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Improving CO_2 Capture Process with Latent Heat Reuse System and Artificial Neural Network Model

Jiasi Sun, Yuka Sakai, Yuki Sato, Yasuki Kansha*

Organization for Programs on Environmental Sciences, Graduate School of Arts and Sciences, The University of Tokyo, 3-8-1 Komaba, Meguro-ku, Tokyo 153-8902 Japan
kansha@global.c.u-tokyo.ac.jp

CO_2 capture is one of the most promising strategies to combat the increasing CO_2 concentration in the atmosphere, but the high energy requirement has prevented its widespread use. A new latent heat reuse system based on pressure swing technology was proposed for the post-combustion CO_2 capture (PCC) process, which can recover more than 50% of the energy from compressed flue gas. As a representative of deep eutectic solvents (DES), reline was adopted as an absorbent for this PCC process and was shown to be suitable for flue gas decarbonization. An artificial neural network (ANN) model was then trained to explore the relationship between the operating parameters of the designed PCC process and their capture results. The ANN model can provide direction for multi-parameters selection as it can quickly predict and find combinations of operational parameters that meet the capture objectives. The result of this work shows a 68.8 % reduction in total capture energy requirement after improvement (1.28 MJ/kg CO_2) compared to the conventional MEA-based capture process (4.1 MJ/kg CO_2).

1. Introduction

Since 2000, the global CO_2 concentration has increased by about 20 ppm per decade, which is about 10 times faster than the average annual rise over the past 800,000 y (Bereiter et al., 2015). This rapid human-driven change is a major cause of global warming, with significant negative impacts on humans and natural systems (IPCC, 2018). In response to the rapid increase in atmospheric CO_2 concentrations, governments have committed to achieving net-zero CO_2 emissions by 2055 - 2080 (Bataille et al., 2018). Among the anthropogenic sources, coal-fired power plants are one of the most dominant CO_2 emissions sources. Coal-fired power plants in Pakistan alone were reported to emit 14,500 t/y CO_2 (Ali et al., 2021). Although countries are now ambitiously developing renewable power resources to replace traditional fossil-based power generation, fossil-based power generation still accounts for about 63 % of the electrical supply (Nimmanterdwong et al., 2022). It will be hard to fully replace coal-fired power plants within a few decades. Therefore, CO_2 capture technology, especially post-combustion CO_2 capture (PCC), has become extremely important for reducing CO_2 emissions, as it can be installed in power plants and can be adapted to different operating conditions.
One obstacle to the widespread usage of PCC technology is its huge energy need. When evaluating absorbents for PCC technology, monoethanolamine (MEA) is considered the industry benchmark because it has been used successfully for more than 50 y with a regeneration energy requirement of 4.1 MJ/kg CO_2 (Kansha et al., 2017). In this work, we chose a typical deep eutectic solvent-reline, consisting of choline chloride and urea in a molar ratio of 1:2, as the CO_2 absorbent. Deep eutectic solvents (DESs) are solutions of Lewis acids and bases that form eutectic mixtures and have been considered as potential CO_2 absorbers due to their almost zero volatility, high thermal stability, high acid gas solubility, and compositional tunability (Kamgar et al., 2017). DESs have proven to show advantages in capturing gas streams with high CO_2 concentration or high pressure, such as biogas and shale gas. While for flue gas, the energy requirement is large (5.12 MJ/kg CO_2) due to its low CO_2 concentration and low pressure (Zhang et al., 2018). The purpose of this work is to explore the potential use of reline for flue gas decarbonization and to reduce the energy requirements of the PCC from process design and proper operating parameters selection.

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2. Research method

2.1 Component definition and thermodynamic specification

In the process of decarbonization of flue gas, various components such as CO_2, H_2O, N_2, and O_2 are involved. Before the flue gas is decarbonized, it undergoes a pre-treatment to remove SO_X, NO_X, and small particles. The flue gas model information of a typical 100 MW coal-fired power plant (flow rate of coal-fired flue gas = 100 kg/s) is listed in Table 1. This PCC process uses reline as absorbent, which is one of the most common DESs used for CO_2 separation and shows a higher CO_2 solubility compared to other DESs (Sarmad et al., 2017). Since reline can be mixed with H_2O in any ratio and is difficult to separate, the H_2O should also be completely removed before the PCC process and be ignored in the simulation. The thermophysical properties of the components other than reline (i.e., CO_2, N_2, and O_2) were calculated using the parameters from the NIST databank in Aspen Plus. In Aspen Plus, reline was defined as a pseudo-component and its physical properties were fitted with a semi-empirical equation using the experimental data. The modelling information of reline were obtained from the work of Ma et al. (2018) and were listed in Table 1.

Table 1. Physical properties of reline and flue gas composition

Property parameters	Equation	
Liquid molar volume (m^3/kmol)	$\rho=0.06358+2.427\times10^{-5}T+1.624\times10^{-8}T^2$	(1)
Viscosity (Pa·s)	$ln\eta=-443.7+26670/T+62.14\ lnT$	(2)
Surface Tension (N/m)	$\sigma=0.09244(1-T_r)^{0.6043}$	(3)
Molar Heat Capacity (m^3/ mol·K)	$V_l=0.06358+2.427\times10^{-5}T+1.624\times10^{-8}T^2$	(4)
Property methods	NRTL-RK	
Critical properties	T_B=445.6 K, T_C=644.4 K, P_C=4.935 MPa, V_C=0.25437 m^3/kmol, ω=0.661, MW=86.58	
Flue gas specification	Flue gas composition	
H_2O (mol%)	7	
N_2 (mol%)	75	
O_2 (mol%)	5	
CO_2 (mol%)	13	
Flue gas feeding temperature (°C)	50	
Flue gas feeding pressure (atm)	1	

2.2 PCC process design with Aspen Plus

For the DESs-based PCC process, the most common capture process is depicted in Figure 1 (Luo et al., 2021). The coal-fired flue gas should first go through a pre-treatment to remove the small particles, SO_X, NO_X, and H_2O. Then, the pressure swing technology was adopted to absorb CO_2 at high pressure and desorbed it at low pressure, as the solubility of CO_2 is different at different pressures. Typically, a multistage compressor is used to compress the flue gas to reach the absorption pressure which consists of compressors and coolers. By cooling after each compression stage, the total energy demand for flue gas compression can be reduced. Still, it accounts for more than 80% total energy requirement of the PCC process. To overcome this large energy demand, a new PCC process was proposed in this work as illustrated in Figure 2, consisting of three parts, including CO_2 absorption, latent heat reuse, and solvent regeneration. This latent heat reuse system was developed based on a three-stage compressor. Instead of using coolers to cool down the flue gas after compression, heater exchangers 1, 2, 3 were used to collect the heat of compression. The residual flue gas (mainly N_2, O_2, and a small amount of CO_2) coming out of the top of the absorber was used as a coolant to absorb some residual heat generated in compressors 1, 2, 3. Since this residual flue gas is already at relatively high pressure (above atmospheric pressure), when it is heated to high temperatures it can be expanded in the turbines (turbines 1, 2, 3) to regenerate electricity. After the residual gas expands in the turbines, its temperature decreases, which makes it a perfect coolant for the whole system. Information about the efficiency of turbines, compressors, vacuum pumps, etc. is also given in Figure 2. Since all compressors (compressors 1, 2, 3) and all turbines (turbines 1, 2, 3) were set to operate at the same efficiency, only the details of compressor 1 and turbine 1 are listed in Figure 2. As for the desorption process, when the solvent was regenerated in the flash tank (stripper), the temperature of the reline increased slightly due to the exotherm of the desorption process. However, even if the temperature of the reline rises only slightly, after hundreds of cycles, the heat accumulates to a certain level that can cause the entire capture process to break down. Therefore, seawater was introduced as a coolant to keep the recycled reline running at a constant temperature. Ullah et al. (2020) investigated a method to produce freshwater by membrane distillation technology using waste heat from a carbon capture process. In this case, using seawater as a coolant is another way to reuse the latent heat.

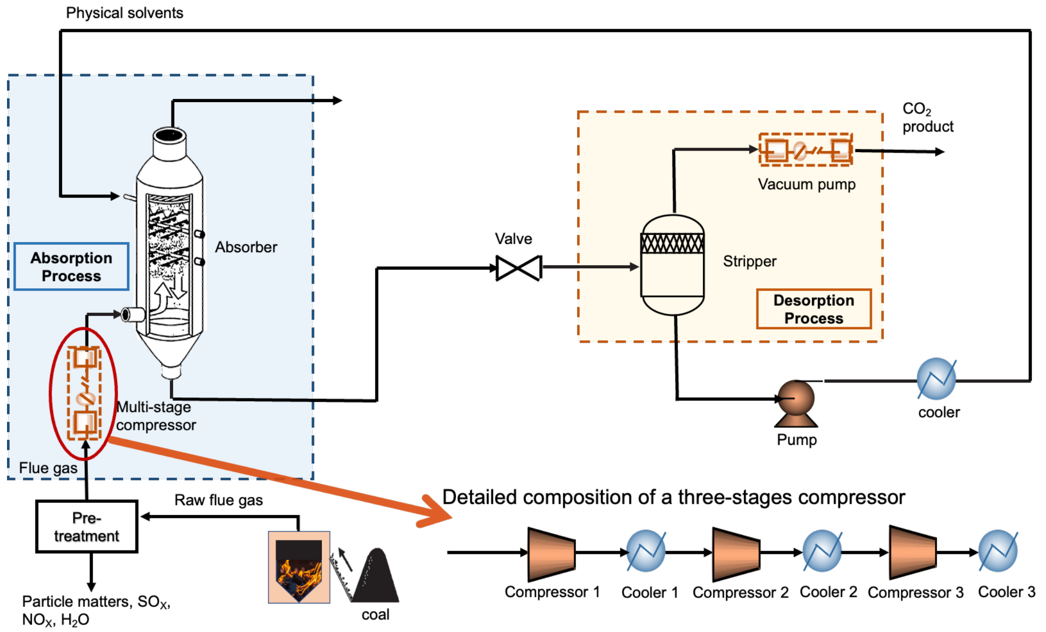

Figure 1: Typical DESs-based PCC process

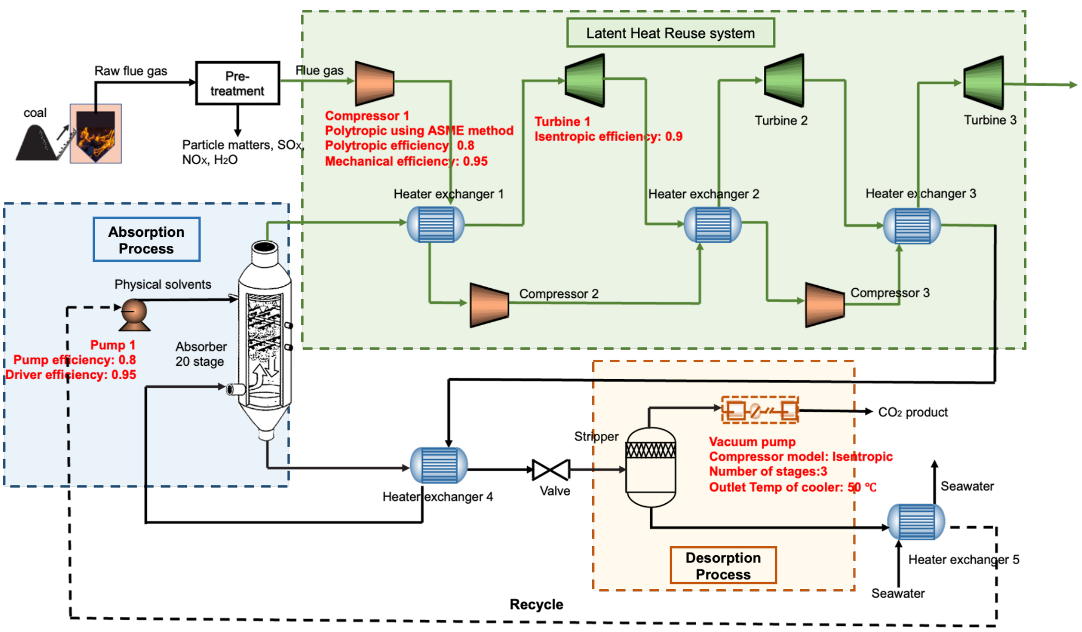

Figure 2: PCC process with latent heat reuse system

2.3 Optimize multiple operating parameters with ANN model

In this designed PCC process, the initial molar ratio (mole amount of CO_2 in the flue gas/mole amount of absorbent), the absorption pressure (atm), and the desorption pressure (atm) are the three main factors affecting the capture results and the total energy need, respectively. These three input parameters can be adjusted in Aspen Plus to find an operating case that achieves the capture target with a relatively low total energy need. The total energy requirement is calculated as Eq (5).

$$W_{total}=W_{pump1}+W_{vacuum\ pump}+\sum_{i=1}^{3} W_{compressor\ i}+\sum_{i=1}^{3} W_{turbine\ i} \tag{5}$$

Where: W_{pump1}, $W_{vacuum\ pump}$, $W_{compressor}$, $W_{turbine}$ represent the work of pumps, compressors, and turbines respectively MW.

The calculation of the loop flow in Aspen Plus requires the calculation of its break flow first to obtain some basic information about the loop stream, then the calculation of the loop flow can be performed, and it is complicated and tedious to calculate all possible scenarios manually. To avoid overly large calculations in Aspen Plus, only 100 random combinations of operating parameters, selected by the Randi function in MATLAB, were calculated to get their output parameters (CO_2 removal rate, CO_2 concentration, and total energy requirement). These 100 sets of data were then used to train an Artificial Neural Network (ANN) model using ANN fitting toolbox in MATLAB. This ANN model which depicts the relationships between input parameters and output parameters was trained using a Bayesian regularization algorithm. In this case, output parameters can be predicted for any combination of input parameters without the necessity to calculate them in Aspen Plus. According to the U.S. Department of Energy recommendations, the capture goal was set to achieve more than 90 % CO_2 removal rate and more than 90 % purity of CO_2 product (Brunetti et al., 2010). The ANN model was used to quickly select the operational conditions that met the capture goal. The results were compared to the value calculated by Aspen Plus to determine the accuracy of the trained ANN model.

3. Results and discussions

3.1 Assessment of ANN model

As previously described, 100 sets of data were trained using the ANN fitting toolbox in MATLAB. The ANN model can also give predictions for these 100 sets of input data. The coefficient of determination (R^2) between these 100 predicted values and the values generated by Aspen Plus was used to determine the number of hidden neurons of the ANN. The R^2 value was controlled to be above 0.99 to maintain the high reliability of the prediction results. The trained ANN model with a two-layer feedforward network was depicted in Figure 3 consisting of 6 sigmoid hidden neurons and 3 linear output neurons. The prediction results of the ANN model and the calculated output of Aspen Plus are demonstrated in Figure 4. The R^2 value for CO_2 concentration, total energy need, and removal rate were 0.9987, 0.9996, and 0.9903. ANN models have shown their advantages in predicting complex processes (e.g., CO_2 capture processes, biomass gasification, etc.), and previous studies have reported satisfactory estimation performance of ANN models (Baruah et al., 2017).

The ANN model was used to select a set of operating conditions that satisfy the capture objective. The detailed operating information and the comparison of ANN prediction results and Aspen Plus results are presented in Table 2. The searching constrains for these three input parameters also listed in Table 2. The maximum deviation between the predicted and true values of the three output values is 1.22 %, so this ANN model can be considered reliable.

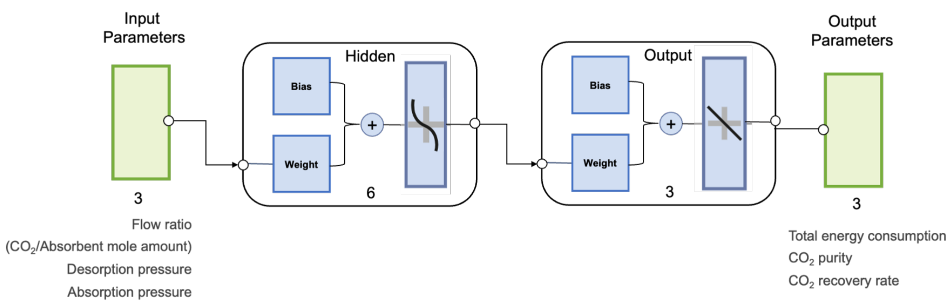

Figure 3: ANN model with a two-layer feedforward network

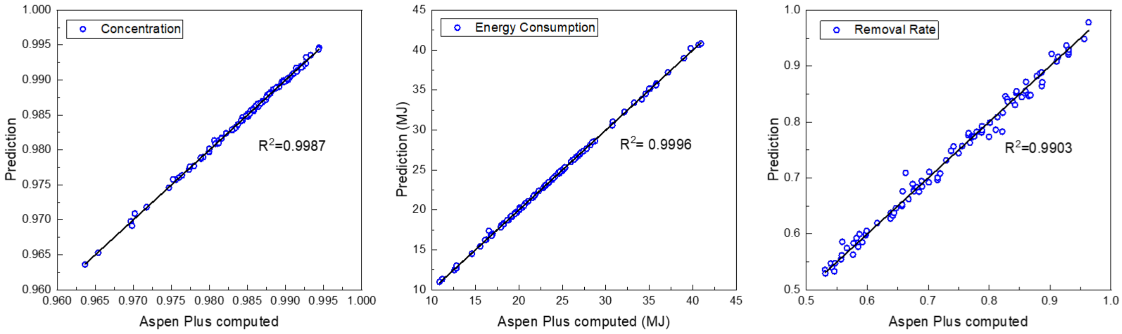

Figure 4: Parity plot of predicted results and the Aspen Plus results

Table 2. Comparison of ANN prediction results and actual results

Operating conditions		Constrains	Output results	Prediction	Real value	Deviation
Absorption pressure	10 atm	1-20 atm	Total energy demand	22.78 MJ	22.90 MJ	1.22 %
Desorption pressure	0.1 atm	0.1-1 atm	CO_2 removal rate	92.29 %	93.43 %	0.49 %
Flow ratio	2.90 %	2-43.53 %	CO_2 purity	99.10 %	99.54 %	0.44 %

3.2 Latent heat reuse system design for PCC process

Figure 5 shows the details of each stream and equipment in the PCC process for this design under the operating conditions described in Table 2. The use of Reline as an absorbent shows great advantages. First, since its vapor pressure is almost zero, the absorbent losses during operation are negligible, which means it can be used repeatedly without the need for an additional refill. Also, the purity of the CO_2 product after separation is high, as N_2 and O_2 are extremely difficult to dissolve in the reline. The biggest concern for the DESs-based PCC process would be the large energy demand. However, 53.3 % of the residual heat generated during flue gas compression can be reused by using this latent heat reuse system. With the help of the ANN model, it was able to quickly find an operation case that meets the capture target with a total energy requirement reduction to 1.28 MJ/kg CO_2, proving its potential for industrial CO_2 capture applications.

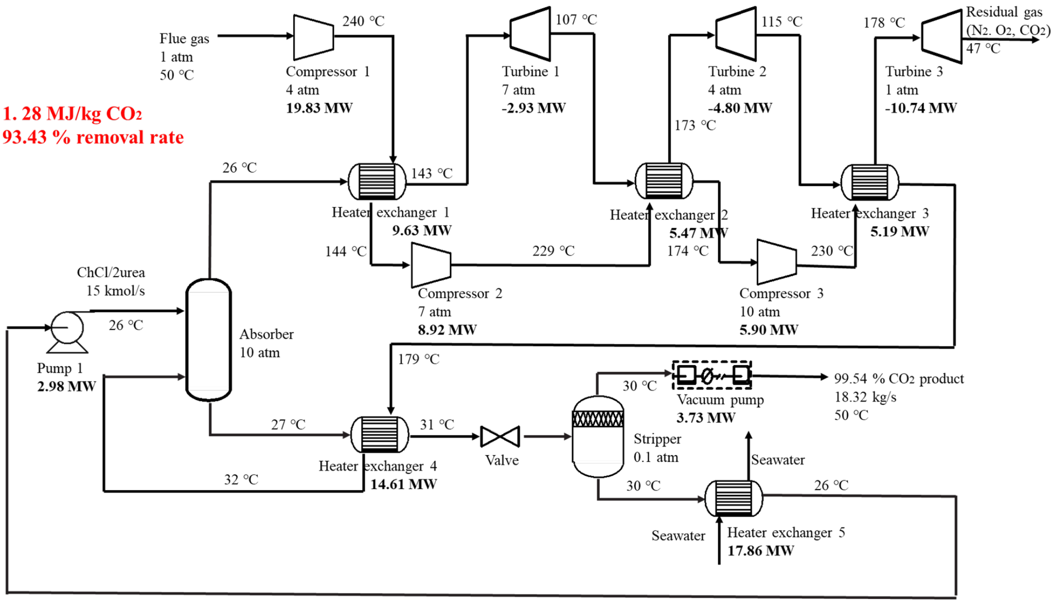

Figure 5: PCC process simulation results under selected condition

4. Conclusion

This work demonstrated the possibility of applying reline to flue gas decarbonization in a PCC process with a latent heat reuse system. This system can recover over 50 % by using the remaining gas to collect latent heat in the heater exchangers and allowing the reheated gas to expand in the turbine to generate electricity. With the ANN model, it is easy to find an operating condition that meets the capture target and reduces its total energy demand to 1.28 MJ/kg CO_2. Compared with the traditional MEA-based PCC process, this can reduce about 68.8 % of energy demand with almost zero absorbent loss. Since flue gas compression still accounts for more than 70 % of the total energy demand, a considerable flow ratio is used in the selected case to reduce the absorption pressure. Since this PCC process with a latent heat reuse system was based on pressure swing technology, it can be applied to other gas decarbonization, such as biomass gas, shale gas, etc., which will have a lower energy demand than the flue gas decarbonization. In this work, the ANN model was certificated as a useful tool for predicting complex processes like the CO_2 capture process. A challenging solution pathway arises when simulating closed process networks, which are computationally demanding and difficult to simulate using traditional methods. With the ANN model, many tedious calculations can be avoided, and it is easy to pre-design the PCC process with highly reliable prediction results.

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