



## **UWL REPOSITORY**

**repository.uwl.ac.uk**

A decision support system for coagulation and flocculation processes using the adaptive neuro-fuzzy inference system

Pouresmaeil, Hossein, Faramarz, Mahdiah G., ZamaniKherad, Mohammad, Gheibi, Mohammad, Fathollahi-Fard, Amir M., Behzadian, Kourosh ORCID logo ORCID: <https://orcid.org/0000-0002-1459-8408> and Tian, Guangdong (2022) A decision support system for coagulation and flocculation processes using the adaptive neuro-fuzzy inference system. *International Journal of Environmental Science and Technology*.

<http://dx.doi.org/10.1007/s13762-021-03848-4>

This is the Accepted Version of the final output.

UWL repository link: <https://repository.uwl.ac.uk/id/eprint/8500/>

**Alternative formats:** If you require this document in an alternative format, please contact: [open.research@uwl.ac.uk](mailto:open.research@uwl.ac.uk)

### **Copyright:**

Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

**Take down policy:** If you believe that this document breaches copyright, please contact us at [open.research@uwl.ac.uk](mailto:open.research@uwl.ac.uk) providing details, and we will remove access to the work immediately and investigate your claim.

### **Rights Retention Statement:**

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

**Hossein Pouresmaeil<sup>1</sup>, Mahdiah G. Faramarz<sup>2</sup>, Mohammad ZamaniKherad<sup>3</sup>, Mohammad Gheibi<sup>4</sup>,  
Amir M. Fathollahi-Fard<sup>5\*</sup>, Kouros Behzadian<sup>6</sup>, Guangdong Tian<sup>7</sup>**

<sup>1</sup>*Department of Environmental Engineering, University of Tehran, Tehran, Iran*

<sup>2</sup>*Department of Building, Civil, and Environmental Engineering, Concordia University, Montreal, Quebec, Canada*

<sup>3</sup>*Department of Civil Engineering, Kharazmi University, Tehran, Iran*

<sup>4</sup>*Department of Civil Engineering, Ferdowsi University of Mashhad, Mashhad, Iran*

<sup>5</sup>*Department of Electrical Engineering, École de Technologie Supérieure, University of Québec, Montréal, Canada*

<sup>6</sup>*Department of Civil Engineering, University of West London, London, UK*

<sup>7</sup>*School of Mechanical Engineering, Shandong University, Jinan, 250061, China*

*\*Corresponding author, email: [amirmohammad.fathollahifard.1@ens.etsmtl.ca](mailto:amirmohammad.fathollahifard.1@ens.etsmtl.ca)*

## **Acknowledgment:**

The authors confirm there is no conflict of interest from authors. They would like to thank the Editor-In-Chief, editorial board and the reviewers who commented on this paper to improve it significantly. We would like to acknowledge that Prof. Hajiaghahi-Keshteli's publications are the main inspiration for our work.

1  
2  
3  
4  
5  
6  
7  
8  
9  
10  
11  
12  
13  
14  
15  
16  
17  
18  
19  
20  
21  
22  
23  
24  
25  
26  
27  
28  
29  
30  
31  
32  
33  
34  
35  
36  
37  
38  
39  
40  
41  
42  
43  
44  
45  
46  
47  
48  
49  
50  
51  
52  
53  
54  
55  
56  
57  
58  
59  
60  
61  
62  
63  
64  
65

# 1 A Decision Support System for Coagulation and Flocculation Processes Using the Adaptive 2 Neuro-fuzzy Inference System

## 3 4 Abstract

5 Decision Support System (DSS) is an approach to have a smart and sustainable management of  
6 facilities for monitoring, predicting and controlling sections. The mentioned platform can be useful  
7 in operation of complex facilities like the Water Treatment Plant (WTP). This study proposes an  
8 Adaptive Neuro-fuzzy Inference System (ANFIS) for prediction of energy consumption and outlet  
9 turbidity according to inlet turbidity and ferric chloride as coagulant in coagulation and  
10 flocculation unit process of WTP. The outcomes of ANFIS model are used in the Petri Net  
11 modelling as a smart conceptual control system. Therefore, the main purpose of this research is  
12 the development of a DSS model for coagulation and flocculation processes in WTP. The results  
13 of quantitative data analysis showed that the correlation coefficients of ANFIS model are more  
14 than 80% meaning that it can reliably predict the outlet turbidity and energy consumption's  
15 variables. With regards to our findings, the first one is to provide a smart and sustainable control  
16 system to be implemented in operations of coagulation and flocculation process in WTPs. It goes  
17 without saying that, our DSS model confirms that the variation of  $15\pm 5\%$  for turbidity values and  
18 the additive coagulant materials (ferric chloride) should be set, on 60-85 and 40-60 kg/day,  
19 respectively for controlling energy consumption and outlet turbidity. At last but not least, the main  
20 benefit from our DSS model is to manage the operation of WTP with a high efficiency and low  
21 human-based errors.

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

## 24 1. Introduction

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

1  
2  
3  
4  
5  
6  
7  
8  
9  
10  
11  
12  
13  
14  
15  
16  
17  
18  
19  
20  
21  
22  
23  
24  
25  
26  
27  
28  
29  
30  
31  
32  
33  
34  
35  
36  
37  
38  
39  
40  
41  
42  
43  
44  
45  
46  
47  
48  
49  
50  
51  
52  
53  
54  
55  
56  
57  
58  
59  
60  
61  
62  
63  
64  
65

31 Therefore, to handle this issue, chlorination disinfection is usually performed on these water  
32 samples before inserting them into the water distribution network in order to prevent secondary  
33 microbiological infections (Berger et al., 2017; Gheibi et al., 2021; Alizadeh et al., 2021; Eftekhari  
34 et al., 2020). However, it should be mentioned that since surface water resources have high  
35 contamination levels, they must be purified through other processes. For the treatment of surface  
36 water, a number of different units are used such as screening, primary disinfection, aeration tank,  
37 active carbon injection, coagulation and flocculation in rapid mixing ponds, rapid sand filtration,  
38 and final disinfection (Eftekhari et al., 2021; Gerhard et al., 2017; McGivney and Kawamura,  
39 2008; Doulabian et al., 2021; Zhang et al., 2020).

40 It goes without saying that the quality of surface water resources in various temporal and  
41 situational conditions may vary due to a set of factors like the concentration of organic material  
42 and minerals, temperature, and pH (Jalali et al., 2021; Shahsavari et al., 2021; Khorrami et al.,  
43 2020; Alipour et al., 2020). Through a classic categorization, the financial expenses of any  
44 treatment plant are separated into two general clusters of investment and operational costs.  
45 Construction costs include expenses for buildings, infrastructures, and facilities, which cannot be  
46 controlled or optimized by the stakeholders. Operation costs of water treatment plants include  
47 annual expenses concerning operation, maintenance, material, energy, amortization, and chemicals  
48 (Zhou et al., 2011). In fact, in situations where the cost of the required chemicals can be predicted,  
49 the costs of water treatment plants can be managed optimally. Predicting the amount of changes  
50 in chemical consumption is a function of management of costs in treatment plants.

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

1  
2  
3  
4  
5  
6  
7  
8  
9  
10  
11  
12  
13  
14  
15  
16  
17  
18  
19  
20  
21  
22  
23  
24  
25  
26  
27  
28  
29  
30  
31  
32  
33  
34  
35  
36  
37  
38  
39  
40  
41  
42  
43  
44  
45  
46  
47  
48  
49  
50  
51  
52  
53  
54  
55  
56  
57  
58  
59  
60  
61  
62  
63  
64  
65

61 area of economical optimization in water treatment and transportation in industrial environments  
62 (Arzate et al., 2012). Through an administrative assessment, in 2013, Igos et al., conducted a cost-  
63 performance analysis on water treatment processes of two treatment plants in Paris, France. To  
64 perform economic and financial analyses (with focus on the water quality), this study employed  
65 an integration of three types of Life Cycle Assessment (LCA) methods including the recipe, step-  
66 wise, and eco-cost ones (Igos et al., 2013). Kislo and Skoczko performed an economic analysis on  
67 a water treatment system in one of the largest cities of Poland during a two-year period 2010-2012.  
68 The capacity of the treatment plant is 600 m<sup>3</sup> per hour and remove parameters such as heavy  
69 metals and turbidity. It is worth mentioning that this treatment plant is fed by 19 wells and carries  
70 out the disinfection operation using the ultra violet disinfection system (Kislo and Skoczko, 2015).

71 Having a look at the recent studies, Marzouk and Elkadi estimated the costs of water  
72 decontamination plant construction utilizing the ANN method. The results of ANN were assessed  
73 and compared to statistics ranking models. It must be noted that the database was provided from  
74 the construction reports of 160 treatment plants in Egypt (Marzouk and Elkadi, 2016). Eggimann  
75 et al. calculated and assessed the financial costs in terms of unit of surface in on-site wastewater  
76 treatment systems using soft computing such as heuristic algorithms. In this study, among the costs  
77 of investment and operation, more emphasis was placed on transportation sections. The main  
78 pointof this study was to compare the cost of Centralized and Decentralized Wastewater  
79 Management Systems (CWMS & DWMS) (Eggimann et al., 2016). In another study, Djukic et al.  
80 analyzed the cost-benefits of infrastructures and cost return rates in wastewater projects in Serbia.  
81 In this study, the EU (European Union) recommended methods were used to carry out financial  
82 research and analyses (Djukic et al., 2016). Elazzouzi et al. studied an economical electronic  
83 coagulation and flocculation process for removal of contaminants. This efficiently-economic  
84 method was used for removal of parameters including Chemical Oxygen Demand, Biological  
85 Oxygen Demand, Total Suspended Solids, Nitrates (NO<sub>3</sub>-), Nitrogen (N), Phosphorus (P) and  
86 fecal coliform (Elazzouzi et al., 2017). As per the reviewed investigations, application of smart  
87 decision-making system is assumed as a research gap which is studied in present research.

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

1  
2  
3  
4  
5  
6  
7  
8  
9  
10  
11  
12  
13  
14  
15  
16  
17  
18  
19  
20  
21  
22  
23  
24  
25  
26  
27  
28  
29  
30  
31  
32  
33  
34  
35  
36  
37  
38  
39  
40  
41  
42  
43  
44  
45  
46  
47  
48  
49  
50  
51  
52  
53  
54  
55  
56  
57  
58  
59  
60  
61  
62  
63  
64  
65

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

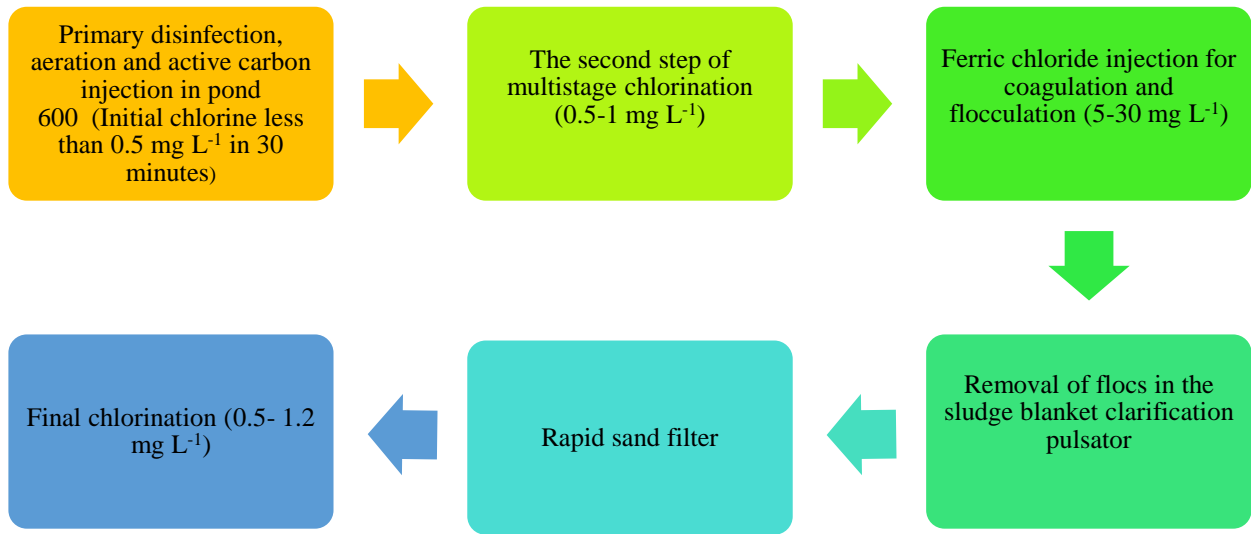
97 The rest of this paper is structured as follows: Section 2 studies the materials and methods of  
98 this research to provide our case study with its details. Section 3 is the results along with the  
99 discussion. Finally, the findings and conclusion along with future research recommendations are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

101 **2. Materials and methods**

102 **2.1. Case Study**

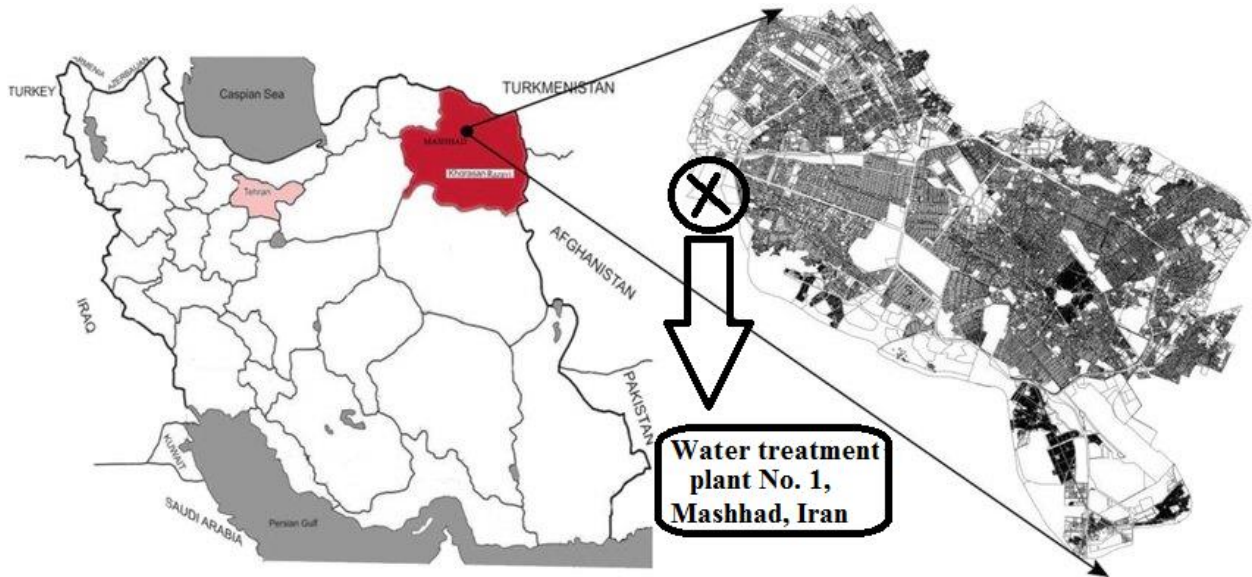
103 Water resources of Mashhad are supplied by groundwater and surface, the former includes Toroq,  
104 Kardeh, Ardak, and Doosti dams. Regarding the treatment processes, groundwater water resources  
105 have much fewer contaminants due to self-purification of the water by nature. Therefore, the costs  
106 of decontamination are not comparable in this case to that of surface water. The mentioned water  
107 resources are standardized, and treating in three treatment plants (No. 1, 2 and 3) prior to providing  
108 the urban water distribution network. The Kardeh and Ardak water resources are refined in  
109 treatment plant No.1, while Toroq and Doosti water resources are treated in treatment plants No.  
110 2 and 3, respectively. In this study, the coagulation and flocculation process behavior of treatment  
111 plant No.1 was supplied by the Kardeh dam. This treatment plant is located in Ab-o-bargh district  
112 and have started working since June, 1992on June, 1992. The nominal capacity of the plant is  
113 96000 m3 per day and is fed by Kardeh dam located in a distance of 40 km from the North-East  
114 of Mashhad. Water is transferred from dam to the treatment plant gravitationally, using 800-  
115 millimeter cast iron ductile pipes with an overall length of 46 km. Treatment process in this plant  
116 includes primary disinfection, aeration for gas outlet, addition of active carbon to remove organic  
117 materials, second step of multistage chlorination, injection of ferric chloride for coagulation and  
118 flocculation, removal of the produced flocs using Super pulsator process, passing through rapid  
119 sand filters, and final chlorination (Figure 1). The location of water treatment plant No. 1, Mashhad  
120 City, Iran is illustrated as per Figure 2.

121



122

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



124

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

## 126 2.2. Research roadmap

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

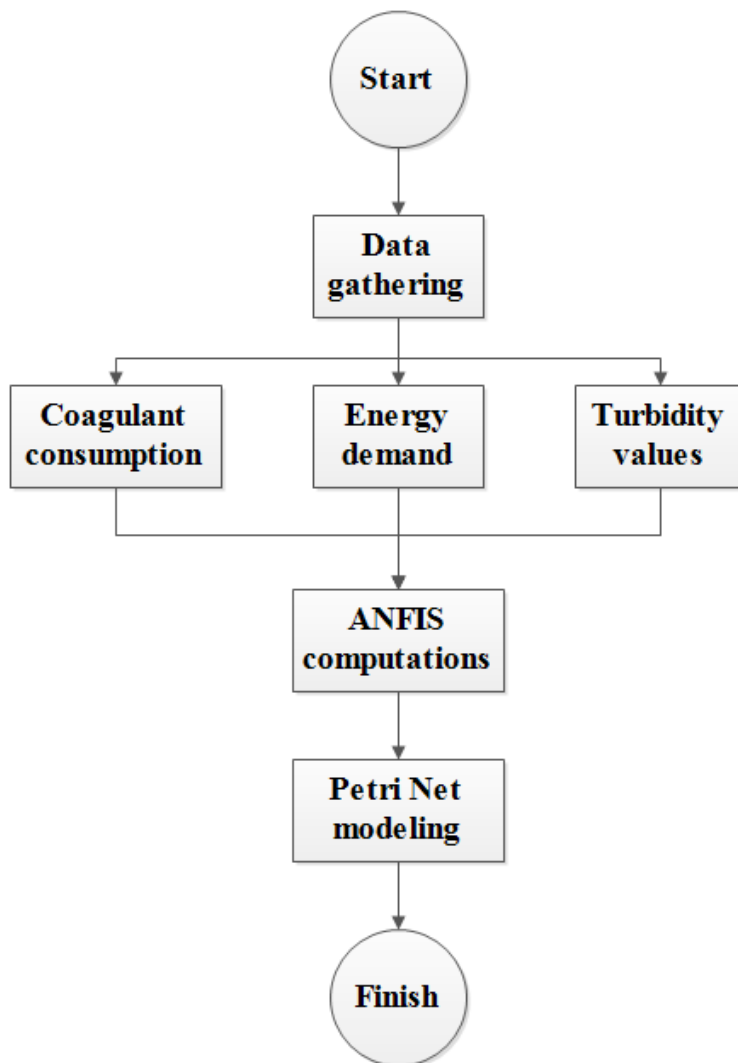
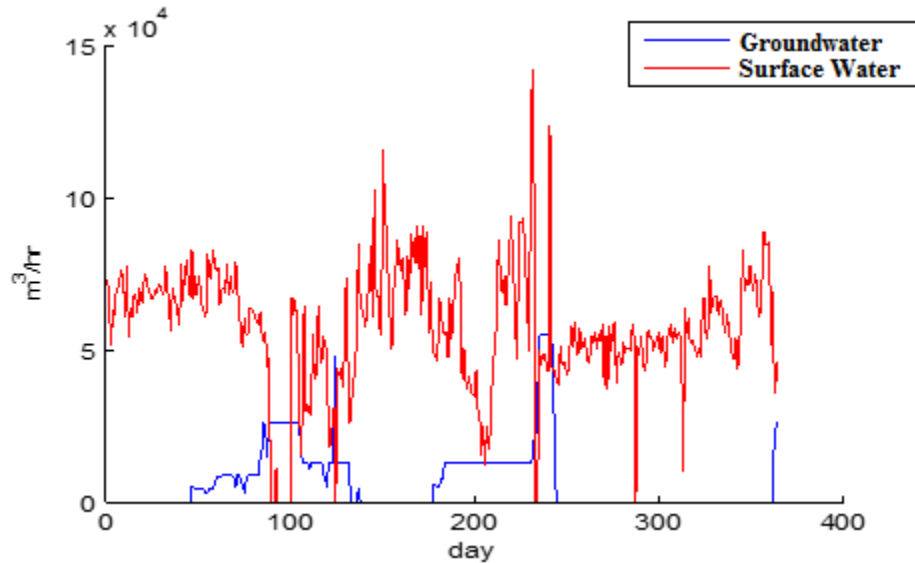


Figure 3. Research roadmap in present study.

### 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

1  
2  
3  
4 144 surface water in the treatment plant. As seen in Figure 4, the extent of surface and groundwater  
5  
6 145 water supplies annual consumption (in 2019) in treatment plant No. 1 is illustrated. All statistical  
7  
8 146 evaluations of present study are done in Excel 2016 software.  
9



10  
11  
12  
13  
14  
15  
16  
17  
18  
19  
20  
21  
22  
23  
24  
25  
26  
27  
28 147  
29  
30 148 Figure 4. The amount of water resources' shares in water treatment No.1, Mashhad, 2019.  
31

## 32 149 **2.4. The Prediction model and design operational pattern**

33  
34  
35 150 The concept of fuzzy cliques was presented and classified by Zadeh (Zadeh, 1997; Zadeh, 2015;  
36  
37 151 Ghadami et al., 2021; Mojtahedi, et al., 2021; Fathollahi-Fard et al., 2021a; Ali et al., 2021). Fuzzy  
38  
39 152 computation is a valuable technique for the systems complicated in difficult subjects which may  
40  
41 153 lead to a set of challenges for various studies such as decision making, assessment and prediction.  
42  
43 154 The fuzzy system is capable of implementing human's language as well as using individual's  
44  
45 155 experiences to progress. Fuzzy logic uses the experiences to develop a prediction of calculations.  
46  
47 156 There are many algorithms such as learning reinforcements which develop fuzzy sets to be learned  
48  
49 157 in various situations (Fathollahi-Fard et al., 2021; Akbarpour et al., 2021). Plus, ANN are achieved  
50  
51 158 through test, train, validation, calibration and verification. The ANN was introduced by  
52  
53 159 McCulloch-Pitts in the 1940s as per compute logical functions (Fathollahi-Fard et al., 2020a). The  
54  
55 160 ANN method makes this conceivable through numerical computing the influences of human brain  
56  
57 161 neurons. The ability to realize the relationships between inputs and outputs along with establishing  
58  
59 162 a complicated model are of significance. Nevertheless, ANN is a black box model and therefore  
60  
61  
62  
63  
64  
65 163 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.

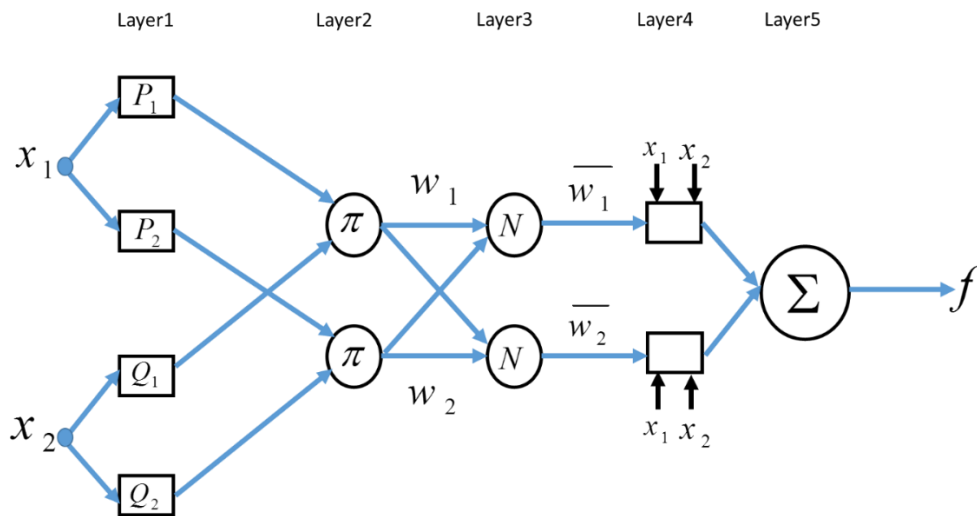


Figure 5. General ANFIS structure (Çaydaş, et al., 2009).

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.

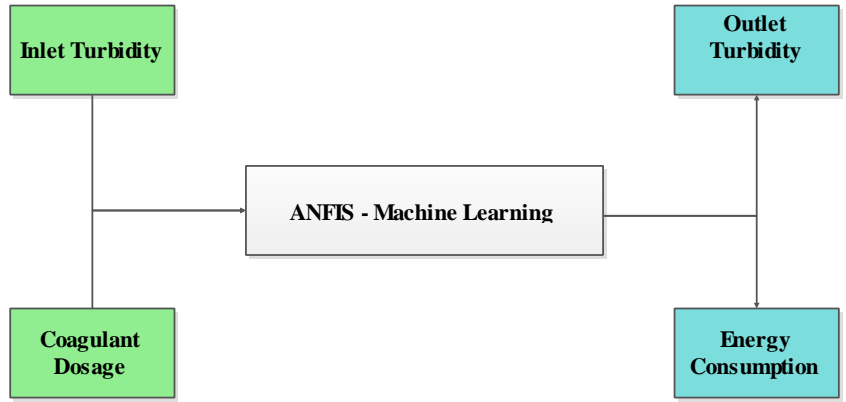


Figure 6. Conceptual model of machine learning in present issue.

### 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.

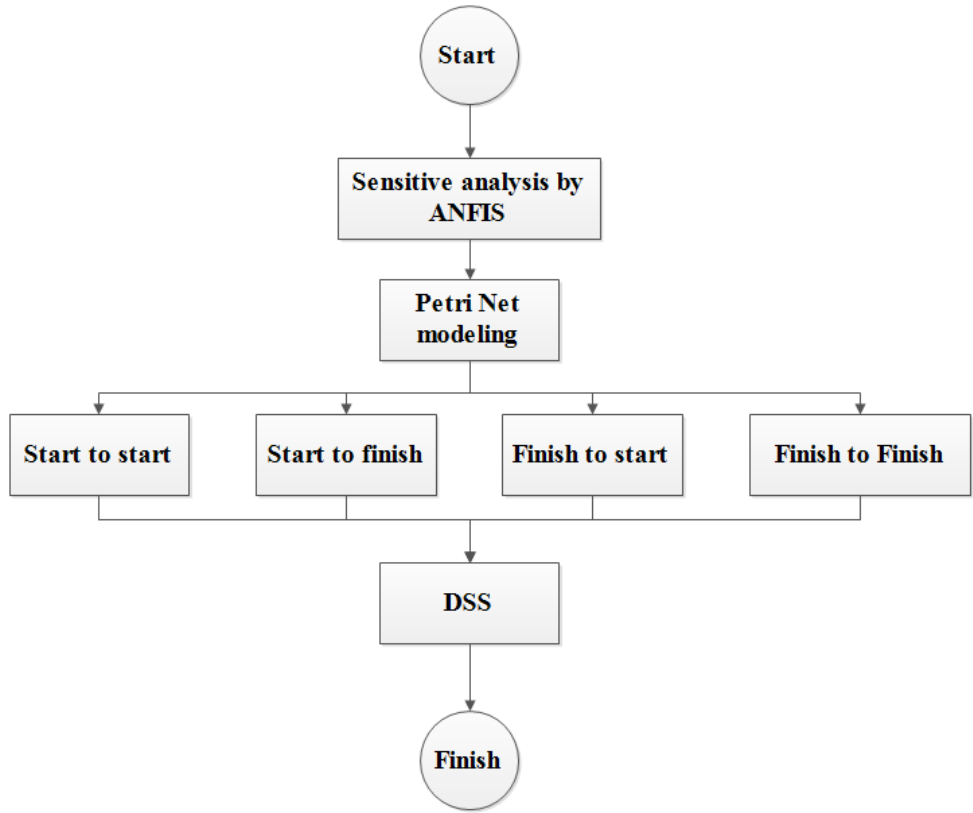


Figure 7. Algorithm of Petri Net modelling in present issue.

### 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

$$f_i = p_1i + q_1j + r_1k + s_1l + t \quad \text{Equation (1)}$$

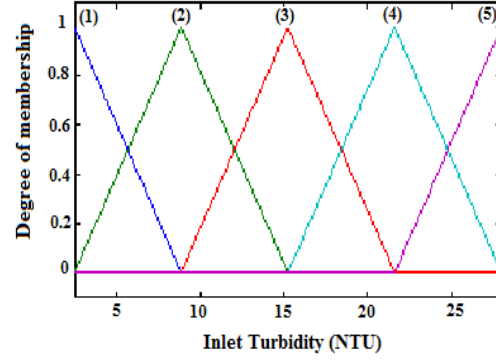
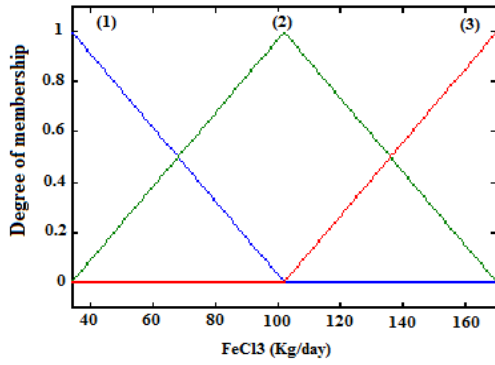
Where  $p_1$ ,  $q_1$ ,  $r_1$ ,  $s_1$  and  $t$  are constant variables. The mentioned constant values are determined through the ANFIS computations and with consideration to weights of each input parameters. Also,  $i$ ,  $j$ ,  $k$ , and  $l$  are the input values of ANFIS model as independent variations 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.



(a)

(b)

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.

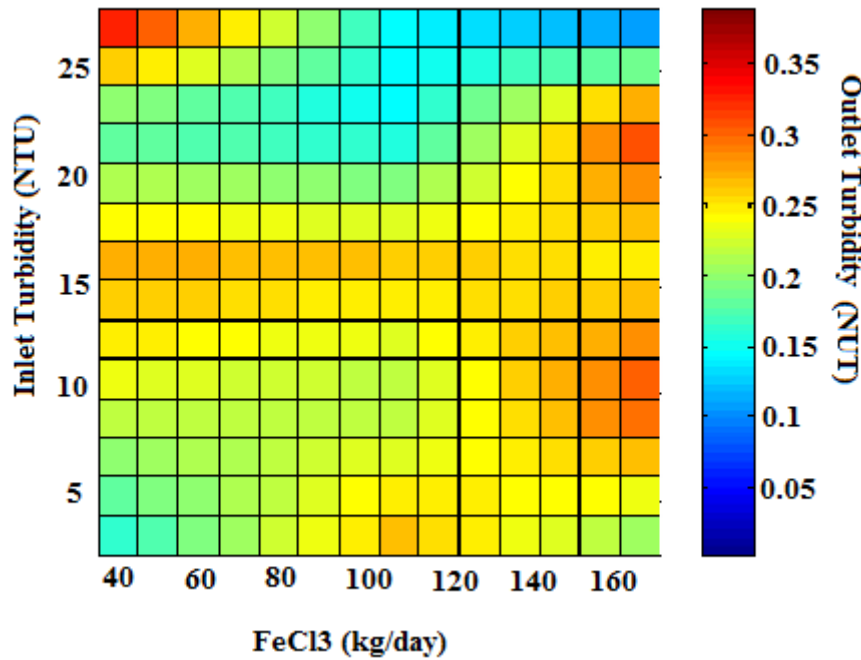
$$Q_i^4 = w_i^* \times f \quad \text{Equation (5)}$$

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

$$Q_i^4 = \sum_i w_i^* \times f = \frac{\sum_i w_i \times f}{\sum_i w_i}$$

Equation (6)

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



241  
 242 Figure 9. Outlet turbidity vs the injected ferric chloride and inlet turbidity.

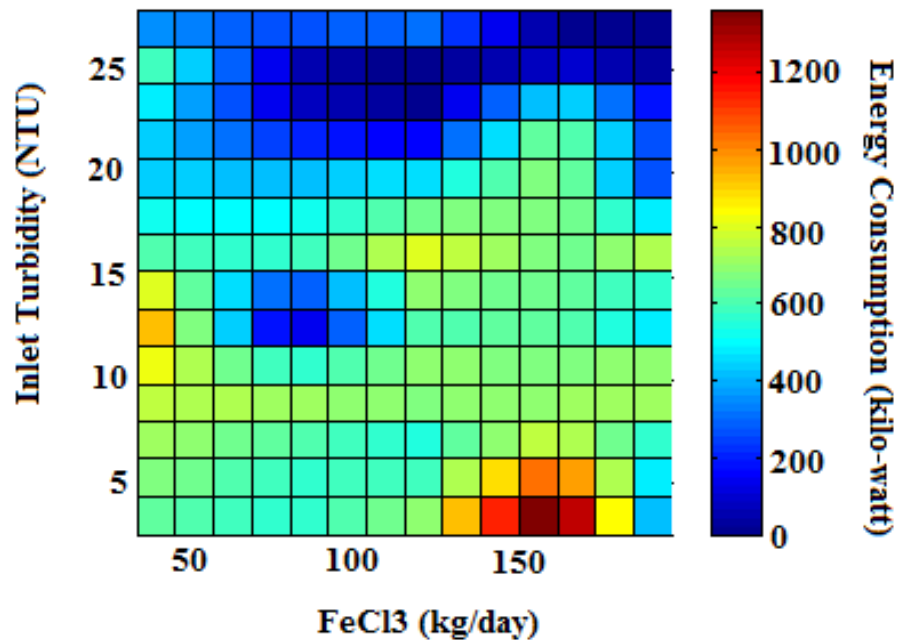


Figure 10. Energy consumed in kilo-watt vs the injected ferric chloride and inlet turbidity.

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<sup>2</sup> was used. If a set of data consists of n members like y<sub>1</sub>: y<sub>n</sub> and the predicted data are shown by f<sub>1</sub>: f<sub>n</sub>, then, the mean of observed data is calculated by Equation 7.

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

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

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

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

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

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

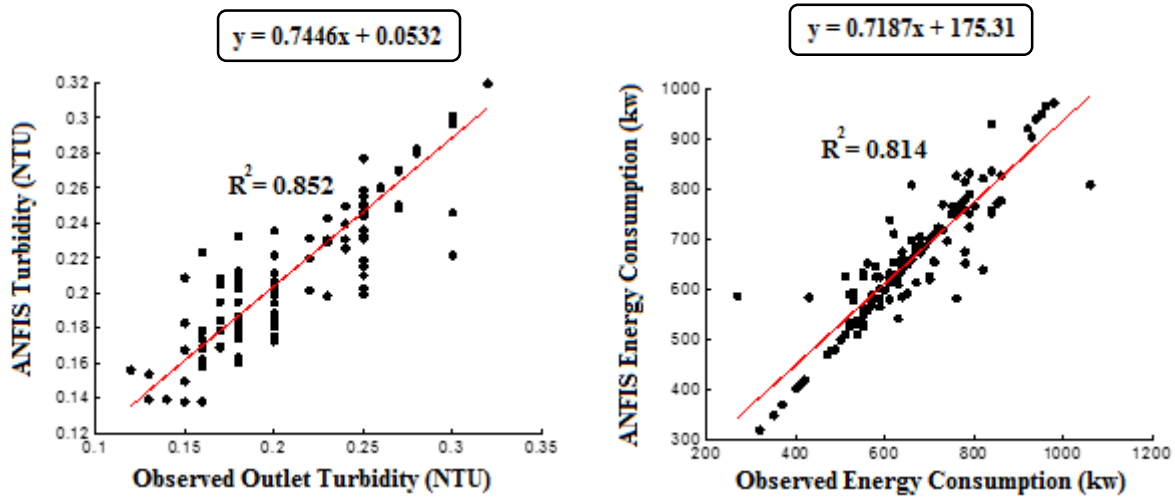
264  
 265 where  $R^2$  and  $\bar{y}$  are correlation coefficient and mean value of records.

266 The calculated coefficients of determination for the proposed models are shown in Table 1. This  
 267 is clear that the earlier R2 amount becomes to 100%, the better is the produced predicted model.  
 268 Accordingly, this model achieved  $R^2 > 80\%$  for both models which are capable of considering a  
 269 consistent model for predicting outlet turbidity and consumed energy. The outcomes of ANFIS  
 270 performance based on regression system is illustrated in Figure 11.

271 Table 1. Coefficient of determination (R2) for various models.

Model	R2
Predicting outlet turbidity	85%
Predicting energy consumption	81%

272  
 273  
 274  
 275



(a) (b)  
 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 (Eftekhari et al., 2021; Fasihi et al., 2021).

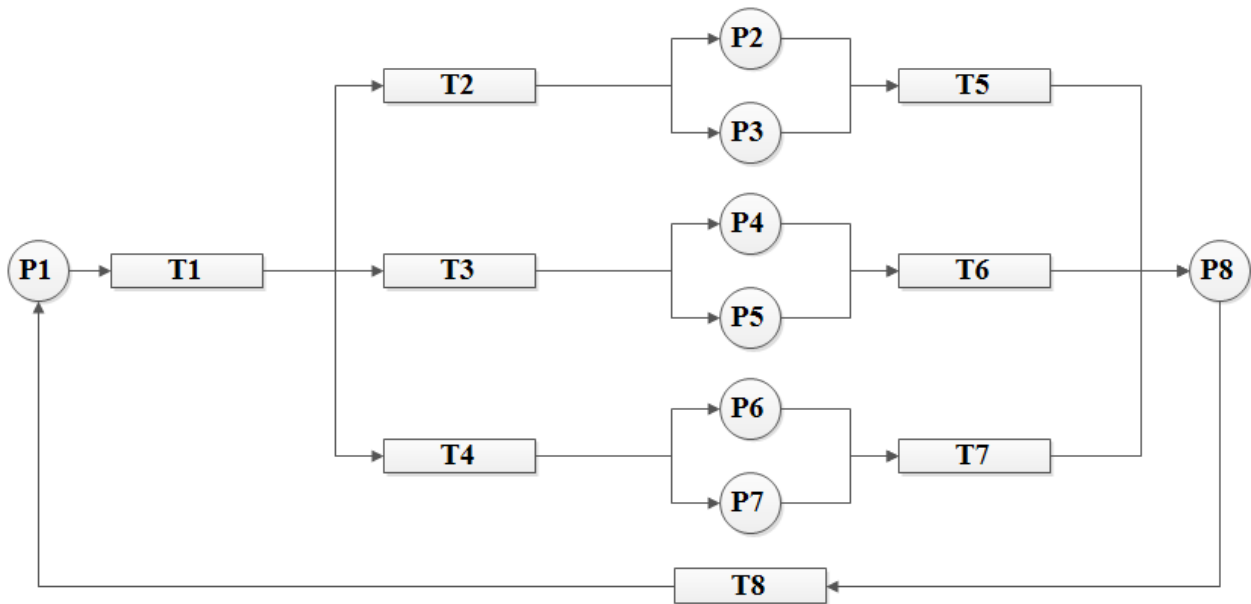
299 • The volume of computations is high and for more than three input parameters, it cannot  
 300 use as real time system and it calculate the outputs with delay (Ghadami et al., 2021).

301 • The ANFIS model is appropriate for single objective problems and due to multi objective  
 302 investigations, other systems are advised (Shakerian et al., 2021; Chouhan et al., 2021).

303 Finally, for future researches, present study suggests to compare outcomes of ANFIS model with  
 304 other classification techniques include Random Tree (RT), Random Forest (RF), and Artificial  
 305 Neural Network (ANN). Therefore, with the declared comparing, the best soft-sensor calculation  
 306 is determined.

### 3.3. Petri Net modelling

309 The pattern of Petri Net modelling is demonstrated according to Figure 12. As per the mentioned  
 310 Figure, in  $15 \pm 5\%$  inlet turbidity values, with adding 60-85 kg/day ferric chloride in the coagulation  
 311 and flocculation reactor, the amount of energy consumption and outlet turbidity are equal to 600  
 312 kw and 0.2 as per Figures 9 and 10. Likewise, in the more than  $15 \pm 5\%$  inlet turbidity, with 50-75  
 313 kg/day coagulant injection the consumed energy and outlet turbidity should control in 300 kw and  
 314 0.15, correspondingly. Finally, according to DSS, the in the less than  $15 \pm 5\%$  inlet turbidity, the  
 315 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  $15\pm 5\%$ ,

1  
2  
3  
4  
5  
6  
7  
8  
9  
10  
11  
12  
13  
14  
15  
16  
17  
18  
19  
20  
21  
22  
23  
24  
25  
26  
27  
28  
29  
30  
31  
32  
33  
34  
35  
36  
37  
38  
39  
40  
41  
42  
43  
44  
45  
46  
47  
48  
49  
50  
51  
52  
53  
54  
55  
56  
57  
58  
59  
60  
61  
62  
63  
64  
65

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.

**References:**

Akbarpour, N., Salehi-Amiri, A., Hajiaghaei-Keshteli, M., & Oliva, D., 2021. An innovative waste management system in a smart city under stochastic optimization using vehicle routing problem. *Soft Comput*, 25(8), 6707-6727.

Ali, S.M., Paul, S.K., Chowdhury, P., Agarwal, R., Fathollahi-Fard, A.M., Jabbour, C.J.C. and Luthra, S., 2021. Modelling of supply chain disruption analytics using an integrated approach: An emerging economy example. *Expert Syst Appl*, 173, 114690.

Alipour, M.H., Kibler, K.M. and Alizadeh, B., 2020. Flow alteration by diversion hydropower in tributaries to the Salween river: a comparative analysis of two streamflow prediction methodologies. *Int J River Basin Manag*, 1-11.

Alizadeh, B., Bafti, A.G., Kamangir, H., Zhang, Y., Wright, D.B. and Franz, K.J., 2021. A novel attention-based LSTM cell post-processor coupled with bayesian optimization for streamflow prediction. *J Hydrol*, 601, 126526.

Amini, M.H., Arab, M., Faramarz, M.G., Ghazikhani, A. and Gheibi, M., 2021. Presenting a soft sensor for monitoring and controlling well health and pump performance using machine learning, statistical analysis, and Petri net modeling. *Environ Sci Pollut Res*, 1-17.

Arzate, E., Huitzil, P., González, A., Martínez, B.E. and Grossmann, I.E., 2012. Automated optimization model to perform sensitivity analysis on cost of investment required to upgrade treatment plants in water networks. In *Computer Aided Chemical Engineering*, 30, 1063-1067.

1  
2  
3  
4 365 Berger, E., Haase, P., Kuemmerlen, M., Leps, M., Schaefer, R.B. and Sundermann, A., 2017. Water quality  
5  
6 366 variables and pollution sources shaping stream macroinvertebrate communities. *Sci Total Environ*,  
7  
8 367 587, 1-10.

9 368 Çaydaş, U., Hasçalık, A. and Ekici, S., 2009. An adaptive neuro-fuzzy inference system (ANFIS) model  
10  
11 369 for wire-EDM. *Expert Syst Appl*, 36(3), 6135-6139.

12 370 Choi, D.J. and Park, H., 2001. A hybrid artificial neural network as a software sensor for optimal control  
13  
14 371 of a wastewater treatment process. *Water Res*, 35(16), 3959-3967.

15  
16 372 Chouhan, V. K., Khan, S. H., & Hajiaghaei-Keshteli, M., 2021. Metaheuristic approaches to design and  
17  
18 373 address multi-echelon sugarcane closed-loop supply chain network. *Soft Comput*, 25(16), 11377-  
19  
20 374 11404.

21  
22 375 Djukic, M., Jovanoski, I., Ivanovic, O.M., Lazic, M. and Bodroza, D., 2016. Cost-benefit analysis of an  
23  
24 376 infrastructure project and a cost-reflective tariff: A case study for investment in wastewater  
25  
26 377 treatment plant in Serbia. *Renew Sustain Energy Rev*, 59, 1419-1425.

27 378 Doulabian, S., Ghasemi Tousi, E., Aghlmand, R., Alizadeh, B., Ghaderi Bafti, A. and Abbasi, A., 2021.  
28  
29 379 Evaluation of integrating swat model into a multi-criteria decision analysis towards reliable  
30  
31 380 rainwater harvesting systems. *Water*, 13(14), 1935.

32 381 Eftekhari, M., Gheibi, M., Azizi-Toupkanloo, H., Hossein-Abadi, Z., Khraisheh, M., Fathollahi-Fard, A.M.  
33  
34 382 and Tian, G., 2021. Statistical optimization, soft computing prediction, mechanistic and empirical  
35  
36 383 evaluation for fundamental appraisal of copper, lead and malachite green adsorption. *J Ind Inf*  
37  
38 384 *Integr*, 23, 100219.

39 385 Eftekhari, M., Akrami, M., Gheibi, M., Azizi-Toupkanloo, H., Fathollahi-Fard, A.M. and Tian, G., 2020.  
40  
41 386 Cadmium and copper heavy metal treatment from water resources by high-performance folic acid-  
42  
43 387 graphene oxide nanocomposite adsorbent and evaluation of adsorptive mechanism using  
44 388 computational intelligence, isotherm, kinetic, and thermodynamic analyses. *Environ Sci Pollut Res*,  
45  
46 389 27(35), 43999-44021.

47 390 Eggimann, S., Truffer, B. and Maurer, M., 2016. Economies of density for on-site waste water treatment.  
48  
49 391 *Water Res*, 101, 476-489.

50  
51 392 Elazzouzi, M., Haboubi, K. and Elyoubi, M.S., 2017. Electrocoagulation flocculation as a low-cost process  
52  
53 393 for pollutants removal from urban wastewater. *Chem Eng Res Des*, 117, 614-626.

54 394 Fasihi, M., Tavakkoli-Moghaddam, R., Najafi, S. E., & Hajiaghaei-Keshteli, M. 2021. Developing a Bi-  
55  
56 395 objective Mathematical Model to Design the Fish Closed-loop Supply Chain. *Int. J. Eng.*, 34(5),  
57  
58 396 1257-1268.

1  
2  
3  
4  
5  
6  
7  
8  
9  
10  
11  
12  
13  
14  
15  
16  
17  
18  
19  
20  
21  
22  
23  
24  
25  
26  
27  
28  
29  
30  
31  
32  
33  
34  
35  
36  
37  
38  
39  
40  
41  
42  
43  
44  
45  
46  
47  
48  
49  
50  
51  
52  
53  
54  
55  
56  
57  
58  
59  
60  
61  
62  
63  
64  
65

397 Fasihi, M., Tavakkoli-Moghaddam, R., Najafi, S. E., & Hajiaghaei, M., 2021. Optimizing a bi-objective  
398 multi-period fish closed-loop supply chain network design by three multi-objective meta-heuristic  
399 algorithms. *Scientia Iranica*.

400 Fathollahi-Fard, A.M., Ahmadi, A. and Al-e-Hashem, S.M., 2020a. Sustainable closed-loop supply chain  
401 network for an integrated water supply and wastewater collection system under uncertainty. *J*  
402 *Environ Manag*, 275, 111277.

403 Fathollahi-Fard, A.M., Hajiaghaei-Keshteli, M. and Tavakkoli-Moghaddam, R., 2020b. Red deer algorithm  
404 (RDA): a new nature-inspired meta-heuristic. *Soft Comput*, 24(19), 14637-14665.

405 Fathollahi-Fard, A.M., Hajiaghaei-Keshteli, M., Tavakkoli-Moghaddam, R. and Smith, N.R., 2021a. Bi-  
406 level programming for home health care supply chain considering outsourcing. *J Ind Inf Integr*,  
407 100246.

408 Fathollahi-Fard, A.M., Hajiaghaei-Keshteli, M., Tian, G. and Li, Z., 2020c. An adaptive Lagrangian  
409 relaxation-based algorithm for a coordinated water supply and wastewater collection network  
410 design problem. *Inf Sci*, 512, 1335-1359.

411 Fathollahi-Fard, A.M., Woodward, L. and Akhrif, O., 2021b. Sustainable distributed permutation flow-  
412 shop scheduling model based on a triple bottom line concept. *J Ind Inf Integr*, 100233.

413 Gerhard, W.A., Choi, W.S., Houck, K.M. and Stewart, J.R., 2017. Water quality at points-of-use in the  
414 Galapagos Islands. *Int J Hyg Environ Health*, 220(2), 485-493.

415 Ghadami, N., Gheibi, M., Kian, Z., Faramarz, M.G., Naghedi, R., Eftekhari, M., Fathollahi-Fard, A.M.,  
416 Dulebenets, M.A. and Tian, G., 2021. Implementation of solar energy in smart cities using an  
417 integration of artificial neural network, photovoltaic system and classical Delphi methods. *Sustain*  
418 *Cities Soc*, 74, 103149.

419 Gheibi, M., Eftekhari, M., Tabrizi, M.G., Fathollahi-Fard, A.M. and Tian, G., 2021. Mechanistic evaluation  
420 of cationic dyes adsorption onto low-cost calcinated aerated autoclaved concrete wastes. *Int J*  
421 *Environ Sci Technol*, 1-16.

422 Gheibi, M., Karrabi, M. and Eftekhari, M., 2019. Designing a smart risk analysis method for gas  
423 chlorination units of water treatment plants with combination of Failure Mode Effects Analysis,  
424 Shannon Entropy, and Petri Net Modeling. *Ecotoxicol Environ Saf*, 171, 600-608.

425 Haimi, H., Mulas, M., Corona, F. and Vahala, R., 2013. Data-derived soft-sensors for biological wastewater  
426 treatment plants: An overview. *Environ Model Softw*, 47, 88-107.

427 Igos, E., Benetto, E., Baudin, I., Tiruta-Barna, L., Mery, Y. and Arbault, D., 2013. Cost-performance  
428 indicator for comparative environmental assessment of water treatment plants. *Sci Total Environ*,  
429 443, 367-374.

1  
2  
3  
4  
5  
6  
7  
8  
9  
10  
11  
12  
13  
14  
15  
16  
17  
18  
19  
20  
21  
22  
23  
24  
25  
26  
27  
28  
29  
30  
31  
32  
33  
34  
35  
36  
37  
38  
39  
40  
41  
42  
43  
44  
45  
46  
47  
48  
49  
50  
51  
52  
53  
54  
55  
56  
57  
58  
59  
60  
61  
62  
63  
64  
65

430 Jalali, F.M., Masoomi, S.R., Azizi, M., Aghlmand, R., Gheibi, M. and Kian, Z., 2021. Determining the  
431 chlorine kinetic behavior in surface water using evolutionary metaheuristic algorithms. *Ann Biol*,  
432 4(1), 026-030.

433 Jang, J.S., 1993. ANFIS: adaptive-network-based fuzzy inference system. *IEEE Trans Sys, Man, Cyber*,  
434 23(3), 665-685.

435 Khorrami, M., Abrishami, S., Maghsoudi, Y., Alizadeh, B. and Perissin, D., 2020. Extreme subsidence in  
436 a populated city (Mashhad) detected by PSInSAR considering groundwater withdrawal and  
437 geotechnical properties. *Sci Rep*, 10(1), 1-16.

438 Kisło, A. and Skoczko, I., 2015. Cost of municipal water treatment plant in the biggest Polish town in  
439 Podlaskie province for the years 2010–2012. *Ecol Eng*, 16(2).

440 Lu, B., Du, X. and Huang, S., 2017. The economic and environmental implications of wastewater  
441 management policy in China: from the LCA perspective. *J Clean Prod*, 142, 3544-3557.

442 Marzouk, M. and Elkadi, M., 2016. Estimating water treatment plants costs using factor analysis and  
443 artificial neural networks. *J Clean Prod*, 112, 4540-4549.

444 McGivney, W. and Kawamura, S., 2008. Cost estimating manual for water treatment facilities. Hoboken,  
445 NJ: John Wiley & Sons.

446 Mohammadi, M., Gheibi, M., Fathollahi-Fard, A.M., Eftekhari, M., Kian, Z. and Tian, G., 2021. A hybrid  
447 computational intelligence approach for bioremediation of amoxicillin based on fungus activities  
448 from soil resources and aflatoxin B1 controls. *Environ Manage*, 299, 113594.

449 Mojtahedi, M., Fathollahi-Fard, A.M., Tavakkoli-Moghaddam, R. and Newton, S., 2021. Sustainable  
450 vehicle routing problem for coordinated solid waste management. *J Ind Inf Integr*, 23, 100220.

451 Mosallanezhad, B., Hajiaghaei-Keshteli, M., & Triki, C. (2021). Shrimp closed-loop supply chain network  
452 design. *Soft Comput*, 25(11), 7399-7422.

453 Muyibi, S.A. and Evison, L.M., 1995. Optimizing physical parameters affecting coagulation of turbid water  
454 with *Moringa oleifera* seeds. *Water Res*, 29(12), 2689-2695.

455 Ndabigengesere, A., Narasiah, K.S. and Talbot, B.G., 1995. Active agents and mechanism of coagulation  
456 of turbid waters using *Moringa oleifera*. *Water Res*, 29(2), 703-710.

457 Pan, J.R., Huang, C., Chen, S. and Chung, Y.C., 1999. Evaluation of a modified chitosan biopolymer for  
458 coagulation of colloidal particles. *Colloids Surf A Physicochem Eng Asp*, 147(3), 359-364.

459 Sadri, E., Harsej, F., Hajiaghaei-Keshteli, M., & Siyahbalaii, J., 2021. Evaluation of the components of  
460 intelligence and greenness in Iranian ports based on network data envelopment analysis (DEA)  
461 approach. *Journal of Modelling in Management*.

1  
2  
3  
4  
5  
6  
7  
8  
9  
10  
11  
12  
13  
14  
15  
16  
17  
18  
19  
20  
21  
22  
23  
24  
25  
26  
27  
28  
29  
30  
31  
32  
33  
34  
35  
36  
37  
38  
39  
40  
41  
42  
43  
44  
45  
46  
47  
48  
49  
50  
51  
52  
53  
54  
55  
56  
57  
58  
59  
60  
61  
62  
63  
64  
65

462 Singh, P., Carliell-Marquet, C. and Kansal, A., 2012. Energy pattern analysis of a wastewater treatment  
463 plant. *Appl Water Sci*, 2(3), 221-226.

464 Shahsavari, M.M., Akrami, M., Gheibi, M., Kaviani, B., Fathollahi-Fard, A.M. and Behzadian, K., 2021.  
465 Constructing a smart framework for supplying the biogas energy in green buildings using an  
466 integration of response surface methodology, artificial intelligence and petri net modelling. *Energy*  
467 *Convers Manag*, 248, 114794.

468 Shahsavari, M.M., Najafzadeh, M., Akrami, M., Kian, Z. and Gheibi, M., 2021. Qualitative Evaluation of  
469 Surface Water Resources Using Iran Water Quality Index (IRWQSI) and National Sanitation  
470 Foundation Water Quality Index (Case Study: Kardeh Dam, Mashhad, Iran). *Ann Environ Sci*  
471 *Toxicol*, 5(1), 030-037.

472 Shakerian, M., Gheibi, M. and Eftekhari, M., 2021. Vortex assisted dispersive solid phase extraction of  
473 thallium followed by electrothermal atomic absorption spectrometry, Adsorption mechanism and  
474 soft computing algorithm prediction. *Int J Environ Anal Chem*, 1-21.

475 Vouk, D., Malus, D. and Halkijevic, I., 2011. Neural networks in economic analyses of wastewater systems.  
476 *Expert Syst Appl*, 38(8), 10031-10035.

477 Zadeh, L.A., 1997. Toward a theory of fuzzy information granulation and its centrality in human reasoning  
478 and fuzzy logic. *Fuzzy Sets Syst*, 90(2), 111-127.

479 Zadeh, L.A., 2015. The information principle. *Inf Sci*, 294, 540-549.

480 Zahedi, A., Salehi-Amiri, A., Hajiaghayi-Keshteli, M., & Diabat, A., 2021. Designing a closed-loop supply  
481 chain network considering multi-task sales agencies and multi-mode transportation. *Soft Comput*,  
482 25(8), 6203-6235.

483 Zhang, Y., Alizadeh, B., Cunha, L., Anderson, R., Curtis, D., Seo, D.J., Yates, D. and Walker, D., 2020,  
484 December. The impacts of ingesting and updating soil moisture-based loss coefficients on HEC-  
485 HMS-based reservoir inflow prediction. *In AGU Fall Meeting Abstracts*, H047-06.

486 Zhang, C., Tian, G., Fathollahi-Fard, A.M., Wang, W., Wu, P. and Li, Z., 2020. Interval-valued  
487 intuitionistic uncertain linguistic cloud petri net and its application to risk assessment for subway  
488 fire accident. *IEEE Trans Auto Sci Eng*.

489 Zhou, T., Wang, Z. and Li, W., 2011. A cost model approach for RO water treatment of power plant.  
490 *Procedia Environ Sci*, 11, 581-588.