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SCREENING OF IONIC LIQUIDS FOR CO_2 CAPTURE USING DATA ANALYTICS TECHNIQUES

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ABSTRACT

Carbon dioxide (CO_2) is the most prominent greenhouse gas (GHG) present in the atmosphere, making it the most accountable for global warming. CO_2 capture is capable of greatly reducing carbon emissions. The current method of CO_2 capture by amine-based solvent has drawbacks, such as high demand for energy and intense corrosion, making it a less reliable method. More attention is given to ionic liquids (ILs) for their negligible vapour pressure, low melting point, and high chemical and thermal stability advantage. This study uses data analytics techniques to develop a predictive model for screening ILs for CO_2 capture, moving away from the experimental approach, which is burdensome, costly, and less environmental-friendly. Data on the properties and parameters of ILs are collected from COSMO-RS software. CO_2 solubility is the function of collected data and developed into 15 models of three different methods: Support Vector Machine (SVM), Neural Networks (NN), and Gaussian Process Regression (GPR). The use of data analytics in this field is new and can provide valuable insight towards CO2 solubility in ILs. The dataset is distributed randomly at 80/20% for training and testing. Each model is evaluated using R-squared and root mean square error (RMSE). The rational Quadratic GPR model shows the lowest RMSE of 0.0002 for training and testing, with R-squared the closest to one. Rational Quadratic GPR is the best model to be used for screening IL for CO_2 capture.

Keywords: *Ionic liquid, carbon capture, data analytics, support vector machine, neural network, gaussian process regression.*

INTRODUCTION

Since the Industrial Revolution, the growth in modernisation, population, and industrialisation has also created growth in the emission of greenhouse gases (GHGs) [1]-[2]. The heat from the Sun's radiation is trapped by GHGs in the Earth's atmosphere contributing to global warming. CO_2, N_2O, and CH_4 are included among these GHGs. According to Islam et al. [1], Carbon dioxide (CO_2) is the most prominent GHG as it is the longest-staying gas on the Earth, making it the most accountable when it comes to global warming. On top of the naturally produced CO_2, serious consumption of fossil fuel and coal has resulted in excessive emission of CO_2 into the environment [3]. Among all GHGs, CO_2 proportion takes up over 70%. Furthermore, CO_2

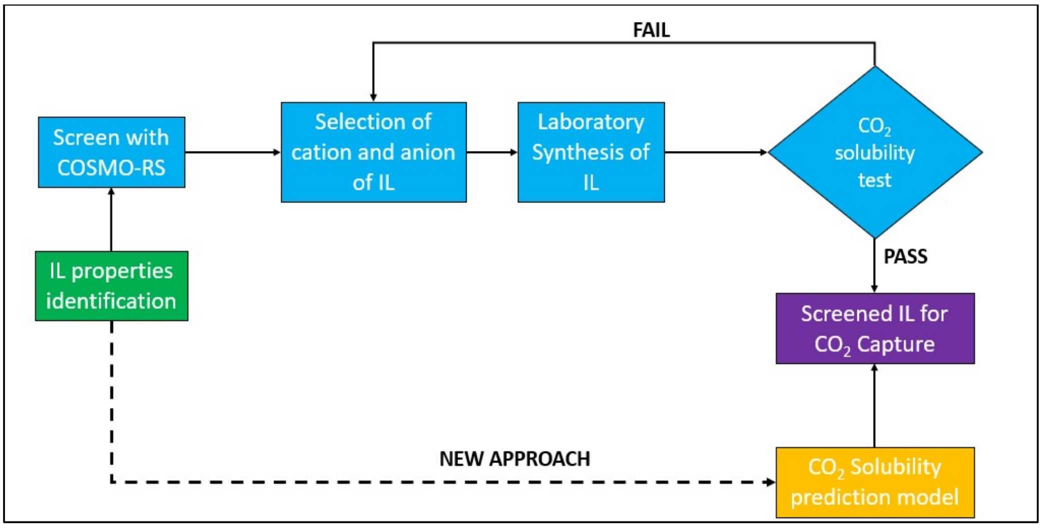

Figure 1 Graphical abstract for screening ILs for CO2 Capture

has the most sources of emissions, including power plants, transportation systems, industrial operations, production services, petroleum businesses, and others [1],[3].

With the increasing concern of global warming, some solutions were proposed to reduce CO_2 emissions. Greater attention was paid to CO_2 capture to achieve the goal of carbon capture, utilisation, and storage (CCUS). The CO_2 capture method by absorption with recoverable solvent is the most favoured and practicable strategy [4]. One of the popular methods is amine-based technologies, such as monoethanolamine (MEA). Amine-based technology for CO_2 capture is currently practised due to the amine nature of high reactivity with CO_2, high thermal stability, and high absorption capacity [3]. Nevertheless, there is still a downside to the amine-based technologies. Constraints such as high demand for energy, solvent loss due to degradation of amine in flue gases, high absorbent make-up rate, and intense corrosion issue cause the method to be less desirable [5]-[6]. These constraints make amine-based technologies require large-high-quality equipment, which is very costly. Besides, serious impacts on the environment and human health can be caused by amine-based solvents.

Researchers are looking for a more efficient technological alternative for CO_2 capture. Utilising greener solvents such as ionic liquids (ILs) will help for a more appropriate strategy. Ils have caught the attention of researchers for their characteristics of negligible vapour pressure, low melting point, and high stability chemically and thermally [6]. Ils can be adjusted according to the condition of CO_2, the type of solutes, and their application by changing the chemical structure, making them friendlier solvents. Ils are considered auspicious competitors with amine-based solvents [7]-[8].

Selecting the appropriate IL for CO_2 capture requires a certain process. Many researchers employed the COSMO-RS method to screen ILs [1],[4],[9]. COSMO-RS is a conductor-liked. The screening model is deemed as a "property explorer" due to its advantage of predicting the properties of several ILs. The input of COSMO-RS only requires the chemical structure of IL molecules. However, this method still has some weaknesses regarding data availability [9]. Extensive work such as ranking, selection, synthesis, validation, and confirmation is still required after COSMO-RS screening, which takes up high labour intensity and time consumption [10]. Extensive work such as ranking, selection, synthesis, validation, and confirmation is still required after COSMO-RS screening, which takes up high labour intensity and time consumption [10]. Therefore, to reduce the burden of screening ILs, robust and efficient correlations are needed to predict the CO_2 solubility and allow rapid screening of fitting ILs for CO_2 capture. In this study, data analytics techniques are used to develop a predictive model for screening of ILs for CO_2 capture hence taking away the experimental approach, which is less reliable, tiresome, and costly.

CO_2 Solubility

CO_2 solubility is a significant property when screening ILs for CO_2 capture. CO_2 will be the outcome (dependent variable) in this study. The solubility of CO_2 of ILs is highly influenced by the type of anion, followed by the type of cation [11]. ILs with the highest CO_2 usually have fluorine as their anions. CO_2 solubility increases when pressure increases and decreases when temperature increases.

CO_2 solubility also decreases when Henry's constant increases. All of these variations are significantly influenced by the type of anion of the IL [12]. The molality of ILs may change their ability to absorb CO_2 and the created solution's physical and chemical properties. Wang et al. [13] studied the effect of molality on some ILs' absorption of CO_2 capability. The researchers found that CO_2 solubility increased with increasing molality until to a point where the solubility has maintained. The authors also found that the nature of cations and anions is a key factor in deciding the absorption ability. Another study by Li et al. [14]researched the relationship between the molality of ILs and their viscosity and CO_2 solubility. The researchers concluded that the viscosity of IL increases as molality increases, while CO_2 solubility fluctuated, initially increased, then decreased with molality increment. The researchers assigned this trend to the difference in the solubility of CO_2 in ILs. Besides, Dong et al. [15] studied the effect of the molality of ILs on their CO_2 solubility. Their research has concluded that CO_2 solubility increases as molality increases; however, it plateaued at higher molalities. They also discovered that the molality of ILs influences the regeneration efficiency of the solvent, with higher molalities creating lower regeneration efficiency. The molality of ILs can affect their physical and chemical properties and their behaviour in various applications. The molality of an IL depends on its nature of cation and anion, with the possibility of effects from other materials such as water.

The CO_2 activity coefficient is an important property that describes the interaction between CO_2 and ILs. Zeng [16] stated that the activity coefficient decreases with increasing temperature and vice versa. The activity coefficient shows the deviation from ideality in a solution. Usually, high activity coefficients indicate high CO_2 solubility. The nature of cation and anion of ILs are key in determining the CO_2 activity coefficient. Zhang et al. [17] also stated that the CO_2 activity coefficient positively relates to CO_2 solubility. The authors also agreed that the properties of cations and anions of ILs play a big role in determining the activity coefficient. The CO_2 activity coefficient is affected by factors such as pressure, temperature, and the nature of components of the IL compounds.

Data Analytics

With the development of technologies, data analytics has made it easier to develop prediction models with the existence of machine learning. Machine learning is defined with 3Vs; 'volume' indicates the huge number of data that can be processed and stored, 'velocity' indicates that data is generated at a faster rate than conventional methods, 'variety' indicates the various sources of data and the nature of it being structured and unstructured [18]. More recent studies have added 'veracity' into the definition, referring to the usefulness of data quality [18]-[19]. Support vector machine (SVM) is a branch of machine learning. It is a supervised learning model with a programmed learning algorithm that analyses regression and classification data. Recent studies still employ SVM to predict CO_2 solubility from ILs [20]-

[21]. Another branch of machine learning is Artificial Neural Networks (ANNs), which are modelled after the human brain. Like biological neurons, ANNs have nodes that are linked to each other with different layers of networks [22]. Balchandani and Dey [7], Daryayehsalameh et al. [24] and Mirarab et al. [25] agreed that feed-forward neural networks (FFNNs) have the highest accuracy among other types of ANNs when it comes to screening ILs for CO_2 capture. Besides, Gaussian process regression (GPR) is also another branch of machine learning that can be used to analyse data. GPR is a common modelling method to establish a non-linear relationship between a system's inputs and outputs [26]. To date, no research has been using GPR to predict the CO_2 solubility of ILs. However, in recent research, GPR was employed to predict IL properties and solubilities of hydrogen sulfide and sulfur dioxide in ILs [27]-[29]. To summarise, several prediction models are available for predicting IL's capability of absorbing CO_2. Data analytics and group contribution methods were developed to predict the CO_2 absorption of ILs. These models are beneficial to identify the most suitable IL for specific CO_2 capture applications.

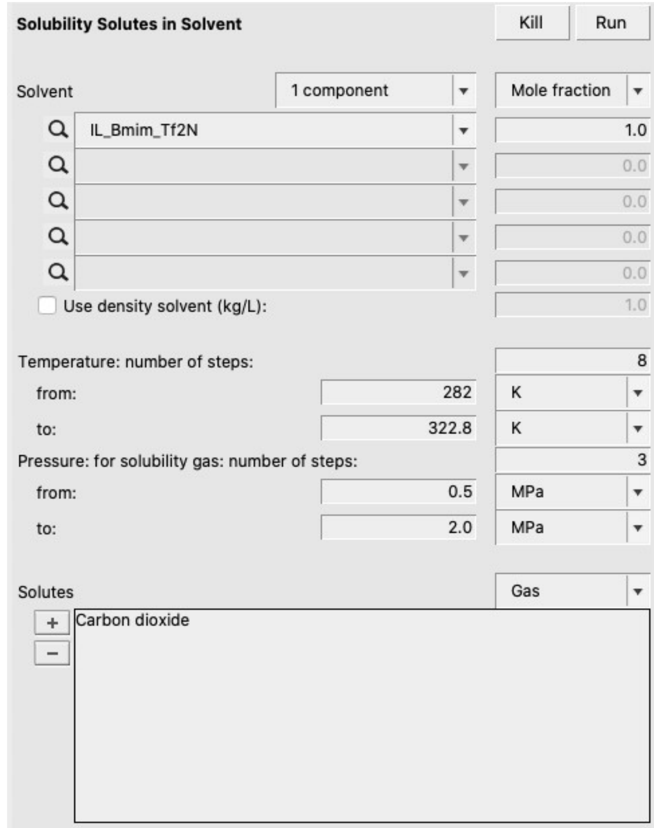

Figure 2 COSMO-RS interface for data collection

Table 1 Summary of IL data

Number of data points						
ILs	Number of data Pressure	Temperature (K)		Molecular Weight (gram/mol)	Molality	CO2 activity coefficient
BMIMAc	144	8	5	1	3	21
BMIMBr	144	8	5	1	3	23
BMIMNO3	144	8	5	1	3	20
EMIMAc	144	8	5	1	3	21
EMIMBr	144	8	5	1	3	23
EMIMNO3	144	8	5	1	3	20
TEAAc	144	8	5	1	3	23
TEABF4	144	8	5	1	3	24
TEABr	144	8	5	1	3	26
TEADHP	144	8	5	1	3	23
TEANO3	144	8	5	1	3	24
TEAOH	144	8	5	1	3	24
TMAAc	144	8	5	1	3	22
TMABF4	144	8	5	1	3	23
TMABr	144	8	5	1	3	24
TMADHP	144	8	5	1	3	20
TMANO3	144	8	5	1	3	24
TMAOH	144	8	5	1	3	19
Grand Total	2592					

Table 2 Types of models

Support Vector Machine (SVM)	Neural Network (NN)	Gaussian Process Regression (GPR)
Linear SVM	Narrow NN	Rational Quadratic GPR
Quadratic SVM	Medium NN	Squared Exponential GPR
Cubic SVM	Wide NN	Matern 5/2 GPR
Fine Gaussian SVM	Bilayered NN	Exponential GPR
Medium Gaussian SVM	Trilayered NN	
Coarse Gaussian SVM		

METHODOLOGY

Data Gathering

Data on the properties of ILs are collected from COSMO-RS software and kept in an Excel spreadsheet. Then, a data management process was carried out to check data quality. This means that any missing data or data with loopholes will be discarded for better-quality data. CO_2 solubility of ionic liquid (mol fraction) will be the dependent variable, while temperature (K), pressure (bar), molecular weight, molality (mol/kg), and COSMO CO_2 activity coefficient will be the independent variable. All the properties were collected for 1-50 bar pressure 298.15-333.15 K and temperature. A summary of the datasets is shown in Table 1. Figure 2 shows the COSMO-RS Interface for Data Collection.

Model Development

Machine learning in prediction modelling allows a model to modify to reduce the error to as low as possible, ensuring the most accurate output. This study used the Regression Learner application in MATLAB R2022b. The input into this application is the dataset of ILs' pressure, temperature, molecular weight, molality, CO_2 activity coefficient, and CO_2 solubility. Within this application, several models can be used to develop prediction models. In this study, Support Vector Machines (SVM), Neural Networks (NN), and Gaussian Process Regression (GPR) are being used. The types of each model are included in Table 2.

For all models, all datasets were distributed randomly into training and testing datasets at the 80/20 division. 80% of the data will be used to train the model, while the remaining 20% will be used to test the model for testing. This split is selected for sufficient training data. The training set must be large enough to provide the model with diverse examples and patterns to learn from. Allocating 80% of the data for training allows the model to capture a significant amount of information and build a reasonably accurate representation of the problem.

Each model was evaluated automatically to check for its accuracy and error. Quantitative evaluation was done immediately to all SVM, NN, and GPR models, then compared to be analysed. R-squared was measured to evaluate the accuracy of each model. As the value of R-squared gets closer to 1, the model is then more accurate. Meanwhile, RMSE will evaluate how much error each model presents, as it estimates the deviation of the actual value of CO_2 solubility from the predicted ones. The formula for R-squared and RMSE are provided as:

$$R^2 = 1 - \frac{RSS}{TSS} \quad (1)$$

$$RMSE = \sqrt{\frac{\sum_{i=1}^{N}(Predicted_i - Actual_i)^2}{N}} \quad (2)$$

where *RSS* is the sum of squares of residuals, *TSS* is the total sum of squares, and *N* is the number of observations.

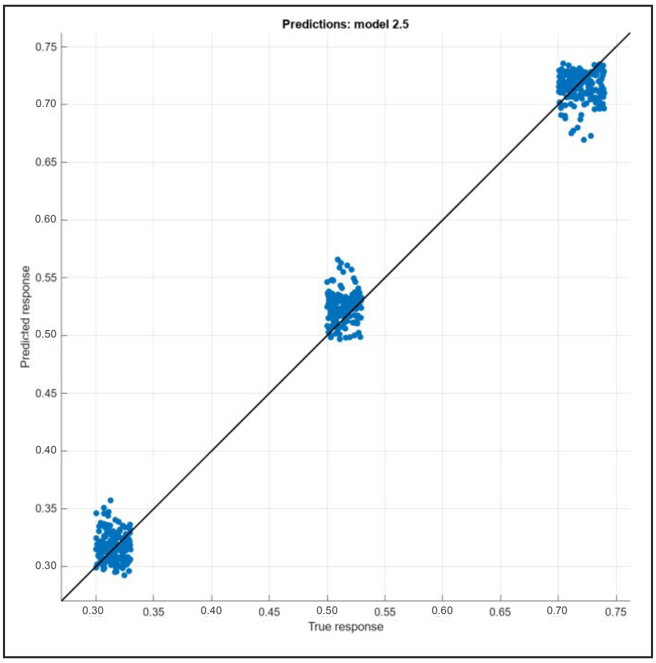

Figure 3 Accuracy plot of Cubic SVM model

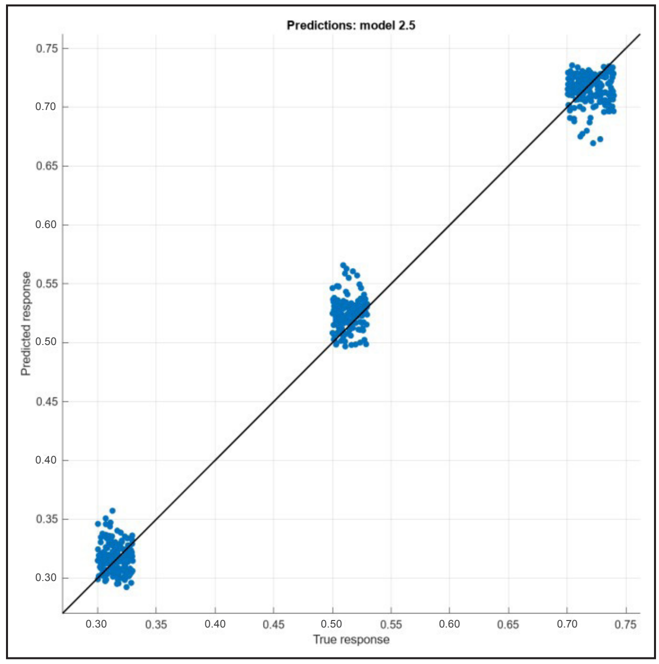

Figure 4 Accuracy plot of Medium Gaussian SVM model

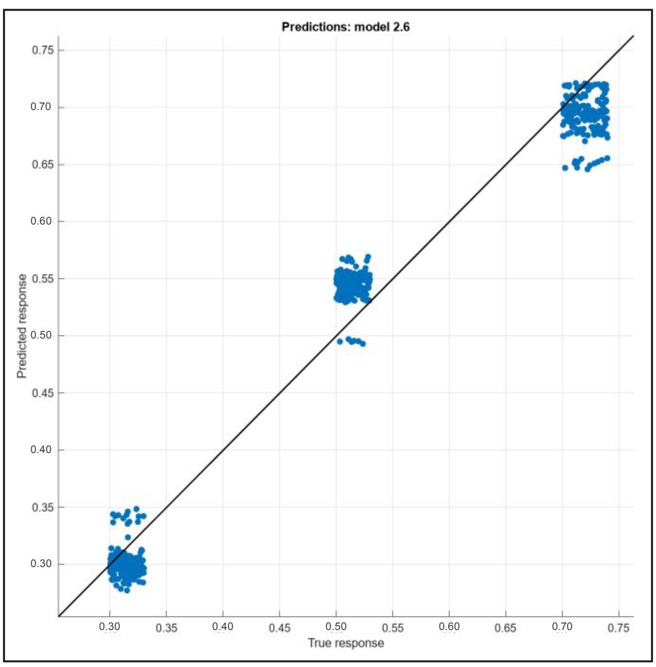

Figure 5 Accuracy plot of Coarse Gaussian SVM model

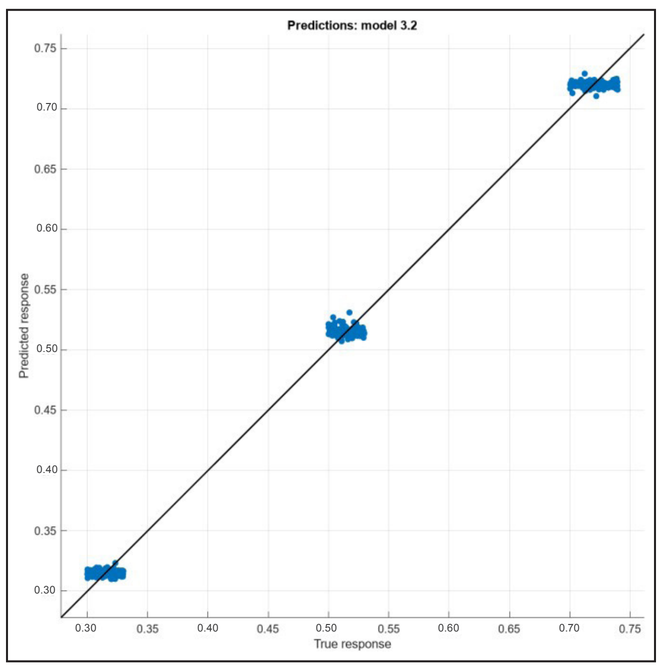

Figure 6 Accuracy plot of Squared Exponential GPR model

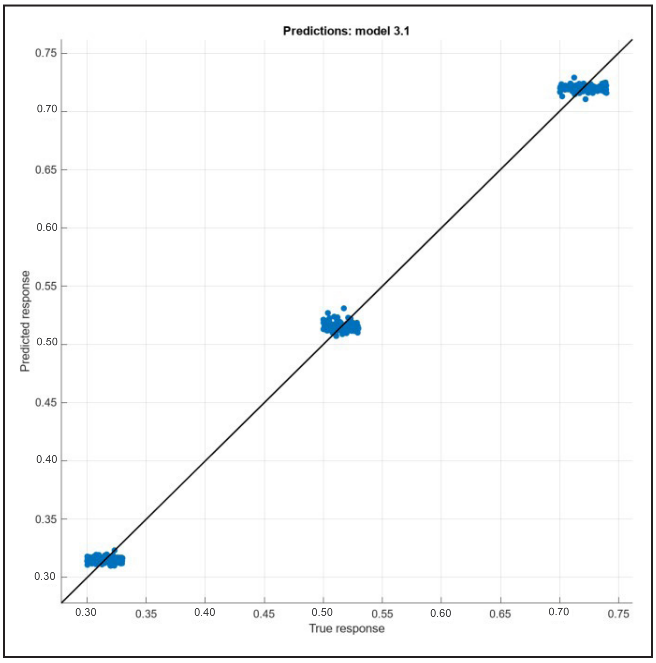

Figure 7 Accuracy plot of Rational Quadratic GPR model

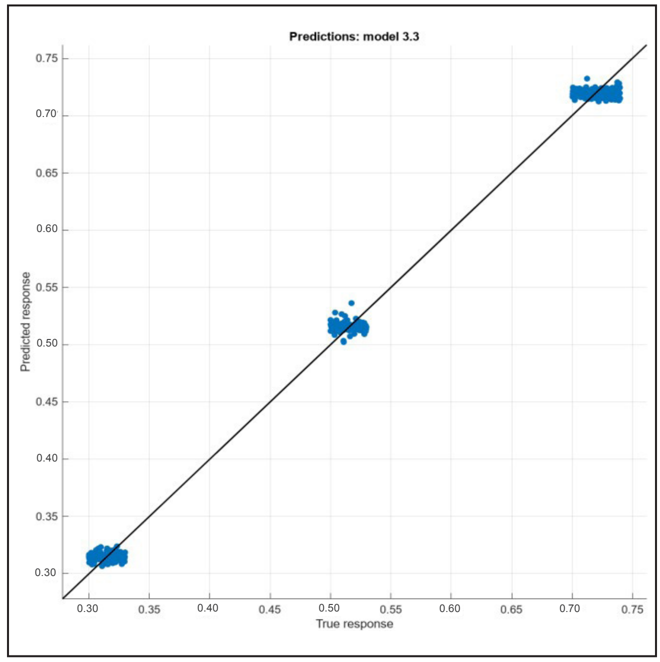

Figure 8 Accuracy plot of Matern 5/2 GPR model

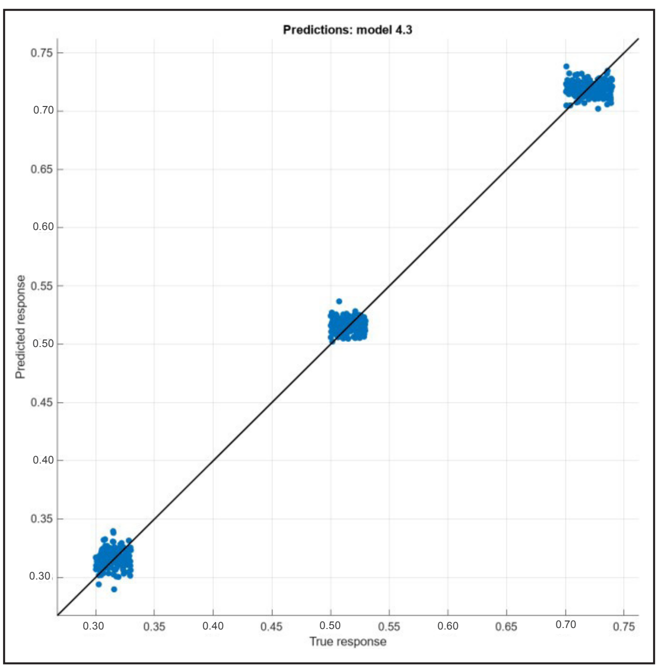

Figure 9 Accuracy plot of Wide NN model

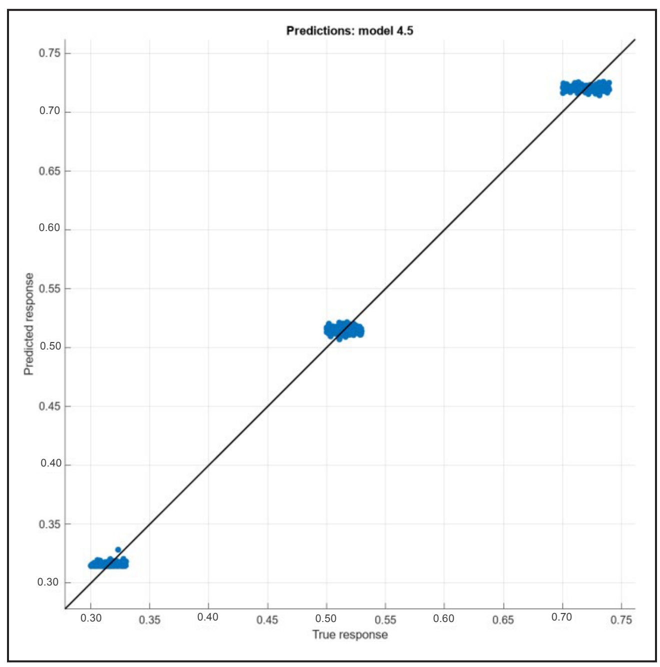

Figure 10 Accuracy plot of Trilayered NN model

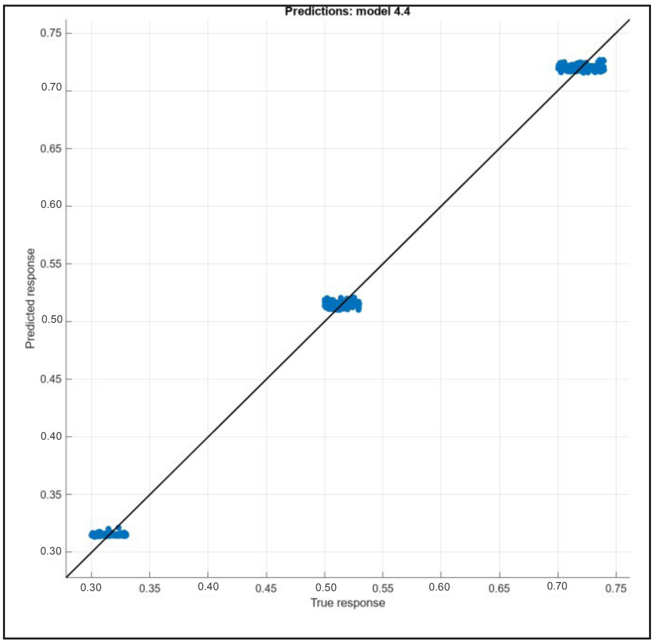

Figure 11 Accuracy plot of Bilayered NN model

RESULTS AND DISCUSSION

The accuracy plot of predicted against actual values was plotted for all fifteen models. Figures 3 to 11 show the accuracy plot of the three best models from each machine learning cluster.

Table 3 Training and Testing RMSE of prediction models

Model Type	RMSE (Train)	RMSE(Test)
Linear SVM	0.062	0.065
Quadratic SVM	0.028	0.028
Cubic SVM	0.022	0.021
Fine Gaussian SVM	0.047	0.041
Medium Gaussian SVM	0.020	0.019
Coarse Gaussian SVM	0.028	0.027
Narrow NN	0.005	0.001
Medium NN	0.001	0.001
Wide NN	0.001	0.001
Bilayered NN	0.001	0.001
Trilayered NN	0.001	0.001
Rational Quadratic GPR	0.0002	0.0002
Squared Exponential GPR	0.0002	0.0002
Matern 5/2 GPR	0.0004	0.0004
Exponential GPR	0.0061	0.005

After each model is tested, the values of RMSE and R-Squared are determined, as shown in Tables 3 and 4. Overall, GPR has the lowest RMSE values, with three out of four of its models having a value of below 0.001. The graphical representation of RMSE for all models is shown in Figure 12. GPR models are also the most accurate, as their R-squared values are close to one.

Table 4 Training and Testing R-Squared of prediction models

Model Type	R-Squared (Train)	R-Squared (Test)
Linear SVM	0.854	0.833
Quadratic SVM	0.969	0.970
Cubic SVM	0.981	0.982
Fine Gaussian SVM	0.918	0.934
Medium Gaussian SVM	0.985	0.985
Coarse Gaussian SVM	0.970	0.970
Narrow NN	0.999	1.000
Medium NN	1.000	1.000
Wide NN	1.000	1.000
Bilayered NN	1.000	1.000
Trilayered NN	1.000	1.000
Rational Quadratic GPR	1.000	1.000
Squared Exponential GPR	1.000	1.000
Matern 5/2 GPR	1.000	1.000
Exponential GPR	0.999	0.999

Rational Quadratic GPR is a non-parametric regression method that widens the standard of GPR by incorporating a rational quadratic covariance function. A covariance function or kernel function plays an important role in deciding the shape of the predicted function. The GPR model in MATLAB is constructed by the mathematical equation shown as:

$$P(y_i|f(x_i), x_i) \sim N(y_i|h(x_i)^T\beta + f(x_i), \sigma^2) \quad (3)$$

where *P* indicates a probabilistic function, *y* is the predicted values, *x* is the independent variables, *f(x)* is the function of the Gaussian Process with kernel function, β is the coefficient estimated from the data, and σ^2 is the error variance.

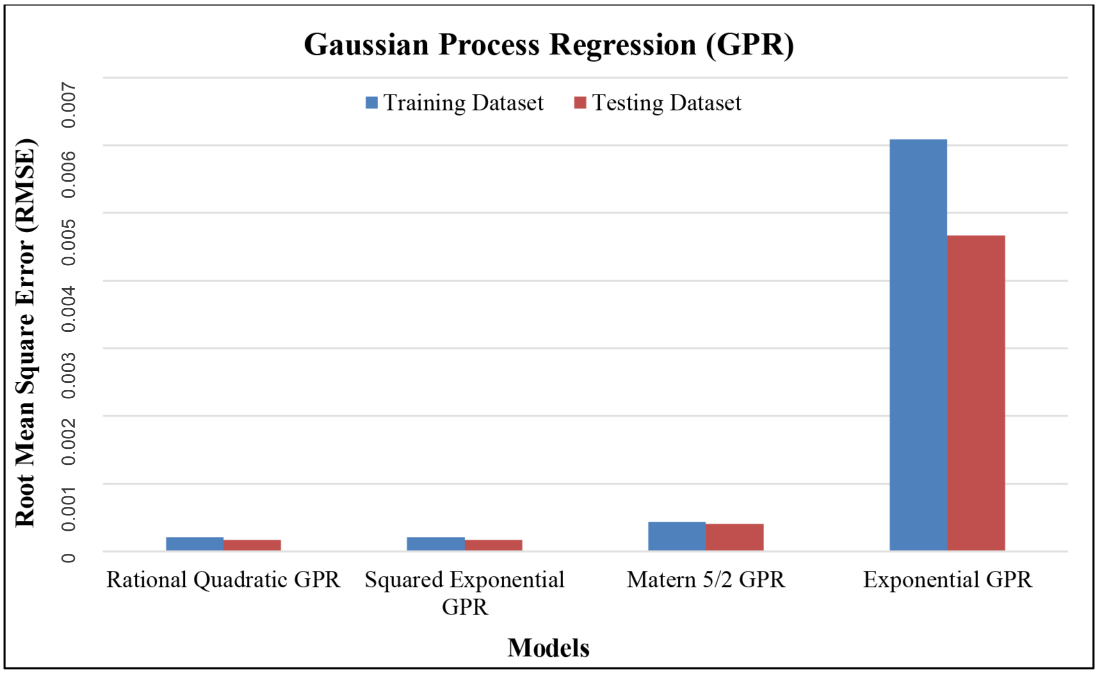

Figure 12 RMSE of GPR Models

The kernel function explains the similarity between any two points in the input space and manages the sleekness and complexity of the prediction model. The rational quadratic covariance function can model the complex and non-stationary relationship between predictors. The kernel function for Rational Quadratic GPR is defined as:

$$K(x_i, x_{i+1}) = {(1 + (|x_i + x_{i+1}|)^2} \Big/ {(2\alpha\sigma^2)^{-\alpha}} \quad (4)$$

One of the benefits of Rational Quadratic GPR is that it can improve the model's ability to capture long-range dependency between predictors and response, creating a better prediction.

The rational Quadratic GPR model has the lowest RMSE values, with 0.00020 and 0.00016 for training and testing, respectively, showing that the model performs very well. The close difference between both values shows that the model is not too complex. A too complex model may cause overfitting of the data as it considers the noise of the data rather than the actual patterns. As a result, the overfitted prediction model may cause new, unseen data to be predicted inaccurately. In this study, the low and close difference RMSE values for both training and testing datasets prove that the model can be used for future screening of IL for CO_2 capture.

Furthermore, Rational Quadratic GPR also has the closest R-squared values to one for both training and testing datasets. The R-squared value is a measure that indicates the proportion of the variance in the response (dependent variable) that is explained by the predictors (independent variables) in a prediction model. R-squared values of 0.999 shows that the predictors strongly explain a huge proportion of the variance in the response. Generally, this indication means that Rational Quadratic GPR is a good fit for the data.

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CONCLUSION

In conclusion, temperature and pressure are the CO_2 absorption parameters relevant to CO_2 capture. Meanwhile, the properties of IL with the highest relevance to CO_2 capture are molecular weight, molality, and CO_2 activity coefficient. 15 models from three machine learning methods were developed to predict the CO_2 absorption potential of ionic liquids. The rational Quadratic GPR model is the most accurate prediction model to screen IL for CO_2 capture. The training and testing RMSE for this model is 0.0002, indicating that the model is performing credibly. In addition, the R-squared values for training and testing models are 0.999, close to 1. Rational Quadratic GPR is capable of being used to screen IL for CO_2 capture. This study is important to reduce the extensive work of screening IL for CO_2 capture. IL with the most appropriate CO_2 absorption potential can be chosen easily and faster, contributing to the effort of reducing CO_2 emission to the environment. Indirectly, this study can help mitigate global warming with the rapid industrialisation that is currently happening.

NOMENCLATURE

bhea	Bis(2-hydroxyethyl)ammonium
bmim	1-butyl-3-methylimidazolium
CO_2	Carbon Dioxide
DBU	1, 8-diazabicyclo[5.4.0]undec-7-ene
emim	1-ethyl-3-methulimidazolium
he	2-hydroxyethanaminium
IL	Ionic Liquid
MLR	Multiple Linear Regression
N4111	Trimethyl-butylammonium
NTf_2	Bis (trifluoromethyl sulfonyl amide
omim	1-octyl-3-methylimidazolium

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