A Supervised Neural Network-based predictive model for petrochemical wastewater treatment dataset

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Abstract- It is understood that water is the most valuable natural resource and as like wastewater treatment plants are necessary base to control the environmental balance where they are installed. To ensure good quality effluents, the dynamic and complicated wastewater treatment procedure must be handled efficiently. A global interest has been prompted in conservation, reuse, and alternative water sources due to growing treats over water supply scarcity. Water utilities are searching for more efficient ways to maintain their resources globally. The development of machine learning techniques is starting to offer real opportunities to operate water treatment systems in more efficient manners. This paperwork shows research as well as its development work implemented to predict the performance of petrochemical wastewater treatment. The data were used from a reputed chemical plant and the predictive models were developed by implementation of Backpropagation Neural Network using sample datasets with the parameters of wastewater dataset.

Keywords- Petrochemical wastewater treatment, Artificial intelligence, Backpropagation neural network, Principal component analysis, Chemical Oxygen Demand, Pollutant Removal Efficiency

I. OVERVIEW

Wastewater treatment is a complex process especially petroleum refineries with requesting ecological management challenges as side-effects can be both unpredictable as well as poisonous [1, 2]. Such kind of wastewater regularly needs a blend of treatment techniques to eliminate oil and different foreign substances before discharge. The main problems such as groundwater defilement; aromatics; grease, oil and biological evacuation, and volatile organic compounds control should be addressed to consent to ecological guidelines and keep a good client image [3-7].

An expanded comprehension of necessities of the petrochemical end-user is acquiring significance as industry needs change owing to sticker guideline and environmental laws and it is important that equipment manufacturers keep level of these prerequisites to benefit on future opportunities. End-users are forced to become aware of what sorts of waste they're making and releasing, and how they can change their present treatment gear to satisfy new needs. Therefore, these all can be overcome from the available data using proper execution of machine learning and data mining techniques [8].

Consequently, the petrochemicals wastewater management system can implement through data-science employing materials big data, data mining and machine learning techniques and significantly reduces the time span between conceptualization to manufacturing [9]. It could be feasible to get a decent plant operation if the administrative control system can respond to the progressions and determinations in the framework and can make the essential moves to re-establish the system's performance. These choices are regularly based on physical, chemical, microbiological principles and on some information. Along these lines, an integrated and distributed artificial intelligence (AI) models seems to be a better choice [10].

This paper deals with the study of the execution of the supervised neural network in order to predict the key attribute for wastewater treatment. Backpropagation neural network (BPNN) is the technique taken for this research study and this technique has been presented by Marvin Minsky in 1961 for solving the credit assignment problem (CAP) [11]. Due to its simplicity of implementation and its efficiency, BPNN has become popular in the case of training neural networks [12, 13]. The BPNN has been made popular by Rumelhart [14]. One of the benefits of BPNN is its ease of programming and its efficiency to manipulate big set of data [15, 16]. Then, another benefit is that layered networks using distinguishable models could perform racial estimations and offer best features such as quick response, learn from experience, and the capacity to classify above the training data [12].

The aim of this work is to increase the diversity of the research for reducing the percentage of pollution of wastewater at the cheap rate. To achieve the aim, study the characteristics and recycle conditions of wastewater from petrochemicals for the manufacturing of necessary elements for industrial purpose using AI techniques by developing supervised neural network based predictive technique. The remaining part of the paper has been arranged as sections: Related studies, Proposed solution, Methodology, Results & Discussions, and Conclusions. Related studies are based on BPNN, and it's some studies related with wastewater treatment process (WWTP). The parameters and its ideas have been introduced in the section of proposed solution. Then, execution of techniques is described in the section of methodology. Next, the experimental strategies are expounded as well as the obtained outcomes are compared and included as graph in result and discussion. The final section is concluded with overall discussion of experiments and its future scope.

II. BACKPROPAGATION NEURAL NETWORK TECHNIQUE AND ITS RELATED STUDIES

Since the proposed technique is a supervised neural network technique and this section discusses some similar approaches. Due to complexity of the relationship between input parameters and output in WWTP, it is difficult to be modelled using statistics [17] and Table 1 showing the studies of applications of BPNN in WWTP. Accordingly, AI models are generally more flexible when comparing with statistical models while modelling complex datasets with possible nonlinearities or missing data [18].

Table I. Few studies relating application of BP neural network in WWTP

Applications	Results	Ref.
Modelling of removal of COD by the Fenton process	Results with correlation coefficient (R^2) of 0.997 as well as Mean Square Error (MSE) 0.000376 are very close by ANN prediction results	[19]
Modelling of discoloration process by neural network	Results showed that the time of activity was the predominant variable as well as response mean temperature was the lesser influent variable	[20]
The removal of humic substances from the aqueous solutions	The ANN model generated determination coefficient of (R^2 = 0.995), standard deviation ratio (0.065), mean absolute error (MAE) is 4.057 and root mean square error (RMSE) is 5.4967	[21]
Prediction of TiO2 photocatalytic efficiency	Overall optimization error was in the normal under 5% and correlations were gained from the dataset with a percentage of 98.57%	[22]
Degradation of polyvinyl alcohol by the photo-Fenton process	R^2 is 0.966 by a comparison between ANN predicted Dissolved organic carbon (DOC) and the experimental DOC	[23]
ANN prediction on azo dye decolorization by UV/H_2O_2	Model gave better predictions of R^2 is 0.996 and mean square error is 0.004	[24]
Colour Removal of Textile Wastewater	RMSE is 0.053 and the R^2 is 0.97	[25]
Modelling of the treatment of wastewater by UV/H_2O_2 process	MSE is 0.0004 and R^2 is 0.998	[26]

BPNN is trained by providing it with input (X) and matching output (y) patterns has been represented in the Figure 1. The input is modelled using real weights (w) and the weights are usually randomly selected. Then, it takes a takes a calculated error using the actual outputs and alters the weights of the various layers backwards from the output layer to the input layer [27, 28] as mentioned in the Equation 1. Finally, keep repeating the process until the desired output is achieved.

$$ErrorB = Actual\ Output - Desired\ Output \quad (1)$$

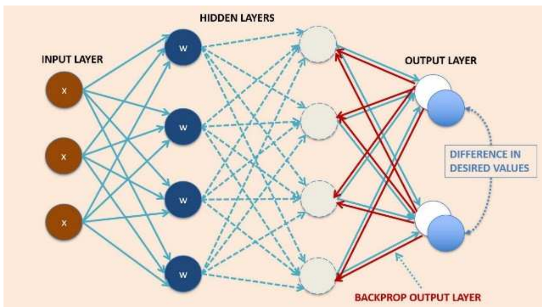

Fig. 1. Backpropagation neural network with supervised learning approach

III. PROPOSED SOLUTION

Water is the most valuable natural resource and wastewater treatment plants are necessary base to control the environmental balance. The development of machine learning techniques is offering real opportunities for operating wastewater treatment systems in more efficient manners. The dataset was collected from a reputed chemical plant and Chemical oxygen demand (COD) removal efficiency is the output parameter or key parameter, and this parameter is getting by the comparison between initial COD and final COD as mentioned in Equation 2.

$$COD\ removal\ efficiency\ (\%) = \frac{\text{COD initial} - \text{COD final}}{\text{COD final}} \times 100 \quad (2)$$

The feature selection technique used for this experiment is Principal component analysis (PCA). It executed on input data to filtrate unrelated arbitrary data. The total number data sets used is 80 were separated into training, validation, and test subsets, each of which contained 40, 20, and 20 sets, respectively. A three-layer BPNN was optimized to predict and simulate the output from the actual output with tangent sigmoid transfer function at hidden layer as well as neurons, and linear transfer function at output layer.

The input and output data of neural network should be normalized or standardized to avoid computational problems and to meet the algorithm necessity and to improve the learning process. There are some common methods providing data normalization [29] and Constant Factor is the normalization technique used here as well as its math equation is shown below.

$$x_n = x_0 / x_{\max} \quad (3)$$

where X_0 represents each value in the given data and X_{max} is the largest among given values as well as X_n is the normalized value.

IV. METHODOLOGY

The entire process of neural network prediction using the proposed technique can be divided into two main stages: (i) forward propagation through the network, and (ii) backward propagation through the network. There are some necessary processes before going through the prediction phase - Fetch dataset (please see Algorithm 1), Normalization (please see Algorithm 2) and assign the size of matrices (please see Algorithm 3)

A. Algorithm 1: Import excel file to fetch dataset

Input layer: X; Output layer: y

1: import LIBRARY

2: book1, book 2 ← OPEN file

3: sheet1, sheet2 ← sheetName

4: X, y ← cell value in sheet1(i, j); for j ← i to 1; for i ← i to j

5: WRITE X, y

B. Algorithm 2: Normalization to maintain the values of input and outputs between 0 and 1

1: import LIBRARY

2: X, y ← X, y elements INTO array

3: X ← X DIV (X to axis = 0)

4: y ← y DIV 1000

5: WRITE X, y

C. Algorithm 3: Assign the size of matrices as well as weights

1: function class NeuralNetwork (object)

2: function init ('self' keyword)

3: self (sizeInput, sizeOutput, sizeHiddenLayer) ← 5, 2, 3

4: self. W1 ← weightMatrix FROM input TO hiddenLayer

5: self. W2 ← weightMatrix FROM hidden TO outputLayer

Forward propagation through the network

A feedforward neural network is an ANN has an input layer, hidden layer and an output layer as shown in Figure 1. Also, this neural network never forms a cycle, and the process is described in Algorithm 4.

D. Algorithm 4: Feed forward propagation and sigmoid normalization

1: function feedForward(self, X)

2: self.z ← np.dot product(X, self.W1)

3: self.z2 ← self.sigmoid function (self.z)

4: self.z3 ← np.dot product(self.z2, self.W2)

5: output ← self.sigmoid function(z3)

6: feedForward ← output

7: function sigmoid (self, s, deriv = False)

8: if deriv equal to True then

9: sigmoid ← s*(1-s)

10: sigmoid ← 1 DIV (1+np.exp(-s))

Backward propagation through the network

This method helps to calculate the gradient of a loss function with respect to all the weights in the network and process is explained in Algorithm 5 and lastly plotting the graph is mentioned in Algorithm 6.

E. Algorithm 5: Backpropagation as well as training the algorithm and prediction

1: function backward (self, X, y, output)

2: self.output_error ← y – output

3: self.output_delta ← self.output_error * self.sigmoid function(output, deriv ← True)

4: self.z2_error ← self.output_delta.dot product (self, W2, T)

5: self.z2_delta ← self.z2_error * self.sigmoid function (self.z2, deriv = True)

6: self.W1 +← X.T.dot product(self, z2_delta)

7: self.W2 +← self.z2.dot product(self, output_delta)

8: function train (self, X, y)

9: output ← self.feedForward(X)

10: self.backward(X, y, output)

11: CREATE OBJECT, NN ← NeuralNetwork () Class Function

12: for i ← 0 to 10000

13: if i MOD 100 equal to 0 then

14: WRITE meanSquareError

15: NN.train (X,y)

16: WRITE input, actualOutput, meanSquareError, predictedOutput

F. *Algorithm 6: Plotting comparison between actual output and predicted output*

1: import library

2: data ← READ file

3: WRITE data

4: X axis, Y axis ← FETCH data

5: PLOT figure

6: PLOT X axis, Y axis FOR setLimit

7: PLOT X axis, Y axis LABEL ← "Number of records", "COD Efficiency"

8: PLOT labelSize, figureSetSize

9: PLOT axesEdgeColor, axesLineWidth, axesFaceColor

10: PLOT fontSize, faceColor, edgeColor

11: DISPLAY GRAPH

V. RESULT AND DICUSSION

The analysis of experimental results for the data sets of petroleum wastewater treatment summarizes as graph in Fig. 3 to show relation between actual output and predicted output. Finally, the mean square error for electrolysis process from the 80 dataset is 0.0025.

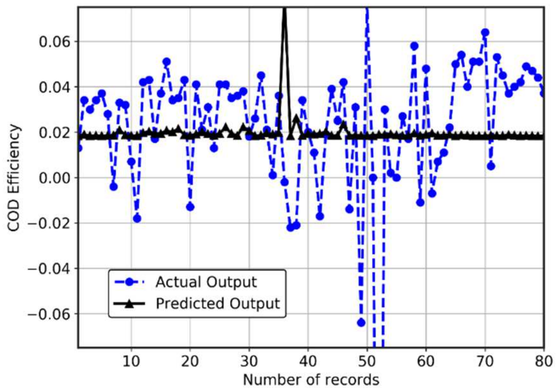

Fig. 3. Comparison of actual and predicted output for the electrolysis process

Up to now, the work is based on the fixed datasets (80), still it can be achieved to predict the output with minor mean square error values. Also, the conventional BPNN is not easy to obtain satisfactory results which gone through small sample conditions, which would prompt overfitting [30]. However, these data are heterogenous and complicated and in future, more performance can be obtained by utilising the big data, with more datasets and more research should be done for application of other AI techniques, for example Support Vector Machine (SVM) and Regression techniques.

VI. CONCLUSIONS

The development of machine learning has been started to offer real opportunities to operate water treatment systems in more efficient manner. A global interest has been prompted in conservation, reuse, alternative water sources due to growing treats over water supply scarcity and it is understood that water is the most valuable natural resource and as like wastewater treatment plants are necessary base to control the ecological balance where they are implemented. The predictive model was developed by implementation of Backpropagation Neural Network using sample datasets having the parameters of electrolysis process and got the mean square error is 0.0025. The output of modelling from BPNN can be used for critical analysis and study the dynamic behaviour of wastewater treatment in petrochemical refineries. Employing Big Data (BD) is the next step in near future, classification and clustering of data, and analytical tools for predicting become more active as well as it will be milestone towards the water industry.

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RFERENCES

[1] S. Lee, J. G. Speight, and S. K. Loyalka, *Handbook of alternative fuel technologies*. crc Press, 2014.
[2] M. E. Ahmed, A. Al-Dhafeeri, and A. Mydlarczyk, "Predominance of attached versus suspended growth in a mixed-growth, continuous-flow biological reactor treating primary-treated petrochemical wastewater," *Arabian Journal for Science and Engineering,* vol. 44, no. 5, pp. 4111-4117, 2019.
[3] I. Oller, S. Malato, and J. Sánchez-Pérez, "Combination of advanced oxidation processes and biological treatments for wastewater decontamination—a review," *Science of the total environment,* vol. 409, no. 20, pp. 4141-4166, 2011.
[4] D. J. Wilson, *Hazardous waste site soil remediation: theory and application of innovative technologies*. Routledge, 2017.
[5] L. Benedetti, G. Dirckx, D. Bixio, C. Thoeye, and P. A. Vanrolleghem, "Environmental and economic performance assessment of the integrated urban wastewater system," *Journal of Environmental Management,* vol. 88, no. 4, pp. 1262-1272, 2008.
[6] R. C. Leitão, A. C. van Haandel, G. Zeeman, and G. Lettinga, "The effects of operational and environmental variations on anaerobic wastewater treatment systems: A review," *Bioresource Technology,* vol. 97, no. 9, pp. 1105-1118, 2006/06/01/ 2006, doi: https://doi.org/10.1016/j.biortech.2004.12.007.
[7] H. Hasheminasab, Y. Gholipour, M. Kharrazi, and D. Streimikiene, "A novel metric of sustainability for petroleum refinery projects," *Journal of Cleaner Production,* vol. 171, pp. 1215-1224, 2018.
[8] S. Tiku, "Wastewater management in the petrochemicals industry," *Industrial WaterWorld,* vol. 6, no. 3, p. 8, 2005.
[9] R. Jose and S. Ramakrishna, "Materials 4.0: Materials big data enabled materials discovery," *Applied Materials Today,* vol. 10, pp. 127-132, 2018.
[10] D. Li, "Perspective for smart factory in petrochemical industry," *Computers & Chemical Engineering,* vol. 91, pp. 136-148, 2016.
[11] F. S. Wong, "Time series forecasting using backpropagation neural networks," *Neurocomputing,* vol. 2, no. 4, pp. 147-159, 1991.
[12] J. A. Cruz-López, V. Boyer, and D. El-Baz, "Training Many Neural Networks in Parallel via Back-Propagation," in *2017 IEEE International Parallel and Distributed Processing Symposium Workshops (IPDPSW)*, 2017: IEEE, pp. 501-509.
[13] P. Vlachas *et al.*, "Backpropagation algorithms and reservoir computing in recurrent neural networks for the forecasting of complex spatiotemporal dynamics," *Neural Networks,* 2020.
[14] D. E. Rumelhart, G. E. Hinton, and R. J. Williams, "Learning internal representations by error propagation," California Univ San Diego La Jolla Inst for Cognitive Science, 1985.
[15] J. Leskovec, A. Rajaraman, and J. D. Ullman, *Mining of massive data sets*. Cambridge university press, 2020.
[16] V. G. Mohan, M. A. Ameedeen, and S. Azad, "A Supervised Learning Neural Network Approach for the Prediction of Supercapacitive Energy Storage Materials," in *Recent Trends in Mechatronics Towards Industry 4.0*: Springer, 2022, pp. 849-858.
[17] N. Bekkari and A. Zeddouri, "Using artificial neural network for predicting and controlling the effluent chemical oxygen demand in wastewater treatment plant," *Management of Environmental Quality: An International Journal,* 2019.
[18] M. G. Karlaftis and E. I. Vlahogianni, "Statistical methods versus neural networks in transportation research: Differences, similarities and some insights," *Transportation Research Part C: Emerging Technologies,* vol. 19, no. 3, pp. 387-399, 2011/06/01/ 2011, doi: https://doi.org/10.1016/j.trc.2010.10.004.
[19] E. S. Elmolla, M. Chaudhuri, and M. M. Eltoukhy, "The use of artificial neural network (ANN) for modeling of COD removal from antibiotic aqueous solution by the Fenton process," *Journal of hazardous materials,* vol. 179, no. 1-3, pp. 127-134, 2010.
[20] O. L. C. Guimarães *et al.*, "Discoloration process modeling by neural network," *Chemical engineering journal,* vol. 140, no. 1-3, pp. 71-76, 2008.
[21] E. Oguz, A. Tortum, and B. Keskinler, "Determination of the apparent rate constants of the degradation of humic substances by ozonation and modeling of the removal of humic substances from the aqueous solutions with neural network," *Journal of hazardous materials,* vol. 157, no. 2-3, pp. 455-463, 2008.
[22] F.-L. Toma, S. Guessasma, D. Klein, G. Montavon, G. Bertrand, and C. Coddet, "Neural computation to predict TiO2 photocatalytic efficiency for nitrogen oxides removal," *Journal of Photochemistry and Photobiology A: chemistry,* vol. 165, no. 1-3, pp. 91-96, 2004.
[23] J. A. Giroto, R. Guardani, A. C. S. Teixeira, and C. A. O. d. Nascimento, "Study on the photo-Fenton degradation of polyvinyl alcohol in aqueous solution," *Chemical Engineering and Processing: Process Intensification,* vol. 45, no. 7, pp. 523-532, 2006.
[24] A. Aleboyeh, M. Kasiri, M. Olya, and H. Aleboyeh, "Prediction of azo dye decolorization by UV/H2O2 using artificial neural networks," *Dyes and Pigments,* vol. 77, no. 2, pp. 288-294, 2008.
[25] R.-F. Yu, H.-W. Chen, W.-P. Cheng, and P.-H. Hsieh, "Dosage control of the Fenton process for color removal of textile wastewater applying ORP monitoring and artificial neural networks," *Journal of Environmental Engineering,* vol. 135, no. 5, pp. 325-332, 2009.
[26] D. Salari, N. Daneshvar, F. Aghazadeh, and A. Khataee, "Application of artificial neural networks for modeling of the treatment of wastewater contaminated with methyl tert-butyl ether (MTBE) by UV/H2O2 process," *Journal of Hazardous Materials,* vol. 125, no. 1-3, pp. 205-210, 2005.
[27] E. S. Elmolla and M. Chaudhuri, "The use of artificial neural network (ANN) for modelling, simulation and prediction of advanced oxidation process performance in recalcitrant wastewater treatment," in *Artificial Neural Networks-Application*: IntechOpen, 2011.
[28] E. Alpaydin, *Introduction to machine learning*. MIT press, 2020.
[29] G. Yaldi, M. A. Taylor, and W. L. Yue, "Forecasting origin-destination matrices by using neural network approach: A comparison of testing performance between back propagation, variable learning rate and levenberg-marquardt algorithms," in *Australasian Transport Research Forum*, 2011.
[30] S. Shi and G. Xu, "Novel performance prediction model of a biofilm system treating domestic wastewater based on stacked denoising auto-encoders deep learning network," *Chemical Engineering Journal,* vol. 347, pp. 280-290, 2018/09/01/ 2018, doi: https://doi.org/10.1016/j.cej.2018.04.087.