

# First-principles based surrogate modeling of pressure swing adsorption processes for CO<sub>2</sub> capture

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**Abstract:** Pressure swing adsorption (PSA) is a highly versatile separate technology and represents a promising option for carbon capture. A dynamic model for a PSA process comprises partial differential equations, which are difficult to use for optimization tasks due to their long computational time and numerical instability problems. A surrogate model for PSA processes which captures the essence of the dynamics to predict key performance measures can enable process optimization to be carried out without the need to evaluate the rigorous model repeatedly. To this end, a surrogate model that predicts energy consumption, removal, purity, and CO<sub>2</sub> avoidance cost for given operating conditions is developed as a system of nonlinear equations. The surrogate model is validated and can be used to find optimal operating conditions without having to carry out time-consuming dynamic simulations. It is expected that the ability of fast-optimization brings further opportunities such as screening of adsorbent candidates in material discovery researches.

**Keywords:** CO<sub>2</sub> capture, pressure swing adsorption, surrogate modeling, first-principle based model, adsorbent performance indicator, process optimization, Bayesian optimization

## 1. INTRODUCTION

Pressure swing adsorption (PSA) is a highly versatile and energy-efficient separation method that can be used for many important industrial separation tasks. For example, it can be used to capture CO<sub>2</sub> from flue gas streams using CO<sub>2</sub>-affinitive adsorbents. Reversible adsorption-regeneration using pressure swing allows effective CO<sub>2</sub> removal. On the other hand, as PSA works with compressed gases, it consumes much electric energy and determination of optimal operating conditions, e.g., pressures for the flue gas and adsorbents, are critical for assessing the bottom-line economics of PSA for given flue gas conditions and separation requirements.

A PSA process is modeled as a system of nonlinear partial differential equations (PDEs). As the operation is inherently dynamic and cyclic, it reaches a cyclic steady-state (CSS) where same dynamic patterns of variables keep repeating. The complex nature of the model hinders its use in tasks like optimizations where the model needs to be evaluated on a repetitive basis. There have been attempts to develop simple surrogate models such as a reduced order model (Agarwal et al, 2009) or artificial neural networks (Sant Anna et al, 2017). In addition, the Bayesian optimization approach with kriging has been used to optimize the process with just a small number of simulations (Hasan et al, 2012). As there is no theoretical basis for the used model structures, these approaches may require a very large number of simulations of the rigorous model to construct reliable surrogates.

At the adsorbent development stage, a performance indicator that can be easily calculated and reflects the performance of the PSA can be highly valuable in searching for good adsorbent materials. Performance indicators like working

capacity, selectivity, efficiency, and product purity have been proposed and simple formulas for evaluating them have been developed by idealizing the adsorption process (Wiersum et al, 2013; Ga et al, 2017). Those performance indicators can be useful but their accuracies in practical environments are questionable given the idealizing assumptions made.

This work proposes a first-principle based surrogate model that can predict some of the key performance indicators that closely match the rigorous simulation data. In addition, the gas uptake profile inside the bed can be predicted by the surrogate model. The model equations are proposed as a system of nonlinear equations to be solved. The surrogate model is validated using the simulation samples from Bayesian optimization.

## 2. PROCESS DESCRIPTION

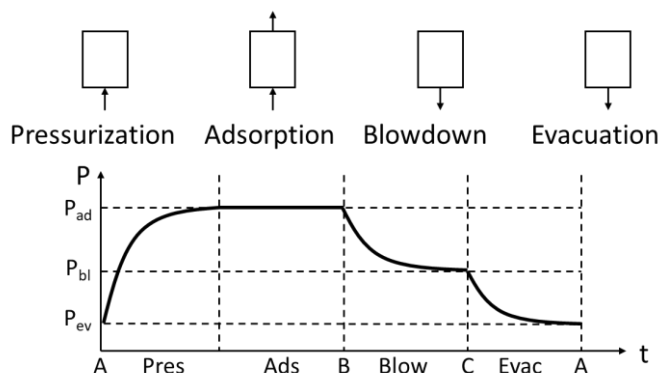


Figure 1. Operation of vacuum cycle.

In this work, the vacuum cycle is chosen as it can give higher purity products than the conventional Skarstorm cycle in a post-combustion CO<sub>2</sub> capture process (Hasan et al, 2012). This cycle consists of 4 steps: pressurization, adsorption, blowdown, and evacuation (Figure 1). In the pressurization step, feed gas is blown to the bed until the bed pressure reaches the maximum, and in the adsorption step, CO<sub>2</sub> in the feed gas is adsorbed until the bed is saturated to point (B). In the blowdown step, the bed pressure is slightly relieved and undesired N<sub>2</sub> in the bed is desorbed to point (C) to maximize the purity. Finally, in the evacuation step, the vacuum pump regenerates the adsorbed CO<sub>2</sub> in the bed and sends it back to point (A).

Compressors and vacuum pumps must be installed for the operation of the vacuum cycle. The adsorption pressure ( $P_{ad}$ ) is always higher than the atmospheric pressure ( $P_{atm}$ ) and the feed gas is compressed. The evacuation pressure ( $P_{ev}$ ) is always lower than  $P_{atm}$  and a vacuum pump extracts the CO<sub>2</sub> in the evacuation step. The blowdown pressure ( $P_{bl}$ ) is between  $P_{ad}$  and  $P_{ev}$  and either above or below  $P_{atm}$ . If  $P_{bl} < P_{atm}$  a vacuum pump is needed; otherwise no equipment is required.

Coal-fired power plant off-gas with CO<sub>2</sub> dry mole fraction of 0.15, temperature as 300 °C, and pressure as 1 bar is selected as a feed gas. Zeolite 13X is selected as the adsorbent of which the isotherm parameters are found in Table 1. It is assumed that the moisture in the flue gas is eliminated beforehand. The captured CO<sub>2</sub> is compressed to a high pressure (120 bar) for transportation. For the purpose of economic evaluation, it is assumed that the electricity price is \$0.079/kWh and the adsorbent price is \$10/kg.

Table 1. Langmuir isotherm parameters for Zeolite 13X (Hasan et al, 2012).

	CO <sub>2</sub>	N <sub>2</sub>
Maximum gas uptake (mol/kg)	9.375	9.375
Henry constant (bar <sup>-1</sup> )	1.8834	0.0399
Heat of adsorption (kJ/mol)	18.9	7.36

### 3. PROCESS MODELING AND SIMULATION

In the rigorous modeling of a vacuum cycle, the following assumptions are made:

- The gas behaves ideally.
- The linear driving force (LDF) model for gas adsorption kinetics holds.
- Adsorbents behave according to the extended Langmuir isotherm.
- The pressure drop is well represented by Ergun's equation.
- All the variables are distributed only along the axial direction.
- Valve equations are used as boundary conditions for the gas velocity.

A set of PDEs including the mass and energy balances are modeled as Eq (1~7)

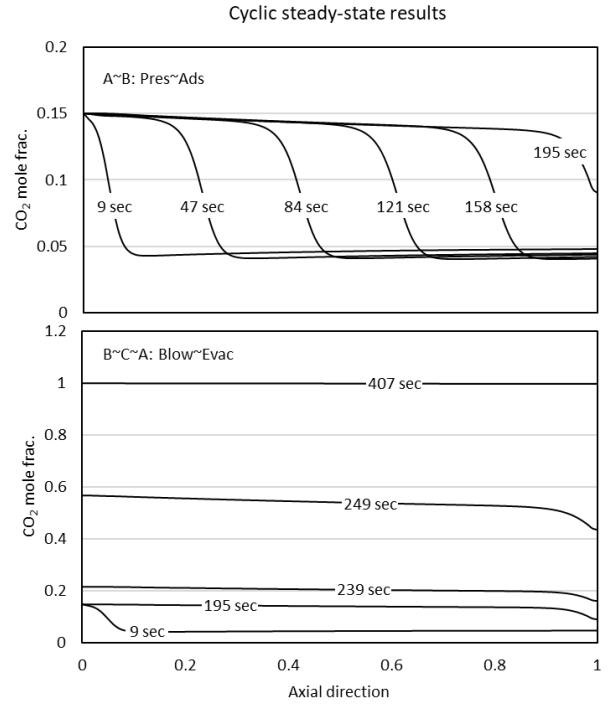


Figure 2. CO<sub>2</sub> mole fraction profile after the cyclic steady state is reached.  $P_{ad} = 1.5$  bar,  $P_{bl} = 1.0$  bar,  $P_{ev} = 0.05$  bar, pressurization step: 0~9 sec, adsorption step: 9~195 sec, blowdown step: 195~239 sec, evacuation step: 239~407 sec. The flue gas is blown at  $z = 0$ .

$$C_i = y_i C \quad (1)$$

$$\frac{\partial C}{\partial t} = -u \frac{\partial C}{\partial z} - C \frac{\partial u}{\partial z} - \frac{1 - \varepsilon}{\varepsilon} \rho_s \sum_{i=1}^2 \frac{\partial q_i}{\partial t} \quad (2)$$

$$\frac{\partial C_i}{\partial t} = D_{ax} \frac{\partial}{\partial z} \left( C \frac{\partial y_i}{\partial z} \right) - \frac{\partial}{\partial z} (C_i u) - \frac{1 - \varepsilon}{\varepsilon} \rho_s \frac{\partial q_i}{\partial t} \quad (3)$$

$$\frac{\partial q_i}{\partial t} = k_i (q_i^* - q_i) \quad (4)$$

$$q_i^* = \frac{q_{m,i} b_i y_i P \exp\left(-\frac{\Delta H_i}{RT}\right)}{1 + \sum_j b_j y_j P \exp\left(-\frac{\Delta H_j}{RT}\right)} \quad (5)$$

$$\begin{aligned} & (\varepsilon \rho_g C_{p,g} + (1 - \varepsilon) \rho_s C_{p,s}) \frac{\partial T}{\partial t} \\ & = (1 - \varepsilon) \rho_s \sum_{i=1}^2 (-\Delta H_i) \frac{\partial q_i}{\partial t} \\ & + \lambda_{ax} \frac{\partial^2 T}{\partial z^2} - \rho_g C_{p,g} \frac{\partial}{\partial z} (uT) \\ & - 2 \frac{h}{R_{in}} (T - T_o) \end{aligned} \quad (6)$$

$$-\frac{\partial P}{\partial z} = 150.0 \frac{(1-\varepsilon)^2}{\varepsilon} \frac{\mu}{d_p^2} u + 1.75 \times 10^{-4} \frac{(1-\varepsilon)\rho_g}{\varepsilon^3} \frac{\rho_g}{d_p} u|u| \quad (7)$$

where  $i$  is the component index ( $i=\text{CO}_2, \text{N}_2$ ),  $y$  is the component mole fraction,  $C$  is the gas molar density,  $u$  is the gas velocity,  $z$  is the dimensionless axial length,  $q$  is the specific gas uptake,  $q_i^*$  is the equilibrium gas uptake,  $\varepsilon$  is the void fraction,  $\rho_s$  is the adsorbent density,  $\rho_g$  is the gas density,  $D_{ax}$  is the axial gas diffusivity,  $k_i$  is the mass transfer coefficient,  $P$  is the pressure,  $T$  is the temperature,  $q_{m,i}$  is the maximum gas uptake,  $b_i$  is the henry constant,  $R$  is the gas constant,  $\Delta H_i$  is the heat of adsorption,  $C_{p,g}$  the gas heat capacity,  $C_{p,s}$  is the adsorbent heat capacity,  $\lambda_{ax}$  is the axial conductivity,  $h$  is the wall heat transfer coefficient,  $R_{in}$  is the bed inner radius,  $T_o$  is the ambient temperature, and  $d_p$  is the particle density.

The PDEs are modeled and simulated in gPROMS using the backward finite difference method. Since all the results should be calculated based on a cyclic steady state reached, the calculation is performed based on the results after 30 cycles are simulated. A test result of the simulation is in Figure 2. It is confirmed that each cycle lasts a few hundreds of seconds, and there is a  $\text{CO}_2$ -saturated region and an unsaturated region during the adsorption step as noted by Ga *et al* (2017), and a high  $\text{CO}_2$  purity value can be attained by the evacuation step.

#### 4. CONSTRUCTION OF A SURROGATE MODEL

The surrogate model is composed of nonlinear equations for mass balances and profiles for the gas uptake and temperature. The decision variables are the operating pressures at each step (adsorption, blowdown, evacuation). The flue gas conditions (pressure, temperature, and  $\text{CO}_2$  mole fractions), adsorbent parameters (Langmuir isotherm parameters, bed porosity, adsorbent density), and cost parameters (electricity price, adsorbent price, compressor price) are input parameters to the model. The outputs of the surrogate model are  $\text{CO}_2$  capture energy (compression energy per 1  $\text{kg}_{\text{CO}_2}$ ),  $\text{CO}_2$  capture rate (captured  $\text{CO}_2$  / total  $\text{CO}_2$  in flue gas),  $\text{CO}_2$  purity of the evacuation step outlet, and  $\text{CO}_2$  avoidance cost (operating cost (\$) per 1  $\text{ton}_{\text{CO}_2}$ ).

To simplify the rigorous model while retaining the key features of the process, several assumptions are made. First, it is assumed that the amounts of  $\text{CO}_2$  and  $\text{N}_2$  in the gas phase are negligible compared to those in the solid phase of adsorbents ( $C_i \ll q_i$ ). Second, gas uptake information is important only at those points where step-step transitions occur (1: evac-pres, 2: ads-blow, 3: blow-evac, see Figure 1). Third, the mass transfer rate is sufficiently fast and the process is operated in equilibrium. The gas uptake in the adsorbents ( $n$ ) is explained as Eq (8)

$$n_{c,i} = (1-\varepsilon)\rho \int_0^1 q_{c,i}(z) dz \quad \forall i, c \quad (8)$$

where  $c$  index stands for the steps of the vacuum cycle (A, B, C). The gas uptake profile in the surrogate model is assumed to be linear as Eq (9)

$$\int_0^1 q_{c,i} dz = \frac{1}{2} q_{c,i}(0) + \frac{1}{2} q_{c,i}(1) \quad \forall i, c \quad (9)$$

so that the surrogate model only considers the edge uptake which can directly be obtained from the edge component partial pressure and temperature. The temperature profile is also assumed to be linear as in Table 2. The surrogate model variable  $\Delta T_{ad}, \Delta T_{bl}, \Delta T_{ev}$  are defined from inter-step energy balance considering the adsorption enthalpy ( $\Delta H_{\text{CO}_2}, \Delta H_{\text{N}_2}$ ) as in Eq (10~12).

$$C_{p,s}\Delta T_{ev} = \Delta H_{\text{CO}_2} (q_{\text{CO}_2,2}(0) - q_{\text{CO}_2,A}(0)) + \Delta H_{\text{N}_2} (q_{\text{N}_2,B}(0) - q_{\text{N}_2,A}(0)) \quad (10)$$

$$C_{p,s}\Delta T_{ad} = \Delta H_{\text{CO}_2} (q_{\text{CO}_2,B}(1) - q_{\text{CO}_2,A}(1)) + \Delta H_{\text{N}_2} (q_{\text{N}_2,B}(1) - q_{\text{N}_2,A}(1)) \quad (11)$$

$$2C_{p,s}\Delta T_{ev} = \Delta H_{\text{CO}_2} (q_{\text{CO}_2,B}(0) - q_{\text{CO}_2,C}(0)) + \Delta H_{\text{N}_2} (q_{\text{N}_2,B}(0) - q_{\text{N}_2,C}(0)) + \Delta H_{\text{CO}_2} (q_{\text{CO}_2,B}(1) - q_{\text{CO}_2,C}(1)) + \Delta H_{\text{N}_2} (q_{\text{N}_2,B}(1) - q_{\text{N}_2,C}(1)) \quad (12)$$

Table 2. Assumed edge temperature in the surrogate model.  $\Delta T_{ad}, \Delta T_{bl}, \Delta T_{ev}$  are surrogate model variables.

Step	$z = 0$	$z = 1$
1	$T_{\text{Feed}} - \Delta T_{ev}$	$T_{\text{Feed}}$
2	$T_{\text{Feed}}$	$T_{\text{Feed}} + \Delta T_{ad}$
3	$T_{\text{Feed}} - \Delta T_{bl}$	$T_{\text{Feed}} + \Delta T_{ad} - \Delta T_{bl}$

In addition, empirical parameters ( $\alpha$  and  $\beta$ ) are introduced for the gas mole fraction calculation as in Eq (13~14),

$$y_{\text{CO}_2,ad,out} = \alpha \frac{P_1}{P_2} y_{\text{CO}_2,A} + (1-\alpha) y_{\text{CO}_2,feed} \quad (13)$$

$$y_{\text{CO}_2,bl,out} = \beta y_{\text{CO}_2,ad,out} + (1-\beta) y_{\text{CO}_2,B} \quad (14)$$

where  $y_{\text{CO}_2,feed}$  is the feed  $\text{CO}_2$  mole fraction,  $y_{\text{CO}_2,ad,out}$  and  $y_{\text{CO}_2,bl,out}$  are the average  $\text{CO}_2$  mole fractions of the outlets in the adsorption and blowdown steps,  $y_{\text{CO}_2,A}$  and  $y_{\text{CO}_2,B}$  are the  $\text{CO}_2$  mole fractions of the outlets at point A and B, respectively. From several tries,  $\alpha = 0.9$  and  $\beta = 0.5$  are selected. The gas phase mole fraction at point 1 can be obtained from Eq 15.

$$\Delta y_A = y_{\text{CO}_2,A} - \frac{\partial n_{\text{CO}_2,A}}{\partial P_{ev,\text{CO}_2}} \left/ \left( \frac{\partial n_{\text{CO}_2,A}}{\partial P_{ev,\text{CO}_2}} + \frac{\partial n_{\text{N}_2,A}}{\partial P_{ev,\text{N}_2}} \right) \right. \quad (15)$$

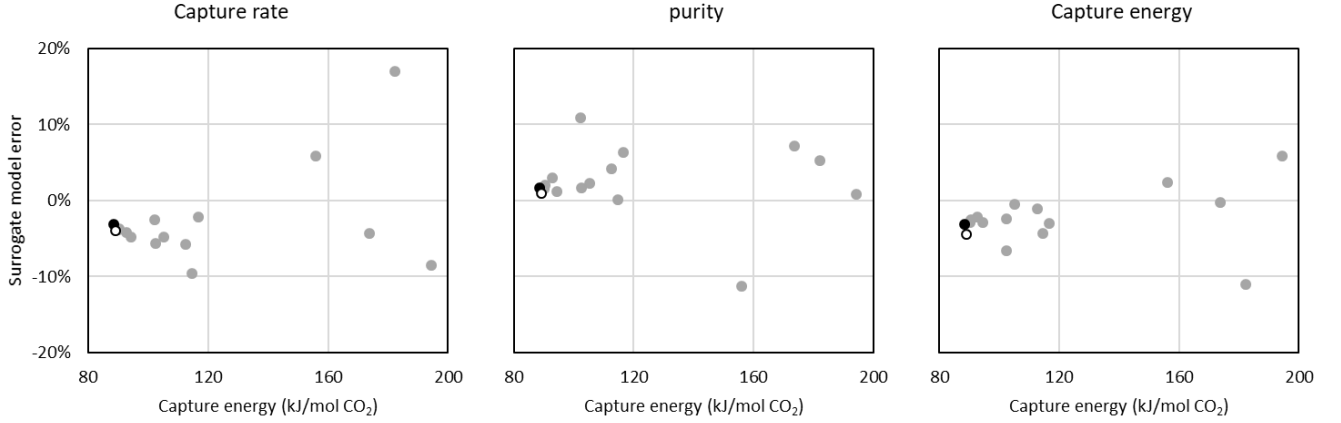


Figure 3. The surrogate model error of key performance indicators for vacuum cycle. The true optimal point found by Bayesian optimization of rigorous model and the expected optimal point by the surrogate model is indicated as black marker and white marker, respectively.

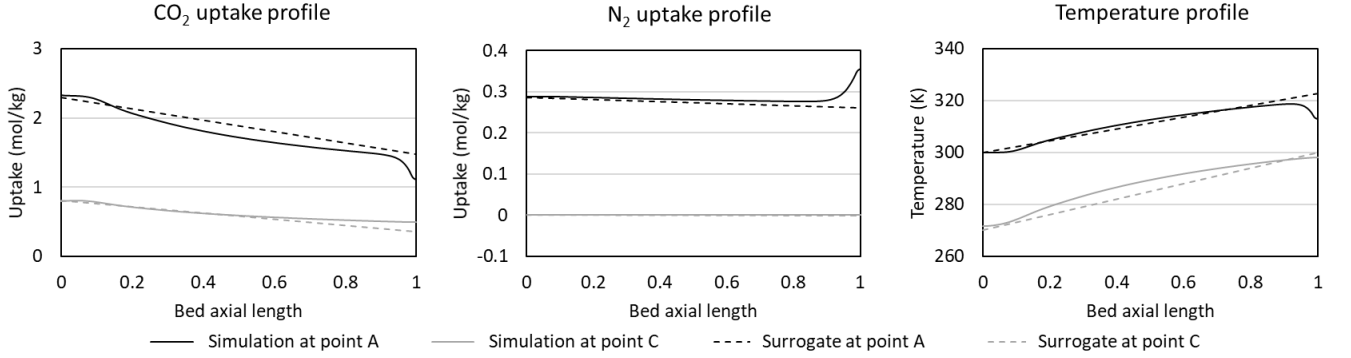


Figure 4. The profile of simulation results and the predicted profile by the surrogate model at points 1 and 3 at the optimal point.

The above equation means that, for the desorption steps, the mole fraction is same as the ratio of the component's mole flux. Here  $\Delta y_A$  is the mole fraction error at point A due to the mass transfer resistance between the gas phase and the solid phase (Eq (4)). Those errors are relaxed in the surrogate model to avoid infeasibility problems but they should be kept small as for the third assumption. Then the surrogate model is determined so as to minimize the mole fraction error with the mass balance equations of the surrogate model as constraints ( $F$ ), where  $v$  are the surrogate model variables and  $p$  are the model parameters.

$$\begin{aligned} & \min \Delta y_A^2 \\ & \text{s. t. } F(v; p) = 0 \end{aligned} \quad (16)$$

Outputs of the surrogate model are defined as below.

$$\begin{aligned} E_{\text{elec}} = 1.3RT_{\text{feed}} & (F_{\text{feed}} \ln(P_{\text{ad}}/P_{\text{feed}}) \\ & + F_{\text{bl}} \max\{0, -\ln P_{\text{bl}}\} \\ & + F_{\text{ev}} \ln(P_{\text{transport}}/P_{\text{feed}})) \end{aligned} \quad (17)$$

$$E_{\text{CAP}} = E_{\text{cycle}}/F_{\text{ev}} \quad (18)$$

$$r_{\text{CAP}} = \frac{F_{\text{ev}} y_{\text{CO}_2, \text{ev}}}{F_{\text{feed}} y_{\text{CO}_2, \text{feed}}} \quad (19)$$

$$\text{AVC} = \frac{f_{\text{OPEX}} E_{\text{cycle}} + f_{\text{CAPEX}} (C_{\text{ads}} + C_{\text{comp}})}{F_{\text{ev}} y_{\text{CO}_2, \text{ev}}} \quad (20)$$

In Eq (17),  $E_{\text{elec}}$  is the electricity consumption rate,  $F$  is the gas flowrate, and  $P_{\text{transport}}$  is the  $\text{CO}_2$  transportation pressure. In Eq (18~19),  $E_{\text{CAP}}$  is the capture energy (kJ/mol  $\text{CO}_2$ ) and  $r_{\text{CAP}}$  is the  $\text{CO}_2$  capture rate, respectively. In Eq (20), AVC is the  $\text{CO}_2$  avoidance cost,  $f_{\text{OPEX}}$  and  $f_{\text{CAPEX}}$  are the cost factors for techno-economic assessment,  $C_{\text{ads}}$  is the cost for adsorbent purchase, and  $C_{\text{comp}}$  is the equipment purchase cost for the compressors.

Overall, the surrogate model contains 30 variables, 29 equality constraints, and four inequality constraints. One degree of freedom is left due to the relaxation of  $\Delta y_A$ . The surrogate model is solved by the nonlinear optimization solver IPOPT version 3.11.1.

## 5. IMPLEMENTATION OF A SURROGATE MODEL

The constructed surrogate model is validated with the rigorous model. The key performance indicators predicted by the surrogate model should be close to the simulated values with the rigorous model. As it is preferred to operate the PSA process near its optimum, the validation should be performed near the optimal point. Operating conditions far from its optimum is costly and may be unrealistic for practical use, and validation of such operating regions is not necessary. The rigorous process model is optimized using a Bayesian optimization technique to find the optimal operating pressure using expected improvements as an acquisition function as Hasan et al. (2012). For all the generated samples, the surrogate model is also solved for the evaluation and the results are compared with the true values from the rigorous model. This procedure allows for more frequent samplings near the optimal point.

The PSA process is first optimized using the rigorous model by reducing the CO<sub>2</sub> avoidance cost, and then optimized again using the surrogate model. Evaluation results by both the rigorous model and the surrogate model at the two optimal points are summarized in Table 3 and Table 4. The two optimal points are very close but the computation times are greatly reduced from one minute to less than 0.1 seconds, indicating that the surrogate model can be used for the optimization of the PSA process. In addition, all the samples generated during the Bayesian optimization are used for calculating the surrogate model prediction error (Figure 3). The surrogate model can predict the key performance indicators very accurately near the optimal point with small errors (consumption energy: -5~0 %, capture rate: -5~-1 %, purity: 0~3 %). The surrogate model slightly underestimates the CO<sub>2</sub> capture rate and the capture energy with less than 5% error. It tends to overestimate the CO<sub>2</sub> purity, but as a very high CO<sub>2</sub> mole fraction value (>95 %) can be attained, this does not appear to be a problem for zeolite 13X.

Table 3. Optimization results of the vacuum process by Bayesian optimization and the evaluation results at the same operating condition by the surrogate model.

	Rigorous model	Surrogate model
$P_{ad}$ (bar)	1.26	
$P_{bl}$ (bar)	0.36	
$P_{ev}$ (bar)	0.022	
Capture energy (kJ/mol CO <sub>2</sub> )	36.7	35.5
Capture rate	0.809	0.783
Purity	0.944	0.959
CO <sub>2</sub> avoidance cost (\$/ton CO <sub>2</sub> )	88.6	87.0
Computation time (s)	74.36	0.061

Table 4. Optimization results of the vacuum process by the surrogate model and the evaluation results at the same operating condition from the rigorous model.

	Rigorous model	Surrogate model
$P_{ad}$ (bar)		1.26
$P_{bl}$ (bar)		0.24
$P_{ev}$ (bar)		0.026
Capture energy (kJ/mol CO <sub>2</sub> )	36.4	34.8
Capture rate	0.763	0.733
Purity	0.970	0.978
CO <sub>2</sub> avoidance cost (\$/ton CO <sub>2</sub> )	89.3	86.3
Computation time (s)	77.58	0.049

The predicted profiles by the surrogate model are compared with the rigorous simulation results (Figure 4). The linear assumption is valid for the gas uptake profile and the temperature profile. The deviation of the profiles at  $z = 1$  at point C is due to the mass transfer resistance. A notable contribution of this work is the ability to predict the temperature profile accurately. The isotherm curve is strongly temperature dependent as shown in Figure 5. In general, if an adsorbent has high CO<sub>2</sub> affinity and CO<sub>2</sub> selectivity, the heat of adsorption is also high and the temperature dependency of the cycle operation is significant. A wrong prediction of the temperature profile leads to inaccurate evaluations of the process. To our best knowledge, known adsorbent performance indicators do not consider this temperature dependency on criteria such as capture energy. In this context, the surrogate model provides useful information that the other indicators do not, avoiding time-consuming (few minutes ~ hours depending on the computational power) rigorous simulations.

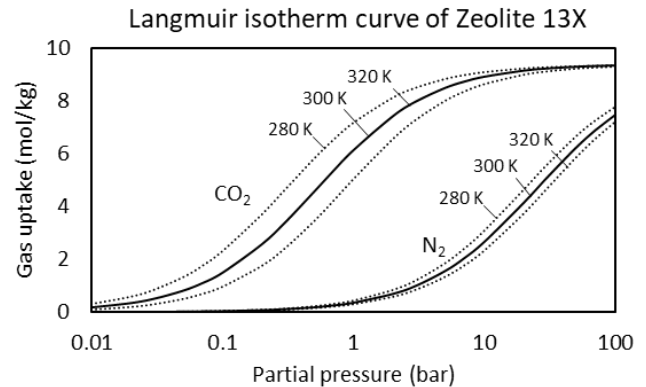


Figure 5. Temperature dependency of isotherm curve for zeolite 13X.

## 6. CONCLUSION AND FUTURE WORK

Simulation of a PSA process requires solving a system of nonlinear partial differential equations and the long computational time associated with it hinders its use in analyses and optimizations of the process. Motivated by this, a surrogate model for a vacuum cycle is developed and validated. The surrogate model comprises a system of nonlinear equations which can be solved much more quickly and easily than the rigorous model. From given adsorbent isotherm parameters, flue gas conditions, and operating conditions, the surrogate model predicts key performance indicators of the process including capture energy, capture rate, purity, and CO<sub>2</sub> avoidance cost. The predicted optimal point by the surrogate model and the true optimal point were shown to be very close, indicating that the surrogate model can replace the rigorous model in process optimizations and analyses, while avoiding long computational times of the latter model.

It is expected that the surrogate model can be used to make quick evaluations of potentials of various adsorbent candidates for CO<sub>2</sub> capture. There are nearly millions of MOFs representing different combinations of metals and organic compounds but most MOFs remain unexamined and screening of them in terms of their potentials as adsorbents is needed. Recently proposed MOFs are carefully designed to lower the capture energy, changing the isotherm curve to a non-Langmuir isotherm, such as the S-shaped isotherms (Ga et al, 2021). It is hoped that the surrogate model can help screen through those MOFs quickly to identify promising ones.

The linear profile assumption is sufficient for a coal-fired power plant off-gas and zeolite 13X; however, there would be some condition that the linear assumption leads to inaccurate predictions. Choices of the empirical parameters in Eq (13~14) can be critical in this regard. A more systematic, data-driven approach to fit the parameters may improve the surrogate model's accuracy in the future.

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