ARTIFICIAL NEURAL NETWORK MODELLING FOR ESTIMATION OF CONCENTRATION OF NI (II) AND CR (VI) PRESENT IN AQUEOUS SOLUTION

S. L. Pandharipande[1], Aarti R. Deshmukh[2] and Rohit Kalnake[2]

[1]Associate Professor, [2]M. Tech. Third Semester,
Department of Chemical Engineering, Laxminarayan Institute of Technology, Rashtrasant Tukdoji Maharaj Nagpur University, Bharat Nagar, Amravati Road, Nagpur, India.

ABSTRACT

Analysis of aqueous solution for determination of metal components is an important task for many professionals including chemical engineers, metallurgists, biologists, geologists etc. and can be done by using sophisticated analytical instruments. It is time consuming and expensive. In present work Artificial neural network has been applied to estimate concentration of Ni (II) and Cr (VI) simultaneously present in aqueous solution with its physical properties such as optical density and pH. Experimental observations for aqueous solutions in the concentration range of 0.247 to 49.38 mg/10ml and 0.353 to 17.67mg/10ml for Ni (II) & Cr (VI) metal ions respectively, have been used in developing ANN models NCO, NCP and NCPO. These are compared for their accuracy of predictions based on the RMSE for training and test data sets. The results are indicative that the ANN model NCPO has high accuracy of prediction for both the data sets .The % relative error for maximum data points predicted is between 5 to 40 using NCPO which is acceptable. The novel feature of this work is estimation of concentration of two heavy metal ions present in the aqueous solution with its physical properties in a single model using ANN.

KEYWORDS: *Artificial Neural Network, modelling, heavy metal ions, analysis, physical property of solution.*

I. INTRODUCTION

Analysis of aqueous solution for determination of metal components is an important subject not only for chemists but for many other professionals including chemical engineers, metallurgists, biologists, geologists etc. The higher concentrations of metallic compounds are harmful to plant, animal & aquatic life cycles. Heavy metals may cause severe health problems & may affect the functioning of vital organs; kidney, nervous system, blood composition, liver, reproductive systems etc [1]. Hence there are restrictions on the concentration of metallic compounds in water to be discharged from the industries. Permissible concentration of heavy metals varies with the type of water & its end use.

The chemical & metallurgical process industries have a special importance of this theme in the context of waste water treatment & its related analysis for metallic ions content & become the basis of the control strategy for chemists & engineers. There are different types of analytical instruments employed industrially in determination of metallic compounds & this includes ICP-MS, HPLC, AAS, GLC, ION chromatography, SEM, TEM etc., among others that are time consuming, expensive and require skilled operators [2].

The paper presents the work carried out with brief introduction to artificial neural network followed by the methodology adopted, results & discussions on the efficacy of the ANN models developed & concludes with the possible future prospects.

II. ARTIFICIAL NEURAL NETWORK

Last two decades has seen advent of Artificial Neural Network which has been successfully applied to various fields of engineering, medical sciences, economics, meteorology, psychology, neurology, mathematics and many others. Neural networks exhibit many advantageous properties for solving complex problems of developing nonlinear multivariable correlation and with speed, accuracy & have the ability to generalize from given training data to unseen data [3].

An Artificial Neural Network (ANN) is a black box modeling tool having its working principle based on the way the biological nervous system processes information. It is composed of a network of largely interconnected neurons working together to solve a specific problem. Multi-Layer Perceptron (MLP) is a type of feed forward neural network. It consists of input & output layers with at least one hidden layer in between them. The numbers of nodes in input & output layers are decided by the number of input & output parameters whereas the number of hidden layers & number of nodes in each hidden layer is decided by the complexity of the multivariable relationship to be developed. Every input signal or its value is altered by a connectionist constant called as weight. The node receives the summation of all the altered input signals & transforms into an output by using a function, either sigmoid or hyperbolic. The layer to layer processing of input signal is carried out which leads to an array of output signals that are compared with their respective known values so as to generate error signal. Delta rule or gradient descent rule is applied for reducing the error further by altering the connectionist weights or constants. The iterative process is terminated by applying the criterion of either reaching a value of desired error or the number of iterations [3, 4].

There are number of applications of ANN, that include, standardization of digital colorimeter[5], estimation of composition of a ternary liquid mixture[2], mass transfer predictions in a fast fluidized bed of fine solids[6], modeling for estimation of hydrodynamics of packed column[7], fault diagnosis in complex chemical plants[8], adsorption study[1, 9], modeling combined VLE of four quaternary mixtures[10] and similar other[11, 12, 13] are also reported.

The objective of the present work is to suggest an effective, low cost & easily accessible method for estimation of the concentrations of two mutually soluble metallic ions simultaneously present in an aqueous solution. Physical property of a solution is dependent upon the concentration of its constituents. In the present work OD & pH are selected as physical properties of the solutions and are to be correlated with the concentrations of Ni (II) & Cr (VI) in the solution.

The selected properties OD & pH can be easily determined in a laboratory with low cost, high accuracy & easily accessible instruments.

The present work aims at developing Artificial Neural Network model in estimation of the concentrations of two mutually soluble metallic ions using the physical properties of the aqueous solution namely optical density (OD) & pH.

III. METHODOLOGY

- Stock solution of aqueous solutions containing Ni (II) and Cr (VI) metallic compounds respectively have been prepared by adding known quantity of commercial grade$NiCl_2$. $(H_2O)_6$ and $K_2Cr_2O_7$ compounds respectively in known volume of distilled water.
- Known volumes of these filtered stock solutions with different proportions have been mixed together for obtaining 51 samples of aqueous solutions containing different concentrations of Ni (II) and Cr (VI).
- All the 51 samples of the solution obtained by addition of the stock solutions are analyzed for its optical density & pH using digital colorimeter & pH meter respectively.

3.1 ANN approach in modeling of estimation of concentration of the Ni (II) and Cr (VI) simultaneously present in the aqueous solution with the physical properties such as optical density and pH:

The accuracy of the ANN model is dependent upon number of factors that include selection of input parameters, the number of hidden layers & number of neurons in each hidden layer among others. Three different ANN models NCO, NCP & NCPO have been developed[14], one model each for correlating input parameters pH and optical density, with two output parameters, concentrations of Ni

(II) and Cr (VI) in aqueous solution and the third model correlating two input parameters pH and optical density with concentrations of Ni (II) and Cr (VI).

- The data generated is divided in two parts one part containing 42 data points as training set and the other with 9 data points as test set.
- The topology of the ANN models NCO, NCP & NCPO developed in the present work is given in table 1.

Table 1. Neural network topology for ANN models

Model code	Number of Neurons					Data points		RMSE	
	Input layer	1st hidden layer	2nd hidden layer	3rd hidden layer	Output layer	Training data set	Test data set	Training data set	Test data set
NCO	1	00	05	05	2	42	9	0.1933	0.2235
NCP	1	00	05	05	2	42	9	0.1968	0.2521
NCPO	2	00	05	05	2	42	9	0.0195	0.0520

Number of iterations = 50000
Input parameters: NCO: OD, NCP: pH, NCPO: pH, OD
Output parameters: For all the Models :Concentration of Ni & Concentration of Cr.

- The architecture of ANN topology for ANN models NCO, NCP & NCPO are shown in Figures 1, 2 and 3 respectively. The snapshot of the elite-ANN© in run mode is shown in Figure 4.

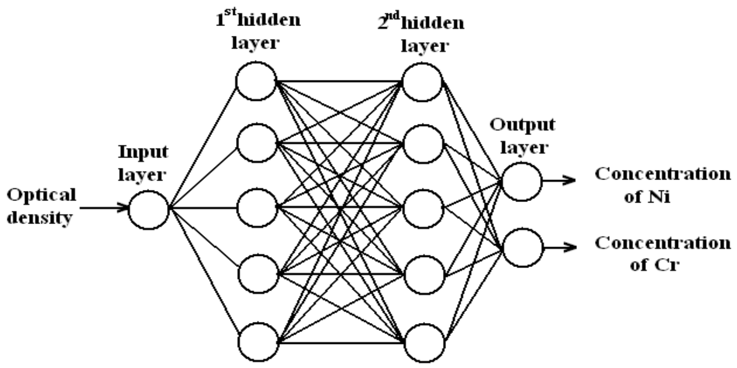

Figure 1. Neural Network Architecture for model NCO

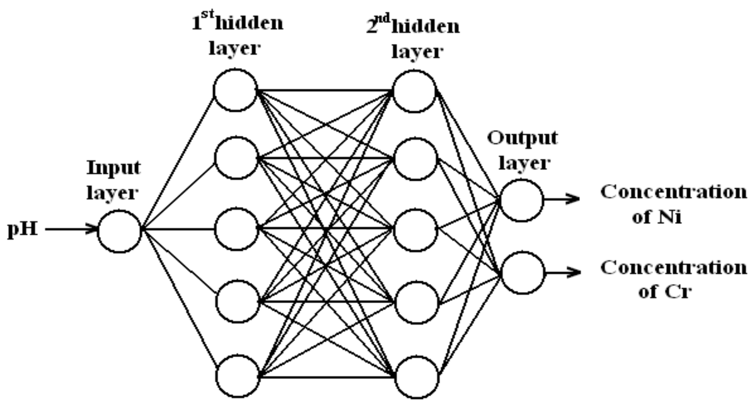

Figure 2. Neural Network Architecture for model NCP

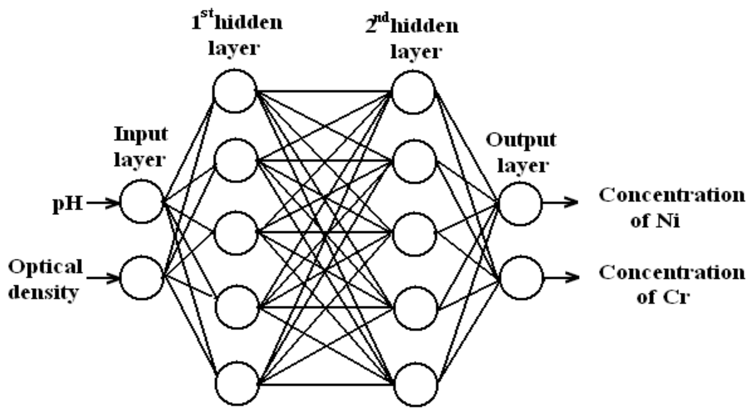

Figure 3. Neural Network Architecture for model NCPO

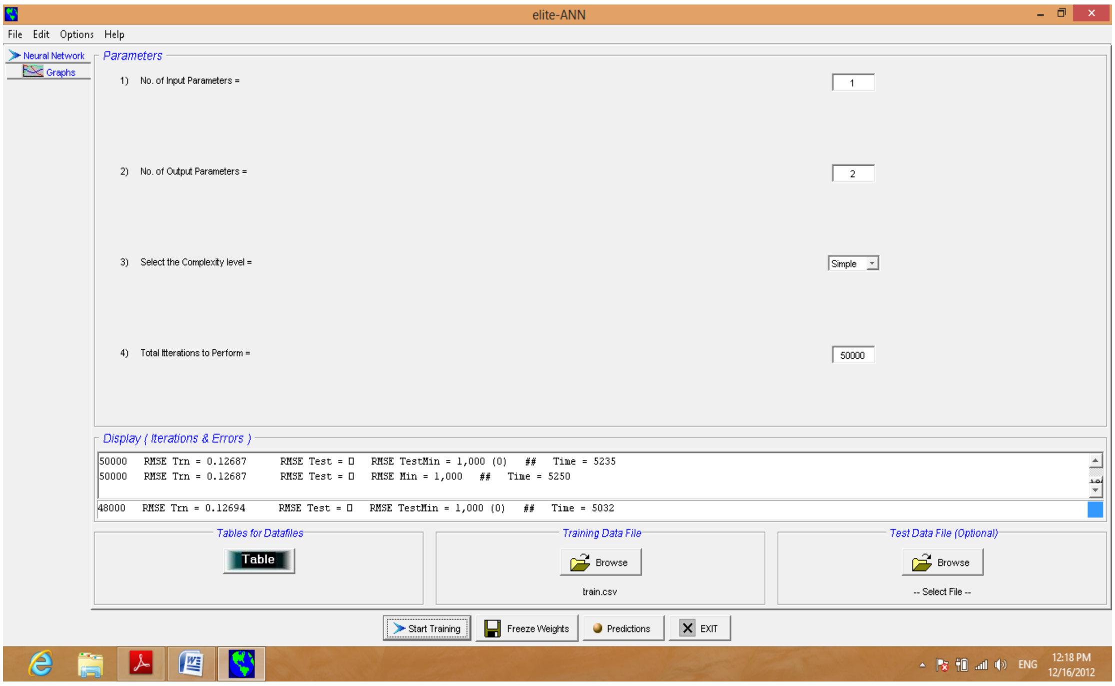

Figure 4. Snapshot of Simulation run

IV. RESULT AND DISCUSSION

- The models developed have been used for prediction of output parameters for given set of input parameters for both the training & test data sets. Comparison of actual and predicted values has also been carried out to arrive at the most suited model.

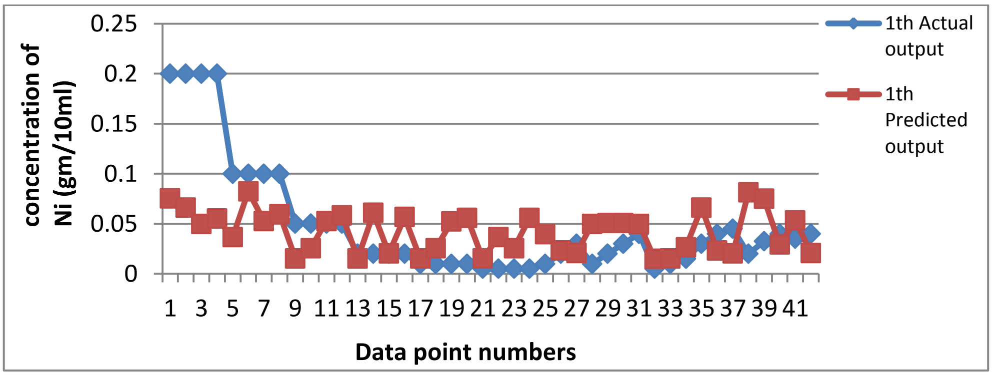

Figure 5. Comparison of actual and predicted output values for concentration of Ni for training data points obtained by model NCO

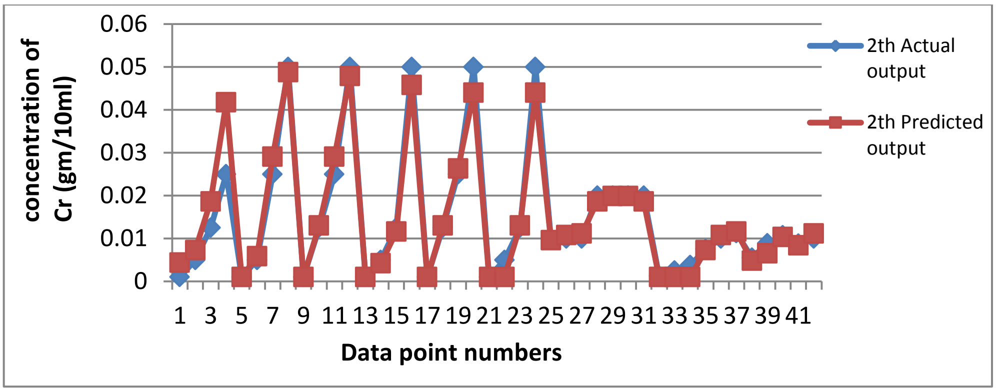

Figure 6. Comparison of actual and predicted output values for concentration of Cr for training data points obtained by model NCO

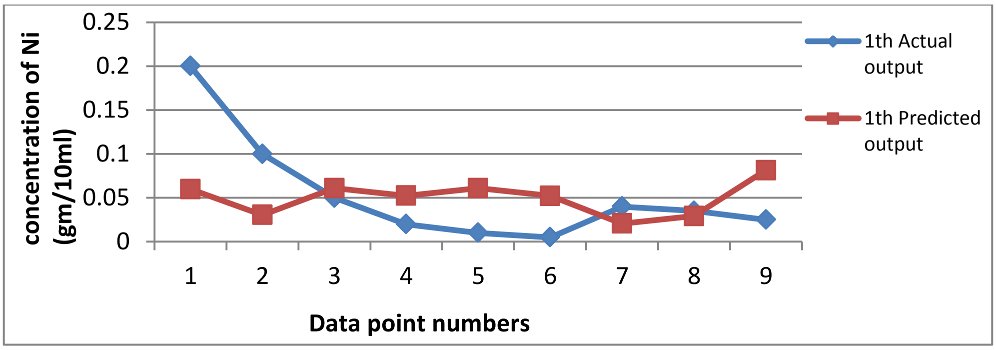

Figure 7. Comparison of actual and predicted output values for concentration of Ni for test data points obtained by model NCO

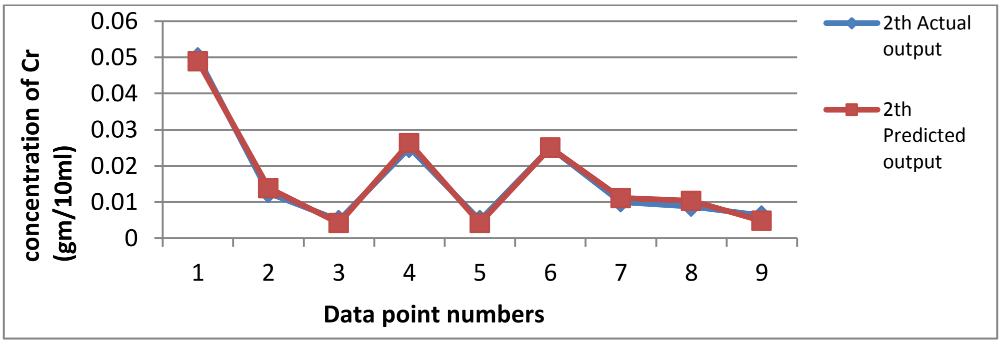

Figure 8. Comparison of actual and predicted output values for concentration of Cr for test data points obtained by model NCO

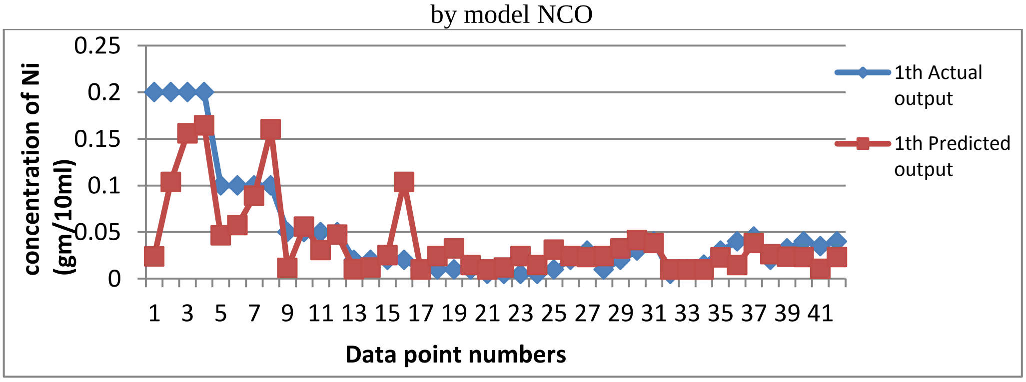

Figure 9. Comparison of actual and predicted output values for concentration of Ni for training data points obtained by model NCP

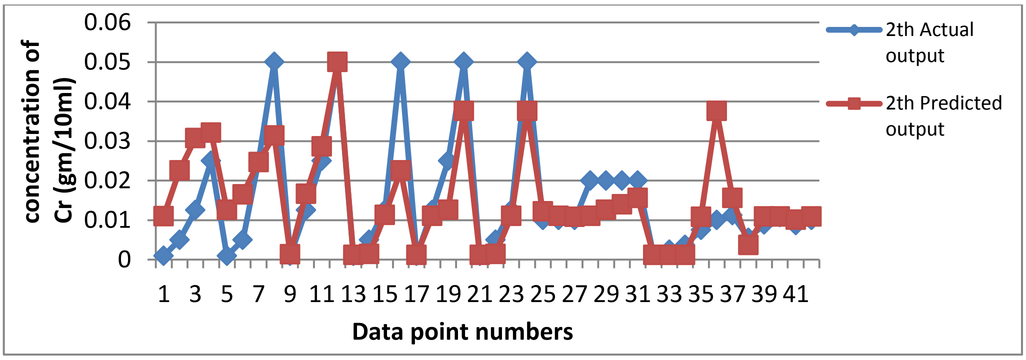

Figure 10. Comparison of actual and predicted output values for concentration of Cr for training data points obtained by model NCP

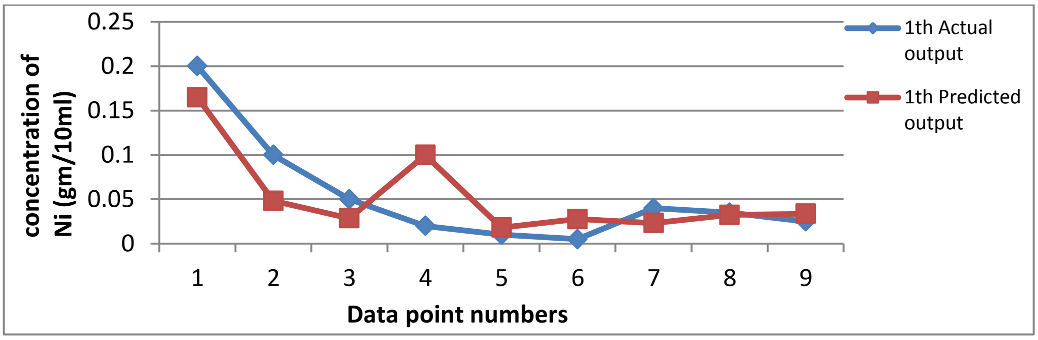

Figure 11. Comparison of actual and predicted output values for concentration of Ni for test data points obtained by model NCP

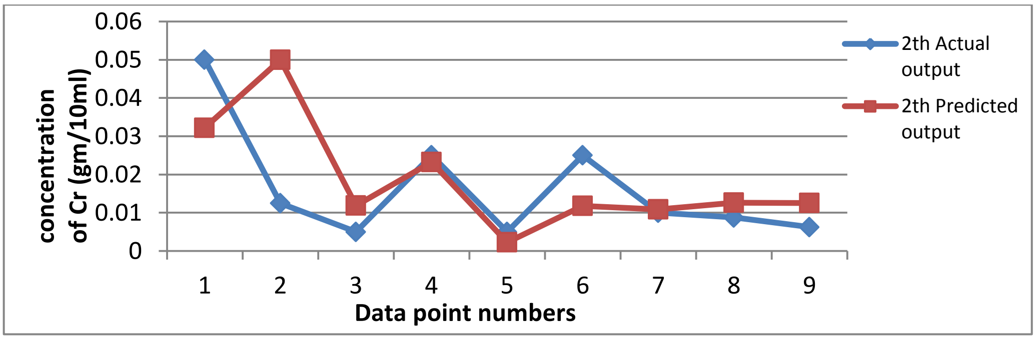

Figure 12. Comparison of actual and predicted output values for concentration of Cr for test data points obtained by model NCP

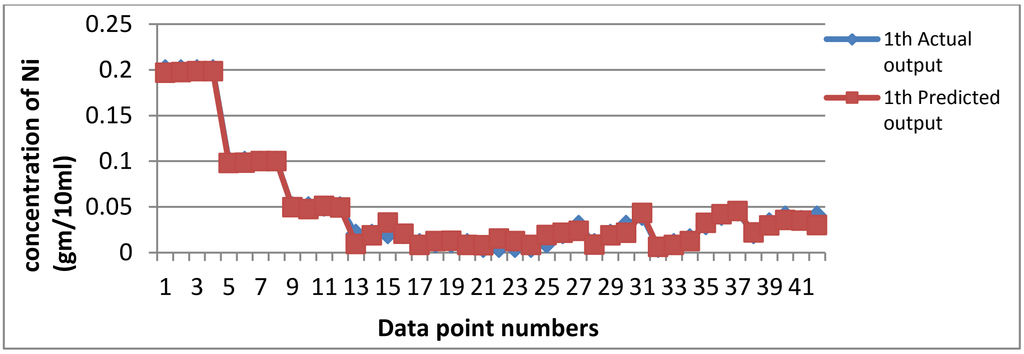

Figure 13. Comparison of actual and predicted output values for concentration of Ni for training data points obtained by model NCPO

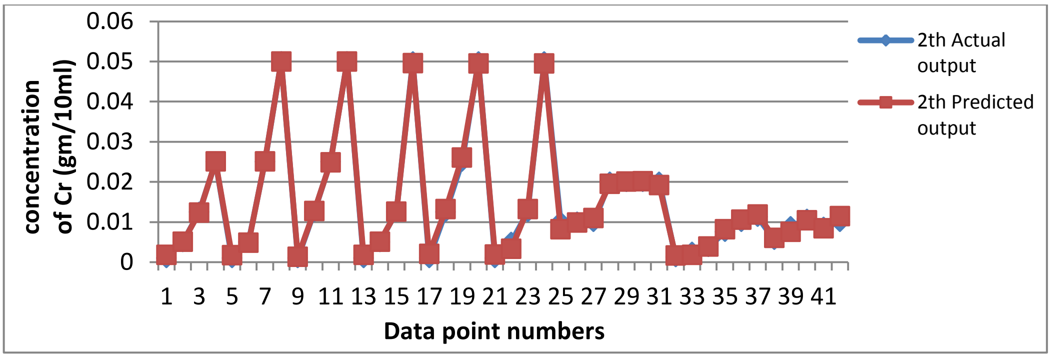

Figure 14. Comparison of actual and predicted output values for concentration of Cr for training data points obtained by model NCPO

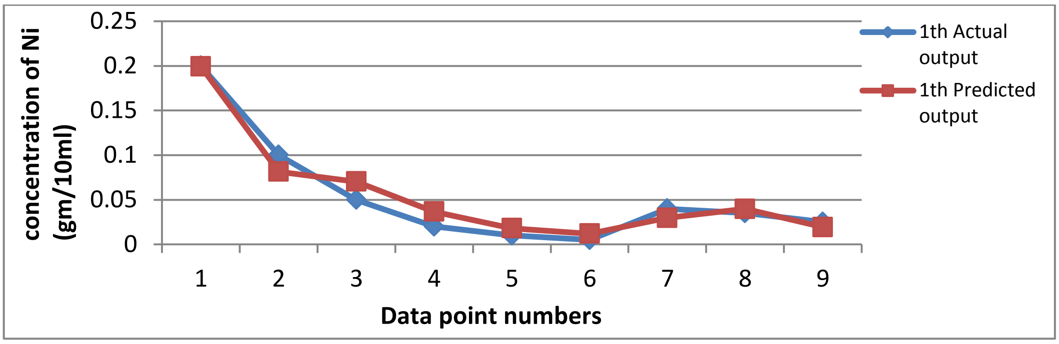

Figure 15. Comparison of actual and predicted output values for concentration of Ni for test data points obtained by model NCPO

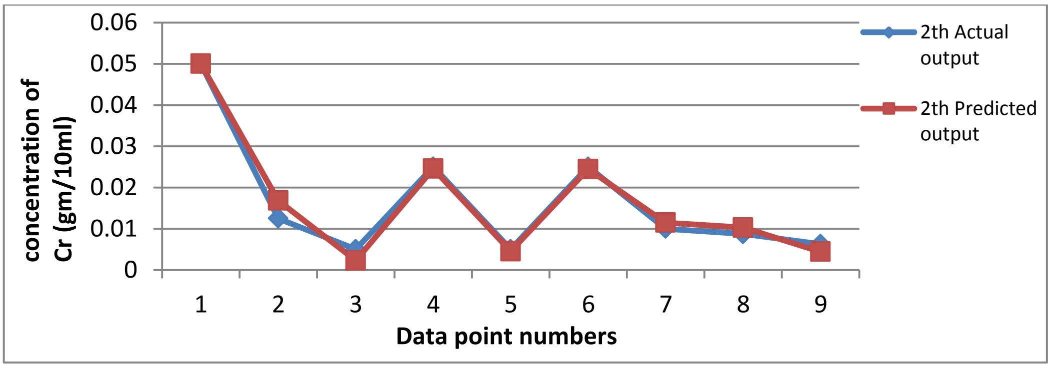

Figure 16. Comparison of actual and predicted output values for concentration of Cr for test data points obtained by model NCPO

- Figures 5 & 6 and 7 & 8 show the comparison for actual and predicted values of concentration of Ni (II) and Cr (VI) for training & test data sets respectively as obtained by ANN model NCO. As can be seen from these graphs there are deviation for prediction of Ni (II) & Cr (VI) concentration for both training & test data set respectively using model NCO.
- Figures 9 & 10 and 11 & 12 show the comparison for values obtained using ANN model NCP.
- The predictions for training data sets have accuracy similar to as obtained by using model NCO. However, the chromium concentrations are predicted fairly accurately by model NCO than model NCP.
- Figure 13 & 14 and 15 & 16 show the comparison for values obtained using ANN model NCPO.

- The nature of graphs depicted in these figures indicts high level of accuracy for predicted values of Ni (II) and Cr (VI) for the both training & test data sets.
- Based on comparisons, it can be inferred that of the three models developed in present work, NCPO is most suitable based on the criterion of RMSE training & test.
- The accuracy claim of NCPO are further substantiated by calculation of % relative error for each data point and is depicted in figure 17 & 18 and 19 & 20 for training and test data set respectively.
- The distribution of % relative error for data point has been carried out in the range of ±5 and ±40 as shown in table2.

Table 2. Distribution of % relative error for data points for ANN model NCPO

Data points	% Relative error = (Actual value –Predicted value)/ Actual value × 100				
	Metal ion	< ± 5	± 5 to ±20	±20 to ±40	>±40
Training data points 42	Ni (II)	19	11	7	5
	Cr (VI)	23	9	3	7
Test Data points 9	Ni	1	1	4	3
	Cr	3	3	2	1

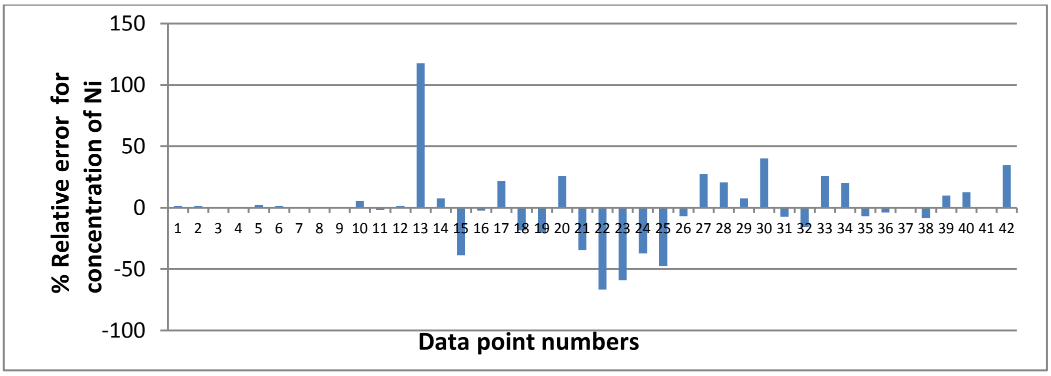

Figure 17. % relative error for estimation of concentration of Ni for ANN model NCPO for training data set

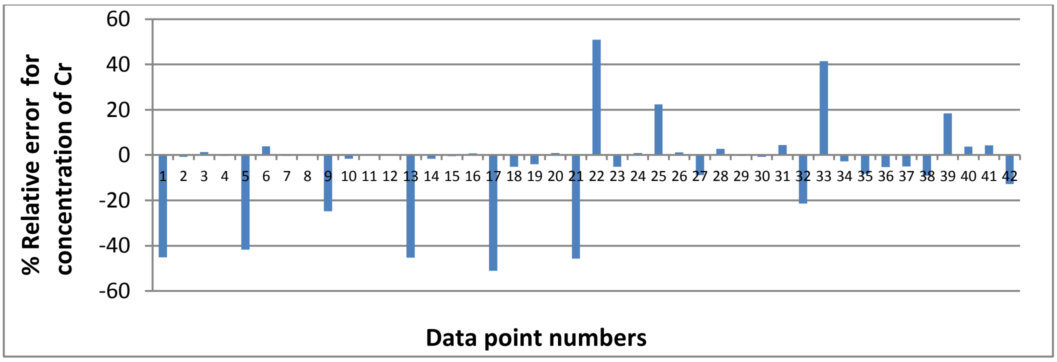

Figure 18. % relative error for estimation of concentration of Cr for ANN model NCPO for training data set

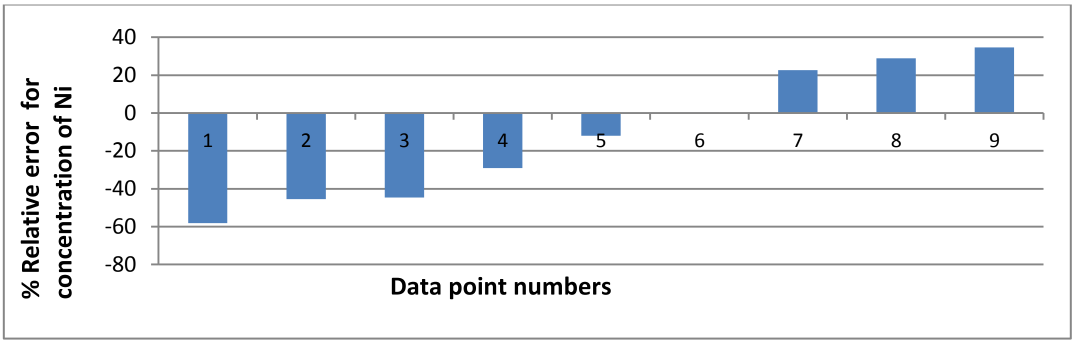

Figure 19. % relative error for estimation of concentration of Ni for ANN model NCPO for test data set

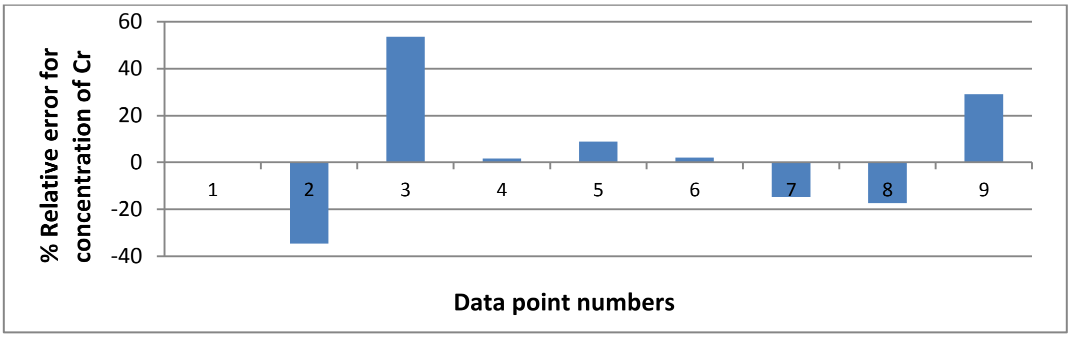

Figure 20. % relative error for estimation of concentration of Cr for ANN model NCPO for test data set

V. FUTURE WORK

The work can be further extended to innumerable situations in industrial processes for estimation of concentration of single and or binary heavy metallic ions present in aqueous solution. There is scope for further studies to explore incorporation of combination of other easily measurable physical properties in developing ANN models.

VI. CONCLUSION

The present work has explored the application of artificial neural network in modeling the concentration of an aqueous solution having two metallic ions simultaneously present with the physical properties optical density and pH. Based on experimental observations, results & discussions, it can be inferred that the present work has been successful in demonstrating the utility of artificial neural network model in estimating concentrations of Ni (II) and Cr (VI) simultaneously present in the aqueous solution in the range 0.247 to 49.38 mg/10ml and 0.353 to 17.67 mg/10ml with its physical properties such as optical density & pH .The ANN models NCO and NCP developed using single physical property optical density and pH respectively, with the concentrations of Ni (II) & Cr (VI) have been observed to be lower in accuracy than the ANN model NCPO developed using two input physical properties optical density & pH. The % relative error for maximum data points predicted is between 5 to 40 using NCPO which is acceptable. The results of this study indicate that the back propagation neural network model NCPO with 2-5-5-2 architecture and Root Mean Square Error (RMSE) of 0.0195 and 0.0520 for prediction of training and test data sets respectively, has the best performance than the other two model.

ACKNOWLEDGEMENTS

Authors are thankful to Director, LIT, Nagpur for the facilities and encouragement provided.

REFERENCES

[1]. Kaan Yetilmezsoy, Sevgi Demirel, (2008) "Artificial neural network (ANN) approach for modeling of Pb(II) adsorption from aqueous solution by Antep pistachio (*Pistacia Vera* L.) shells", *Journal of Hazardous Materials*,Vol.153, pp1288-1300.

[2]. S. L. Pandharipande, Anish M. Shah & Heena Tabassum, (2012) "Artificial Neural Network Modeling for Estimation of Composition of a Ternary Liquid Mixture with its Physical Properties such as Refractive Index, pH and Conductivity", *International Journal of Computer Applications,* Vol. 45, No. 9, pp 26-29.

[3]. Anderson J.A (1999) An Introduction to Neural Networks, Prentice-Hall of India, Pvt Ltd New Delhi.

[4]. Rumelhart D E & McClleland (1986) Back Propagation Training Algorithm Processing, M.I.T Press, Cambridge Massachusetts.

[5]. R. D. Khonde & S. L. Pandharipande, (2011) "Application of Artificial Neural Network for Standardization of Digital Colorimeter", *International Journal of Computer Applications,* ICCIA-5, pp 1-4.

[6]. Zamankhan, P., Malinen, P., Lepomaki, H., (1997) "Application of Neural Networks to Mass Transfer Predictions in a Fast Fluidized Bed of Fine Solids", *AIChE,* Vol. 43, pp 1684-1690.

[7]. S. L. Pandharipande & Ankit Singh (2012) "Optimizing topology in developing artificial neural network model for estimation of hydrodynamics of packed column", *International Journal of Computer Applications*, Vol. 58, No. 3, pp 49-53.

[8]. J. C. Hoskins , K. M. Kaliyur & David M. Himmelblau, (1991) "Fault diagnosis in complex chemical plants using artificial neural networks", *AIChE*, Vol.37, No.1,pp137-141.

[9]. R. D. Khonde & S. L. Pandharipande, (2012) "Artificial Neural Network modeling for adsorption of dyes from aqueous solution using rice husk carbon", *International Journal of Computer Application,* Vol. 41, No.4, pp 1-5.

[10]. Shekhar Pandharipande & Anish M Shah, (2012) "Modeling combined VLE of four quaternary mixtures using artificial neural network", *International Journal of Advances in Engineering, Science and Technology (IJAEST),* Vol. 2, No. 2, pp 169-177.

[11]. S. L. Pandharipande , Aditya Akheramka, Ankit Singh & Anish Shah, (2012) "Artificial Neural Network Modeling of Properties of Crude Fractions with its TBP and Source of Origin and Time", *International Journal of Computer Application,* Vol. 52, No.15, pp 20-25.

[12]. S A Mandavgane, S L Pandharipande & D Subramanian, (2006) "Modeling of desilication of green liquor using artificial neural network", *International journal of chemical technology,* Vol. 13, pp 168-172.

[13]. H.R. Godini, M. Ghadrdan, M.R. Omidkhah & S.S. Madaeni, (2011) "Part II: Prediction of the dialysis process performance using Artificial Neural Network (ANN)", *Desalination*, Vol. 265, pp 11-21.

[14]. Pandharipande S L & Badhe Y P, elite-ANN©, ROC No SW-1471/2004.

AUTHORS

S. L. Pandharipande is working as associate professor in Chemical Engineering department of Laxminarayan Institute of Technology, Rashtrasant Tukadoji Maharaj Nagpur University, Nagpur. He did his masters in 1985 & joined LIT as a Lecturer. He has coauthored three books titled 'Process Calculations', 'Principles of Distillation' & 'Artificial Neural Network'. He has two copyrights 'elite-ANN' & 'elite-GA' to his credit as coworker & has more than 50 papers published in journals of repute.

Aarti R. Deshmukh received the Bachelor of Technology in Chemical Engineering in 2011 from College of Engineering and Technology, Akola, Sant Gadge Baba Amravati University, Amravati. She is currently pursuing the M. Tech. (Chemical Engineering) from Laxminarayan Institute of Technology, Nagpur.

Rohit Kalnake received the Bachelor of Technology in Chemical Engineering in 2011 from Anuradha Engineering College, Chikhali, Sant Gadge Baba Amravati University, Amravati. He is currently pursuing the M. Tech. (Chemical Engineering) from Laxminarayan Institute of Technology, Nagpur.