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A Decision Support System for Coagulation and Flocculation Processes Using the Adaptive Neuro-fuzzy Inference System

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Abstract

Decision Support System (DSS) is an approach to have a smart and sustainable management of facilities for monitoring, predicting and controlling sections. The mentioned platform can be useful in operation of complex facilities like the Water Treatment Plant (WTP). This study proposes an Adaptive Neuro-fuzzy Inference System (ANFIS) for prediction of energy consumption and outlet turbidity according to inlet turbidity and ferric chloride as coagulant in coagulation and flocculation unit process of WTP. The outcomes of ANFIS model are used in the Petri Net modelling as a smart conceptual control system. Therefore, the main purpose of this research is the development of a DSS model for coagulation and flocculation processes in WTP. The results of quantitative data analysis showed that the correlation coefficients of ANFIS model are more than 80% meaning that it can reliably predict the outlet turbidity and energy consumption's variables. With regards to our findings, the first one is to provide a smart and sustainable control system to be implemented in operations of coagulation and flocculation process in WTPs. It goes without saying that, our DSS model confirms that the variation of $15\pm5\%$ for turbidity values and the additive coagulant materials (ferric chloride) should be set, on 60-85 and 40-60 kg/day, respectively for controlling energy consumption and outlet turbidity. At last but not least, the main benefit from our DSS model is to manage the operation of WTP with a high efficiency and low human-based errors.

Keywords: Coagulation and Flocculation, Turbidity, Energy Consumption, Coagulant Material, ANFIS

1. Introduction

Nowadays, the research on sustainability and resiliency aspects of water supply systems are an active research topic (Mosallanezhad et al., 2021; Fasihi et al., 2021). One of the main uses of water supply systems is to provide drinking water considering proper related qualitative standards. As a result, water resources, whether surface or groundwater, must undergo certain treatments based on their contamination levels (Lu et al., 2017). Results of previous research has shown that groundwater water resources contain high amounts of chemical or microbial contaminations.

Therefore, to handle this issue, chlorination disinfection is usually performed on these water samples before inserting them into the water distribution network in order to prevent secondary microbiological infections (Berger et al., 2017; Gheibi et al., 2021; Alizadeh et al., 2021; Eftekhari et al., 2020). However, it should be mentioned that since surface water resources have high contamination levels, they must be purified through other processes. For the treatment of surface water, a number of different units are used such as screening, primary disinfection, aeration tank, active carbon injection, coagulation and flocculation in rapid mixing ponds, rapid sand filtration, and final disinfection (Eftekhari et al., 2021; Gerhard et al., 2017; McGivney and Kawamura, 2008; Doulabian et al., 2021; Zhang et al., 2020).

It goes without saying that the quality of surface water resources in various temporal and situational conditions may vary due to a set of factors like the concentration of organic material and minerals, temperature, and pH (Jalali et al., 2021; Shahsavari et al., 2021; Khorrami et al., 2020; Alipour et al., 2020). Through a classic categorization, the financial expenses of any treatment plant are separated into two general clusters of investment and operational costs. Construction costs include expenses for buildings, infrastructures, and facilities, which cannot be controlled or optimized by the stakeholders. Operation costs of water treatment plants include annual expenses concerning operation, maintenance, material, energy, amortization, and chemicals (Zhou et al., 2011). In fact, in situations where the cost of the required chemicals can be predicted, the costs of water treatment plants can be managed optimally. Predicting the amount of changes in chemical consumption is a function of management of costs in treatment plants.

In 2011, Zhou et al. examined the impact of some effective economical parameters such as water flow, concentration of contaminants in inlet water, and operation aspects on reverse osmosing (RO) method in water treatment. The assessments in this study were carried out using statistical analysis and correlation (through SPSS software) of effective parameters such as water flow, concentration of contaminants in inlet water, and operation aspects (Zhou et al., 2011). Likewise, Vouk et al. performed economic scrutinizing on wastewater gathering and treatment systems using the Artificial Neural Network (ANN) method. In present investigation, an ANN was programmed to estimate a set of expenses including construction, action, and upkeep of wastewater gathering and treatment schemes in rural and urban regions (Vouk et al., 2011). Similarly, in 2012, Arzate et al., also attempted to implement an innovative model (using GAMS environment) in the

area of economical optimization in water treatment and transportation in industrial environments (Arzate et al., 2012). Through an administrative assessment, in 2013, Igos et al., conducted a cost-performance analysis on water treatment processes of two treatment plants in Paris, France. To perform economic and financial analyses (with focus on the water quality), this study employed an integration of three types of Life Cycle Assessment (LCA) methods including the recipe, step-wise, and eco-cost ones (Igos et al., 2013). Kislo and Skoczko performed an economic analysis on a water treatment system in one of the largest cities of Poland during a two-year period 2010-2012. The capacity of the treatment plant is 600 m³ per hour and remove parameters such as heavy metals and turbidity. It is worth mentioning that this treatment plant is fed by 19 wells and carries out the disinfection operation using the ultra violet disinfection system (Kislo and Skoczko, 2015).

Having a look at the recent studies, Marzouk and Elkadi estimated the costs of water decontamination plant construction utilizing the ANN method. The results of ANN were assessed and compared to statistics ranking models. It must be noted that the database was provided from the construction reports of 160 treatment plants in Egypt (Marzouk and Elkadi, 2016). Eggimann et al. calculated and assessed the financial costs in terms of unit of surface in on-site wastewater treatment systems using soft computing such as heuristic algorithms. In this study, among the costs of investment and operation, more emphasis was placed on transportation sections. The main point of this study was to compare the cost of Centralized and Decentralized Wastewater Management Systems (CWMS & DWMS) (Eggimann et al., 2016). In another study, Djukic et al. analyzed the cost-benefits of infrastructures and cost return rates in wastewater projects in Serbia. In this study, the EU (European Union) recommended methods were used to carry out financial research and analyses (Djukic et al., 2016). Elazzouzi et al. studied an economical electronic coagulation and flocculation process for removal of contaminants. This efficiently-economic method was used for removal of parameters including Chemical Oxygen Demand, Biological Oxygen Demand, Total Suspended Solids, Nitrates (NO₃-), Nitrogen (N), Phosphorus (P) and fecal coliform (Elazzouzi et al., 2017). As per the reviewed investigations, application of smart decision-making system is assumed as a research gap which is studied in present research.

All in all, based on what was mentioned above, the purpose of the current research was to first extract, categorize and verify all types of coagulants (for turbidity removal), telemetry data about turbidity and energy consumption (for turbidity removal in coagulation and flocculation process)

in water treatment plants and second to predict, do sensitivity analysis and design a pattern for the outlet turbidity and energy consumption with respect to ferric chloride and the turbidity of raw water. In a nutshell, the purpose of this research is to design energy use and residual turbidity soft sensors in the outlet of water treatment plants by application of Adaptive Neuro-Fuzzy Inference System (ANFIS) among the first studies. Finally, soft sensor model is implemented as a Decision Support System (DSS) using the Petri Net modelling.

The rest of this paper is structured as follows: Section 2 studies the materials and methods of this research to provide our case study with its details. Section 3 is the results along with the discussion. Finally, the findings and conclusion along with future research recommendations are addressed in Section 4.

2. Materials and methods

2.1. Case Study

Water resources of Mashhad are supplied by groundwater and surface, the former includes Toroq, Kardeh, Ardak, and Doosti dams. Regarding the treatment processes, groundwater water resources have much fewer contaminants due to self-purification of the water by nature. Therefore, the costs of decontamination are not comparable in this case to that of surface water. The mentioned water resources are standardized, and treating in three treatment plants (No. 1, 2 and 3) prior to providing the urban water distribution network. The Kardeh and Ardak water resources are refined in treatment plant No.1, while Toroq and Doosti water resources are treated in treatment plants No. 2 and 3, respectively. In this study, the coagulation and flocculation process behavior of treatment plant No.1 was supplied by the Kardeh dam. This treatment plant is located in Ab-o-bargh district and have started working since June, 1992 on June, 1992. The nominal capacity of the plant is 96000 m³ per day and is fed by Kardeh dam located in a distance of 40 km from the North-East of Mashhad. Water is transferred from dam to the treatment plant gravitationally, using 800-millimeter cast iron ductile pipes with an overall length of 46 km. Treatment process in this plant includes primary disinfection, aeration for gas outlet, addition of active carbon to remove organic materials, second step of multistage chlorination, injection of ferric chloride for coagulation and flocculation, removal of the produced flocs using Super pulsator process, passing through rapid sand filters, and final chlorination (Figure 1). The location of water treatment plant No. 1, Mashhad City, Iran is illustrated as per Figure 2.

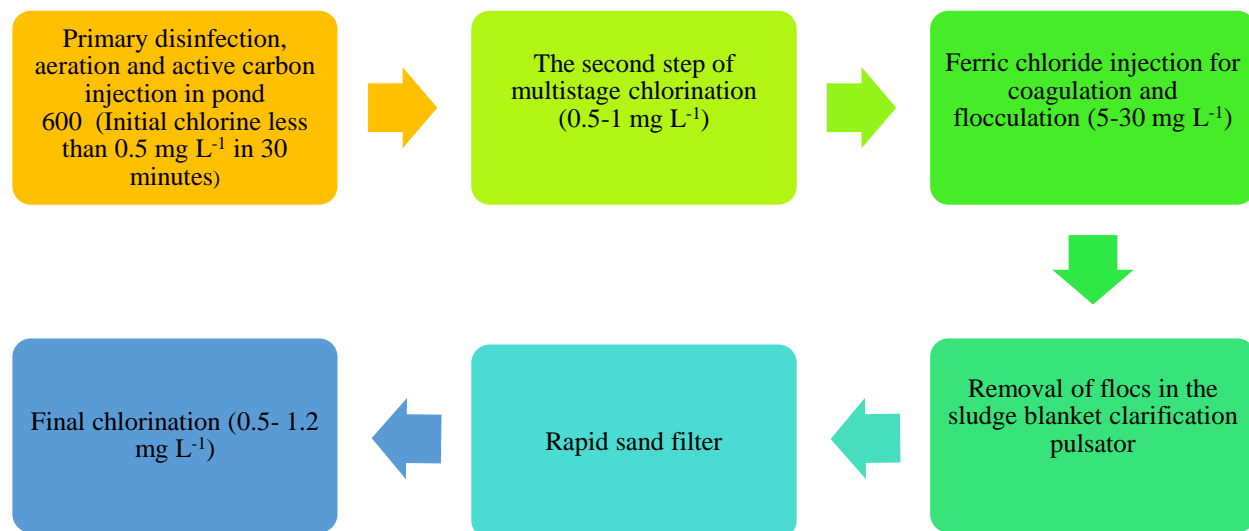


Figure 1. Treatment process of inlet raw water from Kardeh dam in treatment plant No.1, Mashhad, Iran.

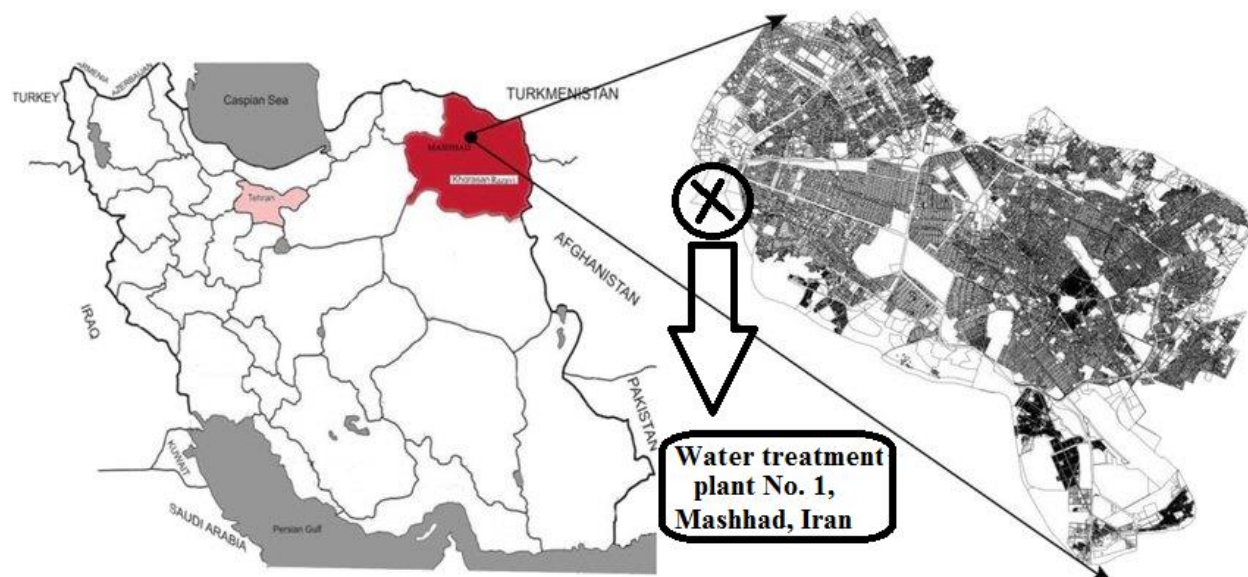


Figure 2. The location of water treatment plant No.1, Mashhad, Iran.

2.2. Research roadmap

The research roadmap of present research is presented in Figure. 3. Also, the mentioned study is divided to three main sections including data gathering and statistical evaluation, ANFIS computations and Petri Net modelling. With regards to this research roadmap, first, available data should be collected from water treatment plant (No. 1) of Mashhad city with the cooperation of Water Management Company. Then, the collected data are categorized in inlet/outlet turbidity amounts, energy and coagulant consumption. In the

following, the categorized data is evaluated by ANFIS model and finally, the outcomes are utilized for implementation in water facilities and controlled by Petri Net conceptual system.

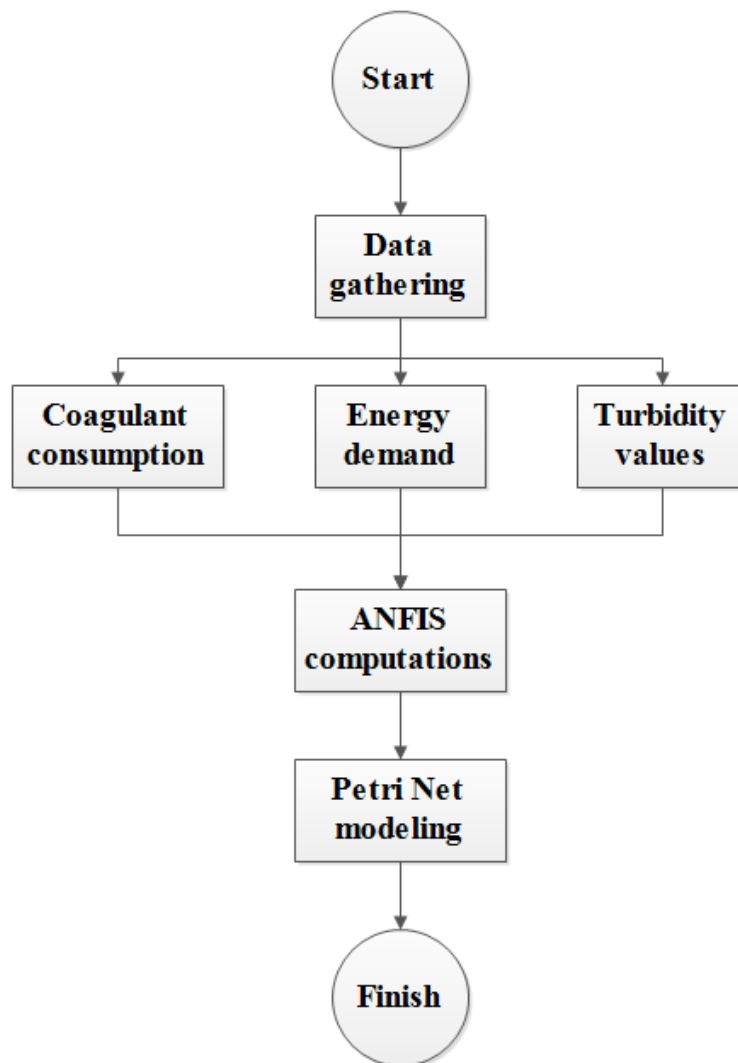


Figure 3. Research roadmap in present study.

2.3. Statistical Data Gathering

In this part of the study, all the records including coagulant (ferric chloride) consumption, consumed energy and automation system outlets (turbidity unit) in treatment plant No. 1 were investigated from the year 2019 until the first half of 2020. During this task, all the statistics results were extracted, categorized, and verified. It is worth mentioning that in treatment plant No.1, in addition to Kardeh dam water supply, Sooran wells water was also chlorinated and following the mixture of these two surface and groundwater water supplies, it was fed into the distribution network. Meanwhile, ferric chloride and active carbon consumption only occurred for the inlet

surface water in the treatment plant. As seen in Figure 4, the extent of surface and groundwater water supplies annual consumption (in 2019) in treatment plant No. 1 is illustrated. All statistical evaluations of present study are done in Excel 2016 software.

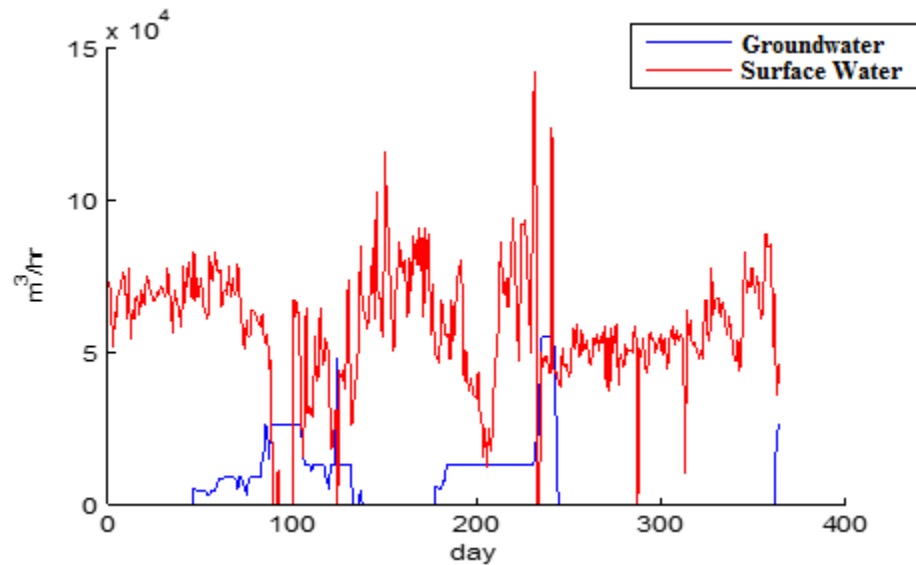


Figure 4. The amount of water resources' shares in water treatment No.1, Mashhad, 2019.

2.4. The Prediction model and design operational pattern

The concept of fuzzy cliques was presented and classified by Zadeh (Zadeh, 1997; Zadeh, 2015; Ghadami et al., 2021; Mojtahedi, et al., 2021; Fathollahi-Fard et al., 2021a; Ali et al., 2021). Fuzzy computation is a valuable technique for the systems complicated in difficult subjects which may lead to a set of challenges for various studies such as decision making, assessment and prediction. The fuzzy system is capable of implementing human's language as well as using individual's experiences to progress. Fuzzy logic uses the experiences to develop a prediction of calculations. There are many algorithms such as learning reinforcements which develop fuzzy sets to be learned in various situations (Fathollahi-Fard et al., 2021; Akbarpour et al., 2021). Plus, ANN are achieved through test, train, validation, calibration and verification. The ANN was introduced by McCulloch-Pitts in the 1940s as per compute logical functions (Fathollahi-Fard et al., 2020a). The ANN method makes this conceivable through numerical computing the influences of human brain neurons. The ability to realize the relationships between inputs and outputs along with establishing a complicated model are of significance. Nevertheless, ANN is a black box model and therefore incapable of displaying an organized formula between entered and purposed data (Fathollahi-Fard

et al., 2021b; Fathollahi-Fard et al., 2020b; Zhang et al., 2020). Integration of fuzzy computation and ANN was a means to overawed the constraints of both methods. In 1993, Jang presented the self-learning competence of fuzzy systems and neural networks instantaneously as a novel soft computing algorithm (Jang, 1993; Fathollahi-Fard et al., 2020c). The mentioned structures are recognized as the ANFIS. In present part, an ANFIS technique is used to forecast the output. In the following Figure 5 demonstrates the ANFIS construction. In the middle layers, the rules have been constructed by the neural network. It should be noted that all computations for machine learning methods include fuzzification, normalization, defuzzification, and output layer are done in MATLAB 2013b software.

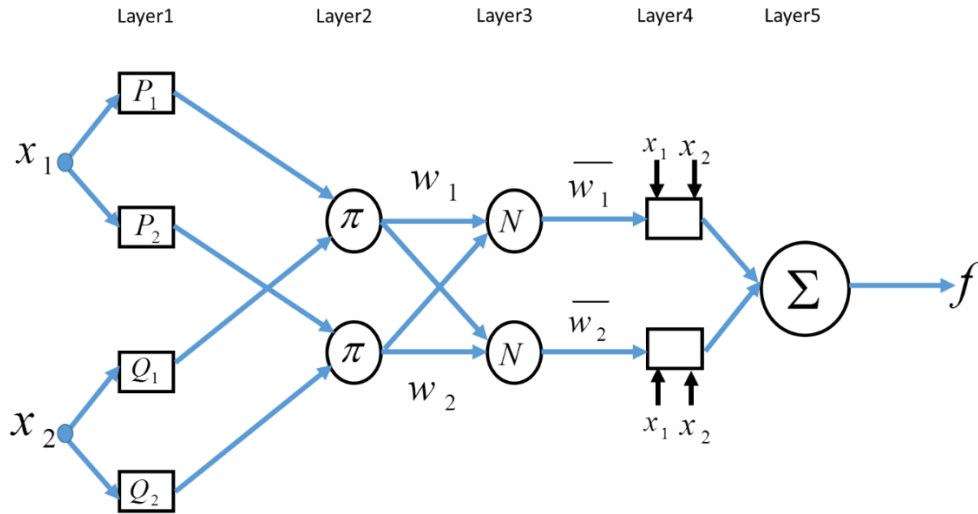


Figure 5. General ANFIS structure (Çaydaş, et al., 2009).

As stated previously, the aim of this research was to predict and design the pattern between inlet turbidity and ferric chloride with respect to outlet turbidity and energy consumption (Figure 6). The designed model can determine the amount of coagulant and energy consumption in normal and abnormal quality situations. On the other hand, operators can evaluate their decisions (before applying them) about coagulant dosage through considering outlet turbidity and energy consumption. In the study, first the largest part of data is considered for training the patterns and rules. Then, based on outputs of trained data, validation of model is discussed by testing procedure through ANFIS computation. Finally, the outcomes of model are used for sensitive analysis of effective factors.

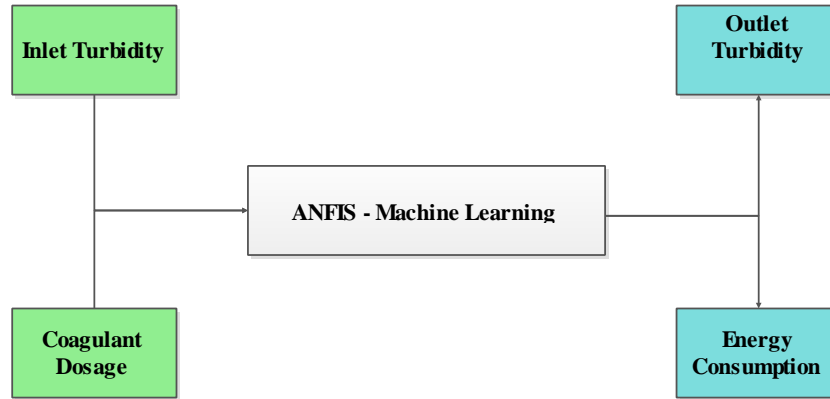


Figure 6. Conceptual model of machine learning in present issue.

2.5. Petri Net modelling

After sensitive analysis by ANFIS model, for creating smart controlling models Petri Net (Amini et al., 2021; Gheibi et al., 2019) concept is utilized. In the declared model, each adjustable factor and conditional values are put in place and transition functions, correspondingly. The algorithm of Petri Net modelling design is shown in Figure 7. In the investigation, E-Draw Max 8.6 is utilized for Petri Net modelling.

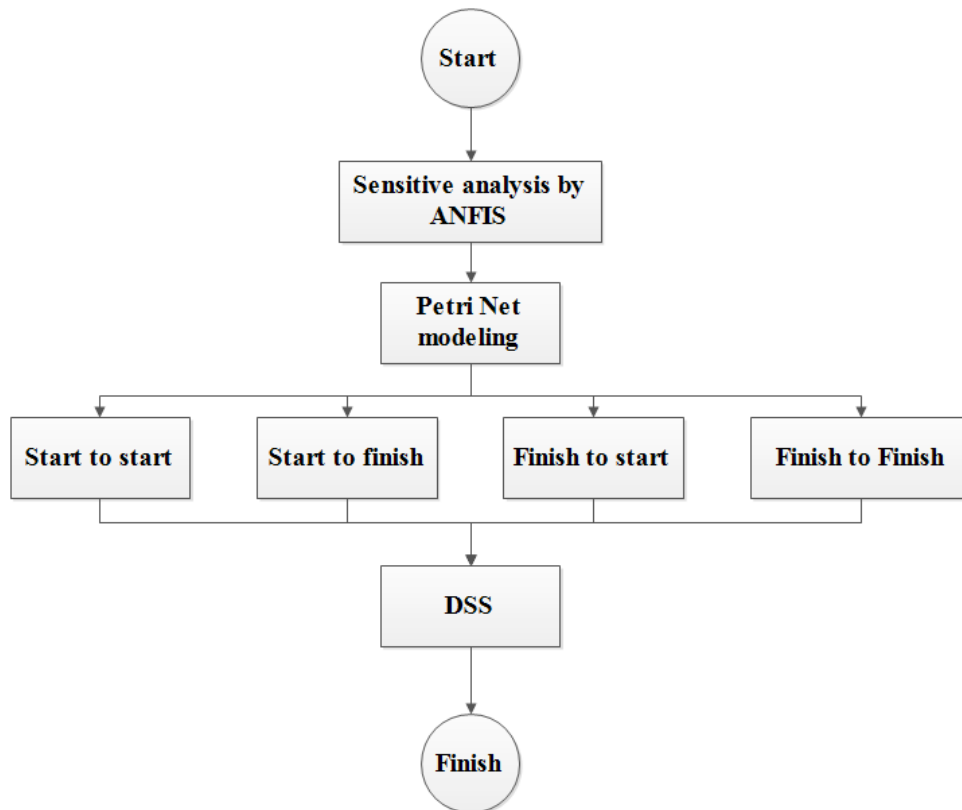


Figure 7. Algorithm of Petri Net modelling in present issue.

3. Results and discussions

3.1. ANFIS modeling

In present investigation, a Sugeno model was applied with two types of initial data prior to using a Takagi–Sugeno type (Çaydaş et al., 2009) fuzzy IF–THEN rules Equation 1.

If Input 1 is f_i , input 2 is f_j , input 3 is f_k , and Input 4 is f_l , then

$$f_i = p_i i + q_i j + r_i k + s_i l + t \quad \text{Equation (1)}$$

Where p_i , q_i , r_i , s_i and t are constant variables. The mentioned constant values are determined through the ANFIS computations and with consideration to weights of each input parameters. Also, i , j , k , and l are the input values of ANFIS model as independent variations which are related to f value as a depended variation.

The first layer of present computation was comprised of two entered variable membership functions (MFs) and then it prepared them for next layer. In the declared layer, each node was completed as a compatible node with an absolute function, where were MFs. Bell-shaped MFs with a maximum value equal to 1 and a minimum value equal to 0 were calculated based on Equation 2.

$$f(x; a, b, c) = \frac{1}{1 + \left(\frac{x - c}{1}\right)^{2b}} \quad \text{Equation (2)}$$

As given in Equation 2, x presents fuzzy variable, a and c convey feet of triangular membership function, and b is related to the tip of the curve.

The proposed system for this equation is illustrated in Figure 8. The first input (ferric chlorine) and the second input (inlet turbidity) are fuzzing by three and five triangular membership functions, respectively. The mentioned functions categorize the input value in regions where 0 and 1 proving this value have no and full associations, correspondingly.

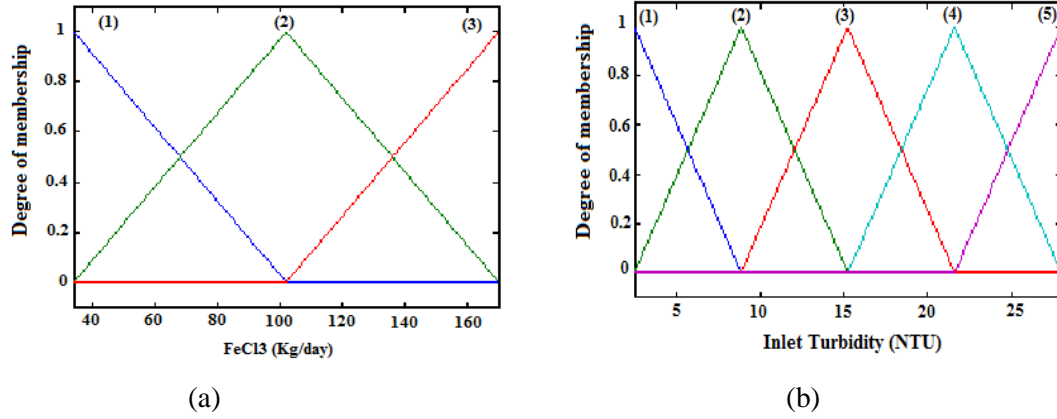


Figure 8. Fuzzy membership functions for inputs (a) Ferric chloride (b) Inlet turbidity.

The next layer called the membership layer assigns the weights for each membership function. The declared layer multiplies the associated signals and calculates them as demonstrated in Equation 3.

$$w_i = \mu(i)_i \times \mu(i)_{i+1} \quad \text{Equation (3)}$$

Where, $\mu(i)$ and w_i are triangular membership function and weight of input variation in the ANFIS model as firing strength.

Rules are made by the Layer 3; hence it is called the layer of rules. Nodes in the mentioned zone normalizes weights of initial parameters and firing strengths are regularized as per Equation 4.

$$w_i^* = \frac{w_i}{w_1 + w_2} \quad \text{Equation (4)}$$

Where, w_i^* presents normalized value of w_i . Likewise, the denominator of the fraction represents the sum of the calculated weights.

Defuzzifying is planned in the fourth zone by implication of the rules and then outcomes are calculated by Equation 5.

$$Q_i^4 = w_i^* \times f \quad \text{Equation (5)}$$

The last section merges all defuzzified inputs and then computes the outcome as the cumulate of received signals as depicted in Equation 6.

$$Q_i^4 = \sum_i w_i^* \times f = \frac{\sum_i w_i \times f}{\sum_i w_i} \quad \text{Equation (6)}$$

Applying present method, the learning system is hired to identify the factors in ANFIS. The policy between the inlet turbidity, ferric chloride with the outlet turbidity and the consumed energy are shown in Figure 9 and Figure 10. According to Figure 9, the efficiency of removal is not always improved by increasing the amount of ferric chloride. Actually, in high levels of turbidity, coagulants can reduce zeta potential between colloid materials better than in low levels of turbidity status. As seen in the upper right corner of the image, in the high level of contamination, ferric chloride removed the pollutant with suitable efficiency. According to other researches, in conditions of low water contaminations, synthetic turbidity with bentonite (Pan et al., 1999) or kaolin (Muyibi and Evison, 1995) is used to increase the contact surface between the coagulant and colloidal compounds (Ndabigengesere et al., 1995).

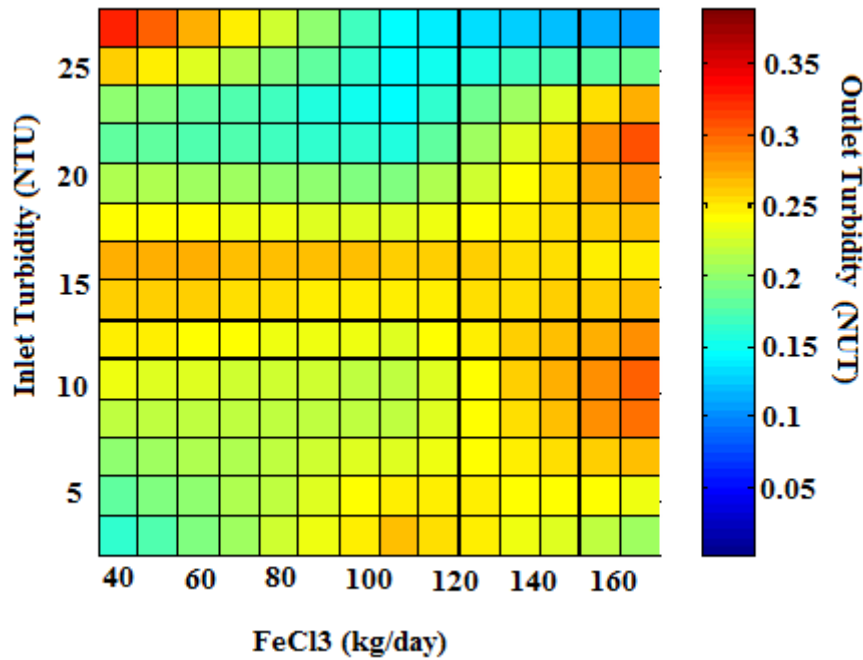


Figure 9. Outlet turbidity vs the injected ferric chloride and inlet turbidity.

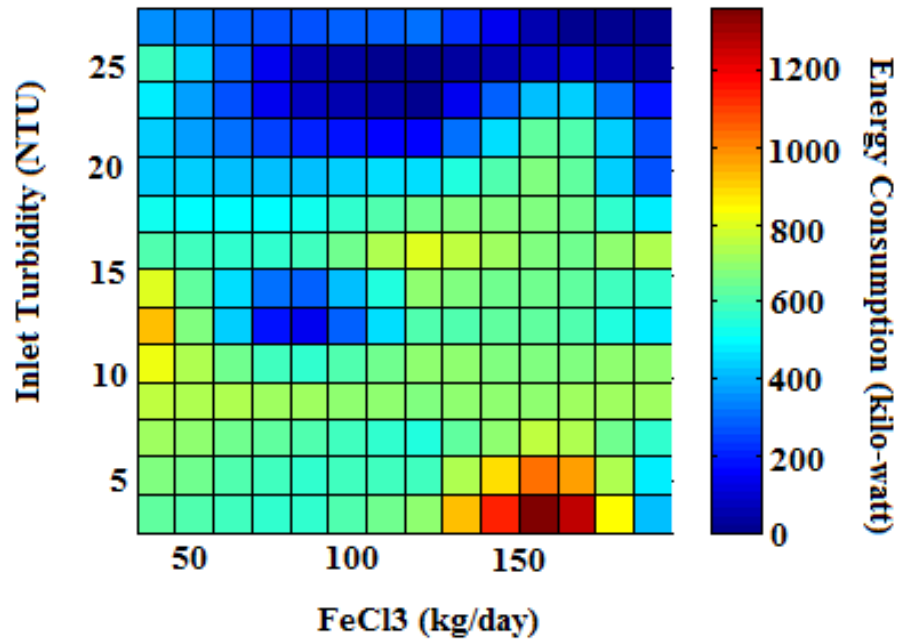


Figure 10. Energy consumed in kilo-watt vs the injected ferric chloride and inlet turbidity.

As shown in the pattern of Figure 9, it turns out that operators can predict the amounts of coagulants and evaluate the probability results with the trial and error method based on machine learning archives. This soft system functions like an assistant for operators in decision making about coagulant dosage. Using soft sensors is an effective tool for operating water and wastewater treatment plants. High technology systems use these soft sensors as decision builders in crisis management (Haimi et al., 2013; Choi and Park, 2001).

As can be seen in Figure 10, the amount of consumed energy increases with increasing the turbidity of water. It is due to the reason that the amount of injectable coagulants and the speed of mixing are in a direct relationship with energy consumption. It is also worth noting that energy pattern analysis is one of the main analytical strategies used energy efficiency optimization systems in water and wastewater decontamination facilities (Singh et al., 2012).

3.2. Evaluation of the models

To evaluate the model discussed in the previous section, the coefficient of determination or R^2 was used. If a set of data consists of n members like $y_1: y_n$ and the predicted data are shown by $f_1: f_n$, then, the mean of observed data is calculated by Equation 7.

$$\bar{y} = \frac{1}{n} \sum_{i=1}^n y_i \quad \text{Equation 7}$$

Where n and y_i are number of records and value of each record.

Using Equation 8 and Equation 9 which show the difference of observed data with the mean and data set with the predicted data, respectively, the coefficient of determination can be calculated by Equation 10.

$$SS_{tot} = \sum_i (y_i - \bar{y})^2 \quad \text{Equation 8}$$

$$SS_{res} = \sum_i (y_i - f_i)^2 \quad \text{Equation 9}$$

$$R^2 = 1 - \frac{SS_{res}}{SS_{tot}} \quad \text{Equation 10}$$

where R^2 and \bar{y} are correlation coefficient and mean value of records.

The calculated coefficients of determination for the proposed models are shown in Table 1. This is clear that the earlier R^2 amount becomes to 100%, the better is the produced predicted model. Accordingly, this model achieved $R^2 > 80\%$ for both models which are capable of considering a consistent model for predicting outlet turbidity and consumed energy. The outcomes of ANFIS performance based on regression system is illustrated in Figure 11.

Table 1. Coefficient of determination (R^2) for various models.

Model	R^2
Predicting outlet turbidity	85%
Predicting energy consumption	81%

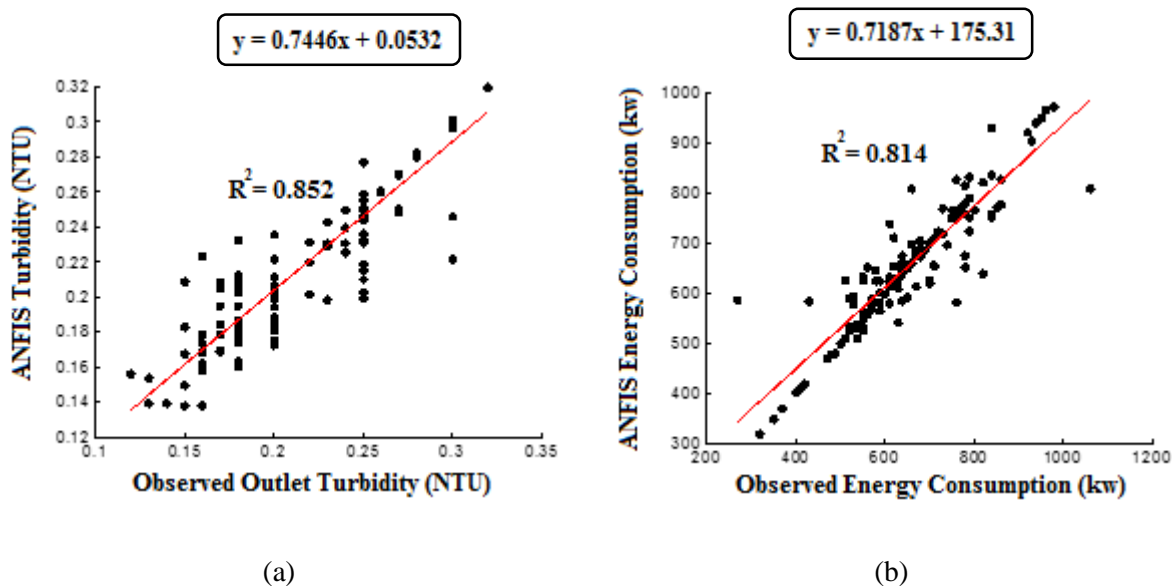


Figure 11. Regression line for all of the proposed ANFIS models (a) outlet turbidity (b) Energy consumption.

The equations of regression process are illustrated in Figure 11. These formulas are useful for reproduction of smart systems for future researches. It goes without saying that the ANFIS model has some advantages and disadvantages in application of water treatment plant and prediction of essential factors for critical units. Likewise, the main advantages are:

- In coagulation and flocculation process, data has high level of fluctuations and ANFIS model can present appropriate robustness and it is so beneficial (Mohammadi et al., 2021; Zahedi et al., 2021).
- ANFIS has hybrid optimization tool for error reduction through train and test computations and it is useful due to estimation of parameters in water treatment systems (Shahsavari et al., 2021; Sadri et al., 2021).
- The type of inputs in ANFIS model of coagulation and flocculation process is far from together and they have different origins. Therefore, with fuzzy procedure, the learning section provide outcomes with high efficiency and precision (Shakerian et al., 2021; Hamdi-Asl et al., 2021).

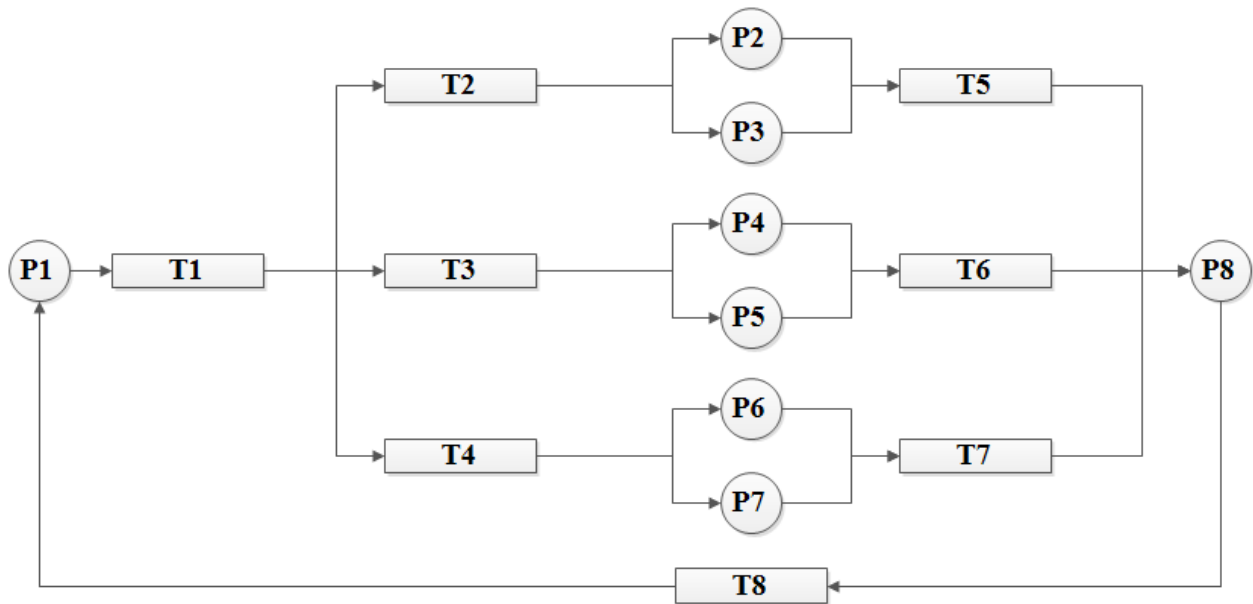
Also, the most noticeable disadvantages of ANFIS model in water treatment plant applications include:

- Through high records of data, this method is so heavy computationally and it needs lots of cost, energy and time (Eftekhar et al., 2021; Fasihi et al., 2021).

- The volume of computations is high and for more than three input parameters, it cannot use as real time system and it calculate the outputs with delay (Ghadami et al., 2021).
 - The ANFIS model is appropriate for single objective problems and due to multi objective investigations, other systems are advised (Shakerian et al., 2021; Chouhan et al., 2021).
- Finally, for future researches, present study suggests to compare outcomes of ANFIS model with other classification techniques include Random Tree (RT), Random Forest (RF), and Artificial Neural Network (ANN). Therefore, with the declared comparing, the best soft-sensor calculation is determined.

3.3. Petri Net modelling

The pattern of Petri Net modelling is demonstrated according to Figure 12. As per the mentioned Figure, in $15 \pm 5\%$ inlet turbidity values, with adding 60-85 kg/day ferric chloride in the coagulation and flocculation reactor, the amount of energy consumption and outlet turbidity are equal to 600 kw and 0.2 as per Figures 9 and 10. Likewise, in the more than $15 \pm 5\%$ inlet turbidity, with 50-75 kg/day coagulant injection the consumed energy and outlet turbidity should control in 300 kw and 0.15, correspondingly. Finally, according to DSS, the in the less than $15 \pm 5\%$ inlet turbidity, the energy demand and outlet turbidity are 500 kw and 0.2 with adding 40-60 kg/day ferric chloride.



P1: Receiving and reading the inlet turbidity value from Online sensors.
P2: Adding 60-85 kg/day coagulant material is the best range.
P3: Outlet turbidity value and energy consumption will be around 0.2 and 600 Kilo-Watt, respectively.
P4: Adding 50-75 kg/day coagulant material is the best range.
P5: Outlet turbidity value and energy consumption will be around 0.15 and 300 Kilo-Watt, respectively.
P6: Adding 40-60 kg/day coagulant material is the best range.
P7: Outlet turbidity value and energy consumption will be around 0.2 and 500 Kilo-Watt, respectively.
P8: Receiving the operators' opinion about existence situation of outlet turbidity and consumed energy.

T1: Is the achieved turbidity value valid with approving by operator?
T2: Is the received turbidity value is around $15 \pm 5\%$?
T3: Is the received turbidity value is more than $15 \pm 5\%$?
T4: Is the received turbidity value is around $15 \pm 5\%$?
T5: Are both P2 and P3 milestones met?
T6: Are both P4 and P5 milestones met?
T7: Are both P6 and P7 milestones met?
T8: Are all operational conditions (P1-P8) appropriate based on operators' opinions?

Figure 12. Schematic plan of Petri Net modelling for coagulation and flocculation process smart DSS.

4. Conclusion and future works

Two of the most common processes in surface water treatment are coagulation and flocculation for removing colloidal materials and turbidity. Operators need to adjust coagulants dosage according to logical criteria. Operators are interested in optimizing chemical materials and energy consumption with respect to high efficiency removal of turbidity. Therefore, they require reliable designed patterns and algorithms for studying coagulation and flocculation behaviors. In this paper, correlational analysis was done on the two inputs and two outputs of a water treatment process. Inputs included the inlet turbidity and the amount of ferric chloride injected into the water. The outputs included the outlet turbidity and the amount of energy spent on this procedure. The ANFIS model was employed in order to organize this practice. The high coefficient of determination value (More than 80%) shows a reliable correlation between the inputs and outputs. In the last section of present study, the Petri Net modelling is utilized for implementation of DSS in water treatment plant No. 1, Mashhad. As per the mentioned technique, every smart order is related to turbidity changes through Petri Net modelling. Based on the declared DSS, in $15 \pm 5\%$,

less and more than it inlet turbidity values, the additive coagulant material (ferric chloride) should be set on 60-85, 60-85 and 40-60 kg/day, respectively. All in all, the main advantages of our ANFIS model are its high accuracy and robustness, while the main disadvantage of our model is to have a high computational time.

It goes without saying that there are several suggestions to improve the contributions of this research in our future works. First, more factors linking with water treatments such as the job opportunities and social justice for workers, can be studied in our model. Using optimization theory and uncertainty for our water systems is another good suggestion. Finally, other programming methods like genetic programming and adaptive search techniques can be suggested to improve the efficiency of our ANFIS model.

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