		20.5066	2.6642	
9	8	2136 FASJAL_clean		20.3505	2.6855	
10	9	346 KAPHAL_clean		20.2424	2.7005	
11	10	1880 FRIMIUN01_clean		20.0279	2.7310	

# Application 1: CO<sub>2</sub> Capture

## Graphical user interface (GUI) for sorbent evaluation

Sorbent\_Ranking\_GUI

New adsorbents (compared with the libraries / unit: bar<sup>-1</sup> & mol/kg & kJ/mol)

Sorbent name	kCO <sub>2</sub>	qCO <sub>2</sub>	H <sub>ad</sub> _CO <sub>2</sub>	kN <sub>2</sub>
1				
2				
3				

Library  
 CoRE MOF library  
 IZA library  
Candidate pool

Feed Conditions

1. Temperature (T<sub>feed</sub>)  
298.15 (Kelvin)
2. CO<sub>2</sub> mol. frac. (y<sub>feed</sub>)  
0.15 (mol/mol)
3. Pressure (P<sub>feed</sub>)  
 1 (bar)

Operating Conditions

4. Target CO<sub>2</sub> purity  
0.9
5. Available lower (or vacuum) pressure (P<sub>low</sub>)  
0.4 (bar)
6. Product pressure (P<sub>prod</sub>)  
 1 (bar)

Filter

7. Minimum saturated loading of CO<sub>2</sub> (q<sub>m\_CO2\_min</sub>)  
 3 (mol/kg)

RUN

Reset all the options Open the library

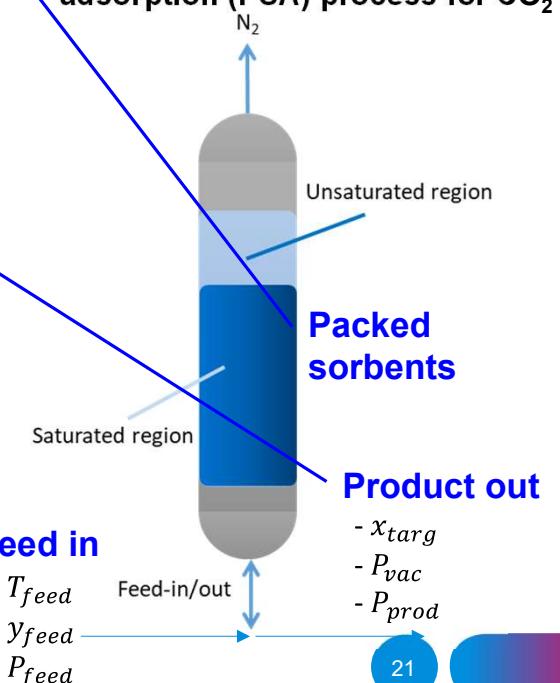
### Parameter library from molecular simulations

- Thousands of candidates:
- CoRE MOF (about MOFs)
  - IZA (about zeolites)

Operating conditions:

Feed conditions:

In a idealized pressure swing adsorption (PSA) process for CO<sub>2</sub>



# Application 1: CO<sub>2</sub> Capture

## Graphical user interface (GUI) for sorbent evaluation

Input GUI for sorbent ranking

Sorbent Ranking GUI

New adsorbents (compared with the libraries / unit: bar<sup>-1</sup> & mol/kg & kJ/mol)

Sorbent name	kCO <sub>2</sub>	qCO <sub>2</sub>	H <sub>ad</sub> CO <sub>2</sub>	kN <sub>2</sub>
1				
2				
3				

Library

- CoRE MOF library
- IZA library
- Candidate pool

Feed Conditions

- 1. Temperature (T<sub>feed</sub>)  
298.15 (Kelvin)
- 2. CO<sub>2</sub> mol. frac. (y<sub>feed</sub>)  
0.15 (mol/mol)
- 3. Pressure (P<sub>feed</sub>)  
 1 (bar)

Operating Conditions

- 4. Target CO<sub>2</sub> purity  
0.9
- 5. Available lower (or vacuum) pressure (P<sub>low</sub>)  
0.4 (bar)
- 6. Product pressure (P<sub>prod</sub>)  
 1 (bar)

Filter

- 7. Minimum saturated loading of CO<sub>2</sub> (q<sub>m\_CO2\_min</sub>)  
 3 (mol/kg)

Output format

- Tables in this window only
- In excel file
- Both of above  Open MS excel

File name (Ranking):  
Ranking.xlsx

File name (Infeasible candidates):  
Infeasible.xlsx

**RUN**

**Reset all the options** **Open the library**

Example ranking result

Ranking of feasible adsorbents

Ranking	ID number	Sorbent can...	CO <sub>2</sub> capture...	Higher press...
1	2169 APD	22.5148	2.4071	
2	2249 NAT	22.5147	2.4071	
3	2233 LOV	22.4644	2.4123	
4	2193 DFT	22.4174	2.4172	
5	326 CUGLTM02_cle...	22.2971	2.4296	
6	1058 KAPGUE_clean'	22.2113	2.4390	
7	328 CUGLTM02_cle...	22.1278	2.4480	
8	960 HAAER_clean'	22.0910	2.4520	
9	1809 RENWEM01_clean'	22.0436	2.4571	
10	327 CUGLTM01_clean'	22.0233	2.4594	
11	2176 AWO	22.0205	2.4597	
12	1059 KAPHAL_clean'	21.8319	2.4806	
13	682 FASJAL_clean'	21.8264	2.4812	
14	615 ESUMOU01_clean'	21.8037	2.4836	
15	1591 NOQLOV01_clean'	21.4976	2.5190	
16	932 GUSNEN01_clean'	21.4947	2.5193	
17	1808 RENWEM_clean'	21.4595	2.5235	
18	614 ESUMOU_clean'	21.2313	2.5507	
19	1274 LIBUJAU_clean'	20.9676	2.5835	
20	240 CDGLGU01_clean'	20.9318	2.5878	
21	1460 MOCJEU_clean'	20.5838	2.6326	
22	2128 ULUPUM01_clean'	20.5626	2.6356	
23	244 CDGLGU12_clean'	20.3211	2.6682	
24	158 BOHGOU_clean'	20.0610	2.7045	
25	685 FAVZEE_clean'	19.4996	2.7876	
26	2281 SOF	19.3944	2.8035	
27	1458 MOCHUI_clean'	19.2230	2.8311	
28	1221 LAXGOH01_clean'	19.0205	2.8641	

Infeasible candidates

ID number	Sorbent can...	Upper limit p...
1924 SIPWUK_clean'	0.8986	
2104 UGUHAG_clean'	0.8984	
148 BICBAU_clean'	0.8983	
336 CUSDIE_clean'	0.8983	
1136 KIPKEB_clean'	0.8969	
804 GATHAL_clean'	0.8956	
771 FOHCAH_clean'	0.8965	
656 FAGFAU_clean'	0.8960	
1521 NANMEW_clean'	0.8951	
1294 LIVTEP_clean'	0.8948	
1430 MIFVEE_clean'	0.8945	
1910 SETWOF_clean'	0.8943	
967 HAZGOF_clean'	0.8935	
1223 LAZGOK_clean'	0.8922	
1984 TARVUD_clean'	0.8920	
731 FIPAM01_clean'	0.8913	
2001 TEHRUU_clean'	0.8911	
757 FUUDOS_clean'	0.8911	
2032 TILDIC_clean'	0.8909	
1584 NOCLUN_clean'	0.8904	
1605 OCIVIH_clean'	0.8903	
60 AGARUW_clean'	0.8903	
1636 OGIVAF_clean'	0.8902	
1291 LIRNEH_clean'	0.8900	
1323 LULHUIW_clean'	0.8898	
1145 KOBPUN_clean'	0.8897	
556 EJONOH_clean'	0.8897	
252 CEHLAD_clean'	0.8897	
1653 OKIIIF_clean'	0.8896	

Candidates that cannot achieve the target purity and their upper bound list ( $x_{upp}$ )

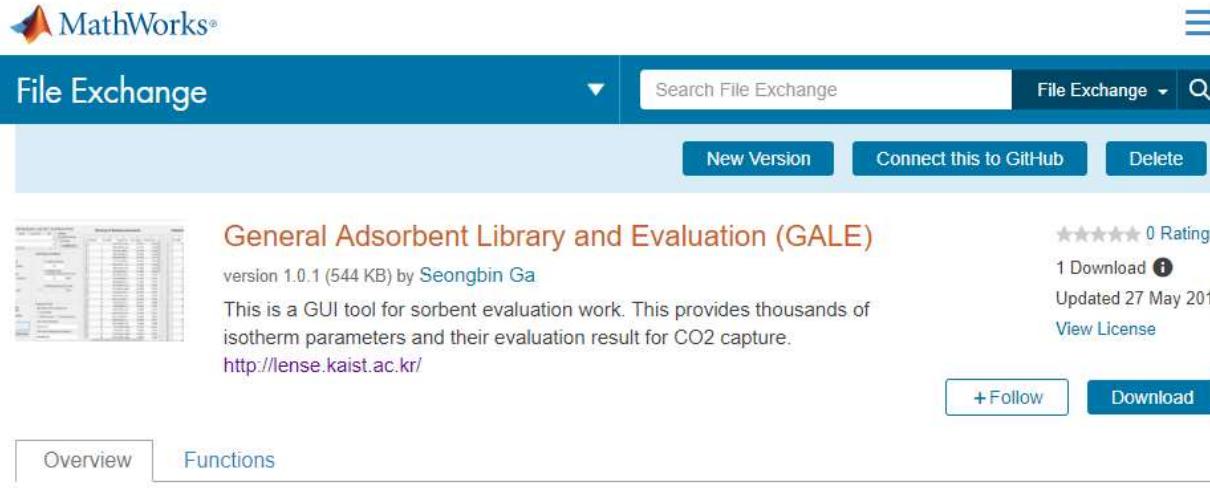
Ranking of adsorbents with quantified performance: efficiency (CO<sub>2</sub> ton/ GJ)

# Application 1: CO<sub>2</sub> Capture

## Graphical user interface (GUI) for sorbent evaluation

Available in File Exchange webpage (MathWorks):

<https://kr.mathworks.com/matlabcentral/fileexchange/71661-general-adsorbent-library-and-evaluation-gale>



The screenshot shows the MathWorks File Exchange interface. At the top, there's a search bar and navigation buttons for 'File Exchange'. Below the search bar, there are buttons for 'New Version', 'Connect this to GitHub', and 'Delete'. The main content area displays a tool named 'General Adsorbent Library and Evaluation (GALE)' by Seongbin Ga, version 1.0.1 (544 KB). It has a rating of 0 stars and 1 download. The description states it's a GUI tool for sorbent evaluation work, providing thousands of isotherm parameters and their evaluation result for CO<sub>2</sub> capture. A link to the source code on lense.kaist.ac.kr is provided. At the bottom of the listing, there are 'Follow' and 'Download' buttons.

Overview Functions

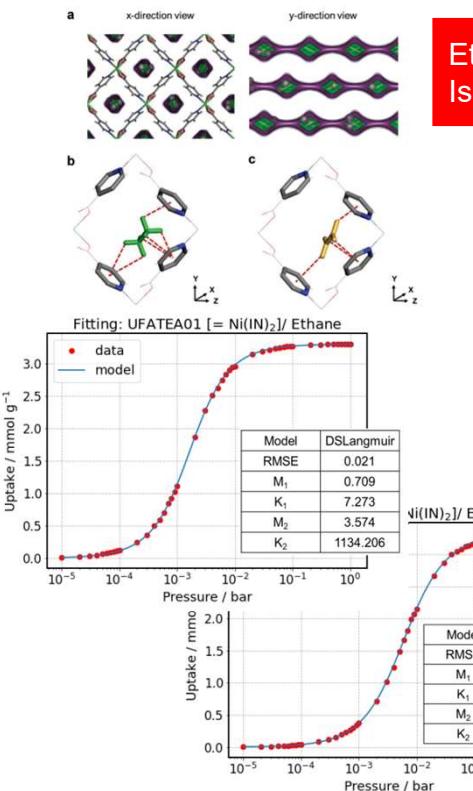
this work developed a software proving both the isotherm parameter library and a computationally efficient function for the process-level evaluation. This software is named General Adsorbent Library and Evaluation (GALE). In GALE, a new type of adsorbent library is provided. This library contains adsorption isotherm parameter sets for thousands of adsorbents. The parameters were found through the molecular simulations using the previous structure libraries. For different temperature and pressures, the uptake values for each adsorbent were found, and then they were parameterized based on a model. Included in the new library are the isotherm parameters, which can be utilized for various applications such as process simulations and estimation of adsorbent

Proposed in  
S. Ga et al., *Comput. Chem. Eng.*, 2020

# Application 2: MOFs for Ethane/ethylene Separation

**Dr. Yongchul Chung**

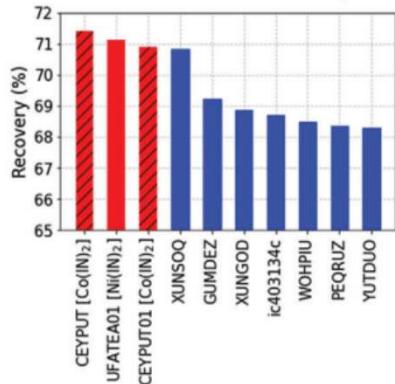
Molecular simulations of 6,830 metal organic frameworks (MOFs) from CoRE MOF database



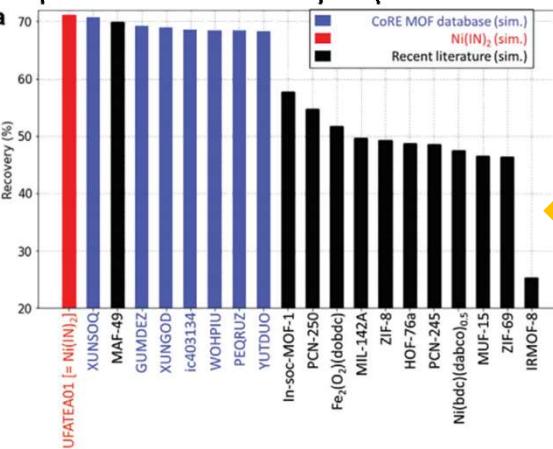
Ethane/ethylene Isotherms

**Dr. Seongbin Ga**

Shortcut method for VSA process



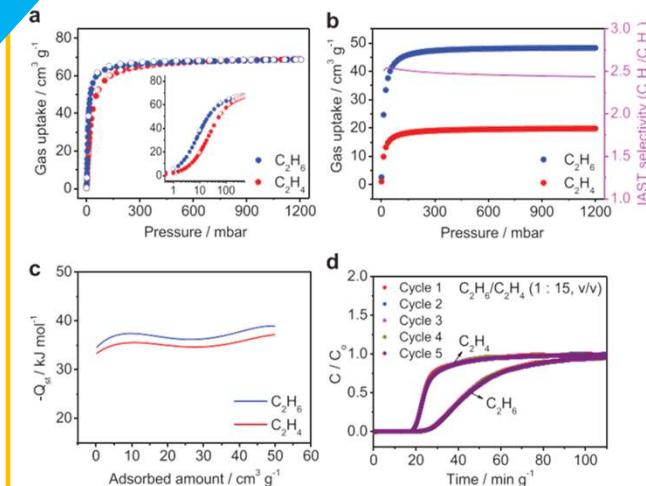
Compare with recently reported MOFs



Best MOFs

**Dr. Chang Seop Hong**

Synthesize of top 3 MOFs, measurement, and durability test



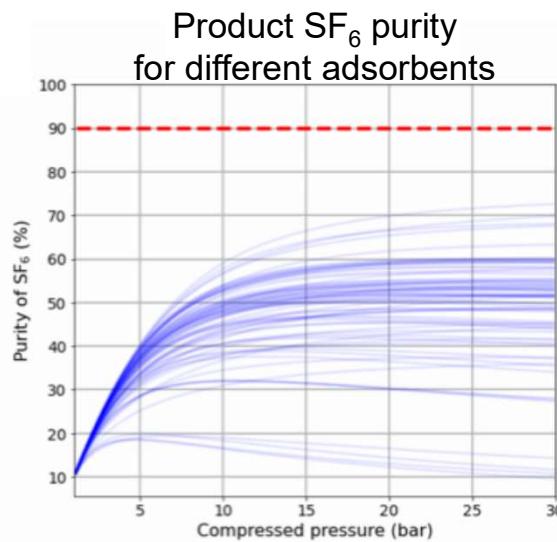
Durable MOFs measured data

Reported in  
Kang et al., *Adv. Sci.*, 2021

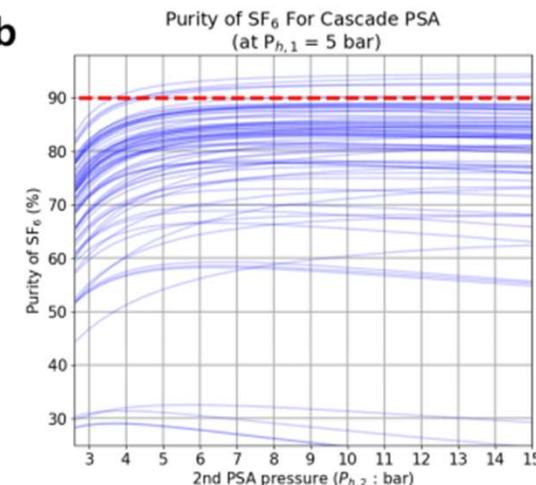
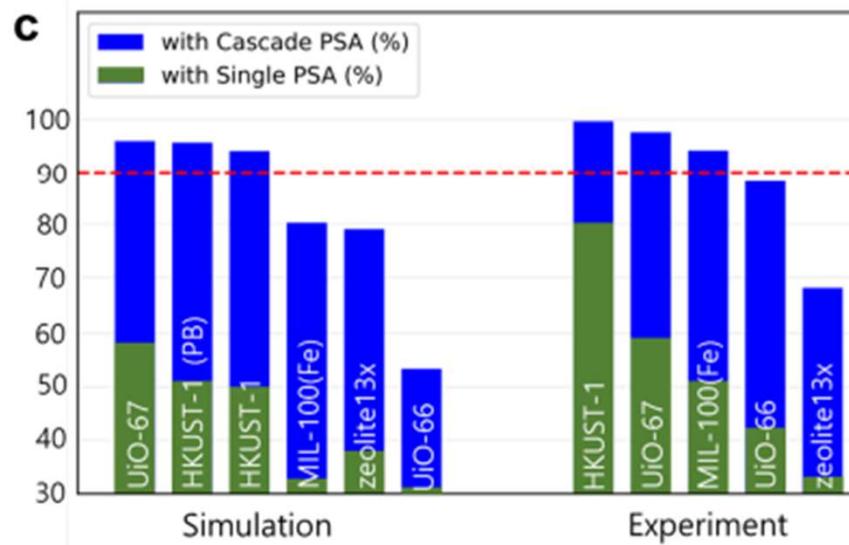
# Application 3: MOFs for $\text{SF}_6/\text{N}_2$ Separation

[Use of CoRE MOF database again for  $\text{SF}_6/\text{N}_2$  separation]

Based on the molecular simulation results (isotherm curves of 2,890 MOFs), we found any of MOFs cannot achieve 90%  $\text{SF}_6$  with a **PSA** process.



Then, we need to use cascade PSA with two trains:



Reported in  
Cha et al., *Chem. Eng. J.*, 2021

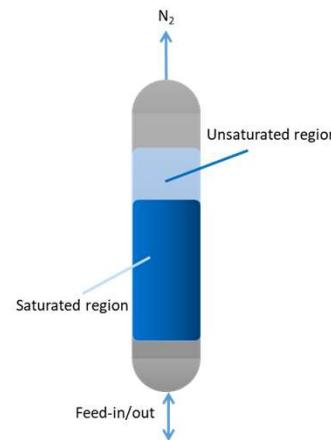
# Summary

## Shortcut evaluation method

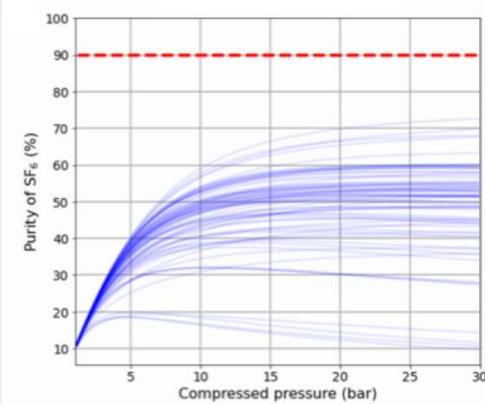
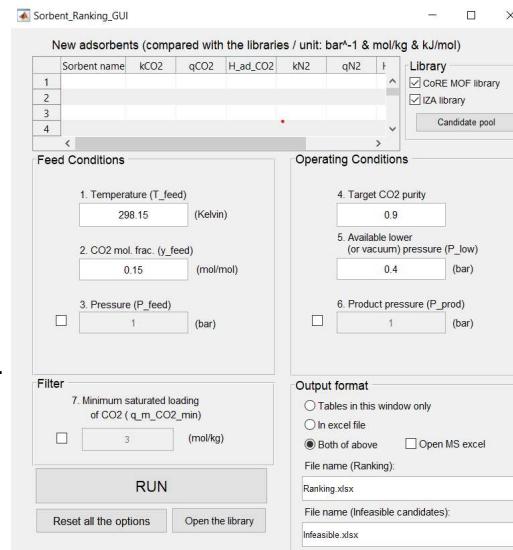
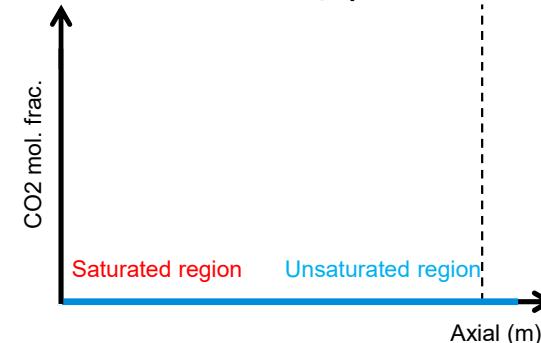
- 1) Shortcut evaluation method has been suggested by assuming an ideal PSA process.
- 2) The method provides quick evaluation with limited information.

## Applications of the shortcut evaluation method

- 1) Adsorbents for CO<sub>2</sub> capture can be evaluated, which is also available in a GUI form.
- 2) MOF screening work found Ni(IN)<sub>2</sub> for C<sub>2</sub> separation, whose durability and separation performance have been tested.
- 3) Through the shortcut method, we found SF<sub>6</sub> separation requires cascade PSA process with at least two PSA trains.



Saturation period



# Table of Contents

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## 1. Shortcut Adsorbent Evaluation Method

1. How adsorption processes work
2. Problems of the existing methods
3. Breakthrough: shortcut method (ideal PSA process)
4. Validation of the process

## 2. Applications to Different Areas

1. For CO<sub>2</sub> capture and graphical user interface (GUI)
2. Ethane/ethylene (C<sub>2</sub>) separation
3. SF<sub>6</sub> capture