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Automated determination of optimal component design for a binary solvent for absorption-based acid gas removal

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Abstract. Natural gases containing impurities, namely carbon dioxide (CO_2), heavy hydrocarbons, hydrogen sulfide (H_2S), and water vapour, need treatment for removing acidic gases (CO_2 and H_2S) to reduce corrosion and enhance the heat capacity of the gas. This gas is commercially known as "sour", and typically, sour gas is any gas that contains significant levels of hydrogen sulfide. The presence of carbon dioxide can affect natural gas quality, which can also lead to CO_2 freezing issues; hence reliable techniques for reducing CO_2 and H_2S from natural gases is necessary. New blends of amines show CO_2 and H_2S uptake capacity comparable to traditional MEA benchmark solutions. This work aimed to create different regression models using open-source software and estimate the best fit model for a given amine solvent. For this purpose, data were obtained from simulation using Aspen HYSYS V12.1 for MDEA (40-45 wt.%), MDEA +PZ (42-50wt.% + 0-2.5wt.%), DEA (21-26wt.%). Regression models for different amine solvent blends were developed and validated. The study showed that the XGB Regression model was best suited for the MDEA solution, while MDEA + PZ and DEA were best suited for multiple linear regression. The data is generated using simulation from ASPEN HYSYS and models were created in python correlating the simulation-generated values with the model results. These models showed low MSE, RMSE and high R^2 values for the tried solvents.

Introduction

Many chemical processes involve the absorption of gases along with chemical reactions (reactive absorption). The reasons for reactive absorption could be purifying flue and tail gases in refineries to meet pollution legislations, removing acidic gases from the feed in fertilizer industries plants, and purification of feed gases to polymerization units in petrochemical industries to prevent poisoning of catalysts. Aqueous amine solutions are solvents traditionally used in the treatment of refinery and synthesis gas streams [1].

Fig. 1 depicts a flow diagram of the amine scrubbing unit for removing CO_2 and H_2S [2]. The purified gas stream contacts the amine-based solvent in a counter-current manner to facilitate acid gas absorption. The concentrated solvent gets separated as acid gas (top product) and regenerated solvent (bottom product) in the distillation column. The absorber regenerates the solvent. The acid gas treatment by amine absorption is energy intensive due to high energy requirements at reboilers in the regenerating distillation columns. The regeneration step captures about 3.3 GJ / t of CO_2 under optimal conditions [3].

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The rapid increasing energy prices have led to research for new solvents and solvent blends, as energy consumption in a process is directly related to the chosen solvent. [4]. The focus on air pollution abatement and the new rules and regulations worldwide mandates the implementation of newer CO_2 and H_2S reactive absorption [5]. Energy generation from fossil fuels in thermal power plants and exhaust gases are the primary supply of CO_2 and account for almost half of greenhouse gases leading to global warming [6]. Acid gases affect the gas−liquid mass switch, which reacts with alkanolamine. Hence, improving gas−liquid mass transfer enhances the acid gas absorption performance [7].

Since there are many factors involved in the energy consumption of a gas treating plant, leveraging statistical modelling to characterize and predict this energy consumption level can be an essential tool for managing and optimizing energy systems. Multivariate regression modelling is one of the most common methodologies for this purpose and can be used to improve energy efficiency (EE) [8]. Statistical modelling helps understand the most significant factors for optimizing energy systems which can be seen in previous studies [9–18].

The ongoing research focuses on finding innovative solvents that can effectively remove CO_2 and H_2S from different gas streams. This paper aims to analyze and compare regression models such as linear, multiple, Ridge and XGB regression in predicting the concentration of H_2S and CO_2.

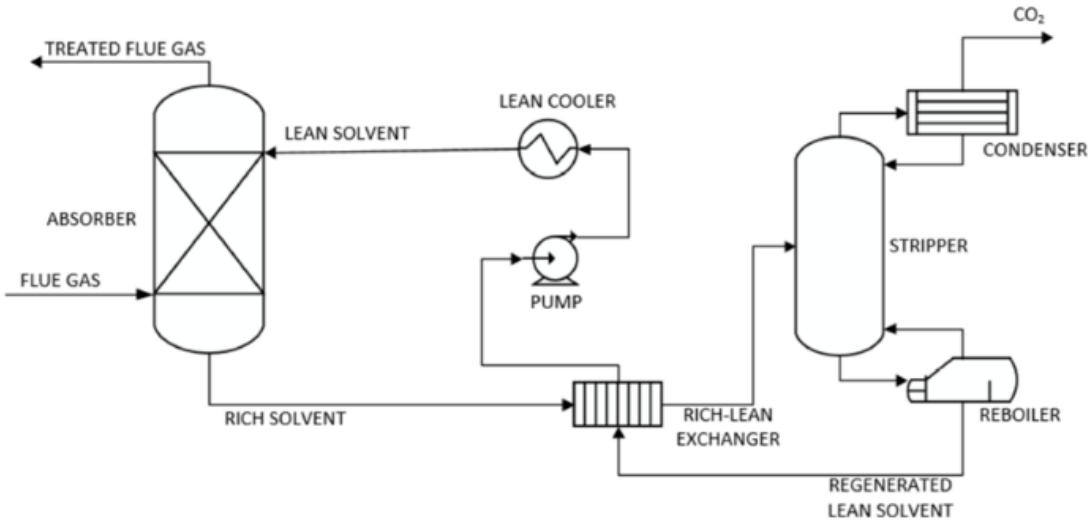

Fig. 1 Typical gas sweetening process by chemical absorption [2]

Methodology

Process flow sheeting

The simulations were conducted for conventional solvents such as MDEA (40-45 wt.%), MDEA +PZ (42-50wt.% + 0-2.5wt.%) and DEA (21-26wt.%) for model and simulation validation. Fig. 2 shows the flowsheet that is developed through Aspen HYSYS V12.1. The case explores the model of a plant that removes H_2S and CO_2 from gas coming from upstream operations. It is a critical operation in the midstream and refining industries to ensure the product gasses meet product quality and emissions standards while operating at optimal conditions.

The flow diagram depicts a packed column (absorber) for removing CO_2 and H_2S from the gas stream. A regenerator (distillation column) regenerates lean amine, and an absorber recycles the

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same. The amine intensity and recirculation are maintained by introducing a replenishment block to estimate the make-up for water.

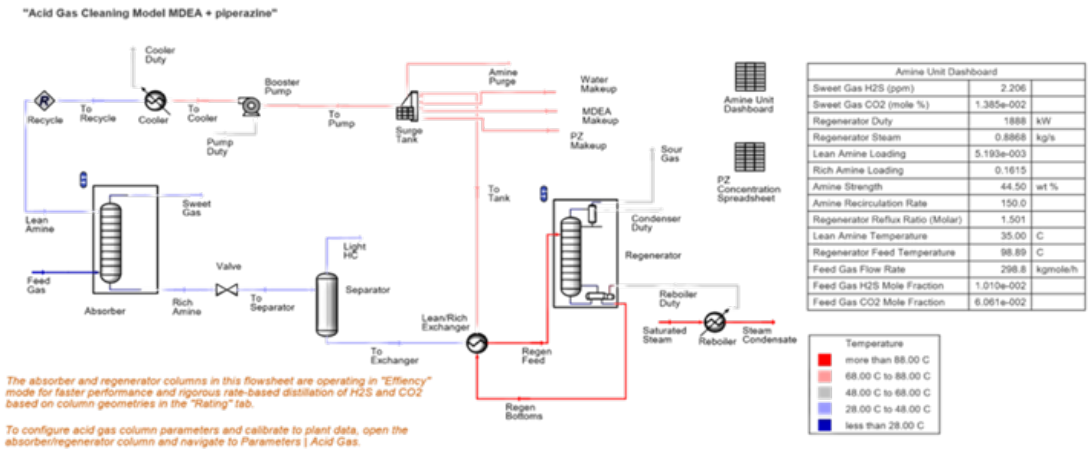

Fig. 2 Flowsheet developed from Aspen HYSYS V12.1

Development of models

Regression models. The choice of the regression analysis technique depends on the data's nature. This paper employs simple, multiple linear, Ridge and XGB regression models for predicting the concentration of H_2S and CO_2. The model of dependent variable y and the independent variables xxi (i=1,2,3...) predicts the trend.

The development of the regression models is a three-step process. First, the data will be collected from various sources and identify the dependent and independent variables in optimization. The multiple parameters are run through python for further regression analysis. Further, RMSE and R^2 quantify are compared to see how well a regression model fits a dataset. Finally, in the simulation, the obtained data is cross verified for model checking.

A design view. For developing regression analysis, the input needs to be made available in the workspace for python to recognize the input and load it into the model. The input can be made available in the base workspace of python by reading from a .xlsx file (excel file) or a .csv data file which is already present in the workspace and accessed through the local device. After the input is loaded, the regression model needs to be run from the coded program.

The input data from excel, as shown in Fig. 3, is used to import any excel data present in the user's pc/laptop and load it into the base workspace of python. The output parameters should be displayed for a specific model for the given data set. For example, if the dependent variable is the absorption efficiency of CO_2, then the R^2, MSE and RMSE values must display the output attributes and their values corresponding to when the dataset is loaded. The plots are also added to the code. When a program is run, its output parameter will be displayed as a graph. The graphical view of the model is shown in Fig. 4.

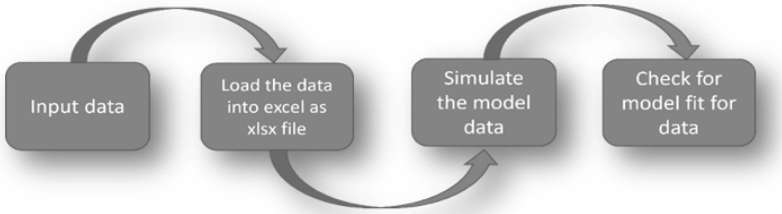

Fig. 3 Block Diagram for developing a Regression model

Fig. 4 Design view of code with markings

Optimization and code view. The coding part for the model is given below. The algorithm block diagram for the code is shown in Fig. 5. The library imported for regression analysis was sklearn, from which the regression model was imported. The program's data was split into two variables, X and Y. X, assigned the parameter to train and tested with the Y variable. The X variables include the parameter, i.e., no of plates, overflow weir height, inlet gas flow rate, pressure, inlet gas-liquid ratio, inlet gas loading, solvent concentration and removal efficiency, and the output variable Y includes the efficiency of a particular solvent.

The test and train were split into 20-80%, and the model was fitted into the X train and Y train by importing the sklearn library. First, the Y test was predicted using the X test, and corresponding values were noted. Then, the full data of X and Y were fitted, model predictions for X were made, and the corresponding values were printed.

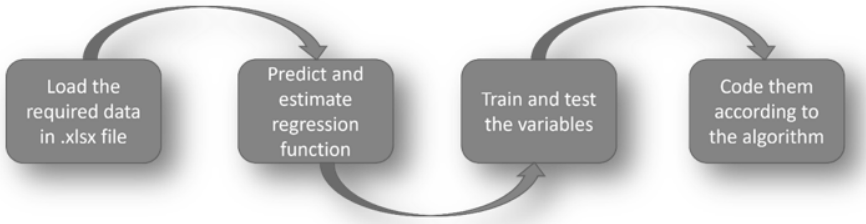

Fig. 5 Block diagram for the code of the application

Results and Discussion

Model simulation results

The CO_2 and H_2S absorption performance of all solvents was ultimately analyzed in terms of the regression analysis to allow practical comparison and future data utilization in process design. Table 1 shows the performance comparison between the models in predicting H_2S and CO_2 in sweet gas while Fig. 6, 7, 8 and 9 shows different graphical representations for other regression models that were coded to get a better understanding of model fit data. This comparison allowed the models to cross-verify with simulated data from ASPEN HYSYS and correlate the model-verified data with simulated generated data .

For the prediction of concentration of H_2S and CO_2 from using MDEA + PZ, it can be observed that high ranges of R^2 values were obtained from linear and multiple regression (0.95 to 0.99) indicating that higher percentage of data is fitted with these proposed models [11]. As for Ridge and XGB regression, based on the coefficient of determination, which largely ranged from 0.53 to 0.93 for Ridge, and 0.07 to 0.1 for XGB regression demonstrates that the H_2S and CO_2 prediction in sweet gas by using MDEA and PZ through Ridge and XGB regression were less accurate.

As for using DEA in predicting the concentration of H_2S and CO_2 in sweet gas, it can be observed that high ranges of R^2 values were obtained from multiple, Ridge and XGB regression, ranging between 0.88 to 0.99. In contrast, low R^2 value is observed through linear regression, ranging from -0.56 to 0.78. As for MSE and RMSE, XGB regression shows promising results for H_2S and CO_2, obtaining MSE values of 0.02 and 0.01, and RMSE value of 0.01 and 0.02. MSE and RMSE can be an indicator on how accurately the model predicts the response and lower values of both MSE and RMSE shows a better fit. Thus, XGB regression suits well for predicting H_2S and CO_2 concentration in sweet gas by using DEA.

It can be observed that high range of R^2 values is obtained from linear, multiple and ridge regression (0.91 to 0.99) in predicting the concentration of H_2S and CO_2 in sweet gas by using MDEA while XGB regression produced a slightly lower range, which is between 0.77 to 0.98 for the R^2. All models showed low range values of MSE (0.001-0.02) and RMSE (0.01-0.086) indicating that all models are able to predict well the values of the response variables.

Table 1: Performance comparison of models

			Linear	**Multiple**	**Ridge**	**XGB**
MDEA + PZ	CO_2	MSE	0.01	0.01	0.01	0.02
		RMSE	0.04	0.02	0.08	0.01
		R^2	0.97	0.99	0.93	0.07
	H_2S	MSE	0.17	0.10	2.51	0.01
		RMSE	0.41	0.31	1.58	0.01
		R^2	0.95	0.98	0.53	0.1
DEA	CO_2	MSE	21.43	1.38	1.43	0.01
		RMSE	4.63	1.17	1.19	0.02
		R^2	-0.56	0.94	0.94	0.99
	H_2S	MSE	5.1	5.0	5.0	0.02
		RMSE	0.45	0.4	2.0	0.01
		R^2	0.78	0.88	0.88	0.99
MDEA	CO_2	MSE	0.001	0.02	0.02	0.01
		RMSE	0.05	0.008	0.01	0.08
		R^2	0.99	0.97	0.99	0.77
	H_2S	MSE	0.03	0.007	0.01	0.01
		RMSE	0.055	0.086	0.09	0.01
		R^2	0.94	0.93	0.91	0.98

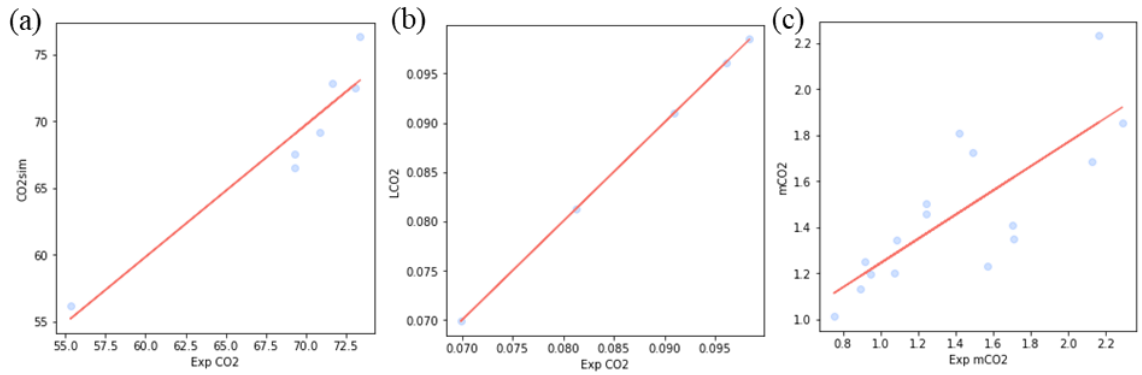

Fig. 1: Linear regression for (a) MDEA+PZ (b) DEA (c) MDEA

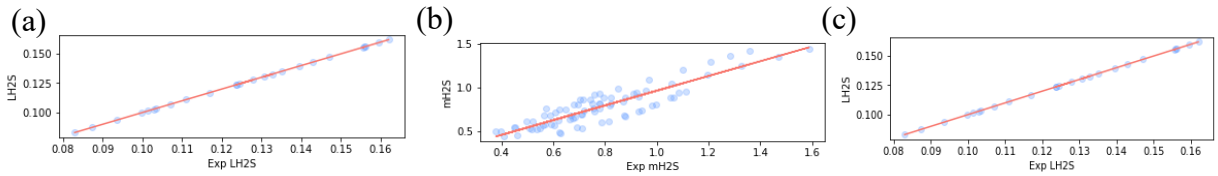

Fig. 2: multi-Linear regression for (a) MDEA+PZ (b) DEA (c) MDEA

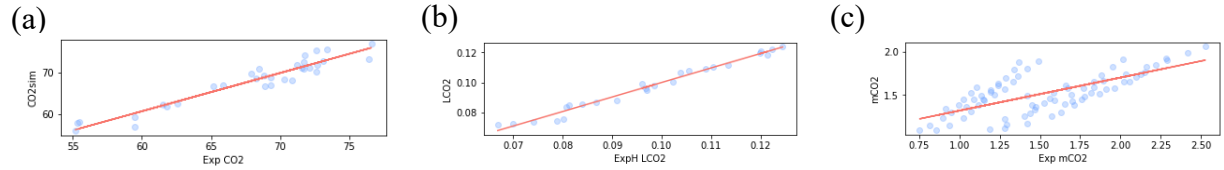

Fig. 3: Ridge regression for (a) MDEA+PZ (b) DEA (c) MDEA

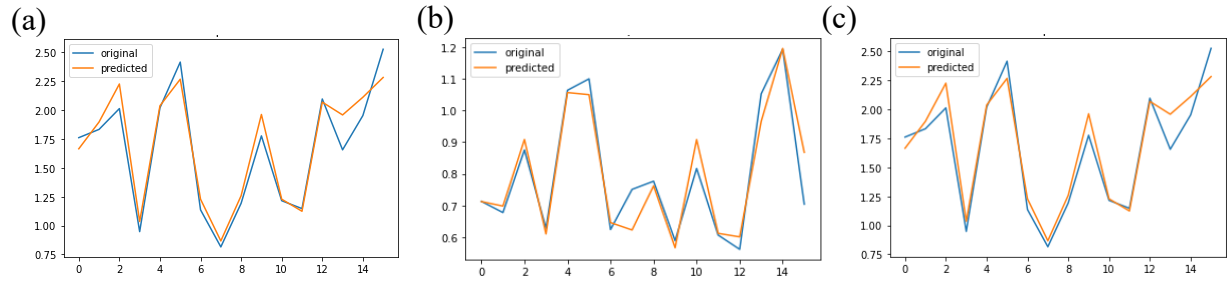

Fig. 4: XGB regression for (a) MDEA+PZ (b) DEA (c) MDEA

Conclusion

This paper aims to analyze and compare regression models such as linear, multiple, Ridge and XGB regression in predicting the concentration of H_2S and CO_2. Acid gas treatment by using solvents such as MDEA (40-45 wt.%), MDEA +PZ (42-50wt.% + 0-2.5wt.%) and DEA (21-26wt.%) were simulated by using Aspen HYSYS 12.1. This study showed that linear and multiple linear regression models were found to be the best fit for MDEA + Piperazine. DEA showed the slightest error for XGB and Ridge regression model for both CO_2 and H2S, and MDEA showed good results from linear, multiple and Ridge regression.

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References

[1] T. Chakravarty, U.K. Phukan, R.H. Weilund, Reaction of acid gases with mixtures of amines, in: 1985.

[2] S.-Y. Oh, M. Binns, H. Cho, J.-K. Kim, Energy minimization of MEA-based CO2 capture process, Appl. Energy. 169 (2016) 353–362. https://doi.org/https://doi.org/10.1016/j.apenergy.2016.02.046

[3] M.R.M. Abu-Zahra, L.H.J. Schneiders, J.P.M. Niederer, P.H.M. Feron, G.F. Versteeg, CO2 capture from power plants: Part I. A parametric study of the technical performance based on monoethanolamine, Int. J. Greenh. Gas Control. 1 (2007) 37–46. https://doi.org/https://doi.org/10.1016/S1750-5836(06)00007-7

[4] D.D.D. Pinto, H. Knuutila, G. Fytianos, G. Haugen, T. Mejdell, H.F. Svendsen, CO2 post combustion capture with a phase change solvent. Pilot plant campaign, Int. J. Greenh. Gas Control. 31 (2014) 153–164. https://doi.org/https://doi.org/10.1016/j.ijggc.2014.10.007

[5] F. Bashipour, S.N. Khorasani, A. Rahimi, H2S Reactive Absorption from Off-Gas in a Spray Column: Insights from Experiments and Modeling, Chem. Eng. Technol. 38 (2015) 2137–2145. https://doi.org/https://doi.org/10.1002/ceat.201500233

[6] J. Ye, C. Jiang, H. Chen, Y. Shen, S. Zhang, L. Wang, J. Chen, Novel Biphasic Solvent with Tunable Phase Separation for CO2 Capture: Role of Water Content in Mechanism, Kinetics, and Energy Penalty, Environ. Sci. Technol. 53 (2019) 4470–4479. https://doi.org/10.1021/acs.est.9b00040

[7] J. Zhan, B. Wang, L. Zhang, B.-C. Sun, J. Fu, G. Chu, H. Zou, Simultaneous Absorption of H2S and CO2 into the MDEA + PZ Aqueous Solution in a Rotating Packed Bed, Ind. Eng. Chem. Res. 59 (2020) 8295–8303. https://doi.org/10.1021/acs.iecr.9b06437

[8] G. Guido, M. Compagnoni, L. Pellegrini, I. Rossetti, Mature versus emerging technologies for CO2 capture in power plants: Key open issues in post-combustion amine scrubbing and in chemical looping combustion, Front. Chem. Sci. Eng. 12 (2018). https://doi.org/10.1007/s11705-017-1698-z

[9] M. Koolivand Salooki, R. Abedini, H. Adib, H. Koolivand, Design of neural network for manipulating gas refinery sweetening regenerator column outputs, Sep. Purif. Technol. 82 (2011) 1–9. https://doi.org/10.1016/j.seppur.2011.07.015

[10] P. Nimmanterdwong, R. Changpun, P. Janthboon, S. Nakrak, H. Gao, Z. Liang, P. Tontiwachwuthikul, T. Sema, Applied Artificial Neural Network for Hydrogen Sulfide Solubility in Natural Gas Purification, ACS Omega. 6 (2021) 31321–31329. https://doi.org/10.1021/acsomega.1c05169

[11] N.F. Salehuddin, M.B. Omar, R. Ibrahim, K. Bingi, A Neural Network-Based Model for Predicting Saybolt Color of Petroleum Products, Sensors. 22 (2022). https://doi.org/10.3390/s22072796

[12] M.H.M Tarik, M.B. Omar, M.F. Abdullah, R. Ibrahim, Optimization of neural network hyperparameters for gas turbine modelling using Bayesian optimization, IET, 2018. https://doi.org/10.1049/cp.2018.1308

[13] Tarik, M. H. M., Omar, M., Abdullah, M. F., & Ibrahim, R. (2017, November). Modelling of dry low emission gas turbine using black-box approach. In TENCON 2017-2017 IEEE Region 10 Conference (pp. 1902-1906). IEEE.

[14] Omar, M. B., Ibrahim, R., Abdullah, M. F., & Tarik, M. H. M. (2020). Modelling of Dry-Low Emission Gas Turbine Fuel System using First Principle Data-Driven Method. Journal of Power Technologies, 100(1).

[15] Omar, M. B., Ibrahim, R., Mantri, R., Chaudhary, J., Ram Selvaraj, K., & Bingi, K. (2022). Smart Grid Stability Prediction Model Using Neural Networks to Handle Missing Inputs. Sensors, 22(12), 4342.

[16] Hakimi, M., Omar, M. B., & Ibrahim, R. (2023). Application of Neural Network in Predicting H2S from an Acid Gas Removal Unit (AGRU) with Different Compositions of Solvents. Sensors, 23(2), 1020.

[17] Rosli, N. S., Ibrahim, R., Ismail, I., & Omar, M. (2022). Modeling of high voltage induction motor cooling system using linear regression mathematical models. Plos one, 17(11), e0276142.

[18] Mahesh, A., Aadhavan, B. A., Meenaa, V. V., Omar, M. B., Ibrahim, R. B., Salehuddin, N. F., & Sujatha, R. (2022, August). Employment of ANN for Predictive Motor Maintenance and Bearing Fault Detection Using Park's Vector Analysis. In 2022 IEEE 5th International Symposium in Robotics and Manufacturing Automation (ROMA) (pp. 1-6). IEEE.