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Research Article

Optimization and Analysis of CO2 Capture in RPB using Cognitive Computing and Evolutionary Algorithm

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ABSTRACT

Due to industrialization, deforestation and many other anthropogenic activities, carbon emission is increasing at a rate of approximately at a rate of 1% in past few years. Now, reduction of atmospheric carbon dioxide (CO2) has become a significant concern and challenge for every country across the globe. This paper is a sincere effort to study, analyse and further optimize, amine based post-combustion carbon (PCC) capture. Monoethanolamine (MEA) in rotating packed beds (RPB) has been extensively studied for CO2 chemical absorption. Enhancing CO2 capturer efficiency necessitates a thorough comprehension of the complex interrelationships within the key parameters. This study focuses on modelling and optimisation of CO2 absorption efficiency in MEA by artificial intelligence and genetic algorithms (GA). Machine learning (ML) and Artificial Neural Networks (ANN) are versatile instruments employed to model and forecast diverse complex and highly non-linear phenomena. The established process models have been established by published steady-state experimental data. Subsequently, SHAP analysis has been applied that reveals the input factors such as solvent concentration, flow rate, and rotational speed are the primary determinants of CO2 absorption in RPB. To assess the model's performance, the acquired results have been examined using statistical measures, including MSE, RMSE, and R2 value. The modelling results have been utilised to optimise CO2 absorption, employing GA under various operating conditions to ascertain the optimal values for the input variables that correlate to maximized CO2 capture.

Keywords: CO2 absorption, machine learning, modeling, optimization.

INTRODUCTION

Humans have known for a long time that the discharge of CO_2, a important greenhouse gas (GHG), causes global warming and damage to the environment. In April, the global surface temperature was recorded at 1.32°C above the 20th-century average of 13.7°C. This temperature is 0.18°C higher than the April 2020 record. Global warming is a worldwide problem that has brought together 195 nations with the shared objective of decreasing global (GHG) emissions and achieving carbon neutrality by 2050. Despite extensive attempts to decrease CO_2 emissions, its concentration has increased by 1.7% worldwide [1]. Carbon capture and storage (CCS) systems offer a way to decrease emissions from an operational fossil fuels power station. Currently, the most economically viable and commercially efficient approach for absorbing CO_2 from power plants is post-combustion carbon (PCC) capture using an amine-based CO_2 absorption technology. In chemical absorption processes, amine-based solvents, particularly monoethanolamine (MEA), are utilised to a great extent since they have proven effective at removing chemicals, do not require an excess of air pressure, and are economical [2], [3], [4]. Rotating Packed Bed (RPB), a intensified process tool, has garnered significant attention in recent years. A notable benefit of RPB is enhanced mass transfer resulting from intense blending at the gas-liquid interface [5], [6]. It has been utilised in various domains, including acid gas absorption, distillation, and nanomaterial synthesis [7], [8], [9]. The liquid is dispersed into minute liquid entities, such as threads, droplets, and films by high-velocity in an RPB, thereby creating a substantial gas-liquid contact area. All of these elements contribute to a significant improvement in mass transfer efficiency [10].

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The effectiveness of the experiment process in RPB has been evaluated using mathematical models [11], [12], [13]. However, studying the fundamental physics of the process necessitates significant time and profound experience in the area. To mitigate this concern, researchers have been employing machine learning (ML) and artificial neural network models (ANN), based on operational data from the process and simulated data for CO_2 absorption in RPB [14], [15]. Artificial intelligence has been applied to validate CO_2 absorption in packed column. Fu et al. [16] employed ANN algorithms, Backpropagation Neural Network (BPNN) and Radial Basis Function Neural Network (RBFNN), to investigate mass transfer in MEA within a packed column. The results acquired from these models have been compared with numerical findings in the literature, revealing that the RBFNN exhibited good performance. Afkhamipour et al. [17] applied a multilayer perceptron neural network (MLPNN) to forecast CO_2 capture in 4-diethylamino-2-butanol (DEAB). The average absolute relative deviation (AARD) between the predicted and actual findings indicates that MLPNN model makes good prediction with an AARD of 5.47%. Wu et al. [18] examine CO_2 absorption through two modelling methodologies: statistical analysis and ANN modelling, employing data from the International Test Centre of CO_2 Capture (ITC) in Regina, Saskatchewan, Canada. The results demonstrate that ANN performs significantly better at predicting CO_2 absorption than statistical analysis. Ashraf et al. [19] employed support vector machine (SVM), and ANN to develop a model with comprehensive hyperparameter optimisation. Additionally, sensitivity analysis based on partial derivatives has been conducted to identify which input features significantly influence CO_2 capture. It has been noted that ANN exhibits strong performance with the existing data.

Further, these methodologies have been also adopted for CO_2 absorption process in RPB. Zhao et al [20] employed LSSVR model to ascertain the mass transfer coefficient in NaOH solution. The findings indicated that the Mean Squared Error (MSE) for the testing set was 0.0012, lowest observed when compared to the ANN, showing higher predictive accuracy and generalisation capability of the model. Shalaby et al. [21] adopted three machine learning techniques based on Gaussian process regression and analysed the outcomes with an ANN model to predict the output of PCC unit. Results indicate that the ANN achieves superior accuracy above 95%. The results collected were utilised to optimise the CO_2 capture mechanism and establish ideal operating parameters. Ardeshiri et al. [22] investigated microfluidic CO_2 absorption by water-lean solvent. The data was utilised to forecast CO_2 absorption efficiency using ANN. The result shows that ANN model performed best with RMSE 0.35, indicating that the ML technique predicts water-lean amine solution CO_2 removal efficiency well.

Reviewing the relevant studies suggests that ANN has been widely used in predictive task, although alternative machine learning algorithms are also applicable. Further, the output of the prediction made by the model can be applied to maximize CO_2 absorption efficiency within a range of optimal conditions. This work employs GPR and a deep network model called BPNN to predict the CO_2 absorption in MEA corresponding to experimental data taken from Nour et al [23]. Also, optimization has been performed to maximize the CO_2 absorption with optimal conditions.

METHODOLOGY

Database information

The CO_2 absorption data in MEA has been gathered from the literature of Nouroddinvand et al. (2021). The experiment utilised a novel design of high-gravity Arc-blade RPB to investigate its impact on CO_2 absorption efficiency with a MEA aqueous solution. The absorption tower is described in the work of Nouroddinvand et al [23]. The WebPlotDigitizer program is utilised to acquire data for the model's input-output variables. The input has been derived from the data acquired via the graph. The comprehensive dataset has 140 observations for input-output variables. The prediction of mole fraction of CO_2 in gas outlet is based on following inputs: MEA concentration (mol/l), rotational speed (RPM), liquid and gas flow rate (l/min), and mole fraction of CO_2 in gas inlet, as illustrated in Table 1. The entire dataset is partitioned in two subsets: training and testing dataset. 30% of entire data is set aside for testing, while 70%s is used for training.

Table 1: Details of parameters and operational variables of experiment conducted in RPB

Parameters and operational variables of RPB	
Axial height (m)	0.098
Inner radius (m), outer radius (m)	0.04, 0.14

Parameters and operational variables of RPB	
Specific surface area of packing (m^{-1})	53.5
Packing porosity	0.9882
CO_2 concentration in gas phase (ppm)	5000-20000
MEA concentration (mol/l)	0.5-2
Flowrate of liquid (l/min)	0.3-0.6
Rotational speed (rpm)	300-1200

Different ML models

Establishing an accurate and dependable analytical relationship to characterise nonlinear processes and connect independent and dependent variables is difficult. Artificial intelligence has gained significant attention in recent times owing to their effectiveness, versatility, accessibility, and the availability of numerous established training methodologies. By employing a suitable learning technique to train these networks, one can determine the relation between inputs-outputs in multivariate nonlinear systems. This paper describes two algorithms: GPR, and ANN.

B.1 Gaussian Process Regression (GPR)

GPR is an adaptable and efficient ML technique designed for regression issues. It is one of a kind because it not only makes predictions, but it also measures how uncertain those forecasts are. GPR is based on Gaussian distributions and Bayes' theorem, and it may adapt to data without requiring a fixed relationship (linear/polynomial) between input and output [24]. The kernel function (covariance function) determines the relationship between data points. It calculates how much effect one data point has on another based on their similarity. GPR employs Bayes' theorem to update its predictions with observed data becomes available. GPR can mathematically represented as Eqn. 1:

Where m(X) - the expected value of the function being modelled, and k(X,X')— the kernel function

$$y = f(m(X), k(X, X')) \quad (1)$$

B.2 Artificial Neural Network (ANN)

ANN employs multilayered architectures known as neural networks to replicate human behaviour through evaluation of data. It comprises numerous basic processing units known as neurones, interacting across various layers. The three layers of an ANN consist of the input, hidden, and output. Data is sent through the input layer, subsequently transmitted to the hidden layer, and finally to the output layer to generate predictions utilising an activation function [25], [26]. The output of each neurone is a function of weight and bias as described by Eqn 2. The output of the ANN model is more in line alongside the real data when the weights given to the neural pathways between the neurones are optimised.

$$\hat{Y} = f(XW + B) \quad (2)$$

Where $\hat{Y}$ is predicted variable and X is input vector, f is activation function, B is bias, and W is associated weights.

C. SHAP analysis

Analysing every input feature on the expected output is crucial. One approach to find the relevance of input features on the prediction is SHAP (SHapley Additive exPlanations) analysis. This approach investigates the significance and function of every value off features in the anticipated output by use of game theory and coalition game reward allocation. The greater the absolute SHAP value of a variable, greater its influence on model prediction [27].

D. Evaluating ML models

Performing statistical analysis is important to predict which model behaves more appropriately. Here, the metrics used for assessment of the two models is Mean Absolute Error (MAE), root mean square error (RMSE), and R^2 value and its mathematical equation is given by Eqn. (3-5). Further analysis have also been made using parity plot between the predicted output, and actual data.

Mean Absolute Error: (3)

$$\sum_{i=1}^{n} \frac{|\alpha^{exp} - \alpha^{pred}|}{n}$$

Root Mean Square Error: (4)

$$\sqrt{\sum_{i=1}^{n} \frac{(\alpha^{exp} - \alpha^{pred})^2}{n}}$$

R2: (5)

$$1 - \frac{\sum_{i=1}^{n} (\alpha^{exp} - \alpha^{pred})^2}{\sum_{i=1}^{n} (\alpha^{exp} - \underline{\alpha})^2} \; where \; \underline{\alpha} = \frac{\sum_{i=1}^{n} \alpha^{exp}}{n}$$

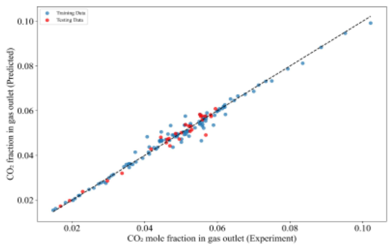
Here, n is total number of observations, η^{exp} denotes the experimental values, and η^{pred} denotes the predicted values

RESULTS AND DISCUSSION

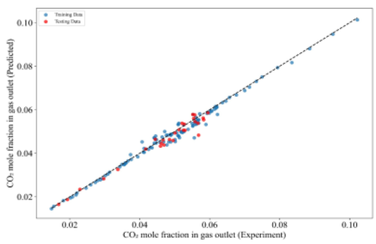
The analysis of the both the models have been performed using statistical analysis and graphical representation as discussed in Section 2.4. The results have been shown in Table 2. It can be observed that RMSE is least for GPR with R^2 value 0.98 which is near to 1. Also, Fig.1 shows that the data is aligned very close to linear line and has least scatter points for GPR. So, it can be concluded that GPR performs better than ANN.

Table 2: Statistical inferences of the models

	GPR	**ANN**
MAE	0.02	0.06
RMSE	0.03	0.078
R- squared value	0.98	0.94



(a)



(b)

Fig. 1. Comparison plot of CO_2 mole fraction in gas outlet (experiment) and CO_2 mole fraction in gas outlet (model predicted) (a) GPR (b) ANN

Further SHAP analysis has been performed to know impact of each input on anticipated output using GPR model. It can be observed from Fig. 2 that among the four input features CO_2 inlet mole fraction has the highest influence on the output as increase in mole fraction of CO_2 enhances mass transfer and hence more absorption. MEA concentration and solvent flowrate also have good influence on the output as this also drives the increase in mass transfer and hence the efficiency. Lastly, we have rotational speed which is least among all but this input is very important operational parameter to be considered.

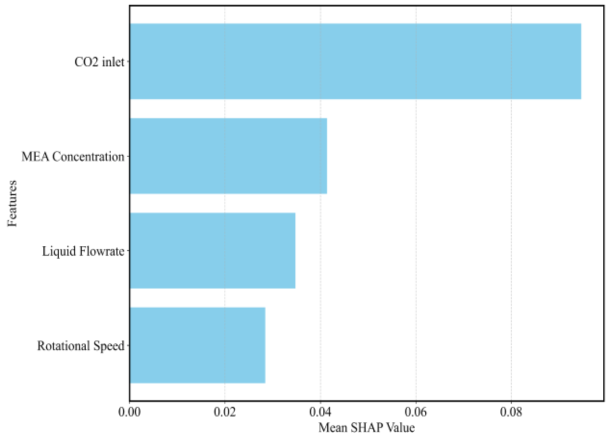


Fig. 2. Impact of input variables on GPR predicted output through SHAP analysis

For better performance, essential operational factors are optimized on the output predicted by the model to maximize CO_2 absorption efficiency. It is essentially desirable to have a model that demonstrates an appropriate generalisation of the mechanism to access the input design space of operating factors and identify the optimum solution. CO_2 absorption efficiency is calculated using Eqn. 6

$$\eta_{CO_2} = \left(\frac{y_{CO_2,in} - y_{CO_2,out}}{y_{CO_2,in}}\right) x100\% \tag{6}$$

Where, η is the absorbption efficiency, $y_{CO_2,in}$, $y_{CO_2,out}$ CO_2 mole fraction in gas inlet and outlet respectively.

Rotor speed for absorber, Concentration of MEA, CO_2 mole fraction (gas inlet), and solvent flowrate are considered as the decision variables of the optimization. The optimization has been performed on all these variables to maximize the CO_2 absorption efficiency. The objective problem is formulated as below by Eqn. (7-11):

$$\eta_{CO_2} \tag{7}$$

$$600 \leq RPM \leq 1300 \tag{8}$$

$$0.25 \leq F_{MEA} \leq 0.65 \tag{9}$$

$$0.25 \leq y_{CO_2,in} \leq 0.3 \tag{10}$$

where, C_{MEA} is MEA concentration, RPM is rotational speed, F_{MEA} is solvent flowrate, and $y_{CO_2,in}$ is mole fraction of CO_2 in gas inlet.

The optimisation has been performed using genetic algorithm. Outcomes exhibit that the maximum efficiency of CO_2 absorption is 90%, with ideal values for the decision variables presented in Table 3. Given the nonlinear interactions of input variables on CO_2 absorption, the established operating values and their variations range can facilitate the attainment of maximum CO_2 capture levels under varying flue gas operating conditions.

Table 3: Optimization summary with optimal values of the variables obtained

	η_{CO_2}	
Decision variables	**Lower and Upper Range**	**Optimal values**
C_{MEA}	0.2, 2.2	2.2
RPM	600, 1300	1000

η_{CO_2}		
Decision variables	**Lower and Upper Range**	**Optimal values**
F_{MEA}	0.25, 0.65	0.56
$y_{CO_2,in}$	0.25, 0.3	0.3

CONCLUSION

This work examines experimental data on CO_2 absorption in MEA using RPB. The modelling has been conducted utilising two Artificial Intelligence methodologies: GPR and ANN. The best predicted model is further amalgamated with optimisation method to enhance CO_2 absorption efficiency. Statistical analysis indicates that GPR outperforms ANN, with an RMSE of 0.03 and a R^2 of 0.98. Additionally, to ascertain the influence of inputs on the projected output, SHAP analysis was conducted, indicating that the CO_2 mole fraction in gas inlet and concentration of solvent MEA are significant factors. The GPR model is combined with an optimisation problem to ascertain the optimal operating parameter for the variables being used that yield maximal CO_2 capture. This work offers a model-driven optimisation system aimed to determine optimal conditions for maximising CO_2 absorption. The findings serve as a valuable reference for the industrial sector in effective application of CO_2 capture utilising MEA, ultimately supporting the goals of carbon neutrality.

REFERENCES

[1] S. Mohammed, F. Eljack, S. Al-Sobhi, and M. K. Kazi, “A systematic review: The role of emerging carbon capture and conversion technologies for energy transition to clean hydrogen,” Apr. 01, 2024, Elsevier Ltd. doi: 10.1016/j.jclepro.2024.141506.

[2] J. Du et al., “Review on post-combustion CO2 capture by amine blended solvents and aqueous ammonia,” Chemical Engineering Journal, vol. 488, p. 150954, May 2024, doi: 10.1016/J.CEJ.2024.150954.

[3] C. Gouedard, D. Picq, F. Launay, and P. L. Carrette, “Amine degradation in CO2 capture. I. A review,” 2012, Elsevier Ltd. doi: 10.1016/j.ijggc.2012.06.015.

[4] C. Nwaoha et al., “Carbon dioxide (CO2) capture: Absorption-desorption capabilities of 2-amino-2-methyl-1-propanol (AMP), piperazine (PZ) and monoethanolamine (MEA) tri-solvent blends,” J Nat Gas Sci Eng, vol. 33, pp. 742–750, Jul. 2016, doi: 10.1016/j.jngse.2016.06.002.

[5] N. Chamchan et al., “Comparison of rotating packed bed and packed bed absorber in pilot plant and model simulation for CO2 capture,” J Taiwan Inst Chem Eng, vol. 73, pp. 20–26, Apr. 2017, doi: 10.1016/j.jtice.2016.08.046.

[6] K. P. Dhaneesh and P. Ranganathan, “A comprehensive review on the hydrodynamics, mass transfer and chemical absorption of CO2 and modelling aspects of rotating packed bed,” Sep Purif Technol, vol. 295, p. 121248, Aug. 2022, doi: 10.1016/j.seppur.2022.121248.

[7] A. Mondal, A. Pramanik, A. Bhowal, and S. Datta, “Distillation studies in rotating packed bed with split packing,” Chemical Engineering Research and Design, vol. 90, no. 4, pp. 453–457, Apr. 2012, doi: 10.1016/j.cherd.2011.08.008.

[8] B. Guo et al., “Research on the preparation technology of polyaniline nanofiber based on high gravity chemical oxidative polymerization,” Aug. 2013. doi: 10.1016/j.cep.2013.05.013.

[9] H. J. Ma and Y. S. Chen, “Evaluation of effectiveness of highly concentrated alkanolamine solutions for capturing CO2 in a rotating packed bed,” International Journal of Greenhouse Gas Control, vol. 55, pp. 55–59, Dec. 2016, doi: 10.1016/j.ijggc.2016.11.009.

[10] J. Zhan et al., “Simultaneous Absorption of H2S and CO2 into the MDEA + PZ Aqueous Solution in a Rotating Packed Bed,” Ind Eng Chem Res, vol. 59, no. 17, pp. 8295–8303, Apr. 2020, doi: 10.1021/acs.iecr.9b06437.

[11] A. Esmaeili, A. Tamuzi, T. N. Borhani, Y. Xiang, and L. Shao, “Modeling of carbon dioxide absorption by solution of piperazine and methyldiethanolamine in a rotating packed bed,” Chem Eng Sci, vol. 248, Feb. 2022, doi: 10.1016/j.ces.2021.117118.

[12] T. N. Borhani, E. Oko, and M. Wang, “Process modelling and analysis of intensified CO2 capture using monoethanolamine (MEA) in rotating packed bed absorber,” J Clean Prod, vol. 204, pp. 1124–1142, Dec. 2018, doi: 10.1016/j.jclepro.2018.09.089.

[13] A. S. Joel, M. Wang, and C. Ramshaw, “Modelling and simulation of intensified absorber for post-combustion CO2 capture using different mass transfer correlations,” Appl Therm Eng, vol. 74, pp. 47–53, Jan. 2015, doi: 10.1016/j.applthermaleng.2014.02.064.

[14] S. Norouzbahari, S. Shahhosseini, and A. Ghaemi, “Modeling of CO2 loading in aqueous solutions of piperazine: Application of an enhanced artificial neural network algorithm,” J Nat Gas Sci Eng, vol. 24, pp. 18–25, May 2015, doi: 10.1016/j.jngse.2015.03.011.

[15] F. Li, J. Zhang, E. Oko, and M. Wang, “Modelling of a post-combustion CO2 capture process using neural networks,” Fuel, vol. 151, pp. 156–163, Jul. 2015, doi: 10.1016/j.fuel.2015.02.038.

[16] D. Fu, Z. Li, and F. Liu, “Experiments and model for the viscosity of carbonated 2-amino-2-methyl-1- propanol and piperazine aqueous solution,” Journal of Chemical Thermodynamics, vol. 68, pp. 20–24, 2014, doi: 10.1016/j.jct.2013.08.025.

[17] M. Afkhamipour and M. Mofarahi, “Modeling and optimization of CO2 capture using 4-diethylamino-2-butanol (DEAB) solution,” International Journal of Greenhouse Gas Control, vol. 49, pp. 24–33, Jun. 2016, doi: 10.1016/j.ijggc.2016.02.019.

[18] Y. Wu, Q. Zhou, and C. W. Chan, “A comparison of two data analysis techniques and their applications for modeling the carbon dioxide capture process,” Eng Appl Artif Intell, vol. 23, no. 8, pp. 1265–1276, Dec. 2010, doi: 10.1016/j.engappai.2010.06.012.

[19] W. M. Ashraf and V. Dua, “Machine learning based modelling and optimization of post-combustion carbon capture process using MEA supporting carbon neutrality,” Digital Chemical Engineering, vol. 8, Sep. 2023, doi: 10.1016/j.dche.2023.100115.

[20] B. Zhao, Y. Su, and W. Tao, “Mass transfer performance of CO2 capture in rotating packed bed: Dimensionless modeling and intelligent prediction,” Appl Energy, vol. 136, pp. 132–142, Dec. 2014, doi: 10.1016/j.apenergy. 2014.08.108.

[21] A. Shalaby, A. Elkamel, P. L. Douglas, Q. Zhu, and Q. P. Zheng, “A machine learning approach for modeling and optimization of a CO2 post-combustion capture unit,” Energy, vol. 215, Jan. 2021, doi: 10.1016/j.energy. 2020.119113.

[22] A. Ardeshiri and H. Rashidi, “Performance of Water-Lean Solvent for Postcombustion Carbon Dioxide Capture in a Process-Intensified Absorber: Experimental, Modeling, and Optimization Using RSM and ML,” Ind Eng Chem Res, vol. 62, no. 48, pp. 20821–20832, Dec. 2023, doi: 10.1021/acs.iecr.3c02397.

[23] V. Mohammadi Nouroddinvand and A. Heidari, “Experimental study of CO2 absorption with MEA solution in a novel Arc-RPB,” Chemical Engineering and Processing - Process Intensification, vol. 165, Aug. 2021, doi: 10.1016/j.cep.2021.108450.

[24] H. Tao et al., “Groundwater level prediction using machine learning models: A comprehensive review,” Jun. 07, 2022, Elsevier B.V. doi: 10.1016/j.neucom.2022.03.014.

[25] R. HECHT-NIELSEN, “Theory of the Backpropagation Neural Network**Based on ‘nonindent’ by Robert Hecht-Nielsen, which appeared in Proceedings of the International Joint Conference on Neural Networks 1, 593–611, June 1989. © 1989 IEEE.,” in Neural Networks for Perception, Elsevier, 1992, pp. 65–93. doi: 10.1016/b978-0-12-741252-8.50010-8.

[26] A. Zahir et al., “Prediction and optimization of liquid dispersion of monoethanolamine in a rotating packed bed for CO2 absorption,” Chemical Engineering Research and Design, vol. 199, pp. 252–267, Nov. 2023, doi: 10.1016/j.cherd.2023.09.031.

[27] D. M. Makarov, Y. A. Fadeeva, V. A. Golubev, and A. M. Kolker, “Designing deep eutectic solvents for efficient CO2 capture: A data-driven screening approach,” Sep Purif Technol, vol. 325, Nov. 2023, doi: 10.1016/j.seppur.2023.124614.