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AI-based Dynamic Modelling for CO_2 Capture

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ABSTRACT

Integrating CO_2 capture with biomass/waste fired combined heat and power plants (CHPs) is a promising method to achieve negative emission. However, the use of versatile biomass/waste and dynamic operation of CHPs result in big fluctuations in the flue gas (FG) and heat input to CO_2 capture. Dynamic modelling is essential to investigate the interactions between key process parameters in producing the dynamic response of the CO_2 capture process. In order to facilitate developing robust control strategies for flexible operation in CO_2 capture plants and optimizing the operation of CO_2 capture plants, artificial intelligence (AI) models are superior to mechanical models due to the easy implementation into the control and optimization. This paper aims to develop an AI model, Informer, to predict the dynamic responses of MEA based CO_2 capture performance from waste-fired CHP plants. Dynamic modelling was first developed in Aspen HYSYS software and validated against the reference. The operation data from the simulated CO_2 capture process was then used to develop and verify Informer. The following variables were employed as inputs: inlet flue gas flow rate, CO_2 concentration in inlet flue gas, lean solvent flow rate, heat input to CO_2 capture. It was found that Informer could predict CO_2 capture rate, reboiler temperature and energy consumption with the mean absolute percentage error of 6.2%, 0.08% and 2.7% respectively.

Keywords: artificial intelligence (AI), dynamic modelling, bioenergy with carbon capture and storage (BECCS), combined heat and power (CHP) plants, energy consumption

NONMENCLATURE

Abbreviations	
BECCS	bioenergy with carbon capture and storage
CHPs	combined heat and power plants
Bio-CHPs	biomass fired combined heat and power plants
Waste-CHPs	waste fired combined heat and power plants
BA-NN	bootstrap aggregated neural networks
LSTF	long sequence time-series forecasting
MAPE	mean absolute percentage error
FG	flue gas
AI	artificial intelligence
DH	District heating
MEA	monoethanolamine
MEA-CA	MEA based chemical absorption
Symbols	
M	mass flowrate
x	volume concentration
Q_{reb}	reboiler heat duty
n	sample size
y_i	the i^{th} predicted value
$\hat{y}_i$	the i^{th} actual value

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1. INTRODUCTION

Negative emission technologies are needed to meet global warming targets by removing CO_2 from the atmosphere. Bioenergy with carbon capture and storage (BECCS), which combines CO_2 capture with bioenergy conversion and utilization, is emerging as the best solution to decarbonize emission-intensive industries and sectors [1]. Integrating BECCS in biomass or waste fired combined heat and power (bio-CHP or waste-CHP) plants is highly possible due to the large amount of CO_2 emission. Among different CO_2 capture technologies, monoethanolamine (MEA) based chemical absorption (MEA-CA) has already been commercialized.

Compared to coal-fired power plants, bio/waste-CHP plants are characterized as more fluctuations in the operation, which are primarily determined by the heat demand [2]. In addition, a wide range of biomass/waste could be used as fuel, which has different properties [3]. The changes in both operation and fuel can lead to big variation in the flue gas (FG) flowrate and composition. Moreover, because there is a competition on heat between heat supply and CO_2 capture, the dynamic change of heat demand will affect the heat input to CO_2 capture. Such fluctuations from CHP plants, including FG flowrate, compositions and the heat input, make it imperative to investigate the dynamic behavior of CO_2 capture by MEA-CA. In order to facilitate the design of control systems and the optimization of operation, it is essential to develop reliable dynamic process models of MEA-CA.

Many research works have focused on the mechanistic models of MEA-CA. For example, Åkesson et al. [4] developed a rate-based dynamic model of MEA-CA using Modelica. In response to the decrease of FG flowrate by 30%, CO_2 removal rate in the absorber was shown to increase rapidly, while more than 1 hour was required for the top temperature of the stripper to rise to a new steady state. However, the establishment of mechanistic models is very time consuming and requires extensive knowledge of the underlying physics of the process. Since numerical optimization typically requires thousands of function evaluations, evaluation of a detailed mechanistic model is typically computationally very demanding. To overcome this problem, artificial intelligence (AI) models can be developed from process operational data and used in plant optimization [5]. However, only a few studies focus on the investigation of AI models. For example, Li et al. [5] developed the bootstrap aggregated neural networks (BA-NN) model for MEA-CA to predict CO_2 capture rate and the flowrate of captured CO_2 by employing the following variables as model inputs: inlet FG flow rate, FG CO_2 concentration, FG pressure, FG temperature, lean solvent flow rate, MEA concentration and temperature of lean solvent. Simulated operation data of CO_2 capture from gPROMS simulation are used to develop and verify BA-NN model. The results showed that BA-NN model is a useful tool to model MEA-CA. However, neural networks need to be trained with large, labeled datasets that were costly and time-consuming to produce for long sequence time-series forecasting (LSTF). In addition, the influence of fluctuations of heat input to CO_2 capture has not been considered, in which energy consumption per unit captured CO_2 is a key indicator. To bridge the knowledge gap, the work aims to develop an accurate AI model for CO_2 capture. Transformers are in many cases replacing convolutional and recurrent neural networks and become the most popular types of deep learning models by using advanced Encoder-decoder structure [6]. Informer is a transformer-based model, which is a very efficient model for long sequence time-series forecasting, and significantly outperforms existing methods [7]. Therefore, the Informer model is selected to predict CO_2 capture rate and energy consumption, by considering the variations of both FG and heat input from waste-CHP plants. The operation data from Aspen HYSYS software is used to build and verify the AI model.

2. METHODS

2.1 System description

A mechanistic dynamic model has been developed for MEA-CA in Aspen HYSYS V12.1, which details can be found in our previous work [8]. The schematic diagram of the system is illustrated in Figure 1. FG enters the absorber from the bottom and contacts counter-currently with a lean MEA solution. After absorption, the rich MEA solution is sent into the stripper, in which CO_2 is regenerated from the top when heat duty is provided to reboiler, and resulted lean MEA solution is recirculated back to the absorber. To make the system run stably, the integral controllers have been integrated to maintain the liquid level of condenser and reboiler. Due to the loss of H_2O and MEA, makeups are added by mass balance. The model is scaled up in this paper in Aspen HYSYS V12.1 to match the flue gas generated from a typical 660 MWe coal-fired power plant. The specifications of absorbers/stripper and the main operating parameters under nominal condition are given in Table 1.

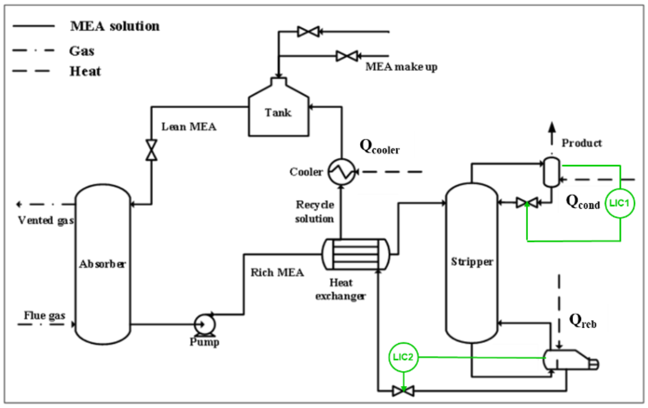

Fig. 1. Flowsheet of MEA-based CO_2 capture

Tab.1. Main specifications and operating parameters

Parameter	Value	Parameter	Value
FG		Absorber	
FG temperature (K)	319.7	Packing height and column diameter (m)	17.4; 8.7
O_2vol% in FG	2.7	Packing type	IMTP# 38MM
H_2Ovol% in FG	4.8	Pressure (kPa)	101.3
Solution		Stripper	
MEA concentration (wt%)	30	Packing height and column diameter (m)	10.9; 4.3
Lean loading	0.287	Packing type	IMTP# 38MM
Solution temperature (K)	314	Condenser pressure (kPa)	159

2.2 Data preparation

The developed MEA-CA model is used as the simulation platform for this study. The CO_2 capture rate (y_1), reboiler temperature (y_2) and energy consumption per unit captured CO_2 (y_3) are three good indicators for the operating performance of the CO_2 absorption and desorption. To predict these indicators, the following important factors are selected as inputs, including FG flow rate (u_1), FG CO_2 concentration (CO_2vol%) (u_2), the lean solvent flow rate (u_3) and the reboiler heat input (u_4).

Random function is used to generate the excitation signal of 4 inputs with step change each 15 mins, as shown in Figure 2, in which the ranges of FG flowrate and FG CO_2vol% are from an actual waste-CHP plant, and the ranges of reboiler heat input and solvent flowrate are determined by the assumption of 50-90% of capture rate. Based on the excitation signal in Fig. 2, the dynamics of CO_2 capture are simulated using the MEA-CA model in the Aspen HYSYS simulator. As outputs, CO_2 capture rate and energy consumption are calculated based on Equation 1 and Equation 2. All input and output data are sampled in every 5 s to form a training set of 12,060 groups of sampled data within 1005 mins.

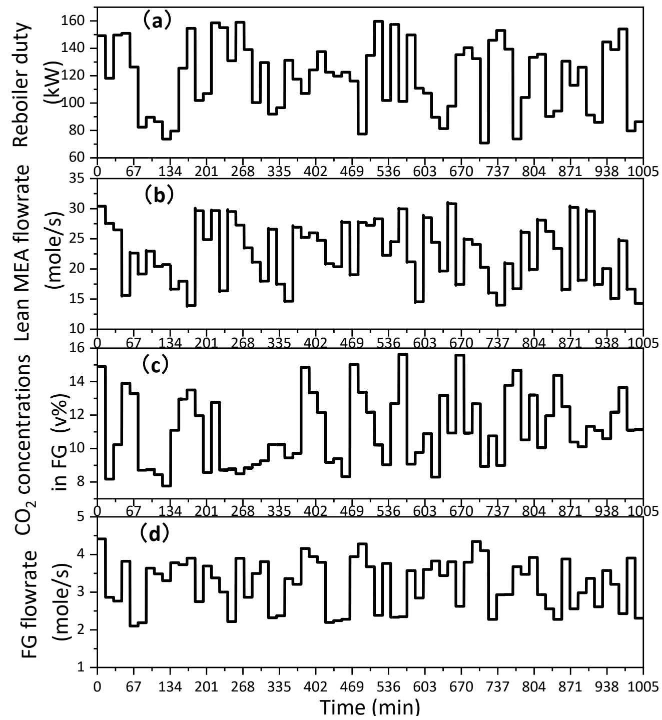

Fig.2. Excitation signal of the four inputs (a) Reboiler duty (b) Lean MEA flowrate (c) FG CO_2vol% (d) FG flowrate

$$CO_2\ capture\ rate = \frac{M_{product} * x_{product}^{CO_2}}{M_{FG} * x_{FG}^{CO_2}} * 100\% \tag{1}$$

$$Energy\ penalty = \frac{Q_{reb}}{M_{product} * x_{product}^{CO_2}} (kJ/kg\ CO_2) \tag{2}$$

where M is the mass flowrate, x is the volume concentration; Q_{reb} is the reboiler heat duty.

2.3 Identification of the Informer model

Informer model was proposed to be beyond efficient Transformer model for LSTF [7], which has a high prediction capacity by capturing precise long term temporal dependency and short term temporal trend efficiently. It shows three distinctive characteristics: (i) a ProbSparse self-attention mechanism makes lower time complexity and reduces memory usage and has excellent performance on sequences' dependency alignment. (ii) the self-attention distilling highlights dominating attention by halving cascading layer input, and efficiently handles extreme long input sequences. (iii) the generative style decoder drastically improves the inference speed of long-sequence predictions by the prediction at one forward operation.

In this study, the Informer model is implemented by Python coding with PyTorch deep learning framework to train the model by using the output values from Aspen HYSYSV12.1. The generated data were split into training data (60%), validation data (20%) and testing data (40%). The data were scaled to zero mean and variance of standard deviation before they were used for model training. Because the temporal complexity of Aspen HYSYSV12.1 is not so much, the model does not need to be constructed deeply as it probably brings overfitting. Thus, we set the number of self-attention layers in encoder and decoder separately as 1. The dimension of feature extraction of layers to be 256. The dimension of the last fully connected layer for output generation is 2048. The dropout rate is 0.1. The learning rate is 0.0001. Also, the patience for early stopping is 10 epochs, which means that as long as the validation loss does not decrease in continuous 10 epochs, the training process will be ended.

3. RESULTS

The mean absolute percentage error (MAPE), defined by Equation 3, is used to evaluate the performances.

$$MAPE = \frac{1}{n}\sum_{i=1}^{n}|(y_i - \hat{y}_i)/\hat{y}_i| \times 100\% \quad (3)$$

where n is the sample size; y_i is the i^{th} predicted value; $\hat{y}_i$ is the i^{th} actual value.

As shown in Figure 3, by using the AI model of Informer, the MAPE is 6.25% for the prediction of CO_2 capture rate. In addition, Informer can portray the character of CO_2 capture rate very well over the range of 60-100%, but higher deviations over the range below 50% and above 125%. As shown in Figure 4 and Figure 5, the MAPE of Informer are 0.08% for the prediction of reboiler T, and 2.7% for the prediction of energy consumption, respectively.

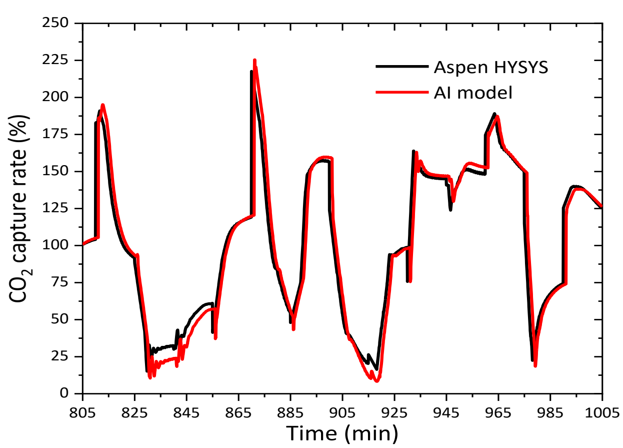

Fig. 3. The result of CO_2 capture rate

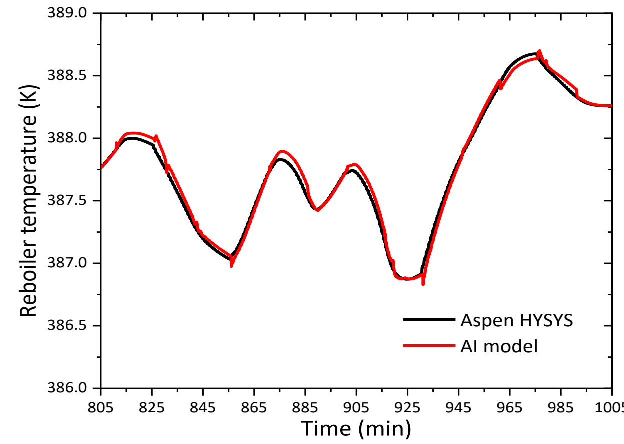

Fig. 4. The result of reboiler temperature

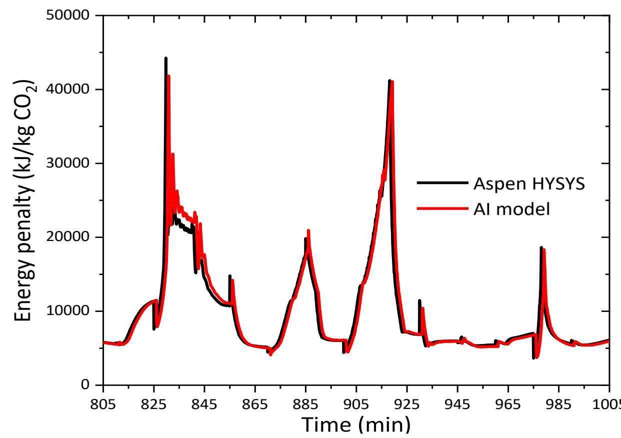

Fig. 5. The result of energy consumption

4. DISCUSSION

The dataset generation from physical model is now used. The operation data from the real test CO_2 capture plant over a long time is expected to update and improve the AI model for future application. Also, the influence of capacity of different CO_2 capture systems on the model development should be considered. For flexible operation of CO_2 capture plants, based on AI models that could track the dynamic response, the AI based controllers are also promising to find the best future control sequence.

5. CONCLUSIONS

An AI model, Informer, is developed to predict the dynamic responses of MEA based CO_2 capture performance from waste-fired CHP plants. By employing the following variables as inputs, inlet flue gas flow rate, CO_2 concentration in inlet flue gas, lean solvent flow rate, heat input to CO_2 capture, it was found that the mean absolute percentage error of Informer is 6.25% for the prediction of CO_2 capture rate, 0.08% for the prediction of reboiler temperature, and 2.7% for the prediction of energy consumption, respectively.

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DECLARATION OF INTEREST STATEMENT

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper. All authors read and approved the final manuscript.

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