Original Article

Machine learning based modelling and optimization of post-combustion carbon capture process using MEA supporting carbon neutrality

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A R T I C L E   I N F O

A B S T R A C T

The role of carbon capture technology using monoethanolamine (MEA) is critical for achieving the carbon-neutrality goal. However, maintaining the efficient operation of the post-combustion carbon capture is challenging considering the hyperdimensional design space and nonlinear characteristics of the process. In this work, CO_2 capture level from the flue gas in the absorption column is investigated for the post-combustion carbon capture process using MEA. Artificial neural network (ANN) and support vector machine (SVM) models are constructed to model CO_2 capture level under extensive hyperparameters tuning. The comparative performance analysis based on external validation test confirmed the superior modelling and generalization ability of ANN for the carbon capture process. Later, partial derivative-based sensitivity analysis is carried out and it is the found that absorbent-based input variables like lean solvent temperature and lean solvent flow rate are the two most significant input variables on CO_2 capture level in the absorption column. The optimization problem with the ANN model embedded in the nonlinear programming-based optimization environment is solved under different operating scenarios to determine the optimum operating ranges for the input variables corresponding to the maximum CO_2 capture level. This research presents the optimum operating conditions for CO_2 removal from the flue gas for the post-combustion carbon capture process using MEA that contributes to achieving the carbon neutrality goal.

Introduction

Climate change is a harsh reality and its dangerous impact on the environment is beginning to be evident in the form of disturbed rain cycles, floods, prolonged summer seasons and elevated sea level. The transition from fossil-fuels to renewable energy systems may not be robust and reliable under the existing state of technology (IEA 2021). Therefore, intensive research is being conducted in decarbonizing the flue gases of fossil-based industrial complexes. Carbon capture is a key carbon removal technology from the flue gases and is presented as one amongst the solutions to achieve carbon-neutrality from the fossil-based industrial systems. In this regard, post combustion carbon capture process using monoethanolamine (MEA) is the most mature form of carbon removal technology and is installed at some industrial stations for decarbonizing the flue gases (IEA 2021). However, the process is energy intensive and requires efficient operation management of the carbon capture system thereby ensuring the higher energy efficiency of the industrial complex.

Post-combustion carbon capture process using MEA is a complex carbon removal process maintained under the large design space of input variables. The mathematical model predicting CO_2 capture level based on the large number of the input variables of the process is quite complex and thus deploying the constructed mathematical model for extensive predictive and optimization analytics can be computationally prohibitive and time intensive. To address this issue, machine learning based modelling algorithms offer an alternative tool to construct an efficient model of the complex and large industrial process that are computationally cheaper to construct, easier to use for predictive analytics, and subsequently be deployed to speed up the optimization analysis.

Artificial neural network (ANN) and support vector machine (SVM) are the two powerful modelling algorithms of machine learning. ANN can approximate any nonlinear output space constructed on large input space with good accuracy and can effectively dig nonlinear patterns from the heap of data (Bishop, 1995). These features enable ANN to be deployed for practical applications ranging from atomic-scale (Uddin et al., 2013) to enterprise-level of industrial complexes (Ashraf et al., 2021) for the operational excellence and improved efficiency of the

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system. Similarly, SVM can also construct the effective functional relationship with the output variable that captures the nonlinearity and interactions among the variables (Singh et al., 2015). This feature is particularly useful for constructing the flexible and efficient models for the multi-scale systems and SVM has been used for a diverse range of practical applications (Ma et al., 2018, Shadloo, 2020, Zendehboudi et al., 2018). However, there are number of challenges to be addressed for the development of an efficient ML based predictive model that include, i) data-collection and visualizing the data-distribution space to ensure the quality of data, ii) elimination of the linearly-dependent input variables, iii) hyperparameters tuning for the development of ML models, iv) evaluation of the predictive performance of the ML model on the unseen dataset etc. More challenges about the ML model development can be studied from (Bishop, 1995, Ashraf et al., 2023).

Over the past few decades, researchers have conducted rigorous research on solvent-based post combustion carbon capture technology. Zhang et al. (Zhang et al., 2009) developed a mechanistic model for the solvent based carbon capture plant and validated it on the pilot plant data from the University of Texas Austin. It was concluded that the high thermal energy spent in the reboiler of stripper could be an obstacle in wide-spread utilization of the carbon-capture plant world-wide. To reduce the thermal duty of the reboiler, Freguia and Rochelle (Freguia and Rochelle, 2003) investigated the sensitivity of the process variables to evaluate the impact of the operating conditions of the CO_2 capture process on the steam requirements in the reboiler. Tatarczuk et al. (Tatarczuk et al., 2015) deployed an inter-heated stripper in the stripper column that modified the solvent recovery process in the column. The results showed that the energy requirements and CO_2 recovery of the process were improved by 8-12% and 8-11% respectively. In another study, Wang et al. (Wang et al., 2011) pointed out in the review study on the post-combustion carbon capture that the effective synchronization of the sub-systems of the carbon capture process like absorption column, flue gas system, stripper column, reboiler, heat-exchangers, condensers etc., can reduce the energy consumption for capturing the CO_2 from the flue gas.

The application of ML models for the process design and operation of post-combustion carbon capture technologies is being widely adopted by the researchers. The potential application of ML models in carbon capture domain is to identify the patterns present in the data that are difficult to capture for the complex operation of carbon capture process. ML algorithms are being applied for the properties evaluation of CO_2 sorbents and oxygen carrying materials, modelling and control of carbon capture process (Bai et al., 2016, Li et al., 2018, Li et al., 2017), predict CO_2 solubilities in solvents and adsorbents (Farmahini et al., 2018, Burns et al., 2020, Pai et al., 2020). Sipöcz et al. (Sipöcz et al., 2011) developed an ANN network to model CO_2 capture level, specific duty and rich load for MEA solvent based carbon capture process using five variables namely inlet flue gas flow, inlet flue gas temperature, CO_2 concentration in the flue gas, reboiler duty and solvent circulation rate. The data from the process simulator CO2SIM was utilized to construct the model. Li et al. (Li et al., 2015) constructed steady-state and dynamic models to model CO_2 capture level of post-combustion MEA based carbon capture process using bootstrap aggregated neural networks. The prediction performance of the models was evaluated to select a well-performing model for CO_2 capture level. Liu et al. (Liu et al., 2022) developed ANN to model CO_2 absorption process with aqueous biphasic absorbents containing diethylethanolamine and diethylenetriamine in a rotating zigzag bed. The flue gas and absorbent conditions like temperature, pressure, flow rate and inlet CO_2 concentration were incorporated to predict mass transfer coefficient and CO_2 absorption efficiency. Shalaby et al. (Shalaby et al., 2021) developed tree and gaussian regression based different models to predict different outputs from carbon capture unit.

In the literature studies, carbon capture in the post-combustion carbon capture process using MEA solution has been investigated by ML approach. The input variables are selected corresponding to the

absorption column and stripper section of the carbon capture process to predict CO_2 capture level using ML based modelling algorithms (Li et al., 2015, Shalaby et al., 2021, Fu et al., 2022). However, the detailed and comprehensive model-based sensitivity (to obtain the insight about the process) and optimization analysis (estimating the optimized values of the input variables corresponding to maximum CO_2 capture level) on the absorption column of the carbon capture is lacking in the literature. Therefore, in this study, we focus only on the absorption column for ANN and SVM based modelling, that is not investigated for carbon capture in the absorption column previously corresponding to the input variables as taken from (Li et al., 2015). Subsequently, the selected ML model is used for carrying out the sensitivity and optimisation analysis for the carbon capture in the absorption column that is not investigated earlier and differentiates this work from the literature studies as cited above. Furthermore, ML model-based sensitivity and optimization analysis supports the utilization of ML for practical engineering applications thereby helping to support carbon neutrality that contributes to the novel aspects of this work as well.

An extensive hyperparameters tuning is carried out to ensure the efficient working of the selected ML algorithms. A rigorous external validation test is performed for the performance comparison of the constructed ML models and subsequently to select a better performing model having excellent prediction and generalization abilities. Partial-derivative based sensitivity analysis is performed to investigate the variables' significance on CO_2 capture level. Furthermore, the developed ML model is embedded in the optimization framework of nonlinear programming technique and the optimization problem under various scenarios is solved to determine the optimal operating ranges of input variables corresponding to maximum CO_2 capture level that is potentially missing in the literature and can be of industrial relevance to achieve efficient operation of carbon capture using the ML based modelling and optimization analysis. This research presents a generic analytical framework incorporating ML model and the optimization technique to determine the optimized conditions for the input variables of the absorption column of carbon capture process that enhances the system's efficiency and contributes to carbon-neutrality target.

Methodology

Fig. 1 shows the key stages of the analysis to optimize the post-combustion carbon capture process using MEA in the absorption column. Four major analysis stages are devised namely data-collection & visualization, ML model development, sensitivity analysis and optimizing the carbon capture process. The detailed description on these stages is provided below.

Data-Collection & Visualization

The MEA based post-combustion carbon capture is the mature carbon removal technology from the flue gas and thus finds its industrial application in power generation, steel, cement and chemical industries. The mathematical model incorporating the various input variables is constructed to model the post-combustion carbon capture process using MEA solution as provided in (Lawal et al., 2009). The description about the carbon capture in the absorption tower can be found in (Li et al., 2015) and the schematic diagram of the process is presented in Fig. 2. An extensive literature survey is conducted to identify the relevant and key important variables for CO_2 removal in the absorption column of carbon capture process (Liu et al., 2022, Fu et al., 2022, Wu et al., 2017, Fu et al., 2014, Quan et al., 2023, Shahsavand et al., 2011). Heat requirement for absorbent generation, circulation amount of MEA, steam consumption in regeneration tower, flue gas flow, liquid to gas ratio, molecular weight of lean liquid are also deployed to predict CO_2 capture amount from the flue gas (Li et al., 2018). However, flue gas and absorbent conditions like temperature, pressure, flow rate and concentration etc., are the relevant variables to model CO_2 capture level from
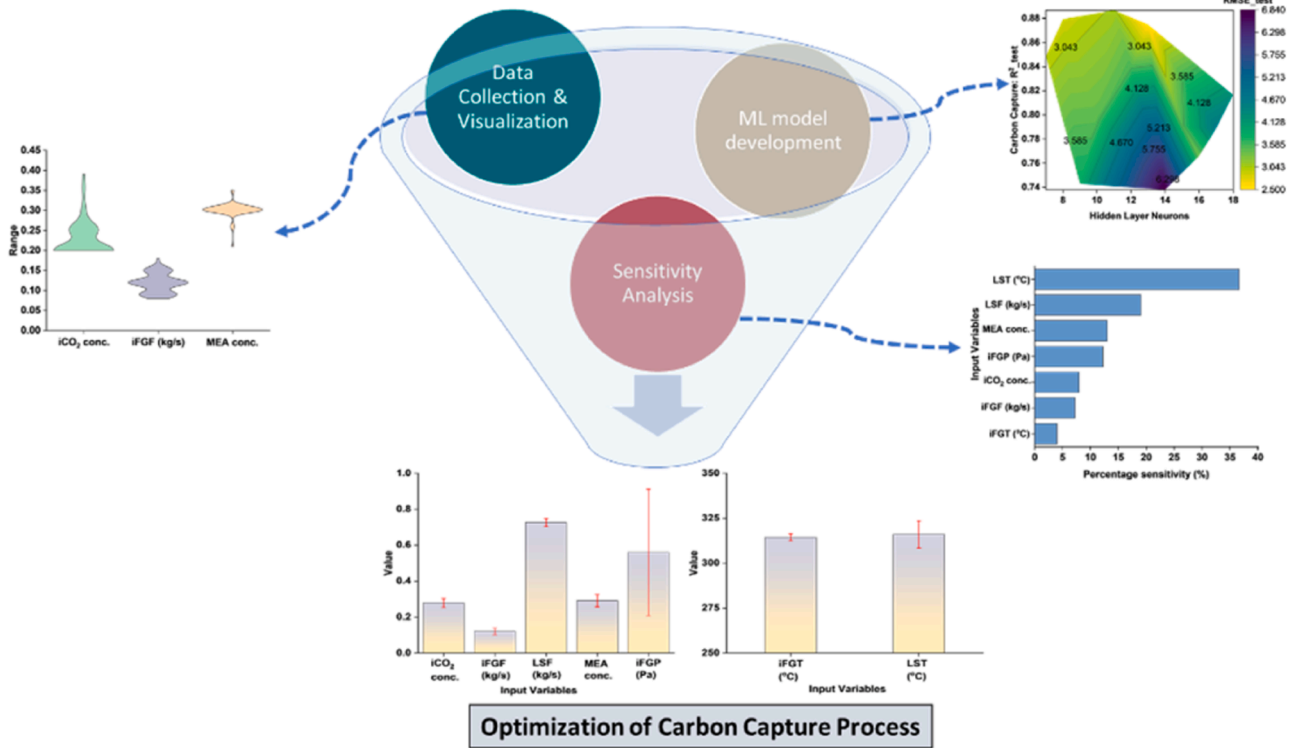
Fig. 1. The proposed methodology to carry out the ML based modelling and optimization analysis for post-combustion carbon capture process using MEA. The key stages in the analysis involves data-collection & visualization, ML model development, sensitivity analysis, and finally, optimizing the carbon capture process.
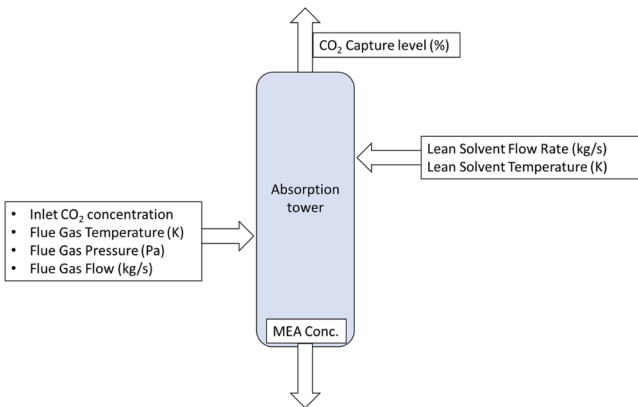

Fig. 2. A general schematic diagram of carbon capture in the absorption tower using MEA solution.

the absorption column. Therefore, the key input variables taken to develop ML model are as follows: a) inlet flue gas flow (kg/s) (iFGF), b) inlet CO_2 concentration (mass fraction) (iCO$_2$ conc.), c) inlet flue gas pressure (Pa) (iFGP), d) inlet flue gas temperature (K) (iFGT), e) lean solvent flowrate (kg/s) (LSF), f) MEA concentration (mass fraction) (MEA conc.), g) lean solvent temperature (K) (LST). Whereas, CO_2 capture level (%) is the output variable considered in this study.

The training dataset is extracted from the figures provided in (Li et al., 2015) as explained in section: Visualizing the input-output space of post combustion carbon capture process using MEA. The hyper-dimensional input space of the process is helpful to control the process and subsequently maintaining the process performance parameters within the designed limits. However, the input variables in the large design-input space may have inter-dependencies, therefore the true independent input variables having significant impact on the process are

required to be identified for the modelling purpose. The selection of the independent input variables is considerably important for the development of a well-performing ML model having effective functional mapping between the input-output variables. To this end, Pearson correlation coefficient is calculated to identify the dependent input variables (Yuan et al., 2021). The mathematical expression of Pearson correlation coefficient is given as:

$$R_{xy} = \frac{\sum_i^N (x_i - \overline{x})(y_i - \overline{y})}{\sqrt{\sum_i^N (x_i - \overline{x})^2}\sqrt{\sum_i^N (y_i - \overline{y})^2}} \quad (1)$$

here, R_{xy} is the Pearson correlation coefficient computed between the variable x and y for the dataset containing N observations. The value of R_{xy} varies from -1 (perfect negative correlation) to +1 (perfect positive correlation). Whereas, zero correlation value indicates the variables' independence. The heat map containing the Pearson correlation coefficient is constructed and the dependent variables (having higher value of correlation coefficient) can be identified and subsequently be eliminated from the list of the input variables. Thus, the independent input variables of the process can be deployed to model the output variable by the ML-based modelling algorithm.

Machine Learning Models

The physics-based mathematical model characterising the output variables with the causal input variables can be constructed depicting the response and behaviour of the system. However, the size of the model gets larger with its improved accuracy and thus the mathematical model-based optimization analysis becomes computationally prohibitive. On the other hand, ML-based models are computationally cheaper and efficient for the modelling and optimization analysis. However, the entire parameters space embedded in the modelling algorithm is to be optimized for the robust prediction and efficient generalization capability of the ML models.

ANN and SVM are the two powerful ML algorithms deployed for modelling output variables having the nonlinear and interactive relationships with the large space of input variables (Ashraf et al., 2020, Ashraf et al., 2022). ANN is an excellent function approximator and can construct the effective functional mapping between the input-output variables (Ashraf et al., 2022). The algorithm can well-generalize the ill-defined problem and dig the hard to extract nonlinearity in the data. Moreover, the memory requirement of the algorithm is low therefore ANN can handle the medium to large datasets of the practical applications (Bishop, 1995). The important hyperparameter to be tuned for the working of the ANN model is to find the optimal number of neurons in the hidden layer and the number of hidden layers (Bourquin et al., 1998). The size of the hidden layer controls the complexity introduced in the ANN algorithm to model the output variable. Too low and too high added complexity can compromise the prediction and generalization performance of the model, thereby requiring an accurate optimization of the hyperparameters. The mathematical expression of ANN model is given as:

$$Y(X_i) = f_2\left(\sum W_2\left[f_1\left(\sum X_i W_1 + b_1\right)\right] + b_2\right) \tag{2}$$

here, X_i is an input vector defined on the number of input variables and $i = 1,2,3,…,N$ equal to the observations. W_1, W_2 and b_1, b_2 are the weight and bias matrices computed at the hidden layer and output layer of ANN network respectively. $\sum X_i W_1 + b_1$ is calculated at each hidden layer neuron of the ANN model and is transformed on the scale of the activation function (f_1). The information from the hidden layer propagates to the output layer and is processed further incorporating W_2, b_2 and f_2 (activation function applied on the output layer of ANN) to simulate the model simulated response $Y(X_i)$. The error is calculated between the actual and model simulated response and the error signal is propagated backward to update the parameters (weights and biases) in an iterative training. The expression for the updated weight and bias is given as follows:

$$W_{new} = W_{old} - \eta \frac{\partial E}{\partial W} \tag{3}$$

$$b_{new} = b_{old} - \eta \frac{\partial E}{\partial b} \tag{4}$$

here, E is the loss function deployed to calculate the deviation between the actual and model-simulated response; η is the learning rate; and $\frac{\partial E}{\partial W}$, $\frac{\partial E}{\partial b}$ are the partial derivative of the loss function with respect to weight and bias respectively. Whereas, W_{new} and b_{new} are the new values of the weight and bias matrices after an update in old values of W_{old} and b_{old} respectively.

SVM is another type of ML based modelling algorithm and can accurately predict the values of the output variables subjected to the designed space of the input variables. SVM model can provide an excellent generalization ability from the data deployed for its development (Ashraf et al., 2021, Muhammad Ashraf et al., 2020). Structural risk minimization principle is used for the SVM model development. The data which is hard to classify through linear hyperplane, the non-linear and complex input space is projected to higher-dimensional data space through the use of kernel and the problem is solved in a linear pattern. The hyperplane separates the data for the prediction efficacy whereas the margin around the hyperplane is maximized since the prediction error is tolerated up to this limit. Gaussian kernel is commonly used for fitting a non-linear hyperplane across the data. Furthermore, SVM incorporates Vapnik's ε-intensive loss function and constructs the approximation problem as an inequality constrained optimization problem to maximize the boundary around the hyperplane (Maddipati et al., 2011). SVM also learns the nonlinear relationship among the variables by solving a convex quadratic programming problem. The mathematical expression for the nonlinear SVM model is given as:

The training dataset for the development of SVM model is represented as:

$$\{(x_i, y_i), \ i = 1, 2, 3, …, N\} \ x_i \ \epsilon \ R^d, \ y_i \ \epsilon \ \{R^d\} \tag{5}$$

where, x_i is the vector of input variables and y_i is the corresponding output variable; $i = 1, 2, 3, …, N$ equal to total number of observations of the training dataset. For nonlinear SVM model, Lagrangian function and non-negative numbers, i.e., α_n and α_n^* are introduced and the loss function is written as:

$$L(\alpha) = \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \left(\alpha_i - \alpha_i^*\right)\left(\alpha_j - \alpha_j^*\right) G(x_i, x_j) + \varepsilon \sum_{i=1}^{N} \left(\alpha_i + \alpha_i^*\right)$$
$$+ \sum_{i=1}^{N} y_i\left(\alpha_i - \alpha_i^*\right) \tag{6}$$

subject to the constraints:

$$\sum_{i=1}^{N} \left(\alpha_n - \alpha_n^*\right) = 0 \tag{7}$$

$$\forall n : 0 \leq \alpha_n \leq C \tag{8}$$

$$\forall n : 0 \leq \alpha_n^* \leq C \tag{9}$$

Here, $G(.)$ is the kernel function that projects the hyperdimensional input space to higher dimensions; ε is epsilon margin around the hyperplane; and C is the penalty parameter. The Karush-Kuhn-Tucker (KKT) conditions are incorporated for developing the optimal solution of the non-linear dual problem of the SVM which are given as:

$$\forall n : \ \alpha_n(\varepsilon + \xi_n - y_n + f(x_n)) = 0 \tag{10}$$

$$\forall n : \ \alpha_n^*(\varepsilon + \xi_n + y_n - f(x_n)) = 0 \tag{11}$$

$$\forall n : \ \xi_n(C - \alpha_n) = 0 \tag{12}$$

$$\forall n : \xi_n^* \left(C - \alpha_n^*\right) = 0 \tag{13}$$

Here, ξ and ξ^* are the slack parameters that tolerate the deviations beyond the ε-tube. Finally, the SVM model can be written as:

$$Y(x) = \sum_{i=1}^{N} \left(\alpha_i + \alpha_i^*\right) G(x_i, x) + b \tag{14}$$

Here, $Y(x)$ is the output variable that can be predicted by the set of input variables (x) and b is the bias value.

Evaluation Criteria

The modelling performance of the ML models should be evaluated on rigorous performance evaluation measures. For this purpose, two statistical measures, namely coefficient of determination (R^2) and root-mean-squared-error (RMSE) are deployed to gauge the modelling accuracy of the developed ML models (Yuan et al., 2021). The mathematical expression of R^2 and RMSE is given as:

$$R^2 = 1 - \frac{\sum_i^N (y_i - \widehat{y}_i)^2}{\sum_i^N (y_i - \overline{y}_i)^2} \tag{15}$$

$$RMSE = \sqrt{\frac{1}{N} \sum_{i=1}^{N} \left(\widehat{y}_i - y_i\right)^2} \tag{16}$$

here, y_i is the actual value of the output variable whereas $\widehat{y}_i$ is the ML model simulated response. Similarly, $\overline{y}_i$ is the mean of y_i and $i = 1,2,3, …,N$ equal to total number of observations. R^2 is a measure of accuracy in predicting the actual values of the output variable by the developed ML model and its value changes from 0 (poor predictability) to 1 (good

functional map between the input and output variable). Whereas, RMSE measures the deviation between ML model simulated responses and the actual values of the output variable.

External validation of the developed ML models

The external validation test is conducted for the comparative performance evaluation of the ML models. The external validation dataset is primarily unseen to the models during their development and contains the observations within the operating ranges of the input variables. Thus, the external validation test is a fair method to evaluate the prediction and generalization performance of the developed models and the external validation test-based performance comparison can help choose a well-performing ML model. Therefore, the external validation test is carried out in this study and a better ML model, in terms of prediction and generalization performance, is selected based on the performance measures (R^2 and RMSE).

Sensitivity analysis

The ML model like ANN is essentially a black box model and it becomes difficult to interpret how the model develops the relationship with the output variable; thereby explaining the prediction process of the ANN is quite challenging. To this end, researchers have reported various sensitivity analysis techniques purposely deployed to get an insight about the parametric dependence as well as significance of the input variables on the output. Neural interpretation diagram, Garson's method, Olden's method, input perturbation etc. are amongst the frequently used sensitivity analysis techniques as reported in literature (Pizarroso et al., 2020). However, these techniques lack in providing the comprehensive information about the interpretability of the ML model in terms of prediction. In this regard, partial derivative-based sensitivity analysis computes the partial derivative of the output variable with respect to the input variables at each sample of the dataset. Thus, the explicit expression for the sensitivity analysis of the ML model can be obtained using partial derivative approach and it provides the robust diagnostic information about the variables' sensitivity compared with previously mentioned techniques (Pizarroso et al., 2020). Therefore, in this study, partial derivative-based sensitivity analysis on the developed ML model is conducted to investigate the input variables' impact on the output variables.

Integrating machine learning model in the optimization framework

The development of a well-performing and flexible machine learning model is an important task for conducting the value-creating analytics using data-driven modelling and optimization approach. A model depicting good generalization of the system is essentially desirable to mine the input design space of operating variables to develop the optimal solution. At the same time, the optimization problem should be written carefully considering the nature of the objective function.

The output variable modelled in this work has the complex interactions with the input variables thereby depicting the nonlinear output space of the objective. Therefore, nonlinear programming (NLP) based optimization technique is used to solve the optimization problem incorporating the developed ML model representing the objective to be optimized. NLP technique is particularly applied when the objective to be optimized is nonlinear and/or the constraints applied on the problem are essentially non-linear. The general expression of NLP problem is given as:

Objective Function: max $f(x)$ subject to:

$$h(x) = 0$$

$$x = x_1, \ x_2, \ldots, x_n \tag{17}$$

$$x \, \epsilon \, X \, \subseteq \, R^n$$

$$x^L \ \leq x \leq x^U$$

where, x is a set of optimization variables defining the objective function $f(x)$. $h(x)$ is the equality constraint representing the ML model (Gueddar and Dua, 2012). x^L and x^U are the lower and upper bounds applied on the design space of the input variables. The objective function represents the output variable of the ML model, i.e., CO_2 capture level. Thus, the NLP based optimization problem is constructed and is solved for several initial guesses to find the optimal solution (operating values of the input variables) corresponding to which the objective function has the maximum value.

Results & Discussion

Data collection and visualizing the data-distribution space of the variables

The mathematical model for the post-combustion carbon capture in the absorption tower using MEA is constructed to model CO_2 capture level (Lawal et al., 2009). The key input variables corresponding to the output variables is presented in the form of input-process-output diagram as presented in Fig. 3. Input variables are shown on the left side while output variable to be modelled on the input variables is shown on the right side of Fig. 3.

WebPlotDigitizer software is used to extract the data for the input-output variables from the figures mentioned in (Li et al., 2015). The value of CO_2 capture level (%) is retained against the operating values of the input variables and the complete dataset containing seventy observations for the input-output variables is compiled from figures as reported in (Li et al., 2015). iFGF, iCO₂ conc., iFGP and iFGT are the variables corresponding to the flue gas and are varied from 0.08 kg/s to 0.18 kg/s, 0.2 to 0.39, 0.12 Pa to 1.06 Pa and 297 K to 329 K respectively in (Li et al., 2015). Whereas, the variables with respect to absorbent, i.e., LST, MEA conc., and LSF have the operating ranges as: 297 K to 332 K, 0.21 to 0.35, and 0.63 kg/s to 0.83 kg/s respectively. In response to the operating conditions of the input variables, CO_2 capture level from the flue gas is changed from 62 % to 100% as reported in (Li et al., 2015). The data-distribution for the input variables as well as output variable is presented in Fig. 4. It is evident that fairly large design space of the input variables is explored to evaluate its effect on CO_2 capture level and the data-distribution profile is reasonable across the operating ranges of the variables that is beneficial for the development of flexible ML model.

In the next step, the dependence among the input variables is investigated by computing the Pearson correlation coefficient. The Pearson correlation coefficient measures the linear correlation between the variables, whereby the variables' linear dependence can be effectively computed. The heat map showing the correlation between the variables of post-combustion carbon capture process using MEA is presented in Fig. 5. The correlation value varies from -0.7 to 0.2 thereby indicating that the strong linear relationship does not exist between the variables (Yuan et al., 2021). Another way for interpreting the small correlation value can be the presence of nonlinear relationships among the variables of carbon capture process.
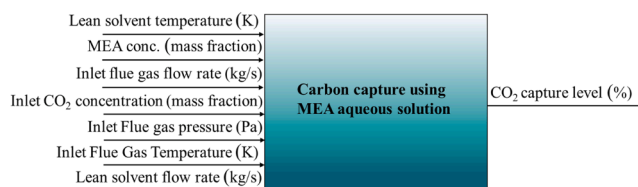

Fig. 3. Input-Process-Output diagram for the post-combustion carbon capture process using MEA. The input variables are enlisted on the left-side and output variable is presented on the right-side of process.
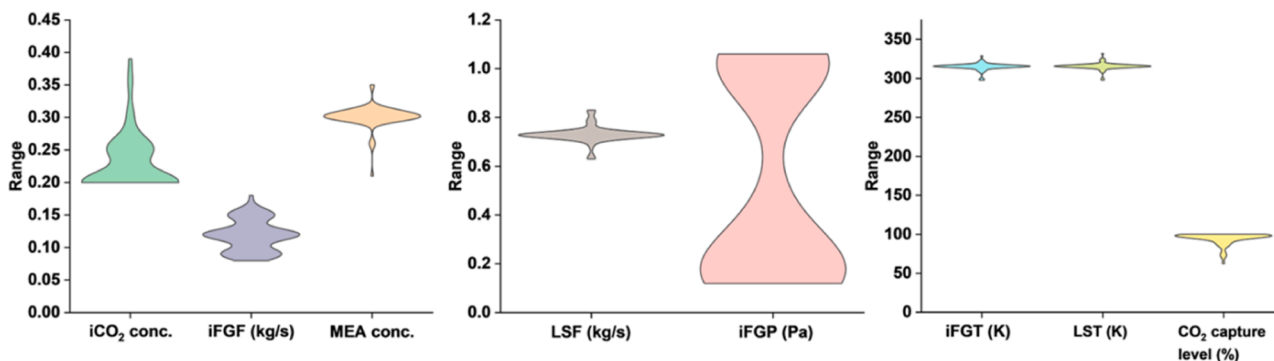
Fig. 4. Visualizing the data-distribution space of variables for the post-combustion carbon capture process using MEA. Good data-distribution is observable for the input and output variables.
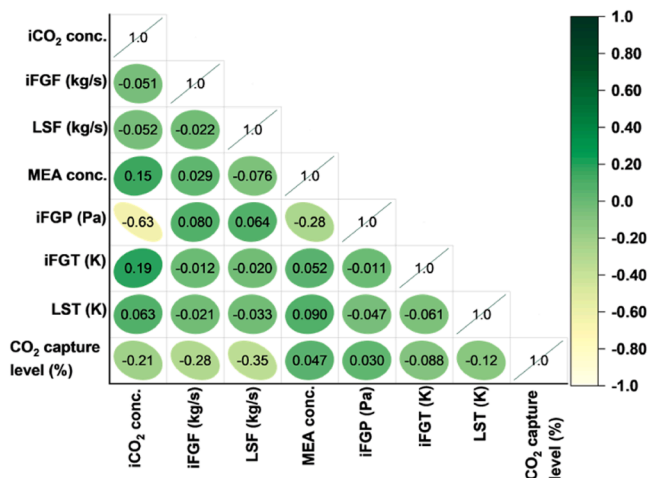

Fig. 5. Pearson correlation coefficient-based heat map constructed for the variables of the carbon capture process using MEA. A small correlation value is observable between the variables indicating the variables' independence.

Development of ANN and SVM model

ANN models are trained on the collected dataset for the carbon capture process. In this work, data split is set as 0.8 and 0.2 for training data and testing data respectively. A shallow multilayer perceptron network containing one hidden layer neuron is developed. It is reported in literature that ANN network consisting of one hidden layer and

having enough number of hidden layer neurons can approximate any non-linear function (Kubat, 1994). The number of neurons in the hidden layer are varied from $1 \times$ to $2.5 \times$ of the number of input layer neurons. Sum of square error is deployed as a loss function with Levenberg-Marquardt algorithm in the architecture of the ANN model for the parametric optimization (weights and biases) since it has stable and fast convergence performance (Yu and Wilamowski, 2018). Moreover, the computational complexity of Levenberg-Marquardt algorithm includes computation of the Jacobian matrix that is comparatively less expensive than that of constructing Hessian matrix (Yu and Wilamowski, 2018). The activation functions applied at the hidden layer and output layer are tangent sigmoidal (to capture the nonlinearity) and linear, respectively. The learning rate is set to 0.01 which is reasonable given the computational time and smooth tuning of the parameters during the network development. The early stopping criteria is made as: minimum gradient achieved $= 1.0 \times 10^{-20}$, maximum validation failure $= 6$ and training epochs $= 10000$. The network training is stopped when either condition of the stopping criteria is met.

ANN models are trained in Matlab 2021b. Fig. 6 shows the performance of ANN models having hidden layer neurons varying from seven to eighteen during training and testing phase. The modelling performance of the models is evaluated on the performance metrics built on R^2 and RMSE. Closely looking the performance of the ANN models in the training and testing phase, it is found that ANN model having eleven neurons in the hidden layer has comparatively higher value of R^2 (R^2_train $= 0.98$, R^2_test $= 0.89$) and lower RMSE (RMSE_train $= 1.2$ % and RMSE_test $= 3.1$ %) in comparison with that of other ANN models. Thus, eleven hidden layer neurons make the optimal size of hidden layer and the resulting ANN model is retained for the external validation test.
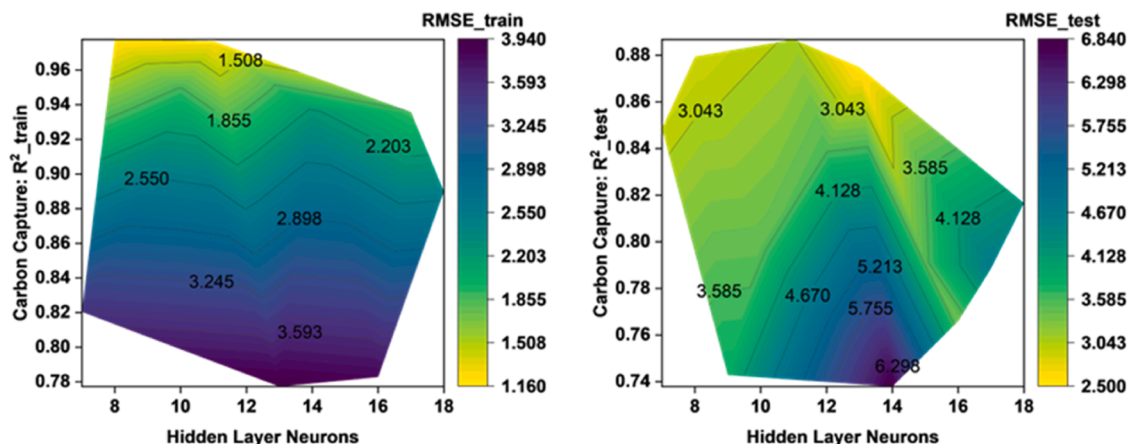

Fig. 6. Tuning of hidden layer neurons for the development of ANN model. R^2 and RMSE are calculated for different architectures of ANN (based on hidden layer neurons) during training and testing phase. ANN model having eleven neurons in the hidden layer has shown comparatively better modelling performance.

The hyperparameters required to be optimized for the SVM model development include epsilon, kernel scale and box constraint. For this purpose, grid-search method is used to systematically construct the combination of hyperparameters from their operating range and subsequently utilize them for the model development. Kernel scale, epsilon, and box constraint are varied between 0.001 to 1000, 0.20859 to 20859.15 and 0.001 to 1000 respectively. Bayesian optimizer along with the expected improvement per second plus acquisition function is deployed for the SVM model development. The mean square error (MSE) between the model-simulated and the actual value is calculated for the given set of hyperparameters values. Finally, the values of hyperparameters are selected corresponding to which MSE is minimum.

Matlab 2021b software is used for SVM model development. In this work, Gaussian kernel function is deployed since the output variable possesses nonlinear characteristics. Extensive combination of hyperparameters are tested in 30 epochs and the optimized values of epsilon, kernel scale and box constraint are 0.540, 1.947 and 974.8 respectively corresponding to the minimum MSE. The performance metrics of the developed SVM model for the training and testing dataset are as follows: R^2_train = 0.99, R^2_test = 0.88 and RMSE_train = 0.58% and RMSE_test = 4.42%. R^2 and RMSE values for the training and testing dataset are reasonable representing the good modelling performance of the developed SVM model.

External Validation of ANN and SVM model and model selection

The ANN and SVM models developed under rigorous hyperparameters optimization are subjected to external validation test. The external validation dataset contains seventeen operating conditions constructed on the ranges of the input variables. The validation dataset is deployed to be predicted from ANN and SVM models; the model-simulated responses are compared with the true CO_2 capture level and the performance metrics are calculated.

Fig. 7 presents the prediction profiles of CO_2 capture level for the external validation dataset by the developed ANN and SVM model. The models-based responses are compared with the true CO_2 level to evaluate their prediction efficacy. The performance metrics for the ANN based predictions for the external dataset are comparatively better than those of SVM, i.e., $R^2_{ANN} = 0.98 > R^2_{SVM} = 0.78$ and $RMSE_{ANN} = 1.28\% < RMSE_{SVM} = 4.41\%$. The comparative predictive performance of the developed ML models for the external validation test confirms the superior modelling capability of ANN, compared with SVM, to model the post-combustion carbon capture process using MEA and thus, is deployed for the subsequent analysis as mentioned in the next section.
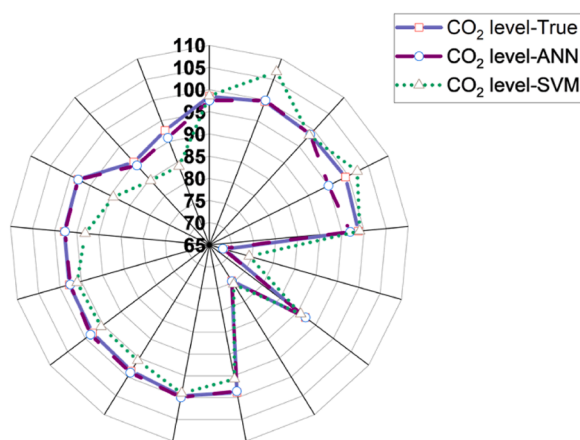
Variables' significance on the carbon capture level

The partial-derivative based sensitivity analysis is conducted to investigate the impact of the input variables on the carbon capture level from the flue gas. Since ANN model has expressed the effective modelling performance, the partial derivative of the model's output is taken with respect to the input variable that signifies the variable's sensitivity on CO_2 capture level. As the tangent hyperbolic activation function is applied on the hidden layer of ANN, the mathematical expression for partial derivative-based sensitivity of input variable (X_p) on the output variable (Y) for the ANN model is given as (Nourani and Fard, 2012):

$$\frac{\partial Y}{\partial X_p} = \sum_{h=1}^{nh} W_2 \left(1 - M^2\right) W_1 \tag{18}$$

here, W_2 is the weight matrix built on the weighted connections from the hidden layer to output layer neuron; W_1 is the weighted connections from the particular input variable (X_p) to the hidden layer neurons; and $\left(1 - M^2\right)$ is the partial derivative of the activation function applied on the hidden layer with respect to the summation computed at the hidden layer neuron.

The variance in the output variable produced as the result of change in the input variable is calculated for the entire dataset (Pizarroso et al., 2020) and the procedure is repeated for all input variables. The percentage significance (r) is calculated accounting for the sensitivity of input variables. Higher is the value of r, the more sensitive is the output variable to the particular input variable and vice versa. The mathematical expression of r is given as:

$$r_i\ (\%) = \frac{\sigma^2_{y_i|x_i}}{\sum_{i=1}^{c} \sigma^2_{y_i|x_i}} \times\ 100 \tag{19}$$

here, $\sigma^2_{y_i|x_i}$ refers to the variance produced in output variable y_i with respect to the input variable x_i; $\sum_{i=1}^{c} \sigma^2_{y_i|x_i}$ is the summation of the variance produced in the output variable with respect to input variables; $i = 1, \ldots, c$ equals to number of input variables. Thus, r is expressed in percentage that measures the percentage contribution of the input variable for explaining the variance of the output variable; thereby the variables' significance is calculated.

Fig. 8 shows the percentage significance of the input variables on CO_2 capture level for post-combustion carbon capture process using MEA. LST turns out to be the most significant variable towards CO_2 capture level and has the r value of 36.6%. The significance of LST towards CO_2 capture level is due to the thermal conditions and subsequently, the reaction kinetics maintained in removing CO_2 from the flue

Fig. 7. The prediction profiles of CO_2 capture level for the external validation dataset by the developed ANN and SVM models. There exists a good agreement between CO_2 level-true and CO_2 level-ANN depicting the excellent modelling and generalization performance by the developed ANN model.
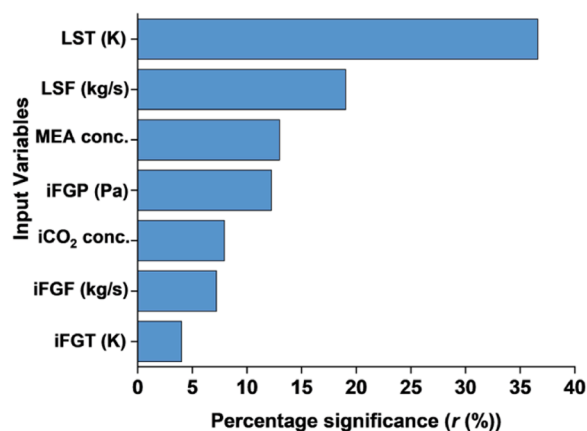

Fig. 8. Partial derivative-based percentage significance of input variables on CO_2 capture level. Two input variables, i.e., LST and LSF are the significant input variables towards CO_2 capture level.

gas. CO_2 absorption in the lean solvent is an exothermic reaction and thus lowering the temperature is advised to enhance the CO_2 capture level from the flue gas (Kazemi and Mehrabani-Zeinabad, 2016). Thus, LST needs to be controlled and maintained in the operating limits carefully to maintain the carbon removal efficiency from the CO_2 rich flue gas. The second most significant variable towards the output variable is LSF having *r* value of 19%. LSF controls the amount of lean solvent being sprayed on CO_2 rich flue gas in counter flow direction in order to clean it. LSF maintains the fresh supply of lean solvent for CO_2 absorption from the flue gas and is an important operation control variable maintaining the carbon capture level in the absorption column of post-combustion carbon capture process (Kazemi and Mehrabani-Zeinabad, 2016). The two input variables like LST and LSF, which represent the input variables with respect to the solvent utilized in the carbon capture process, account for the *r* value of 55.6%. The *r* value for the remaining input variables of carbon capture process, i.e., MEA conc., FGP, iCO_2 conc., iFGF and FGT is 13.0%, 12.2%, 7.9%, 7.2% and 4.0% respectively. The continuous replacement of CO_2 rich solution from the absorption column and solvent recovery in the stripper is synchronized to ensure the enough circulation of lean solvent to the absorption column for CO_2 absorption from the flue gas (Chao et al., 2021). It is important to note that the input variables with respect to lean solvent are more significant to maintain CO_2 capture level than the concentration of CO_2 in the flue gas at the inlet of absorber. Thus, the most significant input variables are required to be carefully monitored and adjusted during the operation in order to effectively control the carbon capture process.

Nonlinear programming-based optimization analysis for maximizing CO_2 capture level

The post-combustion carbon capture process is maintained to keep CO_2 emission level in the flue gas within the tight and strict operating limits of the industrial complexes. The operating input space of carbon capture process is hyperdimensional that is constructed on the input variables. These variables have non-linear interacting relationships, thus maintaining the higher efficiency of the process is a challenging task. In this regard, machine learning based process models like ANN have demonstrated the excellent ability in data-mining and learning the complex dynamics of the hyper-dimensional processes and can well approximate the system with good generalization and prediction efficacy (Uddin et al., 2013, Uddin et al., 2020). Thus, a well-developed ANN model predicting the CO_2 capture level with respect to process control variables of carbon capture process is constructed. Subsequently, the model is integrated within the optimization environment of the NLP technique. Thus, the optimization is formulated as follows:

Objective function:

$$min\ f\ =\ -\ CO_2\ capture\ level\ (\%)\tag{20}$$

Constraints:

$$CO_2\ capture\ level\ (\%)\ -\ 100\ <\ 0$$

$$-1\ \times\ CO_2\ capture\ level(\%)\ +\ 62\ <\ 0$$

Bounds:

$$297 \le LST\ (K) \le 332$$

$$0.21 \le MEA \le 0.35$$

$$0.08 \le iFGF(kg\ /\ s) \le\ 0.18$$

$$0.2 \le iCO_2\ conc. \le 0.39$$

$$0.12 \le iFGP\ (Pa) \le 1.06$$

$$297 \le iFGT\ (K) \le 329$$

$$0.63 \le LSF\ (kg\ /\ s) \le 0.83$$

The optimization problem (20) for maximizing the carbon capture level is solved by interior point solver in MATLAB 2021 b version and the optimal operating values of the input variables are determined. Fig. 9 shows the operating values of the input variables determined by solving the NLP based optimization problem under different initial conditions for the carbon capture process. The operating values are calculated corresponding to maximum CO_2 capture level (100 %) of the carbon capture process. Furthermore, the range in the operating values of the input variables is also measured with respect to the different starting conditions for the NLP based optimization problem. A tight confidence bound around the optimal values of the input variables except iFGP of the carbon capture process is observed. It indicates that iFGP can be maintained within the estimated bound and the maximum carbon capture level can be achieved. However, the remaining input variables are required to be controlled within the bounds to achieve the optimal performance of the carbon capture process. The operating values of the input variables determined from the NLP based optimization analysis are: iCO_2 conc. = 0.28 ± 0.02; iFGF = 0.12 ± 0.02 kg/s, LSF = 0.72 ± 0.02 kg/s, MEA conc. = 0.29 ± 0.03, iFGP = 0.56 ± 0.3 Pa, iFGT = 314.3 ± 1.96 K, and LST = 316 ± 7.53 K. Considering the nonlinear interactions among the input variables, the optimizer has determined the optimized values that are not essentially the minimum or maximum operating bound of the input variables; therefore signifying the effectiveness of the determined operating ranges of input variables for the maximum CO_2 capture level. Thus, the operating values of the input variables can be determined by NLP based optimization technique thereby ensuring the maximum CO_2 capture level for the nonlinear and complex carbon capture process.

Similarly, the maximum carbon capture level from the flue gas is investigated by NLP approach under the different conditions of the flue gas. Three operating scenarios considering the different operating values of the flue gas based variables like iCO_2 conc., iFGF, iFGP and iFGT are considered which are as follows: a) iCO_2 conc. = 0.2, iFGF = 0.08 kg/s, iFGP = 0.12 Pa, iFGT = 298 K, b) iCO_2 conc. = 0.23, iFGF = 0.12 kg/s, iFGP = 0.54 Pa, iFGT = 315 K, c) iCO_2 conc. = 0.39, iFGF = 0.18 kg/s, iFGP = 1.06 Pa, and iFGT = 329 K. Thus, the flue gas-based variables are held at constant values in the three scenarios and the resulting optimization problem is solved by NLP under different starting conditions to determine the optimized values of the remaining input variables of carbon capture process corresponding to the maximum CO_2 capture level. Fig. 10 shows the optimized values of LSF, MEA conc., and LST determined by the NLP based optimization analysis to achieve maximum CO_2 capture level corresponding to the three constructed operating scenarios. Referring to Fig. 10(a), the estimated optimized values of input variables are as follows: LSF = 0.74 ± 0.03 kg/s, MEA conc. = 0.30 ± 0.02, and LST = 316 ± 7 K. Whereas, the optimized values of the variables corresponding to the maximum CO_2 capture level for scenario (b) and scenario (c) are: LSF = 0.72 ± 0.02 kg/s, MEA conc. = 0.28 ± 0.02, LST = 316 ± 7 K, and LSF = 0.72 ± 0.03 kg/s, MEA conc. = 0.28 ± 0.01, and LST = 315 ± 5 K. Since, there exists nonlinear interactions among LSF, MEA conc. and LST (Kazemi and Mehrabani-Zeinabad, 2016), the determined operating values of the input variables along with the range of variability can help achieve maximum CO_2 capture level under different operating conditions of the flue gas.

Conclusions

The efficient operation of post-combustion carbon capture process is critical to ensure higher carbon removal from the flue gas, contributing to the carbon neutrality goal. In this work, CO_2 capture level in the absorption tower is modelled on the relevant input variables (lean solvent temperature (K), MEA concentration (mass fraction), inlet flue gas flow rate (kg/s), inlet CO_2 concentration (mass fraction), inlet flue gas pressure (Pa), inlet flue gas temperature (K), and lean solvent flowrate
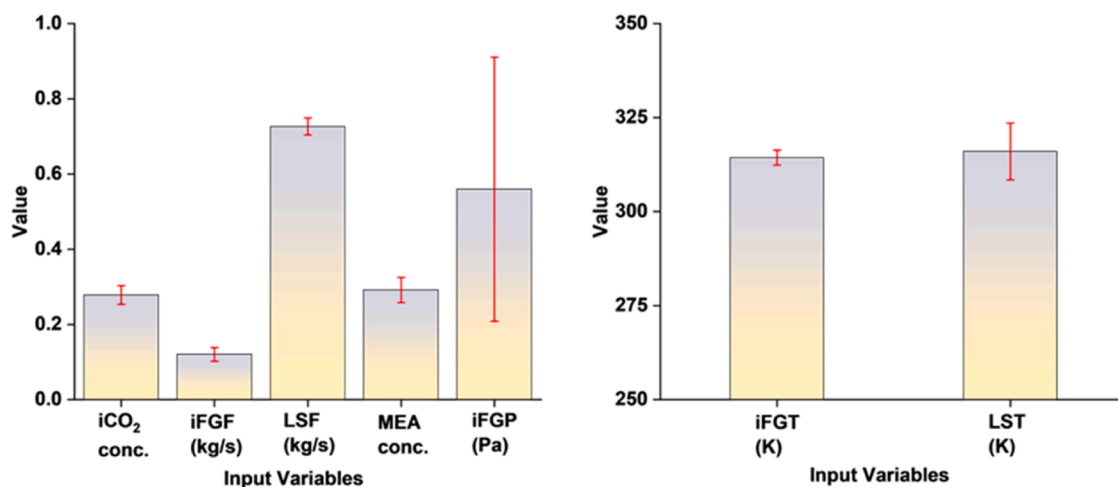
Fig. 9. NLP based optimization problem integrating the developed ANN model for CO_2 capture level is solved and the optimum operating conditions for the input variables are determined for the maximum CO_2 capture level for post-combustion carbon capture process using MEA.
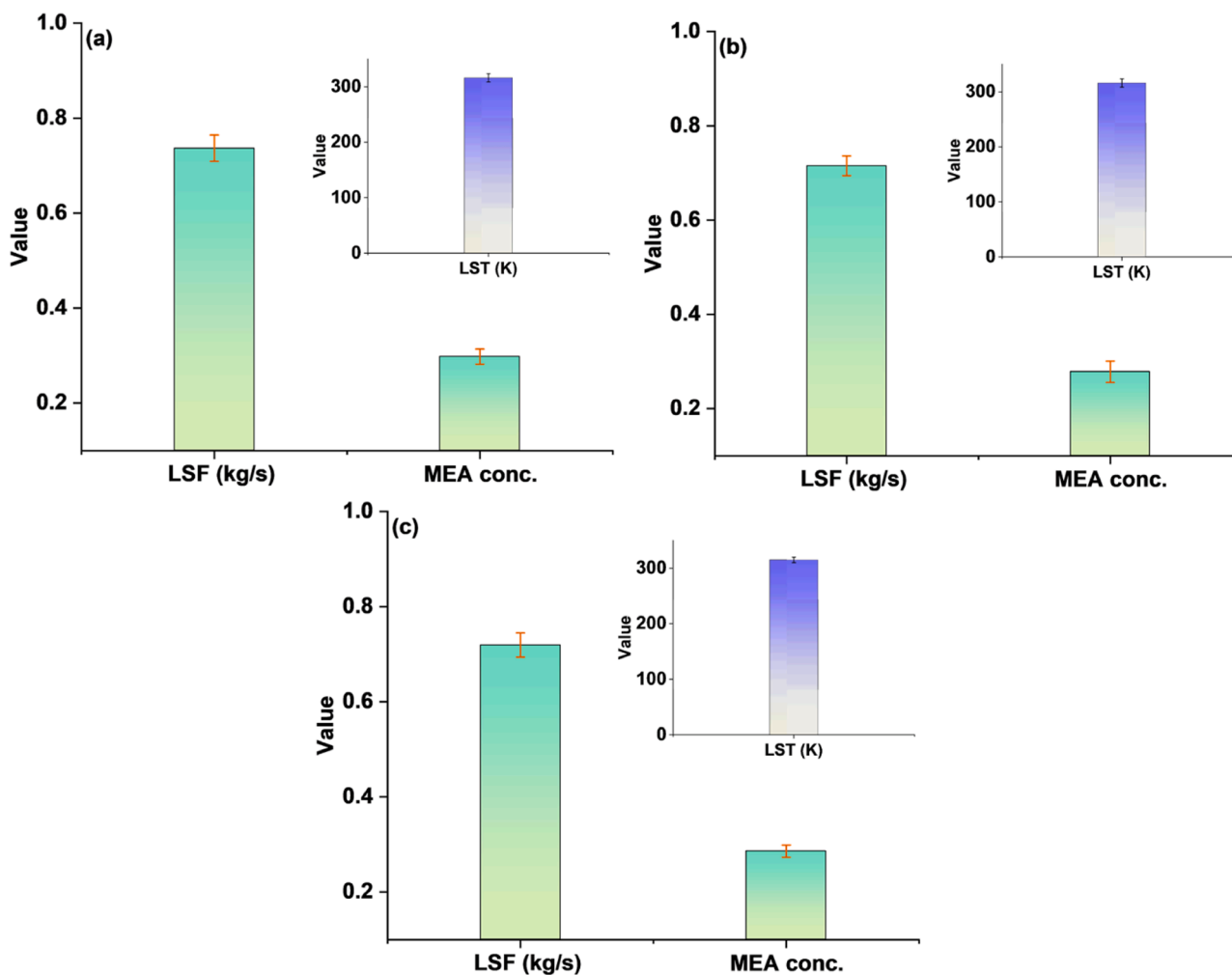

Fig. 10. Maximizing the carbon capture level for different conditions of the flue gas: a) iCO_2 conc. = 0.2, iFGF = 0.08 kg/s, iFGP = 0.12 Pa, iFGT = 298 K, b) iCO_2 conc. = 0.23, iFGF = 0.12 kg/s, iFGP = 0.54 Pa, iFGT = 315 K, and c) iCO_2 conc. = 0.39, iFGF = 0.18 kg/s, iFGP = 1.06 Pa, iFGT = 329 K.

(kg/s)) by ML model for the post-combustion carbon capture process using MEA. Two ML based models, i.e., ANN and SVM are trained under rigorous hyperparameters optimization. The comparative prediction performance of the two models evaluated on external validation dataset reveals the superior modelling performance of ANN. The partial derivative-based sensitivity analysis is carried out and it is found that lean solvent temperature and lean solvent flow rate are the two most significant input variables contributing the percentage significance

value of 55.6% towards the prediction of CO_2 capture level. The ANN model is integrated within the nonlinear programming-based optimization environment and the optimum operating conditions for the input variables corresponding to maximum CO_2 capture level are determined. The optimum operating ranges for the input variables are: iCO_2 conc. $= 0.28 \pm 0.02$; iFGF $= 0.12 \pm 0.02$ kg/s, LSF $= 0.72 \pm 0.02$ kg/s, MEA conc. $= 0.29 \pm 0.03$, iFGP $= 0.56 \pm 0.3$ Pa, iFGT $= 314.3 \pm 1.96$ K, and LST $= 316 \pm 7.53$ K. Furthermore, the optimized values of the LSF, MEA conc., and LST are determined by the NLP approach under three scenarios constructed on the operating values of iCO_2 conc., iFGF, iFGP, and iFGT. This research provides the insight about the carbon capture process as well as the general model-based optimization framework to obtain the optimized operating conditions for the maximum CO_2 capture level that the industrial community can consult with for the optimum operation of carbon capture process using MEA and contributes to carbon-neutrality goal. While the focus of this work has been on the absorption column, the future work will take into account other aspects, such as the stripper, of the whole carbon capture process, for ML based modelling, sensitivity analysis and optimisation.

Code Availability

The code developed in this research to perform different tasks can be provided on request.

Declaration of Competing Interest

The authors declare no competing financial benefits and personal relationships have influenced the findings of the paper.

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