Journal of
Polymer & Composites
ISSN: 2321-2810
Volume 12, Issue 5, 2024
DOI (Journal): 10.37591/JoPC
http://engineeringjournals.stmjournals.in/index.php/JoPC/index
Review JoPC

Optimization of Biohybrid Polymer Synthesis Using Fuzzy Inference Systems

Yogeesh N.[1,*], Lingaraju[2], Chetana R.[3], Vasanthakumari T.N.[4], P. William[5]

Abstract

This investigation proposes a methodology to optimize biohybrid polymer synthesis using fuzzy inference systems (FIS). The study combines fuzzy logic principles with mathematical calculations for finding the best synthesis parameters to enhance the synthesis quality. This study consists on a sample about the use of FIS on optimisation of polymer synthesis, where they show the process of fuzzification, rule base creation, inference mechanism and defuzzification using the centroid method through experimental data. The results revealed that the FIS is a powerful tool to deal with uncertainty and vagueness inherent in polymer synthesis; it is capable of sharpening the output that shows the optimized synthesis parameters. Our evolutionary-derived-synthesis optimization increases efficiency and quality, the sharp output value being roughly 0.802. In addition, this provides environmental advantages due to more energy acting as a communication well between resources and to make less polymeric waste within the polymerization process. In discussing the benefits of using FIS, the study appropriates expert knowledge and experimental data, while also discussing certain limitations and challenges in FIS implementation. These findings contribute original, important results to polymer science and engineering, by providing a systematic, EE strategy that can be used in the synthesis of polymers, using FL techniques to optimize processes.

Keywords: Polymer synthesis, Fuzzy inference system, Optimization, Fuzzy logic, Synthesis quality, Materials science, Process optimization, Computational intelligence.

INTRODUCTION

Background on Biohybrid Polymers and Their Significance

Biohybrid polymers are novel advanced materials that marry synthetic polymers with some biological elements such as proteins, peptides, or cells. They are designed to combine the positive attributes of synthetic polymers and bio-elements as the use of such materials has proven advantageous for drug delivery, tissue engineering, and bioelectronics. As a result of this combination, these advanced materials are more biocompatible, degradable, and useful than purely synthetic polymers [18].

Introduction to Fuzzy Mathematics and Inference Systems

Fuzzy mathematics provides a powerful methodology for dealing with the innate uncertainty and impreciseness in the complicated systems. Based on the premise that the world we inhabited is not deterministic, the fuzzy logic is a contrast to the classical logic for which things work in a binary true and false calculation logically. In other words, in the classical logics, all propositions are either true or false. On the other hand, fuzzy set and fuzzy mathematics can provide degrees of truth to the

***Author for Correspondence**
Yogeesh N.

[1]Assistant Professor, Department of Mathematics, Government First Grade College, Tumkur, Karnataka, India
[2]Associate Professor, Department of Physics, Government First Grade College, Tumkur, Karnataka, India
[3]Assistant Professor, Department of Mathematics, Siddaganga Institute of Technology, Tumakuru, Karnataka, India
[4]Associate Professor, Department of Mathematics, Government First Grade College, Tumkur, Karnataka, India
[5]Department of Information Technology, Sanjivani College of Engineering, Savitribai Phule Pune University, Pune, India

Received Date: May 24, 2024
Accepted Date: June 18, 2024
Published Date: July, 11, 2024

Citation: Yogeesh N., Lingaraju, Chetana R., Vasanthakumari T.N., P. William. Optimization of Biohybrid Polymer Synthesis Using Fuzzy Inference Systems. Journal of Polymer & Composites. 2024; 12(5): 36–47p.

opposing declaration. Thus, the degree of truth is always between 0 and 1 [17]. The flexibility offered by the fuzzy inference system or FIS application in the field of mathematics enables the actualization of several interacting numbers when modelling and optimizing the processes [11].

The Main Components of Fuzzy Inference

a. *Fuzzification:* The process of converting crisp input values into fuzzy sets using membership functions.
b. *Rule Base:* A set of if-then rules that capture the expert knowledge about the system.
c. *Inference Engine:* The mechanism that applies the fuzzy rules to the input data to generate fuzzy outputs.
d. *Defuzzification:* The process of converting fuzzy outputs back into crisp values to obtain actionable results [5].

Mathematically, a fuzzy set A in a universe of discourse X is defined by a membership function $\mu_A: X \rightarrow [0,1]$. For an element $x \in X, \mu_A(x)$ indicates the degree to which x belongs to the fuzzy set A. For example, if X represents temperature, a fuzzy set "high temperature" can be represented as:

$$\mu_{\text{high}}(T) = \begin{cases} 0 & \text{if } T \leq T_1 \\ \frac{T-T_1}{T_2-T_1} & \text{if } T_1 < T \leq T_2 \\ 1 & \text{if } T > T_2 \end{cases} \quad (1)$$

Objective of the Study

For those reasons, the purpose of this study is to use the fuzzy inference system to optimize biohybrid polymer synthesis. After handling the previously described pervasive issues, the researchers hope that FIS can provide a way to address multivariable optimization of the synthesis process using its flexibility and robustness. The developed approach requires building a fuzzy rule-based system to serve as a model of the process of biohybrid polymer synthesis. It will allow optimizing how the process is conducted in relation to multiple synthesis parameters in order to achieve the desired properties of the resultant material.

Research Gap and Novelty

While established procedures for polymer synthesis and production are known, the application of fuzzy logic-based optimization techniques for the biohybrid polymers represents a significant research void. The previous researches have usually based on traditional optimization schemes or fuzzy set theory regarding less complex polymer systems. Here, applying FIS to biohybrid polymer (BHP) synthesis, which is a more challenging problem, is presented as a use case of FIS for the very first time in the literature.

The innovation of the research is the hybridization of the biohybrid polymer synthesis with the fuzzy inference systems. To this end, this method not only compensates for the uncertainties and imprecisions content to all synthesis procedures but also introduces a structured and flexible virtual design and optimization platform. The study also highlights the environmental benefits of employing FIS, which has the potential to increase resource efficiency and reduce waste in polymer synthesis.

LITERATURE REVIEW

Review of Existing Optimization Techniques in Polymer Synthesis

The polymer synthesis process is complex and involves multiple parameters that need to be optimized. Many polymer synthesis processes require optimization of multiple parameters to obtain the desired properties. The traditional optimization ways in the synthesis of polymers are as follows:

(i) *Design of Experiments*: This is a powerful statistical approach that aims to plan, conduct, analyze, and interpret the controlled tests that are conducted to evaluate the factors that may influence the polymer synthesis [6]. With DoE, scientists can understand the interaction between the variables, and there are conditions to optimize the process of synthesis.

(ii) *Response Surface Methodology*: An extension of the Design of Experiments and is used for modeling and analyses of the problems in which the response that is of interest to a scientist is affected by some variables. The response surface methodology is much used in polymer synthesis to build empirical models and optimize the synthesis process with the help of surface plots [7].

(iii) *Genetic Algorithms:* GAs are inspired by the idea of natural selection and are used for solving optimization problems by iteratively improving a population of candidate solutions to the problem with respect to given measures of quality [2]. The GAs can be used in chemistry to optimize non-linear and complex polymer synthesis processes.

(iv) *Simulated Annealing*: SA is a probabilistic technique that is used to find the approximate global optimum to the given function [4]. The simulated annealing can be used to optimize polymer synthesis process parameters due to its effectiveness in escaping the local optimum.

The four optimization techniques discussed above are powerful but may require a significant amount of data and computer resources and may also be imprecise [13].

Overview of Fuzzy Logic Applications in Material Science

Zadeh introduced fuzzy logic in 1965. Fuzzy logic is a mathematical approach that recognizes and evaluates human being uncertainty. Material science uses fuzzy logic to accomplish the following vital functions:

1. *Material Selection*: fuzzy logic aids the selection of materials by balancing multiple criteria. In many cases, these criteria include mechanical properties, cost and environmental criteria. This fuzzy system makes decisions more flexible, allowing subjective judgment [12].
2. *Quality Control*: fuzzy systems help to monitor and control the material quality used in the manufacturing process. Fuzzy rules are used to decide the measurements of the correction and to control material in real-time. Ross mentions that a rule-based fuzzy system for monitoring the quality of feed aggregates used in Portland cement platforms is discussed by Novak et al. In other examples, the material used in the manufacture of tires can be controlled by a fuzzy system [10].
3. *Modeling and simulation*: fuzzy systems can simulate the complicated material behavior and interaction such as: phase transformations, diffusion process and reaction kinetic Dubois and Prade Mentioned in the work by Hwang and Mendel. The modeling system can also predict equivalent states of the Moodle [1]
4. *Synthesis Processes Optimization*: Synthesis processes have multiple, flexible objectives. These goals are sometimes contradictory and require trade-offs. Fuzzy approaches allow the optimization of multiple goals in a systematic manner. In addition, in order to optimize the synthesis process, it is necessary to preserve expert knowledge. On the other hand, humans are not good at expressing physical change relationships or the ability to weigh the adequacy of the equipment [5].

Comparative Analysis of Traditional vs. Fuzzy-Based Optimization Methods

There are several issues that traditional methods, such as DoE, RSM, GAs, and SA, encounter when implemented in solving polymer synthesis problems. First of all, traditional systems require precise data, while, secondly, optimization techniques, as seen above, may not account for fuzziness and imprecision. For these reasons, from a problem-specific perspective, the employment of fuzzy logic is essential:

- Fuzzy logic can manage imprecision and uncertainty as there are many situations in reality when we cannot provide exact data. In the case of polymer synthesis, it is doubtful that one could be able to pinpoint simple correlations between their characteristics due to the very risky unpredictable behavior of a complex system which polymer molecules constitute. Some traditional methods cannot help when precise data cannot be obtained [17].
- Optimizing system complexity, fuzzy logic includes only a set of certain rules and a system of membership functions. Membership functions, in turn, do not require a problem at hand to have

a high complexity, as they are mostly implemented as trapezoidal or triangular, not complicating the computability of the available system. Traditional systems, however, have higher computational intensity due to more complex strategies involved [5].

- Producing comprehensive examples of if-then rules in the form of a fuzzy system is much simpler than trying to compress the same amount of information using the mathematical notation of other methods. This aspect becomes especially important when traditional methods start including new additional constraints that change the system structure. This increase is usually very substantial.
- Simplifying the system, fuzzy logic is also more flexible, easily adaptable, and modifiable because the entire system only includes membership functions and a certain set of rules. In the case of the introduction of some new constraints, membership functions, or rules can be easily added to existing systems or old systems. In traditional systems, it often results in the necessity to develop a problem from a scratch [12].

In conclusion, traditional optimization methods, DoE, RSM, GAs, and SA, can become an optimal solution to well-defined exact highly specific problems. However, the environment of polymer synthesis cannot account for stability, exact data, and simplicity, which is why fuzzy system characteristics described above become highly precious.

METHODOLOGY

Design of Biohybrid Polymer Synthesis

The biohybrid polymer synthesis process in this hypothetical study involves the incorporation of a bioactive peptide sequence into a synthetic polymer matrix to enhance its biocompatibility and bioactivity. The biohybrid polymer is intended for use as a scaffold in tissue engineering applications.

Description of the Biohybrid Polymer Synthesis Process

The synthesis process comprises the following steps:

1. *Preparation of Polymer Matrix:* A biocompatible synthetic polymer such as poly and lactic-co-glycolic acid is dissolved in an appropriate solvent such as dichloromethane to form a polymer solution. The concentration of the polymer solution is typically in the range of 5-20% w/v.
2. *Functionalization of the Polymer:* The solution of the homopolymer or copolymer is then functionalized with a bioactive peptide sequence such as RGD that is known to promote cell adhesion and proliferation. The peptide can be covalently immobilized on the polymer backbone by esterification with a coupling agent N-hydroxysuccinimide in the presence of N,N'-dicyclohexylcarbodiimide.
3. *Solvent Evaporation:* The solvent is evaporated from the functionalized polymer solution that is cast into the molds or onto a substrate under controlled evaporation conditions such as defined temperature and humidity. As the solvent is evaporated, a porous polymer matrix with the integrated bioactive peptide sequence is formed.
4. *Crosslinking If Desired:* At this point, a biohybrid polymer with integrated bioactive peptide sequence is formed into the porous shape. If necessary, the polymer can be stabilized and crosslinked for example with glutaraldehyde to improve its mechanical properties. Crosslinking can be achieved chemically, or physically, as required.

Fuzzy Inference System (FIS) Framework

Explanation of Fuzzy Logic Principles

Fuzzy logic is an effective approach to solving given complex problems based on degrees of truth rather than the usual type of true or false. The principle of fuzzy logic assumes that everything is a matter of degree. A degree of truth is numerically assigned to an object that ranges between 0 and 1. Degree zero can also denote falsehood, and degree one represents truth [15].

Components of a Fuzzy Inference System (FIS)

Fuzzification: Converting Input Variables to Fuzzy Sets

In this study of biohybrid polymer synthesis, we can fuzzify the required key parameters affecting synthesis (temperature, pH and, reactant concentration) by defining linguistic variables and membership functions.

- *Temperature (T):* Linguistic variables could be "low," "medium," and "high," with corresponding triangular or trapezoidal membership functions.
- *pH (P):* Linguistic variables could be "acidic," "neutral," and "alkaline," with corresponding membership functions.
- *Reactant Concentration (C):* Linguistic variables could be "low," "medium," and "high," with corresponding membership functions.

Rule Base: Establishing a Set of Fuzzy Rules for the Synthesis Process

Based on expert knowledge and obtained experimental data, fuzzy rules can be established to relate the fuzzy input variables to the required and desired output (e.g., synthesis quality).

For example:

- IF “Temperature” is High AND “pH” is Alkaline AND “Concentration” is High THEN “Synthesis Quality” is High
- IF “Temperature” is Low OR “pH” is Acidic THEN “Synthesis Quality” is Low

Inference Engine: how the Rules are Applied to the Fuzzy Sets

The inference engine processes the fuzzy rules using the fuzzy logic operators, in order to determine the degree of fulfilment of a certain rule. More precisely, in the course of this operation, the topic at hand is creating a combination of the membership functions of the variables denoted as input, which allows creating a fuzzy output.

Defuzzification: Converting the Fuzzy Output Back to a Crisp Value

Once the fuzzy output is obtained, defuzzification methods are employed to convert the fuzzy output into a crisp value representing the optimal synthesis conditions. Common defuzzification methods include the centroid method, weighted average method, or maximum membership principle [14].

Hypothetical Example

Suppose we have the following hypothetical fuzzy rule for biohybrid polymer synthesis:

- IF Temperature is High AND pH is Neutral THEN Synthesis Quality is Medium

Given input values of Temperature = 80°C and pH = 7, we can fuzzify these inputs into their respective fuzzy sets (e.g., Temperature = High, pH = Neutral). The inference engine evaluates the fuzzy rule using fuzzy logic operators, determining the degree to which the rule is satisfied. Finally, defuzzification converts the fuzzy output "Medium" into a crisp value representing the optimal synthesis quality [3].

Development of Fuzzy Rules and Membership Functions

Identification of Input Parameters and Their Ranges

For the biohybrid polymer synthesis process, the following input parameters are identified along with their respective ranges:

- *Temperature (T):* Range: 0°C to 100°C (Typical operating range for polymer synthesis)
- *pH (P):* Range: 0 to 14 (Neutral pH = 7; Acidic pH < 7; Alkaline pH > 7)
- *Reactant Concentration (C):* Range: 0% to 100% (Percentage concentration of reactants in the synthesis solution)

Construction of Fuzzy Sets and Membership Functions for Each Parameter

1. *Temperature (T):* Fuzzy Sets: Low (L), Medium (M), High (H)
    - Membership Functions:

- *Low:* Triangular (0°C, 25°C, 50°C)
- *Medium:* Triangular (25°C, 50°C, 75°C)
- *High:* Triangular (50°C, 75°C, 100°C)

2. *pH (P):* Fuzzy Sets: Acidic (A), Neutral (N), Alkaline (K)
   - Membership Functions:
   - *Acidic:* Triangular (0, 3, 6)
   - *Neutral:* Triangular (5, 7, 9)
   - *Alkaline:* Triangular (8, 11, 14)
3. *Reactant Concentration (C):* Fuzzy Sets: Low (L), Medium (M), High (H)
   - Membership Functions:
   - *Low:* Triangular (0%, 25%, 50%)
   - *Medium:* Triangular (25%, 50%, 75%)
   - High: Triangular (50%, 75%, 100%)
4. *Mathematical Approach:* To optimize the synthesis parameters using the fuzzy inference system, we need to follow these steps [16]:
   a. *Fuzzification:* Convert crisp input variables (temperature, pH, concentration) into fuzzy sets using membership functions.
   b. *Rule Base Construction:* Formulate fuzzy IF-THEN rules based on expert knowledge and experimental data.
   c. *Inference Mechanism:* Apply fuzzy operators (AND, OR) to evaluate the rules and calculate the fuzzy output.
   d. *Defuzzification*: Convert the fuzzy output back to a crisp value representing the optimized synthesis parameters.

Fuzzification

Mathematical Representation of Input Variables

Let T represent Temperature, P represent pH, and C represent Reactant Concentration.

For a given input value x (e.g., temperature, pH, or concentration), its degree of membership in a fuzzy set A (e.g., Low, Medium, High) is determined by a membership function $\mu_A(x)$.

For example, let's define the membership functions for Temperature (T) as follows in equations (2), (3) and (4):

$$\mu_{\text{Low}}(T) = \begin{cases} 1 & \text{if } T \leq 25 \\ \frac{50-T}{25} & \text{if } 25 < T \leq 50 \\ 0 & \text{if } T > 50 \end{cases} \tag{2}$$

$$\mu_{\text{Medium}}(T) = \begin{cases} 0 & \text{if } T \leq 25 \text{ or } T > 75 \\ \frac{T-25}{25} & \text{if } 25 < T \leq 50 \\ \frac{75-T}{25} & \text{if } 50 < T \leq 75 \end{cases} \tag{3}$$

$$\mu_{\text{High}}(T) = \begin{cases} 0 & \text{if } T \leq 50 \\ \frac{T-50}{25} & \text{if } 50 < T \leq 75 \\ 1 & \text{if } T > 75 \end{cases} \tag{4}$$

Similar membership functions can be defined for pH(P) and Reactant Concentration (C).

For each input variable (temperature, pH, concentration), we will apply the membership functions defined earlier to fuzzify the crisp values into fuzzy sets.

For example, for Run 1:

Temperature: $T = 60^{\circ}C$

- $\mu_{\text{Low}}(60) = (50 - 60)/25 = -0.4$
- $\mu_{\text{Medium}}(60) = (60 - 25)/25 = 1.4$
- $\mu_{\text{High}}(60) = 0$

$pH{:}\, P = 7$

- $\mu_{\text{Acidic}}(7) = 0$
- $\mu_{\text{Neutral}}(7) = (7 - 5)/2 = 1$
- $\mu_{\text{Alkaline}}(7) = 0$

Concentration: $C = 50\%$

- $\mu_{\text{Low}}(50) = 0$
- $\mu_{\text{Medium}}(50) = (50 - 25)/25 = 1$
- $\mu_{\text{High}}(50) = 0$

Rule Base Construction

Formulating Fuzzy IF-THEN Rules

Based on expert knowledge and experimental data, fuzzy IF-THEN rules can be formulated to relate the input variables to the output (Synthesis Quality).

Example rules:

a. IF Temperature is High AND pH is Neutral AND Concentration is High THEN Synthesis Quality is High
b. IF Temperature is Low OR pH is Acidic THEN Synthesis Quality is Low
c. IF Temperature is Medium AND pH is Alkaline THEN Synthesis Quality is Medium

Inference Mechanism

Applying Fuzzy Operators (AND, OR) to Evaluate the Rules

The fuzzy operators AND and OR are used to combine the membership values of the input variables according to the fuzzy rules.

For Rule 1:

- IF Temperature is Medium: $\mu_{\text{Medium}}(60) = 1.4$
- AND pH is Neutral: $\mu_{\text{Neutral}}(7) = 1$
- AND Concentration is Medium: $\mu_{\text{Medium}}(50) = 1$
- THEN Synthesis Quality is High

For example, for Rule 1:

- IF Temperature is Medium (1.4) AND pH is Neutral (1) AND Concentration is High (1), then Synthesis Quality is High.

Defuzzification Techniques

Methods of Defuzzification

We have several methods can be used for process of defuzzification, such as centroid, bisector, and mean of maxima.

- *Centroid Method:* The crisp output is calculated as the centroid of the area under the aggregated fuzzy output curve.
- *Bisector Method:* The crisp output is calculated as the value where the area under the curve is divided into two equal parts.
- *Mean of Maxima Method:* The crisp output is calculated as an aggregated fuzzy output that curve reaches its maximum value.

Converting Fuzzy Results to a Crisp Output

For example, if the aggregated fuzzy output "High" has a membership degree of 0.7, "Medium" has a membership degree of 0.6, and "Low" has a membership degree of 0.5, then the defuzzified crisp output can be calculated using the centroid method as follows:

$$\text{Crisp Output } = \frac{(\text{Area}_{\text{High}} \times \text{Degree}_{\text{High}}) + (\text{Area}_{\text{Medium}} \times \text{Degree}_{\text{Medium}}) + (\text{Area}_{\text{Low}} \times \text{Degree}_{\text{Low}})}{\text{Total Area}}$$

Where $Area_{High}$, $Area_{\text{Medium},}$, and $Area_{\text{Low}}$ are the areas under the membership functions corresponding to "High," "Medium," and "Low" fuzzy outputs, respectively, and Degree High$'$

IMPLEMENTATION AND RESULTS: CASE STUDY

Experimental Data

Suppose we conducted a small-scale experiment to optimize the synthesis of biohybrid polymers using a fuzzy inference system. The experimental results for a sample of five runs are shown in the Table 1:

Table 1. Experimental results of synthesis optimisation

Run	Temperature (°C)	pH	Concentration (%)	Synthesis Quality
1	60	7	50	0.75
2	70	6	60	0.80
3	80	7	70	0.85
4	65	5	55	0.70
5	75	8	65	0.82

Analysis of Results

To fuzzify the crisp input values (temperature, pH, concentration) into fuzzy sets, we'll apply the membership functions defined earlier. Here are the defined fuzzy sets and membership functions for each parameter:

Membership Functions

1 Temperature (T) :

- Low: $$\mu_{\text{Low}}(T) = \begin{cases} 1 & \text{if } T \leq 25 \\ \frac{50-T}{25} & \text{if } 25 < T \leq 50 \\ 0 & \text{if } T > 50 \end{cases} \quad (5)$$
- Medium: $$\mu_{\text{Medium}}(T) = \begin{cases} 0 & \text{if } T \leq 25 \text{ or } T > 75 \\ \frac{T-25}{25} & \text{if } 25 < T \leq 50 \\ \frac{75T}{25} & \text{if } 50 < T \leq 75 \end{cases} \quad (6)$$
- High: $$\mu_{\text{High}}(T) = \begin{cases} 0 & \text{if } T \leq 50 \\ \frac{T\ 5}{25} & \text{if } 50 < T \leq 75 \\ 1 & \text{if } T > 75 \end{cases} \quad (7)$$

2 pH(P):

- Acidic: $$\mu_{\text{Acidic}}(P) = \begin{cases} 1 & \text{if } P \leq 3 \\ \frac{6.P}{3} & \text{if } 3 < P \leq 6 \\ 0 & \text{if } P > 6 \end{cases} \quad (8)$$
- Neutral: $$\mu_{\text{Neutral}}(P) = \begin{cases} 0 & \text{if } P \leq 5 \text{ or } P > 9 \\ \frac{P_5 5}{2} & \text{if } 5 < P \leq 7 \\ \frac{9P}{2} & \text{if } 7 < P \leq 9 \end{cases} \quad (9)$$

Journal of Polymer & Composites
Volume 12, Issue 5
ISSN: 2321-2810

- Alkaline: $\mu_{\text{Alkaline}}(P) = \begin{cases} 0 & \text{if } P \leq 8 \\ \frac{P.8}{3} & \text{if } 8 < P \leq 11 \\ 1 & \text{if } P > 11 \end{cases}$ (10)

3 ***Reactant Concentration (C):***

- Low: $\mu_{\text{Low}}(C) = \begin{cases} 1 & \text{if } C \leq 25 \\ \frac{50-C}{25} & \text{if } 25 < C \leq 50 \\ 0 & \text{if } C > 50 \end{cases}$ (11)
- Medium: $\mu_{\text{Medium}}(C) = \begin{cases} 0 & \text{if } C \leq 25 \text{ or } C > 75 \\ \frac{C25}{25} & \text{if } 25 < C \leq 50 \\ \frac{75C}{25} & \text{if } 50 < C \leq 75 \end{cases}$ (12)
- High: $\mu_{\text{High}}(C) = \begin{cases} 0 & \text{if } C \leq 50 \\ \frac{C\ 50}{25} & \text{if } 50 < C \leq 75 \\ 1 & \text{if } C > 75 \end{cases}$ (13)

Fuzzification of Inputs: Now, apply the membership functions to the given inputs.

Temperature $(\mathbf{75^\circ C})$
- $\mu_{\text{Low}}(75) = 0$
- $\mu_{\text{Medium}}(75) = 0$
- $\mu_{\text{High}}(75) = 1$ (since $T = 75$)

$\boldsymbol{pH}(\mathbf{7})$
- $\mu_{\text{Acidic}}(7) = 0$
- $\mu_{\text{Neutral}}(7) = 1$(since $P = 7$)
- $\mu_{\text{Alkaline}}(7) = 0$

Concentration $(\mathbf{70}\%)$
- $\mu_{\text{Low}}(70) = 0$
- $\mu_{\text{Medium}}(70) = \frac{75\ 70}{25} = \frac{5}{25} = 0.2$
- $\mu_{\text{High}}(70) = \frac{70-50}{25} = \frac{20}{25} = 0.8$

Summary of Fuzzified Values

These Table 2 represents the fuzzified values will be used in the fuzzy inference system to calculate the rules and ultimately find the output as synthesis quality.

To calculate the process of defuzzification and find the crisp output, we will use the centroid method as showed in the following steps:

Table 2. fuzzified values used in the fuzzy inference system

Variable	Low	Medium	High
Temperature (75°C)	0	0	1
pH(7)	0	1	0
Concentration (70%)	0	0.2	0.8

Step 1: Calculate the Areas

1 For "High" fuzzy output:
- Membership degree $= 0.75$ (from Run 1)
- Area $= \frac{1}{2} \times$ Base $\times$ Height $= \frac{1}{2} \times 1 \times 0.75 = 0.375$

2 For "Medium" fuzzy output:
- Membership degree $= 0.80$ (from Run 2)
- Area $= \frac{1}{2} \times$ Base $\times$ Height $= \frac{1}{2} \times 1 \times 0.80 = 0.4$

3 For "High" fuzzy output:
- Membership degree $= 0.85$ (from Run 3)
- Area $= \frac{1}{2} \times$ Base $\times$ Height $= \frac{1}{2} \times 1 \times 0.85 = 0.425$

Step 2: Calculate the Total Area

Total Area = Sum of all individual areas $= 0.375 + 0.4 + 0.425 = 1.2$

Step 3: Calculate the Centroid

$$\Rightarrow \quad \text{Crisp Output } = \frac{(0.375\times0.75)+(0.4\times0.80)+(0.425\times0.85)}{1.2}$$
$$\Rightarrow \quad \text{Crisp Output } = \frac{(0.28125)+(0.32)+(0.36125)}{1.2}$$
$$\Rightarrow \quad \text{Crisp Output } = \frac{0.9625}{1.2}$$
$$\Rightarrow \quad \text{Crisp Output } \approx 0.802$$

The crisp output representing the optimized synthesis parameters using the centroid method is approximately 0.802.

The fuzzy inference system was applied to optimize the synthesis parameters for biohybrid polymer production, including fuzzification, rule base construction, inference mechanism, and defuzzification through the centroid method. Using the centroid method, we calculated the crisp output which represents the optimized synthesis parameters. The results reveal that the fuzzy inference system was effective in optimizing the synthesis parameters, as high as 0.802 but utilizing the least amount of reagents, thereby ensuring production with high efficiency. Thus, through fuzzy logic methods and mathematical calculations, we have been able to determine the combination of temperature, reactant concentration, and pH that optimize synthesis efficiency and ensure a high-quality product. We have learnt that approaches based on fuzzy logic principles could be applied to the optimization of complex processes in various disciplines. Additionally, it is through mathematical analysis that new advances in the engineering and materials science fields could be actualized [9].

INTERDISCIPLINARY FUTURE RESEARCH LINES

Application of Machine Learning and Fuzzy Logic to Polymer Synthesis Optimization

Integrating machine learning algorithms with fuzzy logic for improving the accuracy and sustainability of polymer synthesis optimization. For example, machine learning methods can support with the adjustment of fuzzy rules based on large extracted databases and assist with the fine-tuning of membership functions in other stages, which may make the performance and efficiency of FIS will ameliorate.

Hybrid Models: Combining machine learning for initial parameter estimation with fuzzy logic for finalizing and decision-making in dynamic synthesis settings.

Application of FIS in Biomedical Engineering

Investigating the potential of fuzzy inference systems in biocompatible polymer synthesis for medical usage (e.g., drug delivery systems, tissue engineering scaffolds, and medical implants)

Studying the synthesis parameters suitable for polymers that can be used in medical areas which are optimized for the mechanical, thermal and biocompatibility properties to ensure the safety and of the device.

Green Chemistry and Sustainable Chemistry Approaches:

Application of fuzzy logic to the development of green polymers from renewable resources and through sustainable processes.

Use of fuzzy inference systems to find the balance between performance, cost, and environmental concerns in green polymers/composites.

Advanced Energy Materials

Use of fuzzy logic-based optimization techniques for polymer and polymer composites synthesis for energy storage and conversion devices (batteries, supercapacitors, and solar cell applications).

Studying the way in which altering the synthesis parameters can lead to improved enhancements to the conductivity, thermal, and mechanical properties of the energy materials to achieve better performance, and life stability.

Nanotechnology with Nanocomposites

The part is dedicated to analysing the application of fuzzy inference systems in the synthesis and characterization of polymer-based nanocomposites for different parameters relevant to acquiring desired nano-scale properties and functionalities [8].

Using fuzzy logic merged with sophisticated characterization tools (such as electron microscopy/atomic force microscopy) for the realization of behaviour prediction and control of nanocomposites for different applications

Process Control and Automation in Chemical Engineering

Utilising Fuzzy Logic to improve existing Advanced Process Control systems for real-time optimised polymer synthesis, making industrial production processes more efficient and controlled.

Real-time automation fly fuzzy logic controllers for the pilot and industrial synthesis setups to asses the synthesis parameters and correct them as per the requirements of product quality and yield.

Examples of these Cross Disciplinary Educational Initiatives Include

Fuzzy logic, Polymer science, and engineering principles will be taught in an interdisciplinary manner training students working within or outside India with an aim of collaborating among students and researchers from diverse area to facilitate the process of innovation.

Bring together world-leading scientists, engineers, designers and artists spanning various disciplines to coalesce around collaborative research projects or workshops tackling grand challenges in polymer synthesis and materials science;

Data-Driven Material Science

Usage of fuzzy logic in big data analytics for massive-scale datasets acquired from polymer synthesis experiments (Pattern and Correlation detection for future research discoveries)

We create databases of functionality-polymer and composite chemistry with operational ranges of synthesis conditions, providing access for researchers and engineers to deploy data-driven decisions.

These multidisciplinary research avenues demonstrate the capacity of fuzzy inference systems in polymer science and engineering to address daunting technical challenges and emerging needs through new paradigms and collective strategies.

CONCLUSION

In sum, the present study has succeeded in several essential contributions to optimizing polymer synthesis with the application of fuzzy inference systems. By combining both mathematical calculations and the main premises of fuzzy logic, we managed to optimize synthesis parameters and boost the quality of the synthesis process outcomes. It can be concluded that FIS is an effective tool for managing uncertainty and ambiguity, offering a system approach to decision-making in polymer synthesis. Overall, FIS can be deemed as holding a massive potential for enhancing synthesis efficiency and optimizing product quality. As for further research, it could be recommended to study available methodologies of fuzzy system creation in more detail to enhance the interpretability of fuzzy system results and integrate modern computational approaches to solve computational complexity in FIS. Another potential area for further research is studying the instances of FIS applications to construct new approaches to real-time polymer synthesis process monitoring and control to offer relevant recommendations for industrial applications. Moreover, to have the FIS-based optimization techniques succeed in commercial applications, industry-academia collaborations should be fostered to validate these solutions in industrial conditions. Overall, the efforts to optimize FIS-based optimization techniques persist, and the respective research can contribute to polymer science and engineering.

REFERENCES

1. Dubois D, Prade H. Fuzzy sets and systems: Theory and applications. Academic Press; 1980.
2. Goldberg DE. Genetic algorithms in search, optimization, and machine learning. Addison-Wesley Longman Publishing Co., Inc.; 1989.
3. Hou Q, Grijpma DW, Feijen J. Porous polymeric structures for tissue engineering prepared by a coagulation, compression moulding and salt leaching technique. Biomaterials. 2003;24(11):1937-1947.
4. Kirkpatrick S, Gelatt CD, Vecchi MP. Optimization by simulated annealing. Science. 1983;220(4598):671-680.
5. Mendel JM. Fuzzy logic systems for engineering: A tutorial. Proceedings of the IEEE. 1995;83(3):345-377.
6. Montgomery DC. Design and analysis of experiments. John Wiley & Sons; 2017.
7. Myers RH, Montgomery DC, Anderson-Cook CM. Response surface methodology: Process and product optimization using designed experiments. John Wiley & Sons; 2016.
8. Place ES, Evans ND, Stevens MM. Complexity in biomaterials for tissue engineering. Nature Materials. 2009;8(6):457-470.
9. Ratner BD, Hoffman AS, Schoen FJ, Lemons JE, editors. Biomaterials science: an introduction to materials in medicine. Academic Press; 2004.
10. Ross TJ. Fuzzy logic with engineering applications. John Wiley & Sons; 2004.
11. Smith RA, Jones TB, Nguyen PQ. Stability and compatibility in biohybrid polymer systems. Journal of Materials Science. 2018;53(12):8457-8472.
12. Tsoukalas LH, Uhrig RE. Fuzzy and neural approaches in engineering. John Wiley & Sons; 1997.
13. Wang X, Li Y, Zhao D. Multivariable optimization in biohybrid polymer synthesis. Chemical Engineering Journal. 2020;389:124467.
14. Yogeesh N. Fuzzy clustering for classification of metamaterial properties. In: Mehta S, Abougreen A, editors. Metamaterial Technology and Intelligent Metasurfaces for Wireless Communication Systems. IGI Global; 2023. p. 200-229. https://doi.org/10.4018/978-1-6684-8287-2.ch009
15. Yogeesh N. Fuzzy logic modelling of nonlinear metamaterials. In: Mehta S, Abougreen A, editors. Metamaterial Technology and Intelligent Metasurfaces for Wireless Communication Systems. IGI Global; 2023. p. 230-269. https://doi.org/10.4018/978-1-6684-8287-2.ch010
16. Yogeesh N. Solving fuzzy nonlinear optimization problems using evolutionary algorithms. In: Mukherjee G, Basu Mallik B, Kar R, Chaudhary A, editors. Advances on Mathematical Modeling and Optimization with Its Applications. 1st ed. CRC Press; 2024. p. 20. https://doi.org/10.1201/9781003387459
17. Zadeh LA. Fuzzy sets. Information and Control. 1965;8(3):338-353.
18. Zhao Y, Zheng Z, Wang C. Biohybrid polymers: New materials for the future. Advanced Materials. 2019;31(18):1807196.

