International Journal of Recent Technology and Engineering (IJRTE)
ISSN: 2277-3878, Volume-8 Issue-3, September 2019

Optimization and Assessment of Residual Chlorine using Response Surface Methodology (RSM) and Artificial Neural Network (ANN) Modeling

Manahel Mohammad Al-Araimi, Varghese Manappallil Joy, Lakkim Setty Nageswara Rao, Shaik Feroz

Abstract*: Water polluted with microorganisms and pathogens is one of the most significant hazards to public health. Potential microorganisms unsafe to human health can be destroyed through effective disinfection. To stop the re-growth of microorganisms, it is also advisable to take care of the residual disinfectant in the water distribution networks. The most frequently used cleanser material is chlorine. When the chlorine dosage is too low, there will be a deficiency of enough residues at the end of the water network system, leading to re-growth of microorganisms. Addition of an excessive amount of chlorine will lead to corrosion of the pipeline network and also the development of disinfection by-products (DBPs) including carcinogens. Thus, to determine the best rate of chlorine dosage, it is essential to model the system to forecast chlorine decay within the network. In this research study, two major modeling and optimization strategies were employed to assess the optimum dosage of chlorine for municipal water disinfection and also to predict residual chlorine at any predetermined node within the water distribution network. Artificial neural network (ANN) modeling techniques were used to forecast chlorine concentrations in different nodes in the urban water distribution system in Muscat, the capital of the Sultanate of Oman. One-year dataset from one of the distribution system was used for conducting network modeling in this study. The input factors to RSM model considered were pH, chlorine dosage and time. Response variables for RSM model were fixed as total organic carbon (TOC), Biological oxygen demand (BOD) and residual chlorine An Artificial neural network (ANN) model for residual chlorine was created with pH, inlet-concentration of chlorine and initial temperature as input parameters and residual chlorine in the piping network as an output parameter. The ANN model created using these data can be employed to forecast residual chlorine value in the urban water network at any given specific location. The results from this study utilizing the uniqueness of an ANN model to predict residual chlorine and water quality parameters have the potential to detect complex, higher-order behavior between input and output parameters exist in urban water distribution system.

Keywords: Chlorine-Disinfection; Artificial Neural Network; Municipal Water Distribution Network Modeling, Response Surface Methodology (RSM)

Manuscript published on 30 September 2019
* Correspondence Author
Manahel Mohammad Al-Araimi* , MIE Dept., College of Engineering, National University of Science and Technology, Muscat ,Oman
Varghese.M.J*, CCCI, College of Engineering, National University of Science and Technology, Muscat ,Oman, E-mail:varghesemj@yahoo.com
Lakkim Setty Nageswara Rao, MIE Dept., College of Engineering, National University of Science and Technology, Muscat ,Oman.
Shaik Feroz, College of Engineering, National University of Science and Technology, Muscat ,Oman

I. INTRODUCTION

Chlorine is one of the most widely accepted disinfectants used in the treatment process of drinking water pollutant remediation across the world. When suitably employed at the end of the treatment process, the goal is to eliminate pathogens. When exiting the treatment plant, the chlorine flows across the piping network within water distribution system; it experiences a sequence of chemical reactions. Majorly there are two types of reactions occur in the piping network, viz: the first one is the reactions within the bulk of water and the second one is the reactions with the pipe inner-wall. Water needs a residual amount of chlorine to guarantee microbiological steadiness during transport through the circulation system. However, the chemical reaction of excess-chlorine with organic mixtures may lead to the formation of secondary products of disinfectant (DBPs), some of which are even carcinogens [1]. The more the dosage of chlorine and the bigger the amount of organic matter contained in the water, great chance for the formation of DBPs. It is very common at drinking water facilities that the major challenges facing is balancing the benefits and disadvantages of chlorine-disinfection.

To maintain optimum chlorine-concentration throughout the water circulation network, it is necessary to add chlorine at different locations in the circulation system through chlorine booster-stations. They must ensure that adequate doses of chlorine to sustain microbiological quality and reduce the development of DBP through the distribution system. The residual chlorine concentration may become too low at locations far from chlorination points, in the distribution system. Since number of parameters and factors involved, residual chlorine decay is a complex type of phenomenon [2]. The input factors may be linked to the final quality of the treated water and the operating criterion in the treatment plant or in the water circulation system and characteristics of the piping system.

Disinfection is one of the important pretreatment methods used to destroy microorganisms that cause waterborne diseases and inhibit bio fouling. There are many types of methods of disinfection, including chemical, electrical, ultrasonic, ultraviolet and thermal radiation [3].

Among these methods, the most popular ones are chemical means. These include chemical agents such as species of ozone and chlorine such as hypochlorite, chloramines and chlorine dioxide. Water adulterated with microorganisms and pathogens is one of the most important hazards to public health. Potential microorganisms dangerous to human health can be destroyed through disinfection. To stop the regrowth of microorganisms, it is also advisable to take care of the residual disinfectant in the urban water circulation system. Frequently used type of cleanser is chlorine due to its universal disinfection qualities. When the dosage of chlorine is considerably low, there will not be enough residues at the farthest location in water network system, leading to re-growth of microorganisms[3]. On the other hand, the addition of an excessive amount of chlorine will promote corrosion of the piping system and also the generation of disinfectant by-products, including carcinogens. Thus, to compute the optimum rate of chlorine doses, it is vital to generate a model to forecast chlorine degradation within the piping network system. The solution lies in accurate modelling of the complex interaction between parameters of water distribution system [4]. After reverse osmosis (RO) desalination procedures at water producing plants, it is transferred to various customers. The Omani Standard ensures a prescribed quantity of chlorine for the drinkable water. The problem is the safeguard measures to shield water quality parameters during this transfer, which may take considerable amount of time, making it free from any bacteriological pollution. The level of chlorine could reduce during the distribution process, depending on the time duration and the influence of other parameters like presence of organic matter, temperature or due to piping material. Hence it is a common practice that after desalination, the water is chlorinated to attain the Omani Standards (where the value of free-chlorine range between 0.2mg/l and 0.5mg/l).

Chlorine is one of the chemical disinfectants most commonly used for municipal water disinfection and decontamination. It reacts and produces hypochloric and hydrochloric acids when added to water. Hypochloric acid partially dissociates and oxidizes the microorganisms, which are more effective at low pH. Chlorine decay means a decrease in chlorine concentration in drinking water as it moves from the water treatment plant to the end of the distribution network. Once disinfection has been completed at the water treatment plant, the chlorine will continue to react with any organic or inorganic material that may be available in intermediate reservoirs or distribution pipes (e.g. organic sediments, corroded metals, pipe fittings, pipe materials, bacterial slimes etc). The chlorine concentration at the end of the network will be usually less than the concentration in the water plant [1]. This phenomenon can happen because of various reasons: viz: type of material used in distribution pipes or tanks and duration of water remains in the distribution system. Modeling techniques like the artificial neural network is successfully employed in predicting residual chlorine at any particular node within the water distribution system

II. MATERIALS AND METHODS

In this research study, two major strategies of real-time data modeling and optimization were employed to assess the optimum dosage of chlorine for municipal water disinfection and also to predict residual chlorine at any predetermined node within the water distribution network. Real-time data for one year were collected from the Public Authority of Water, Muscat, Oman to model the water distribution network by using an artificial neural network (ANN) techniques. Factors like initial chlorine dosage, temperature and pH were used as input variables to ANN and residual chlorine concentration at selected nodes were fixed as the output of the ANN. The network model is created by mapping, one-year data of these three input parameters to the output parameter, which is residual chlorine. ANN model was created using MATLAB neural network tool box. The created ANN model was used for predicting new values of residual chlorine for a given combination of input parameters. Test prediction conducted using ANN model showed less than 1 % error.

Design of experiments (DOE) integrated with response surface statistical regression methodology (RSM) was employed to compute the optimum initial chlorine dosage to municipal water for effective disinfection treatment. The input factors to RSM model considered were pH, chlorine dosage and time. Response variables for RSM model were fixed as Total Organic Carbon (TOC), Biological Oxygen Demand (BOD) and residual chlorine. For RSM modeling a total of 17 experiments were done as per the design matrix is shown in Table 1. Input variables such as pH, chlorine dose and contact time are varied in the range of 4-8, 1-2 mg/L and 30-60 min respectively.

Artificial neural networks techniques are stimulated by biological type of neural system. In this modeling strategy, the weighted sum of the inputs arriving at each neuron is allowed to pass over an activation-function from which the output signals are being generated [5]. A supplementary bias value is incorporated to the weighted sum for enhancing or minimizing the added input supplied to the activation function. The architecture of the network and synaptic connection between the processing units determines the synthesis of function. Most of the ANN architectures used in engineering problems modeling utilizes feed-forward networking where the model is trained with input-output data using error-back-propagation algorithm. The input node or neuron number is equal to the number of input factors. ANN input layer nodes or neurons represent the input variables or independent factors and the number of output layer neurons represents the response factors or independent variables [6]. The purpose of the hidden layers is to accomplish nonlinear conversions of the input data space and is typically used for network calculation purpose. Rodriguez et al. have demonstrated that a three-layer perceptron of ANN employing sigmoid transfer-function is capable of mapping and generalizing any function of real-world importance [2].

In the present research study, for ANN model development, following input factors were selected, viz: temperature, initial chlorine concentration and pH.

Output layer comprise of a single neuron which represents the residual chlorine response variable. The input layer of ANN consists of three neurons which represent the number of independent factors. Fig.1 represents the schematic diagram of three-layered feed-forward ANN network architecture with three input nodes, ten hidden neurons and a single output neuron. The number of neurons in the hidden layer is a random choice and based on the error value between target and ANN output.

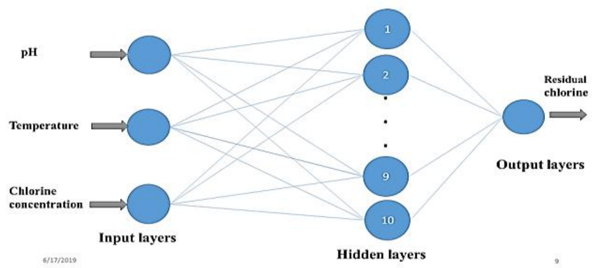

Figure 1 : Three-layered feed-forward ANN network architecture consist of three input nodes, ten hidden neurons and a single output neuron

Before ANN modeling, design of experiments (DOE) integrated with response surface statistical methodology (RSM) was employed to compute the optimum initial chlorine dosage to municipal water for effective disinfection treatment. Design of experiment (DOE) is a systematic empirical method to determine the interactive relationship between process input factors and quantify how it affects the response variables of the process through statistical analysis. The regression equations developed and validated with various statistical techniques are used to find cause-and-effect relationships between input and response variables associated with the process. This information is needed to manage process inputs to optimize the output. Controllable input factors or x factors are those parameters which can be changed in an experiment or process. These parameters which cannot be changed are uncontrollable input factors. Responses or output measures are the elements of the outcome of the process

Response Surface Method of modeling is a typical statistical methodology that utilizes empirical data attained from a statistically designed matrix in order to optimize the output response of a process. Statistical modeling is performed in any process in which the output parameter of interest is affected by numerous input factors [7]. Mainly, response surface optimization methodology is executed by practicing three sequential steps viz., carrying out the empirical and statistically considered experimentation, approximating regression coefficients of input variables in a mathematical model and in the final step predicting the responses accurately after verifying the adequacy of the model [8].Response Surface statistical Methodology aid to compute the interactive relationships among and between output factors called dependent response variables (Y) and input factors known as independent factors (X's). A typical RSM surface design called Central Composite Design (CCD) was utilised in the present modeling study. This statistical technique is suitable for fitting a quadratic surface and aid to optimize the effective response parameters and regression coefficients by performing minimum number of experiments. The model created will enable to analyze the interaction between input parameters and quantify how each factors influence the response variable [9]. In general, the Central Composite Design (CCD) consists of a 2^k factorial runs with 2k axial runs and k_c central runs where 'k' indicates the number of input parameters. The center points are utilized to evaluate the random process variation called pure error which demonstrate the reproducibility within the experimentation and data generation. Thus, for the initial optimization study comprising three independent parameters (n = 3), seventeen number (17) of experiments were required in total. The sequence of experimental runs was randomized to minimize the influence of uncontrollable factors. The outcome from each run was populated into the Design Expert software to associate the response parameters with input factors. The experimental second degree polynomial regression equation for a response that explains its behavior is given by a second-order quadratic equation.

ANOVA statistical methodology was used to model the system characterized by independent input factors and dependent output response and to optimize the process by determining the coefficients and statistical regression parameters. The statistical experimentation design as identified by the Design-Expert software is demonstrated in Table 1.

III. RESULTS AND DISCUSSION

Figure 3, (a), (b) and (c) shows the response surface plots generated by Design-Expert software for responses Residual chlorine, BOD % removal and TOC % removal, respectively. In these figures, the response surfaces corresponding to the output residual chlorine is depicted as a function of initial chlorine dosage and pH, BOD % removal as a function of time and dosage and TOC % degradation as a function of input dosage and time. The regression model equations for each of these responses are shown in equations (1), (2) and (3).

$$\text{TOC \% Removal} = +89.94 - 2.10A + 3.80B - 0.6000C \tag{1}$$

$$\text{BOD \%Removal} = +86.82 - 2.40A + 1.40B - 0.2000C + 3.50AB + 5.75AC - 0.7500\,BC \tag{2}$$

$$\text{Residual Chlorine} = +0.2247 - 0.001A + 0.0850B - 0.0250\,C \tag{3}$$

For 17 runs of DOE generated experimental work, input variables such as pH, chlorine dosage and reaction time are varied in the range of 4-8, 1-2 mg/L and 30-60 minutes respectively. In each of these runs, all the three response values were measured and populated to the Design-Expert DOE matrix. Subsequently, the regression models that are shown in Eq (1), (2) and (3) were developed by the software and statistically validated the significance by ANOVA technique. By analyzing coefficient values of each factor in Equation (1),

it can be established that factor C (Reaction time) has more

Table 1 Statistical Experimental Design Matrix with Empirically Calculated Response Variables

Run	Design-Space Type	A:pH	B:Dosage mg/L	C:Time Minutes	D:TOC ppm	BOD ppm	Residual Chlorine
1	Axial	6	2	45	94	92	0.36
2	Factorial	8	2	30	91	80	0.32
3	Factorial	4	2	60	96	90	0.37
4	Axial	8	1.5	45	91	87	0.12
5	Axial	6	1.5	30	94	90	0.18
6	Factorial	4	1	60	91	76	0.03
7	Factorial	4	1	30	90	94	0.2
8	Center	6	1.5	45	84	80	0.28
9	Axial	6	1	45	80	82	0.27
10	Axial	6	1.5	60	80	90	0.13
11	Center	6	1.5	45	91	87	0.34
12	Center	6	1.5	45	91	85	0.11
13	Factorial	4	2	30	95	96	0.35
14	Factorial	8	1	60	87	97	0.16
15	Factorial	8	2	60	94	82	0.29
16	Factorial	8	1	30	84	77	0.18
17	Axial	4	1.5	45	96	91	0.13

influence on TOC % Removal, compared to factor A (pH) and factor B (Dosage). The negative value of the coefficient of factor C (-0.60) indicates that as the reaction time increases from its center value (45 minutes) to maximum value (60 minutes), TOC % removal will be decreased by six units. By analyzing Eq (2), it can be observed that the interaction between pH and Time (AC interaction with highest coefficient +5.75 compared to other factors) has the largest effect on BOD % Removal. From Eq (3), it can be deducted that factor B (Chlorine dosage) has more influence on the value of residual chlorine.

Optimization studies using desirability function is performed to determine the optimum values of TOC % removal, BOD % removal and Residual chlorine using Design-Expert software. The optimum conditions obtained as pH (4), dosage (1.408 mg/l), reaction time (30 min) in this method. At optimum set point TOC % degradation, BOD % degradation and COD removal rates found to be 91.94 %, 94.13 % and 0.235 respectively. ANN network model was generated using initial chlorine concentration, pH, and temperature as independent input variables, ten neurons or nodes in the hidden layer, and residual chlorine as the dependent output neuron. Through MATLAB neural network toolbox ANN network model was created by using one-year real-time input-output data collected from a water distribution network in Muscat, Oman. Neural network training was operated with a hidden layer containing 10 neurons and was being trained until the mean squared error between target and model output became the least.

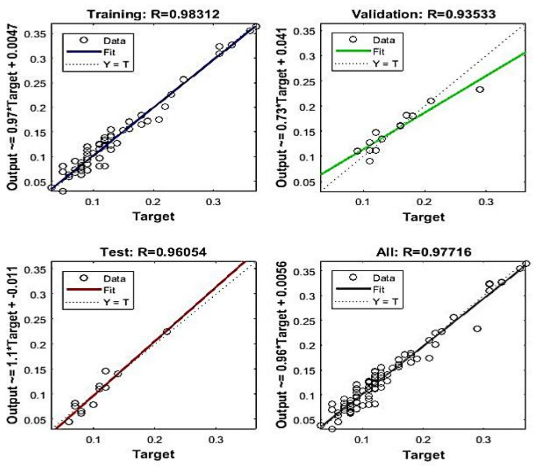

Figure 2: Comparison between ANN network model outputvalues and target values of residual chlorine

The data collected from the Public Authority of Water were split into three groups consist of data for training, testing and validation. At the validation stage, generalizations of the artificial neural network were verified with respect to the desired value or the value required mapping residual chlorine as the target. Figure 2 shows the comparison between ANN network model output values and target values of residual chlorine. High correlation coefficient value for training, validation and testing as well as overall comparison depicts that the model is good enough to predict the value of residual chlorine at any predetermined

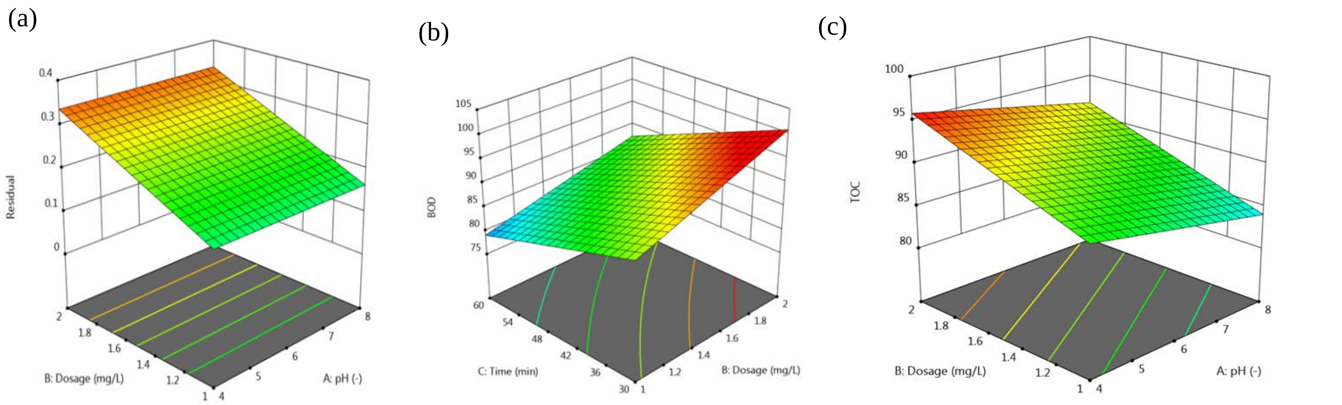

Figure 3: **Response surfaces corresponding to (a) Residual chlorine as a function of initial chlorine dosage and pH (b) BOD % Degradation as a function of Time and dosage (c) TOC % Degradation as a function of pH and Dosage**

location within the water distribution network. The confirmation runs with new data shown that the error between target and output was less than 1 %. This error value is in good agreement with the previous study conducted for residual chlorine prediction in the urban network [2].

IV. CONCLUSION

Chlorination in urban water networks is always a challenging task. Determining optimum chlorine is essential to prevent over-chlorination as well as under-chlorination. While over-chlorination may lead to the generation of disinfection bye-products, some of which are even carcinogens, under-chlorination may lead to poor disinfection. In this research, artificial neural networks modeling technique was employed to predict chlorine concentrations at any selected node within the urban water distribution network. A one-year dataset from real-time urban water distribution network was used to model the residual chlorine concentration at any selected node within the system. Initial optimization study for chlorine disinfection was conducted using the design of experiments (DOE) and response surface methods (RSM). An Artificial neural networking (ANN) model for residual chlorine is created with pH, inlet-concentration of chlorine from the desalination plant and initial temperature as input parameters. This data can be used to forecast the residual chlorine value in the municipal water circulation network at any given specific location. The findings from this study will help the operator to determine the exact amount of chlorine dosage to be fed at the input locations so that there will not be any excess amount or any lower concentration leading to insufficient disinfection at any locations within the urban water distribution piping network. The results from this study demonstrate the uniqueness of an ANN model to predict residual chlorine, which has the potential to detect complex, non-linear behavior between data. The statistical/ANN model created in this study will help engineers to ensure safe-supply of potable water to the end users free of pathogens and cancer causing disinfection bye-products.

REFERENCES

1. I. E. Karadirek, S. Kara, A. Muhammetoglu, H. Muhammetoglu, and S. Soyupak, “Management of chlorine dosing rates in urban water distribution networks using online continuous monitoring and modeling,” Urban Water J., vol. 13, no. 4, pp. 345–359, 2016.
2. M. J. Rodriguez and J. B. Sérodes, “Assessing empirical linear and non-linear modelling of residual chlorine in urban drinking water systems,” Environ. Model. Softw., vol. 14, no. 1, pp. 93–102, 1998.
3. M. Zounemat-Kermani, A. Ramezani-Charmahineh, J. Adamowski, and O. Kisi, “Investigating the management performance of disinfection analysis of water distribution networks using data mining approaches,” Environ. Monit. Assess., vol. 190, no. 7, 2018.
4. M. Gibbs, N. Morgan, H. Maier, G. Dandy, M. Holmes, and J. Nixon, “Use of artificial neural networks for modelling chlorine residuals in water distribution systems,” … 2003 Proc. …, no. April 2014, pp. 789–794, 2003.
5. M. S. Bhatti, D. Kapoor, R. K. Kalia, A. S. Reddy, and A. K. Thukral, “RSM and ANN modeling for electrocoagulation of copper from simulated wastewater: Multi objective optimization using genetic algorithm approach,” Desalination, vol. 274, no. 1–3, pp. 74–80, 2011.
6. E. Betiku and S. O. Ajala, “Modeling and optimization of Thevetia peruviana (yellow oleander) oil biodiesel synthesis via Musa paradisiacal (plantain) peels as heterogeneous base catalyst: A case of artificial neural network vs. response surface methodology,” Ind. Crops Prod., vol. 53, pp. 314–322, 2014.
7. S. Chatterjee, A. Kumar, S. Basu, and S. Dutta, “Application of Response Surface Methodology for Methylene Blue dye removal from aqueous solution using low cost adsorbent,” Chem. Eng. J., vol. 181–182, pp. 289–299, 2012.
8. Y. Xie, L. Chen, and R. Liu, “Oxidation of AOX and organic compounds in pharmaceutical wastewater in RSM-optimized-Fenton system,” Chemosphere, vol. 155, pp. 217–224, 2016.
9. M. B. Kasiri, H. Aleboyeh, and A. Aleboyeh, “Modeling and optimization of heterogeneous photo-fenton process with response surface methodology and artificial neural networks,” Environ. Sci. Technol., vol. 42, no. 21, pp. 7970–7975, 2008.

AUTHORS PROFILE

Manahel Mohammad Alaraimi was born in Muscat Oman on September 4, 1991. Presently she is working as lab Instructor at College of Engineering, National University of Science and Technology, Oman. She earned her BSc degree in Chemical Engineering from Caledonian College of Engineering, Oman in 2015. She published one paper as part of her Bachelor degree thesis in Water treatment field. Currently she is doing MSc in Process Engineering at College of Engineering, National University of Science and Technology, Oman.

Dr. Nageswara Rao Lakkimsetty is presently working as Assistant Professor in Department of Mechanical & Industrial Engineering (Chemical Engineering) at College of Engineering, National University of Science and Technology, Muscat, Sultanate of Oman. Dr. Rao has obtained his doctorate in the field of Chemical Engineering from Sri Venkateswara University, India in the year 2013. He has worked with various organizations for 17 years which includes 8 years of research experience. Dr. Rao has 70 research publications to his credit in journals and 60 conferences of international/ National repute. He is a life member of the American Institute of Chemical Engineers, Indian Institute of Chemical Engineers, Institution of Engineers and I.S.T.E. His has a significant contribution as a peer reviewer for various reputed journals. Dr. Rao has interest includes advanced separation processes, Biochemical Engineering Nano-based treatment of wastewater & Environmental engineering.

Prof. Dr. Shaik. Feroz worked as professor at Caledonian college of Engineering, Oman from 2005 to 2017 and currently providing Research Consultancy to College of Engineering, National University of Science & Technology, Oman. Prior to this he has worked with various organizations including 5 years in industry. He has obtained his doctorate in the field of Chemical Engineering from Andhra University, India and Post Doc Research Fellow from Leibniz University, Germany. He has total experience of 25 years in teaching, research and industry. Prof. Feroz has expertise in process engineering, handling of shift activities, plant design and trouble shooting, quality control using advance analytical equipment, wastewater treatment, solar energy systems (PV & CSP) for desalination, hot water systems and water treatment, synthesis of nano photo catalysts, simultaneous treatment of wastewater and production of hydrogen, environmental impact assessment, design, delivery and management of industrial based training programs related to chemical and process engineering. Professor Feroz has more than 150 publications to his credit in journals and conferences of international repute and supervised 4 PhD research works with another 4 on-going. He is a life member of Indian Institute of Chemical Engineers and Institution of Engineers, India. He is also a member of Oman Society of Engineers and Environmental Society of Oman. Professor Feroz is associated as the Principal Investigator/CO-Investigator to a number of research projects and also involved as "Technology transfer agent" by Innovation Research Center, Sultanate of Oman. His has a significant contribution as Editorial member and peer reviewer for various reputed international journals and conferences. He was awarded "Best Researcher" by the Caledonian College of Engineering for the year 2014. Professor Feroz developed research links with various international research centers and his research interest includes solar nano-photocatalysis, solar desalination, solar photocatalytic hydrogen production and environmental engineering.

Mr. Varghese Manappallil Joy is currently employed as Research Assistant and a faculty in MSc-Process Engineering (Program affiliated with University of South Carolina, USA) with College of Engineering, National University of Science and Technology, Muscat, Sultanate of Oman. He has worked with various organizations for 24 years which includes 7 years of research experience He is currently pursuing his PhD in Chemical Engineering with National Institute of Technology-Durgapur (NIT Durgapur), West Bengal, India. He has co-authored more than 25 publications in Environmental Engineering, Nanotechnology, Renewable Energy, Reverse Osmosis (RO) pretreatment, Water and wastewater treatment and Solar Nano Photocatalysis Research areas. He has been involved in various funded research projects awarded from The Research Council (TRC), Oman. He has undergone training in Japan for operation and maintenance of highly sophisticated analytical equipment with SCHIMADZU, JAPAN.