A Study of Soft Computing Techniques in Chemical Reactions

RAMJEET SINGH YADAV

Department of Computer Science and Engineering
Ashoka Institute of Technology and Management, Varanasi 221007, Uttar Pradesh, India
ramjeetsinghy@gmail.com

Abstract. This research paper describes the fuzzy logic and hybrid fuzzy logic-based systems, which are utilized to create knowledge-based frameworks in chemical engineering. In this study, we have proposed fuzzy logic-based methods such as subtractive clustering (SC) and integrated approach of SC with artificial neural network fuzzy inference system (SC-ANFIS) for calculating the rate of chemical reactions. The root mean square error (in both training and testing data) of SC-ANIFIS is less as compared to existing FCM method. So, the proposed methods give better results as compared to the exiting methods such as classical fuzzy logic and fuzzy C-means (FCM).

Keywords: Classical logic, Fuzzy Logic, ANFIS, SC, SC-ANFIS.

(Received January 30th, 2021 / Accepted May 18th, 2021)

1 Introduction

In the recent years, fuzzy logic and hybrid methods have been demonstrated to be effective methods for decision-making frameworks. These methods are based on the fuzzy set and have been utilized in a few chemical reactions.

The chemical engineering is the discipline of engineering that validates the applications of physical sciences with mathematics. Control system based intelligent technique is a control framework with the extreme degree of independence in terms of self-learning, self-configuration, thinking, data arranging and decision-making and moreover the capacity to extricate the most profitable data from unstructured and loud information from any powerfully complex framework and environment [20].

Complex mechanical forms such as clump chemical reactors, blast furnaces, cement ovens and fundamental of oxygen in steel making, are troublesome to control naturally. Generally, the handle controls to regulate the quality and amount of the items to be delivered were used by the human administrators in the past. [11].

Ranganath Muthu and Elamin EI kanzi have proposed a fuzzy logic based controller for simulation of pH neutralization process [13]. A real-time execution of the fuzzy logic controller (FLC) was performed to control the fluid level of a circular tank. Control of fluid level in a circular tank is profoundly non-linear due to varied range of cross-sectional areas of the level framework with alteration in shape [18]. The investigated endeavors to upgrade the capacity of the fuzzy logic controller in controlling wastewater treatment framework, highlights the pH parameter in manufacturing wastewater treatment plants [16]. Abolpour showed that a fuzzy logic suggests the lime-enhancement and hydrogen reuction by cuprous sulfide. They discovered a well-defined relationship between the crucial factors [2, 1].

Morteza Sadegh Amalnik presented the advancement of fuzzy logic controller to include the insights in the electrochemical machining (ECM) process. Fuzzy logic techniques were utilized to construct a fuzzy logic controller framework, which controls nourish rate of the device and the stream rate of the electrolyte [4].

We concentrate on the suggestions of individual express when it delivers reasons for the things. For us, a contention is a list of suggestions, called the premises, taken after by a word such as "therefore" or "so" and at that point, another suggestion called the conclusion [15]. Researchers have described a non-iterative method for solving fuzzy reactions that have the ability to obtain and select solutions of different quality [6].

Taking into the view that the differential equation is a vital instrument to describe and get it's real-world form, it is imperative to analyze the behavior of a chemical reaction by utilizing differential equation. First-order differential equations are examined in chemistry [19]. Creators of [17] have examined the energy of chemical reactions by utilizing the isothermal calorimetric information. A bundle of response kinetics is displayed and portrayed in [14]. A consistent state estimation approach for equation rate conditions is displayed in [9]. In accordance with this approach, coupled differential equations are changed into a system of arithmetical conditions, one for each species within the responses.

After thorough review of modeling/calculation of coefficient rate of chemical reactions, we have found that the fuzzy inference system techniques have very rarely been used for calculating the rate of chemical reactions by changing the temperature and other properties of particles/substance of the reaction. Keeping this point into consideration, in this paper we have tried to search the desirable reaction rate in fuzzy environment with artificial neural network. In this context, we have proposed subtractive clustering-adaptive neuro fuzzy inference system (SC-ANFIS). SC-ANFIS method automatically converts the crisp data into fuzzy set and also calculates the coefficient rate of chemical reactions.

2 Approximate Reasoning in Fuzzy Logic

The thought of linguistic fuzzy models of mimicking the human way was considered and proposed by Zadeh in his spearheading work [24]. Induction in approximate reasoning is the sharp differentiation to deduce in classical logic. Induction in surmised thinking is computation [15] with fuzzy sets that speaks the meaning of a certain set of fuzzy recommendations. Approximate reasoning with fuzzy sets envelops a wide assortment of deduction plans and has been promptly connected in numerous fields like decision making, expert system, medical science, computer engineering and other branch of engineering [5].

2.1 Fuzzy Set

In crisp set, the elements are either completely belonged to a set or not completely belong to a set. But in a fuzzy set, elements are partially belonged to a set called universal set. The universal set is also known as universe of discourse. The true value of every element in a set is calculated by a characteristic function. This characteristic function is known as membership function and denoted by μ_A, where A is the crisp set or universe of discourse. The formula of characteristic function or membership function is given as:

$$\mu_A : X \to [0, 1] \tag{1}$$

Fuzzy logic is the extension of a classical logic. The value of membership function lies in between 0 to 1 [24].

2.2 IF-THEN Rule

In classical logic, the IF-THEN rule is given by in the forms of: IF statement and THEN statement. The IF part is known as premise part whereas, THEN part is known as conclusion part [22].

2.3 Approximate Reasoning Models

There are two types of models of approximate reasoning: (1) **Linguistic fuzzy model:** This model has both premise part as well as conclusion part and referred as fuzzy statement. (2) **Fuzzy relational model:** Fuzzy relational model is an extension of linguistic model in which premise statement is connected by a number of diverse consequent statements from beginning to end in a fuzzy relation [25, 12, 8].

2.4 Fuzzy Relation

Fuzzy relation

Fuzzy relation is a fuzzy set which is defined by the cartesian product of fuzzy sets on the universe of discourse X.

Fuzzy Cartesian product

The cartesian product of fuzzy set *A* and *B* is represented by fuzzy relation *R* and denoted by $A \times B$. Relation *R* is given by the following relation [10, 21]:

$$R = A \times B \subseteq X \times Y \tag{2}$$

Membership function of fuzzy relation *R* is defined as

$$\mu_R\,(x, y) = \mu_{(A\times B)}\,(x, y) = min\,[\mu_A(x), \mu_A(y)] \tag{3}$$

There are various methods available for the calculation of implication in fuzzy relation for chemical reactions. Let us consider *A* and *B* are two fuzzy sets and *R* is relation given by the following equation:

$$B = A \circ R \tag{4}$$

3 Fuzzy C-Means Clustering (FCM) Method

The fuzzy C-means (clustering algorithms) are frequently used to identify the clusters. The objective (criterion) function of the fuzzy C-means (FCM) is referred as:

$$f_b(U,Z) = \sum_{i=1}^{C}\sum_{k=1}^{N}\left(\mu_{C_i}(x_k)\right)^m \|x_k - z_i\|^2 \tag{5}$$

Where U = fuzzy partition of the dataset X created by $C_1, C_2, \ldots, C_k$; x_k = Point in data space, $= 1, 2, \ldots, N$, N = Number of data points, m = Weighing parameters that find out the measure of fuzziness up to which the biased membership values of a cluster influences the result of clustering, z_i = final cluster center, $i = 1, 2, \ldots, c$, c = Number of fuzzy rules, $\mu_i k \in [0,1]$ = Grade of fuzzy membership of the k^{th} data points belong to the i^{th} fuzzy set, $\mu_i k$ is restricted as follows [1]:

$$\sum_{i=1}^{C} \mu_{ik} = 1, 2, \ldots, N \tag{6}$$

Algorithm

Step 1: The preliminary cluster centers for all $k = 1, 2, \ldots, N$ and $i = 1, 2, \ldots, c$. Initial fuzzy C partition ($U = [\mu_{ik}]$) used to represent membership value for the i^{th} cluster center.

Step 2: To compute the following equation:

$$z_i = \frac{\sum_{k=1}^{N} z_k(\mu_{ik})^m}{\sum_{k=1}^{N}(\mu_{ik})^m},\ i = 1, 2, \ldots, c \tag{7}$$

Step 3: To iteratively recalculates (update) U to adjust cluster centers of the following equation:

$$\mu_{ik} = \left[\sum_{j=1}^{c}\left(\frac{x_k - z_i}{x_k - z_j}\right)^{\frac{2}{m-1}}\right]^{-1} \tag{8}$$

$$i = 1, 2, \ldots, c \;\; k = 1, 2, \ldots, N$$

Step 4: To check for termination criteria if

$$\|U_k - U_{k-1}\| < \varepsilon \tag{9}$$

Stop else, let $k = k + 1$ and go to step 2.

Step 5: To recognize conclusion parameters with the help of orthogonal least squares (OLS) technique.

4 Subtractive Clustering Method

Subtractive clustering is an extension of mountain method proposed by Chiu [7, 23].

$$D_i = \sum_{j=1}^{N} exp\left(-\frac{\|x_i - x_j\|^2}{(\frac{r_a}{2})^2}\right) \tag{10}$$

$[x_1, x-2, \ldots, x_N]$ = Data points space. The radius of hypercube is denoted by r_a and $r_a \in [0,\infty]$. The neighboring compactness of the cluster is also known as hypercube. The formula for updating the cluster center is as follows:

$$D_i = D_i - D_{c1}\sum_{j-1}^{N} exp\left(-\frac{\|x_i - x_{c1}\|^2}{(\frac{r_b}{2})^2}\right) \tag{11}$$

Where x_{c1} denotes the first cluster center, D_{c1} denotes the largest density and $r_b \in [0,\infty]$. The value of r_b is $1.5r_a$.

5 Subtractive Clustering-Artificial Neural Fuzzy Inference System (SC-ANFIS)

The SC-ANFIS is an integrated method of subtractive clustering and artificial neural network. The subtractive clustering is based on fuzzy set. Therefore, the integrated SC based fuzzy method with back-propagation learning gives very good results [3].

6 Experimental Results

In chemical engineering discipline, the chemical reactions happen at distinctive level of rates. These rates of reactions depend upon a few key components of chemical reactions. In the proposed method, the utilization of fuzzy logic method and reasoning of approximations are used to assess the rate of chemical reaction at which the chemical response is performed. The chemical reactions are characterized in terms of different variables. The strategy is outlined by utilizing inaccurate information in terms of data which is in the form of implications and conditional propositions. Fuzzy proposition logic method includes variables on which rate of reaction depends and measures the rate of chemical reactions with response to these factors. The rate of chemical reaction depends on the key features such as temperature and particles size. Essentially, the rate of chemical reaction also depends upon the recurrence of the collisions between particles. The rate of chemical reaction will be fast if the collision between particles is frequent and vice versa. The collision between particles and the rate of chemical reaction (frequency) increases with increasing the particles size and temperature. Every chemical reaction has both minimum and maximum range of rate. The variation from the boundaries can make genuine issues. Underneath the boundary no chemical reactions will occur and over it is exceptionally dangerous.

6.1 Existing Fuzzy C-Means Clustering (FCM) [M. Jafarli, 2020]

M. Jafarli describes the implementation and testing of the calculation of coefficient rate of chemical reaction of proposed work by using fuzzy C-means clustering [10]. This method automatically generates the fuzzy membership function for the calculation of coefficient rate of chemical reaction. Department of Chemistry, Banarus Hindu University (BHU), Varanasi is the source of dataset. For the purpose of experimental results and discussion, we have taken 50 dataset for training purpose and 20 datasets for the testing purpose of the fuzzy C-means clustering (FCM) method. These datasets are shown in table 7 and 8. The features of these data are concentration of particles and coefficient rate of chemical reactions. The Mamdani fuzzy inference system has five input variables namely very low, low, medium, high and very high and five output variables namely very slow, slow, medium, high and very high. These input and output variables connected through IF-THEN fuzzy inference rule. Table 1 shows the input variables namely very low, low, medium, high and very high. These are the linguistic variables representing the fuzzy sets. Table 2 shows the output variables namely very slow, slow, medium, high and very high. These are the linguistic variables representing the fuzzy sets.

Table 1: Membership function of input variables (Concentration of particles)

S.No.	Membership Function	Membership Value
1	Very Low	(0.0478, 0.8395)
2	Low	(0.0812, 0.6451)
3	Medium	(0.1230, 0.4366)
4	High	(0.0374, 0.9460)
5	Very High	(0.04418, 0.9944)

The fuzzy IF-THEN rules are given below:

1. If the concentration of particles is very low then the rate of reaction is very slow.

2. If the concentration of particles is low then the rate of reaction is slow.

Table 2: Membership function of output variables (Rate of chemical reaction)

S.No.	Membership Function	Membership Value
1	Very Slow	(0.0001566, 0.0002575)
2	Slow	0.0001489 0.0004127
3	Medium	(0.000142, 0.0004948)
4	High	[0.0007833 0.001193
5	Very High	0.0008341 0.0005899

3. If the concentration of particles is medium then the rate of reaction is also medium.

4. If the concentration of particles is high then the rate of reaction is also high.

5. If concentration of particles is very high then the rate of reaction is also very high.

The objective function suggests the suitability of the fuzzy C-means clustering method. The value of objective function of fuzzy C-means clustering (FCM) method is 0.024337, after 29 iterations. These twenty nine iterations are stopping criteria of FCM method. Figure 1 shows objective function values of FCM model, which gain after twenty nine iterations. This shows that after 10 iterations, the value of objective is saturated, i.e. reaches the stopping criterion of FCM algorithms.

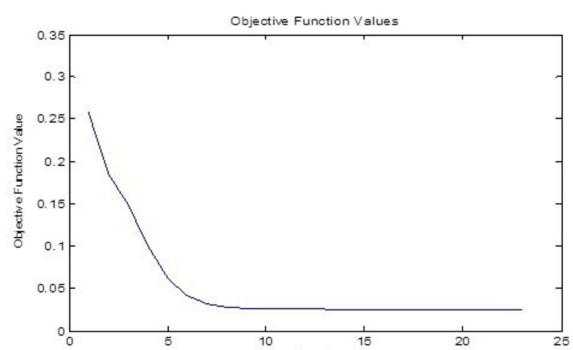

Figure 1: Objective function values

For accuracy evaluation of FCM model, we have used root mean square error (RMSE) method. The RMSE of FCM is 2.8549×10^{-4} for training datasets and 2.9462×10^{-4} is for testing datasets, respectively.

6.2 Proposed Methods

In this section, we have proposed two methods namely subtractive clustering (SC) and subtractive clustering-artificial neural fuzzy inference system (SC-ANFIS) methods for calculating the coefficient rate of chemical reactions. The SC-ANFIS method has high learning capability due to artificial neural network. So, this proposed method is very efficient for calculating the rate of chemical reactions. The experimental results and discussion of these two proposed methods are given below:

Subtractive Clustering (SC) Method

The implementation and testing of SC to calculate the coefficient rate of chemical reactions have been described in this section. The SC method automatically generates the fuzzy membership function to calculate the coefficient rate of chemical reactions. For experimental results and discussion of the SC method, we have taken 50 dataset for training purpose and 20 datasets for the testing purpose. These datasets are shown in table 7 and 8. The features of these data are concentration of particles and coefficient rate. Table 3 shows the input variables namely low, medium and high. Table 4 shows the output variables namely slow, medium and high. The experimental result of SC method is shown in table 7 and 8 for training and testing datasets, respectively. Figure 2 shows the surface viewer of input (concentration of particles) and output (rate of reaction) variables.

Table 3: Membership function of input variables (Concentration of particles)

S.No.	Membership Function	Membership Value
1	Low	(0.1096, 0.5517)
2	Medium	(0.1096, 0.9499)
3	High	(0.1096, 0.9987)

In Sugeno-type fuzzy inference, linear membership function is used for output variables. Functions with linear relationship with input output variables are listed in table 4.

Table 4: Membership function of output variables (Rate of chemical reaction)

S.No.	Membership Function	Membership Value
1	Slow	(0.112400, -0.029770)
2	Medium	(0.238000, -0.310100)
3	High	(-0.001466, 0.001063)

The fuzzy IF-THEN rules are given below:

1. If the concentration of particles is low then the rate of reaction is slow.
2. If the concentration of particles is medium then the rate of reaction is also medium.
3. If the concentration of particles is high then the rate of reaction is also high.

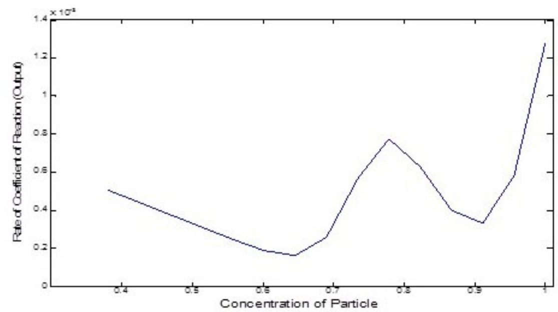

Figure 2: Surface viewer of input (concentration of particles) and output (rate of reaction) variables

The training error of the output of subtractive fuzzy inference system is as follows:

Training Error $= 2.5249 \times 10^{-4}$

The testing error of the output of subtractive fuzzy inference system is as follows:

Testing Error $= 2.6453 \times 10^{-4}$

Both, training root mean square error and testing root mean square error are less as compared to the existing fuzzy C-means clustering method [10]. Due to this reason, we can say that the proposed subtractive clustering method predicts the better results as compared to the fuzzy C-means clustering method for calculating the coefficient rate of chemical reactions

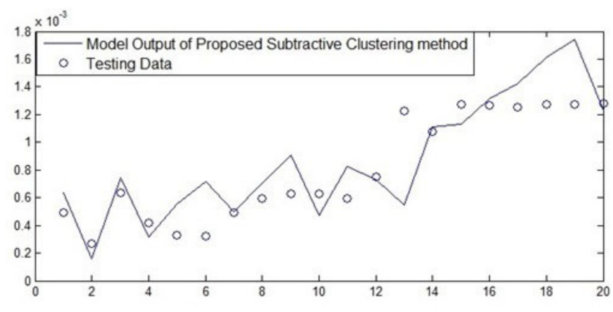

Figure 3: Proposed subtractive clustering based model output and testing dataset

The coefficient rate of chemical reactions (original laboratory results and results of subtractive clustering method) has been classified into slow, medium and high. The proposed model (SC) has been trained with the help of 50 training datasets and tested with 25 datasets (Table 7 and 8). The MATLAB software has been utilized for calculating the coefficient rate of chemical reactions. The experimental results of sub-subtractive clustering method and testing datasets are shown in figure 3. The subtractive clustering based model output and testing dataset are shown as circles solid lines, respectively. After comparing the results of training error (RMSE) and testing error (RMSE), it was found that both errors are less as compared to existing fuzzy C-means clustering method [10]. Due to this reason, we can say that the proposed subtractive clustering method gives better result of coefficient rates of chemical reactions as compared to the fuzzy C-means clustering method (M. Jafarli, 2020 method) [10] in chemical engineering.

The plotted figure 3 shows that the subtractive based fuzzy inference system does not perform well as compared to the testing datasets. This is the over-fitting condition of subtractive clustering method. We can solve this problem with help of artificial neural network. At this point, we have proposed SC-ANFIS model to calculate the coefficient rate of chemical reaction. The SC-ANFIS model has high level learning capability due to artificial neural network method. The experimental results and discussion of SC-ANFIS method are given in below section:

Subtractive Clustering based ANFIS (SC-ANFIS) Method

The implementation and testing of SC-ANFIS results have been described in this section to calculate the coefficient rate of chemical reactions. The SC-ANFIS method automatically generates the fuzzy membership function to calculate the coefficient rate of chemical reactions. For the purpose of experimental results and discussion of the SC-ANFIS method, we have taken 50 datasets for training purpose and 25 datasets for the testing purpose. These datasets are shown in table 7 and 8. The table 5 shows the input variables namely low, medium and high. The table 6 shows the output variables namely slow, medium and high. The features of these data are concentration of the particles and coefficient rate. The experimental results of SC-ANFIS method are shown in table 7 and 8. Figure 4 shows the SC-ANFIS based Sugeno fuzzy inference system to calculate the coefficient rate of chemical reactions. This Sugeno fuzzy inference system has the three inputs and one output. The three inputs map into one output with the help of IF-THEN fuzzy rules. The fuzzy IF-THEN rules are given below:

1. If the concentration of particles is low then the rate of reaction is slow.

2. If the concentration of particles is medium then the rate of reaction is also medium.

3. If the concentration of particles is high then the rate of reaction is also high

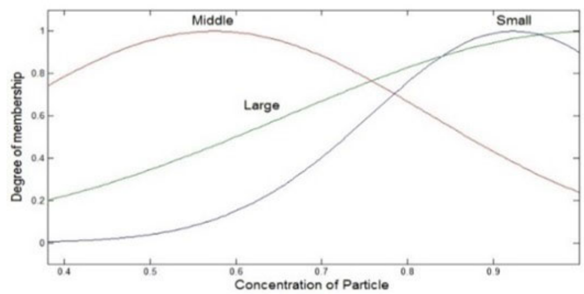

Figure 4: Membership function (Input) of concentration of particles

Table 5: Membership function of input variables (Concentration of particles)

S.No.	Membership Function	Membership Value
1	Low	(0.1661, 0.9233)
2	Medium	(0.2508, 0.5744)
3	High	(0.3559, 1.019)

Table 6: Membership function of output variables (Rate of chemical reaction)

S.No.	Membership Function	Membership Value (m, c)
1	Slow	(-0.005982, 0.01959)
2	Medium	(-0.06837, 0.06022)
3	High	(0.1104, -0.1035)

The surface viewer of input (concentration of particles) and output (rate of reaction) variables are given in figure 5. This surface viewer shows the better results of the proposed SC-ANFIS model.

The training error of the output of subtractive based ANFIS fuzzy inference system is as follows:

Training Error $= 2.3112 \times 10^{-4}$

The testing error of the output of subtractive based ANFIS fuzzy inference system is as follows:

Testing Error $= 2.3852 \times 10^{-4}$

The coefficient rate of chemical reactions (original laboratory results and results of SC-ANFIS method) is

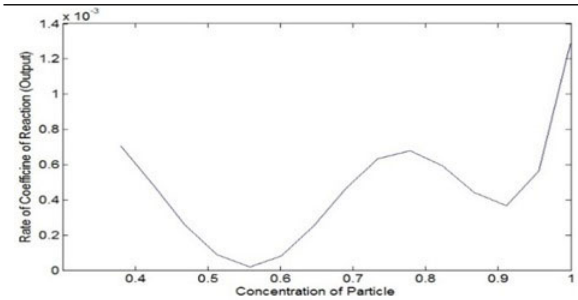

Figure 5: Surface viewer of input (concentration of particles) and output (rate of reaction) variables

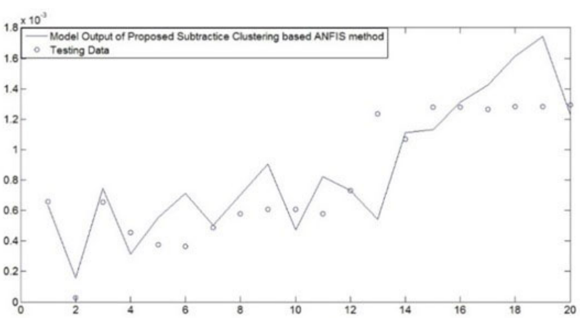

Figure 6: Proposed subtractive clustering based ANFIS model?s output and testing dataset

shown in table 7 for input and table 8 for output. The MATLAB software has been utilized for calculating the coefficient rate of chemical reactions. The experimental results of SC-ANFIS method and testing datasets are shown in figure 6. The proposed SC-ANFIS based model's output and testing dataset are shown as circles and solid lines, respectively. The results of SC-ANFIS of training error (RMSE) and testing error (RMSE) were found to be less as compared to existing FCM clustering method and SC method. Therefore, the SC-ANFIS method displays the better result as compared to the FCM clustering method and SC method to calculate the coefficient rate of chemical reactions.

The results of coefficient rates of existing methods such as FCM and SC are shown in table 7 and 8. These two tables also include the results of proposed SC-ANFIS method and it is clear from the data that SC-ANFIS method proved to be better as compared to the existing FCM and SC methods.

The figure 7 and 8 shows the output of coefficient of existing FMC method, SC method and SC-ANFIS method for the training datasets and testing datasets, respectively. The table 8 shows the comparative reaction rate of existing FCM method with SC method and SC-ANFIS method for testing datasets. According to table 8, the proposed SC-ANFIS method gives the better result as compared to the other two methods.

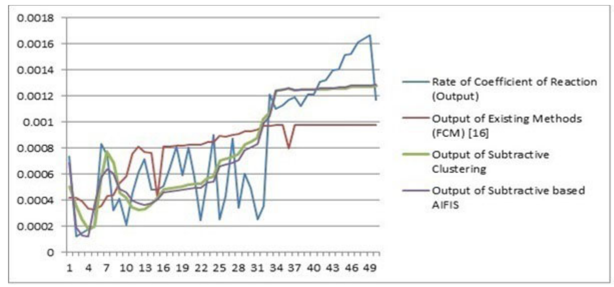

Figure 7: Output of coefficient rate of existing FCM method, SC method and SC-ANFIS method for the training datasets

The figure 8 shows the output of coefficient rate of existing method i.e. FCM, SC methods and SC-ANFIS method for testing the datasets. The figure 8 also shows that SC-ANFIS gives the better results as compared to FCM and SC methods.

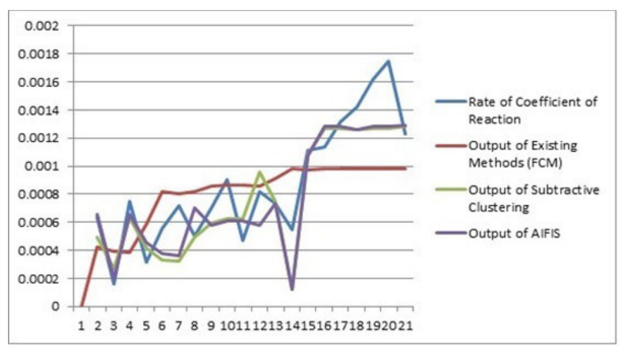

Figure 8: Output of coefficient rate of existing FCM method, SC method and SC-ANFIS method for the testing datasets

The results of SC-ANFIS for training error (RMSE) and testing error (RMSE) are less as compared to existing FCM method and subtractive clustering method (Table 9). So, we can say that the proposed SC-ANFIS method gives better result as compared to the existing FCM and SC methods for the calculation of coefficient rate of chemical reactions.

7 Conclusion

Fuzzy logic is a multivalued logic that has more than two values such as one, zero etc. The base of fuzzy logic is fuzzy set with extension of classical logic. This research work describes the details of crisp set, classical logic, fuzzy sets, fuzzy logic, approximate reasoning

Table 7: Rate of reaction of existing FCM method, SC method and SC-ANFIS method for training datasets.

S.No.	Concentration of Particles	Coefficient rate of Chemical Reaction	Output of Existing FCM Method	Output of SC Method	Output of SC-AIFIS Method
1	0.380121	0.000733	0.000422	0.000506	0.000690
2	0.473818	0.000122	0.000421	0.000368	0.000190
3	0.551682	0.000149	0.000388	0.000254	0.000132
4	0.618118	0.000178	0.000339	0.000172	0.000123
5	0.673823	0.000195	0.000332	0.000200	0.000355
6	0.732832	0.000834	0.000360	0.000556	0.000579
7	0.773471	0.000741	0.000431	0.000772	0.000643
8	0.813412	0.000321	0.000439	0.000686	0.000606
9	0.854541	0.000412	0.000530	0.000456	0.000487
10	0.862317	0.000211	0.000583	0.000419	0.000462
11	0.882471	0.000451	0.000758	0.000348	0.000401
12	0.892471	0.000614	0.000815	0.000329	0.000379
13	0.913214	0.000714	0.000772	0.000334	0.000361
14	0.924712	0.000481	0.000764	0.000366	0.000375
15	0.935236	0.000482	0.000422	0.000417	0.000408
16	0.944776	0.000512	0.000810	0.000483	0.000458
17	0.945787	0.000641	0.000813	0.000491	0.000465
18	0.946681	0.000814	0.000816	0.000498	0.000471
19	0.947821	0.000589	0.000820	0.000508	0.000479
20	0.948932	0.000805	0.000824	0.000517	0.000487
21	0.949932	0.000573	0.000828	0.000526	0.000495
22	0.949993	0.000247	0.000828	0.000527	0.000495
23	0.954521	0.000573	0.000845	0.000570	0.000533
24	0.955532	0.000901	0.000849	0.000580	0.000542
25	0.966612	0.000256	0.000894	0.000708	0.000663
26	0.967652	0.000432	0.000889	0.000721	0.000676
27	0.968632	0.000872	0.000903	0.000734	0.000689
28	0.969954	0.000342	0.000909	0.000752	0.000707
29	0.975412	0.000604	0.000931	0.000831	0.000787
30	0.976541	0.000492	0.000931	0.000848	0.000805
31	0.978412	0.000251	0.000941	0.000877	0.000836
32	0.986781	0.000354	0.000968	0.001020	0.000990
33	0.989841	0.001211	0.000968	0.001080	0.001050
34	0.997819	0.001101	0.000979	0.001240	0.001240
35	0.998416	0.001131	0.000979	0.001250	0.001250
36	0.998823	0.001172	0.000797	0.001260	0.001260
37	0.998161	0.001192	0.000979	0.001240	0.001250
38	0.998312	0.001121	0.000979	0.001250	0.001250
39	0.998413	0.001211	0.000979	0.001250	0.001250
40	0.998511	0.001211	0.000979	0.001250	0.001250
41	0.998641	0.001311	0.000979	0.001250	0.001260
42	0.998705	0.001321	0.000979	0.001250	0.001260
43	0.998815	0.001401	0.000979	0.001260	0.001260
44	0.998964	0.001405	0.000979	0.001260	0.001270
45	0.999124	0.001515	0.000979	0.001260	0.001270
46	0.999354	0.001521	0.000979	0.001270	0.001280
47	0.999461	0.001611	0.000979	0.001270	0.001280
48	0.999473	0.001641	0.000979	0.001270	0.001280
49	0.999614	0.001668	0.000979	0.001270	0.001280
50	0.999854	0.001171	0.000979	0.001280	0.001290

Table 8: Rate of reaction of existing FCM method, SC method and SC-ANFIS method for testing datasets.

S.No.	Concentration of Particles	Coefficient rate of Chemical Reaction	Output of Existing FCM Method	Output of SC Method	Output of SC-AIFIS Method
1	0.390131	0.000633	0.000422	0.000491	0.000659
2	0.541682	0.000158	0.000395	0.000269	0.000198
3	0.742832	0.000745	0.000383	0.000633	0.000653
4	0.862481	0.000314	0.000585	0.000419	0.000457
5	0.892581	0.000554	0.000816	0.000329	0.000376
6	0.902537	0.000714	0.000804	0.000323	0.000365
7	0.946337	0.000501	0.000815	0.000495	0.000706
8	0.956893	0.000701	0.000854	0.000594	0.000577
9	0.959933	0.000905	0.000866	0.000627	0.000608
10	0.959964	0.000474	0.000866	0.000628	0.000609
11	0.956872	0.000822	0.000854	0.000954	0.000577
12	0.969974	0.000733	0.000909	0.000752	0.000730
13	0.997541	0.000544	0.000979	0.000123	0.000123
14	0.989984	0.001113	0.000974	0.001080	0.001070
15	0.999514	0.001132	0.000979	0.001270	0.001280
16	0.999456	0.001312	0.000979	0.001270	0.001280
17	0.998806	0.001423	0.000979	0.001260	0.001260
18	0.999584	0.001614	0.000979	0.001270	0.001280
19	0.999594	0.001745	0.000979	0.001270	0.001280
20	0.999999	0.001228	0.000979	0.001280	0.001290

Table 9: RMSE of existing FCM method, SC Method and AIFIS method.

S.N.	Training and Testing Error (RMSE)	Existing FCM Method	SC Method	SC-AIFIS Method
1	Training (RMSE)	2.8549×10^{-4}	2.5249×10^{-4}	2.3112×10^{-4}
2	Testing (RMSE)	2.9462×10^{-4}	2.6453×10^{-4}	2.3852×10^{-4}

and various techniques behind the fuzzy logic like hybrid neuro-fuzzy systems. This research work also explains the applications of fuzzy logic and integration of artificial neural network to chemical reactions for calculating the reactions rate. The strategy is exceptionally basic and effective based on the modus ponens and modus tollens. It can be connected to diverse chemical parting and synthesis of chemical reactions together with (AND) and (OR) logic operations of antecedent and consequent statements to get superior result. The significance of such concept would appear to be imperative and much more investigation is required in the future. Now, we have also proposed two methods i.e. subtractive clustering method and SC-ANFIS method for calculating coefficient rate of chemical reactions in chemical industry and other related engineering branch. After comparing the results, it is found that SC-ANFIS method gives the better result in comparison to existing FCM method and SC method. Therefore, we conclude that the SC-ANFIS is the best method for calculating the coefficient rate of chemical reactions. This proposed method is very useful for controlling rate of chemical reactions in nuclear reactor and other chemical engineering process.

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