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ABSTRACT

of the dissertation for the degree of Doctor of Philosophy

EVALUATION OF ISOTHERMAI CHEMICAL REACTIONS RATE AND ITS STABILITY USING FUZZY LOGIC

Speciality: 3303.01 - Chemical technology and engineering

Field of science: technical

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The work was performed at the department "Technology of Organic Substances and High-Molecular Compounds" of the Azerbaijan State Oil and Industry University

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GENERAL DESCRIPTION OF THE DISSERTATION

The actuality of the topic. The basis of the mechanism of a chemical reaction is its rate law. It describes the relation between the reaction rate and the concentration of chemical reagents.

The aim of this thesis is to develop methods and models for determining the rate constant of isothermal chemical reactions under conditions of uncertainty. The development of such tools can be very useful in the control of industrial processes as well as in the study of the reaction mechanisms. Determination of the more adequate values of the rate constants makes it possible to determine the optimal conditions for the design of the reactor, including the necessary parameters of the chemical reaction.

Experimental data contains several types of errors, including temperature variation, impurities in the reactants , and human errors.

The nature of information is one of the factors required to control chemical processes. So that, it is difficult to control the behavior of chemical processes when information is insufficient. This is due to the inability to accurately determine the parameters that characterize the process.

If these processes are characterized by large amounts of data, their monitoring requires from the researcher new practical knowledge related to applied chemistry and information technology. In such cases, it is important to extract useful knowledge from the data. On the other hand, many years of experimentation and millions of data on chemical reactions have been put into databases compiled in the scientific literature. Instead of conducting experiments, it is important to obtain information from data using modern technology-based methods that take into account uncertainty and predict the rate stability of chemical reactions. In order to solve this problem, "computational chemistry", the fuzzy logic that is the basis of soft computing technology, were used.

Modeling of two chemical reactions is described as an example. Fuzzy velocity equations (fuzzy differential equations) were solved to obtain an analytical concentration related to time profiles.

The results of computer experiments have shown that the suggested tools are very effective, faster and more adequate

tools for determining the true rate constants of reactions.

The suggested methodology can be used to determine the rate constant of any complex reaction at a given temperature. The proposed tools do not depend on the nature of the reaction, only the rate equations and initial conditions must be changed for any new reaction.

Goal and tasks of the dissertation. The purpose of the dissertation is to evaluate isothermal chemical reactions on the basis of fuzzy logic, taking into consideration the uncertain behavior of the rate constant and stability.

The object and subject of research.İnvestigation of the isothermal chemical reactions under uncertainty using fuzzy logic methods, analysis of stable reaction rate constant of chemical reactions.

Research methods. The research methods, like the Soft Computing technology, solution of fuzzy differential equations, the method of fuzzy inference, the method of clustering fuzzy C-means were applied in the dissertation.

The computer simulation was carried out in the MATLAB environment and the accuracy and efficiency of the results obtained were confirmed.

Main highlights, brought forward for dissertation defense.

The following main highlights and results of the dissertation are brought forward for defense:

- Mathematical analysis of systems of isothermal chemical reactions in uncertain conditions;
- Creation of the fuzzy IF ... THEN model to determine the rate constant in isothermal chemical reactions;
- Investigate of the quality of the suggested fuzzy models;
- Study of fuzzy stability of isothermal chemical reactions at different values of the rate constant;
- Implementation of the sensitivity analysis of the proposed fuzzy models;
- Study of a fuzzy model of the decomposition reaction of hydrogen

peroxide;
- Study of a fuzzy model of the alkylation reaction.

Scientific findings. The main scientific findings obtained in the dissertation are:

- ✓ For the determination of the rate constant of isothermal reactions occurring in an environment of uncertainty , a fuzzy IF .. THEN model has been developed;
- ✓ A multicriterial study of the quality of the suggested fuzzy model was carried out.
- ✓ Dynamic behavior of isothermal chemical reaction described by fuzzy differential equationin in different values of the rate constant was analyzed.
- ✓ The fuzzy stability of isothermal chemical reactions characterized by uncertainty has been investigated for the first time.
- ✓ The obtained theoretical results were applied to analyze the reactions of hydrogen peroxide and alkylation.

Theoretical and practical significance of the dissertation work. The mathematical analysis of isothermal chemical reaction systems was carried out under conditions of uncertainty. A fuzzy mathematical model of an isothermal chemical reaction was built, a fuzzy model was created to determine the rate constant of an isothermal reaction, and analysis of fuzzy stability and sensitivity of isothermal chemical reactions was studied. This allows the user to determine the desired stable behavior of the chemical reactor. An experimental study of fuzzy models of isothermal chemical reactions has been carried out. A fuzzy model of the reaction of decomposition of hydrogen peroxide and the reaction of alkylation of propylene and benzene was studied. The study of the quality of fuzzy models proves the validity and effectiveness of the suggested models. The proposed approach is more adequate to the real environment of complex chemical reactions, because it allows to take into consideration their fuzzy uncertainty.

Realization of the results of dissertation work. The scientific results obtained in the dissertation can be applied to other similar reactions.

Approbation of the dissertation. Main scientific and practical results of the dissertation were presented in the ICAFS-2018- "Thirteenth International Conference on the Application of Fuzzy Systems and Soft Computing" (Warsaw, 2018), ICSCCW-2019- "Tenth International Conference on the Theory and Application of Soft Computing with Words and Perceptions (Czech), 2019), ICAFS-2020- "14th International Conference on Applications of Fuzzy Systems, Soft Computing and Artificial Intelligence Tools (Montenegro, Budva, 2020), APCE-2020-" engineering "(Baku, 2020), GTDOEK -" Online conference of young researchers and doctoral students, "The conference dedicated to the 100th anniversary of the Azerbaijan State Oil and Industry University (ASOIU) ".

Published works. According to the results of the study, 8 works were published, including: 5 articles, 4 of them without co-authors, 4 were published abroad; 3 conference materials, 1 of them abroad, 2 without co-authors.

Name of the organization within which the dissertation work is carried out. The work was performed at the department "Technology of Organic Substances and High-Molecular Compounds" of the Azerbaijan State Oil and Industry University.

Structure and volume of the dissertation. The dissertation manuscript consists of an introduction, five chapters, results, references and appendices. The total volume of the dissertation is 166 pages: the main part of the work, including 29 figures, 21 tables, 5 appendices and a list of 96 sources, the total volume of the dissertation is 165090 characters.

The introduction substantiates the relevance of the problem under study, summarizes the main goals and problems that need to be addressed, provides scientific novelties and a practical assessment of the research.

In the first chapter, the issues of mathematical analysis of isothermal chemical reaction systems under uncertain conditions are considered and the formal statement of the problem is determined.

Based on the analysis of scientific literature of recent years, it has been proved that the technology of fuzzy logic is one of the most successful technologies for the development of methods for investigation complex chemical processes. Thus, fuzzy logic is a technology that can be used to solve real-world problems and can be used in chemical engineering to evaluate decomposition, combustion, separation, input and output rates in chemical reactions, and risk management in chemical reactions. Here are the factors that influence the reaction rate - temperature, the values of the factors that influence the stability and instability of the reaction, and so on. may be characterized by uncertainty. Certain conceptual work is underway in this area. The use of fuzzy logic in chemical processes is a challenging problem and is in the focus of analysts' attention. The following conclusions were made from a review of studies on the analysis of isothermal chemical reactions in different environments.

There are a lot of literatures on stochastic modeling of chemical reactions. However, most of small articles deal with simulation-based methods. Others are more technical in nature and require a high level of mathematical knowledge to understand. On the other hand, since a person (researcher) is involved in the management of complex chemical processes, these processes involve not only probabilistic uncertainty, but also higher-order uncertainty.

When it is impossible to determine the reaction rate using classical rigid mathematical methods, preference should be given to human-centered mathematical computational methods.

Such problems are solved by a person who makes decisions based on linguistic information. The scientific review showed that the work carried out in this direction in the scientific literature, and the results obtained are in an embryonic state, there is a great need to extend them, to obtain new scientific results.

The second chapter provides an overview of fuzzy logic. Here are the basic concepts of fuzzy sets, fuzzy numbers, fuzzy differential equations, fuzzy If-Then type models. They were used to model fuzzy knowledge expression for relationship between information expressed in natural language and behavioral aspects in a reaction and to analyze the results obtained from the models, to study the stability of a fuzzy differential equation describing a chemical process. Some definitions of the fuzzy logic used in dissertation is given below.

Fuzzy set[1]**.**Let X be universal set, whose elements are denoted x. The inclusion of elements $A \subset X$ subset is often expressed through $\mu_A : X \to \{0,1\}$ a characteristic function, that is,

$$\mu_A(x) = \begin{cases} 1, & x \in A \\ 0, & x \notin A \end{cases}$$

Where {0,1} is called a valuation set. If the valuation set is taken from the real interval [0,1], no {0,1} then A is called a fuzzy set. In this case $\mu_A(x)$ is called membership functions. As closer the value of $\mu_A(x)$ is to 1 , so much x belongs to set A. A is completely characterized by the set of pair:

$$A = \{x, \mu_A(x)), x \in X\}$$

Fuzzy number[1]**.** A fuzzy number A is a fuzzy set A with membership function $\mu_A : R \to [0,1]$ on R which possesses the following properties: A is convex, normal set and the support is bounded set and for every $\alpha \in (0,1]$ α-cut is bounded interval. The fuzzy number A is represented as

$$A = \int_R \mu_A(x)/x$$

α **-cut**[1] **.** If A fuzzy number, then its α-cut is

$$A^\alpha = [a_1^\alpha, a_2^\alpha]$$

shaped number. Here $A^\alpha = \{x / \mu_A(x) \geq \alpha\}$.

Fuzzy point[1]**.** Fuzzy point $\tilde{x}_0$ is a convex fuzzy subset of R^n. Fuzzy point in R is characterized by kernel x_0 whose precise location is only approximately known. A crisp point $x_0 \in R^n$ is the kernel, from which membership function decreases in all directions monotonically.

Fuzzy equation[1]**.** If f_1 and f_2 are the arithmetic expressions

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[1] Aliev R.A., Aliev R.R. Soft Computing and its Applications //World Scientific, – 2001. – 444 p

(elements of $x \in R^1$, variables and mathematical construction created using $+,-,\times,:$ operations which connect them), Q fuzzy relation, then

$$f_1 \, Q \, f_2$$

is called fuzzy equation possessed fuzzy relation.

For instance, Q relation can be given $Q \underset{=}{\Delta}$ “approximately equals”.

If f_1 and f_2 are fuzzy terms , R is crisp mathematical relation, then the following equations can be define using α-cut

$$\left(\bigcup_{\alpha} \alpha f_1^{\alpha}\right) R \left(\bigcup_{\alpha} \alpha f_2^{\alpha}\right) = \left(\bigcup_{\alpha} \alpha[\delta_{f_1}, \gamma_{f_1}]\right) Q \left(\bigcup_{\alpha} \alpha[\delta_{f_2}, \gamma_{f_2}]\right) \tag{1}$$

where

$$\delta_{f_1} \underset{=}{\Delta} \delta_{f_1}(\alpha); \;\; \delta_{f_2} \underset{=}{\Delta} \delta_{f_2}(\alpha); \;\; \gamma_{f_1} \underset{=}{\Delta} \gamma_{f_1}(\alpha); \;\; \gamma_{f_2} \underset{=}{\Delta} \gamma_{f_2}(\alpha);$$

$\delta_f(\alpha) = \mu_+^{-1}(\alpha)$, $\gamma_f(\alpha) = \mu_-^{-1}(\alpha)$, $\mu_+^{-1}(\alpha)$, $\mu_-^{-1}(\alpha)$ $\mu_f(x)$ respectively inverse function of the increasing and decreasing part of the membership function.

For solving $f_1 \, R \, f_2$ type equations bringing it into form (1), it can be solve separately on δ_x and γ_x .

Fuzzy differential equations[1].

Let, $\tilde{f}(t,\tilde{y})$ be a fuzzy function of a crisp variable t and fuzzy variable $\tilde{y}$ **.** The equation

$$\tilde{y}' = \tilde{f}(t,\tilde{y}), \quad -\infty < t < \infty$$

is called a first order fuzzy differential equation. This equation can be replaced by

$$(\underline{y})'(t) = \underline{f}(t,y), \;\; (\overline{y})'(t) = \overline{f}(t,y); \qquad y(t_0) = y_0 .$$

Here $\underline{y}(t)$ and $\overline{y}(t)$ are upper and lower endpoints of $[\tilde{y}(t)]^{\alpha}$ respectively.

Denoting

$\underline{f}(t,y) = F(t, \underline{y}(t), \overline{y}(t))$; $\overline{f}(t,y) = G(t, \underline{y}(t), \overline{y}(t))$

One can write

$$(\underline{y})'(t) = F(t, \underline{y}(t), \overline{y}(t)), \quad (\overline{y})'(t) = G(t, \underline{y}(t), \overline{y}(t)),$$

$$\underline{y}(t_0) = \underline{y}_0, \qquad \overline{y}(t_0) = \overline{y}_0$$

Solution of the system can be obtained by solving the integral system:

$$\underline{y}(t) = \underline{y}_0 + \int_{t_0}^{t} F[s, \underline{y}(s), \overline{y}(s)]\, ds,$$

$$\overline{y}(t) = \overline{y}_0 + \int_{t_0}^{t} G[s, \underline{y}(s), \overline{y}(s)]\, ds$$

Linguistic variable[1]. Lingustic variable is defined by the set

$$(x,\ T(x),\ U,\ G,\ M)$$

where x is the name of variable, $T(x)$ is the term set of x variable, that is set of names of linguistical value of x variable, thus, each such value u is a variable receiving values in a universal set U. G is a syntactic rule (usually in form of a gramma) generating linguistic terms. M is a semantic rule that assigns to each lingustic term its meaning, which is a fuzzy set on X.

IF ... THEN type fuzzy model[1]. This model is described by the following type rules in the form of production rules:

G_1: IF x is A_1, Then y is B_1,

G_2: IF x is A_2, Then y is B_2,

…

G_n: IF x is A_n, Then y is B_n.

where x – input variable, y – output variable, A= $\{A_1, A_2 ... A_n\}$ and B= $\{B_1, B_2 ... B_n\}$ are membership functions on linguistical terms of values x and y variables.

The third chapter deals with the creation of a fuzzy model of isothermal chemical reaction and a fuzzy model for determining the rate constant of isothermal reaction.The goal is to determine the reaction rate constant using a fuzzy model and analyze the result achieved during testing of this model, i.e, the behavior of the isothermal chemical reaction expressed by the differential equation, using obtained rate constant.

A process of creating a linguistic model expressing the relationship between the rate constant and decayed concentration using data available in the scientific literature is described below.

A fragment of the information about relation between the decayed concentration and the reaction rate is given in Table 1.

FCM clustering method is used to design IF-THEN fuzzy model from dataset.

For this the input (decayed concentration) and output (reaction rate constant) of the obtained model should be described linguistically in the form of granules.

Table 1.

Decayed consentration and reaction rate constant

Data	Decayed consentration	reaction rate constant
1	0,381217	8,33E-05
2	0,472708	0,000111
3	0,550671	0,000139
…	…	…
34	0,996849	0,001
37	0,99805	0,001083
38	0,998338	0,001111
...	...	...

Linguistical representation of the variables on fuzzy models as "code book" are given in Figure 1 and Figure 2.

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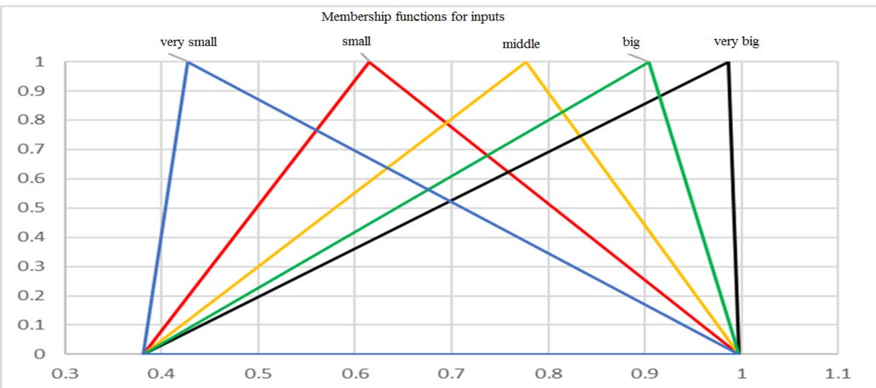

Figure 1.Graphical representation of the membership functions for decayed concentration

Values of triangular fuzzy number for input and output linguistical variable of the model are given in Table 2. Clustering process is performed in Matlab environment using FCM algorithm by data described in Table 1

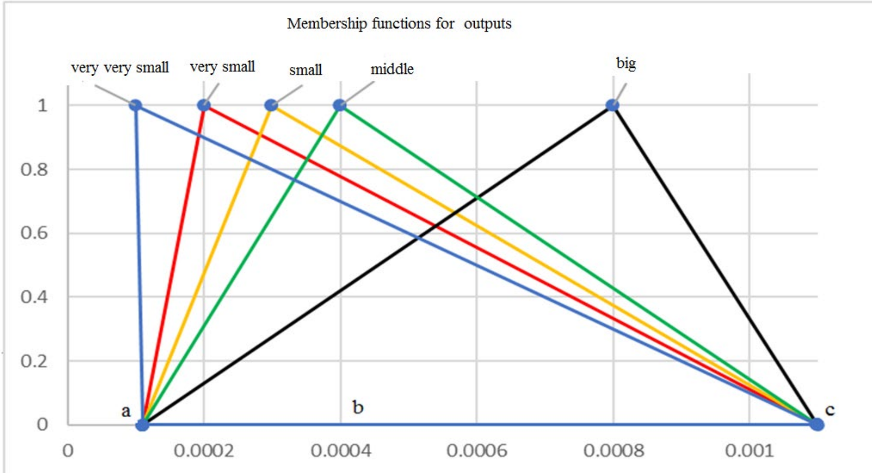

Figure 2. Graphical representation of the membership functions for reaction rate constant

Values of triangular fuzzy number for input and output linguistical variable of the model are given in Table 2.

Clustering process is performed in Matlab environment using FCM algorithm by data described in Table 1.

Table 2.

Fuzzy numbers for linguistical values of the input and output variables

Decayed consentration	Fuzzy number Tr(a,b,c)	reaction rate constant	Fuzzy number Tr(a,b,c)
Very small	(0.3812,0.427,0.998)	Very very small	(0.00011,0.0001,0.0011)
Small	(0.3812,0.6152,0.998)	Very small	(0.00011,0.0002,0.0011)
Average	(0.3812,0.7768,0.998)	Small	(0.00011,0.0003,0.0011)
Big	(0.3812,0.9036,0.998)	Average	(0.00011,0.0004,0.0011)
Very big	(0.3812,0.9867,0.998)	Big	(0.00011,0.0008,0.0011)

The input and outputs of the rule are represented by Triangular fuzzy number Tr(a,b,c).

$$Tr((a,b,c),x)=\begin{cases}\frac{x-a}{b-a}; a \le x < b\\ 1; \quad x=b\\ \frac{c-x}{c-b}; b < x \le c\end{cases}$$

where a, b, c are parameters of triangular fuzzy number.
For computer simulation selected value of FCM parameters are: Cluster numbers = 5, Max iteration = 1000, fuzzification exponent = 2, Min. Improvement = 0,000001.

Centers of clusters and their membership functions are given in Tables 3 and 4 respectively.

Table 3.

Center of clusters

0.6152	0.0002
0.7768	0.0003
0.9867	0.0008
0.9036	0.0004
0.4271	0.0001

Table 4.

Fragment of the values of the membership functions

Cluster 1	Cluster 2	Cluster 3	Cluster 4	Cluster 5
0.0361	0.0126	0.0054	0.0072	0.9387
0.0897	0.0197	0.0069	0.0098	0.8739
0.6761	0.2183	0.0237	0.0438	0.0381
0.1839	0.6985	0.0299	0.0636	0.0241
0.0084	0.9771	0.0037	0.0093	0.0016
	…	…		…
0.0007	0.0021	0.9853	0.0116	0.0003
0.0008	0.0023	0.9841	0.0125	0.0003
0.0008	0.0024	0.9830	0.0134	0.0004

Constructed fuzzy model using FCM approach consists of 5 rules, one input and one output:
If Decayed concentration is small Then reaction rate constant is very small;
If Decayed concentration is average Then reaction rate constant is small;
If Decayed concentration is very big Then reaction rate constant is very big;
If Decayed concentration is big Then reaction rate constant is average;
If Decayed concentration is very small Then reaction rate constant is very very small;

In this type fuzzy model, the number of rules and the number of inputs and outputs can be any. These parameters should be such that the quality of the resulting fuzzy model is close to optimal. This issue is also discussed in this chapter.

Numerous tests have been simulated to verify the performance and effectiveness of the model. If crisp or fuzzy values of variables are given as input to a fuzzy model, fuzzy inference tools are used to find the value of the output variable. In our case, the Mamdani inference method is used in the Matlab environment.

Test.1. IF Decayed concentration is 0.6897 THEN rate constant is 0.000528(Figure 3).

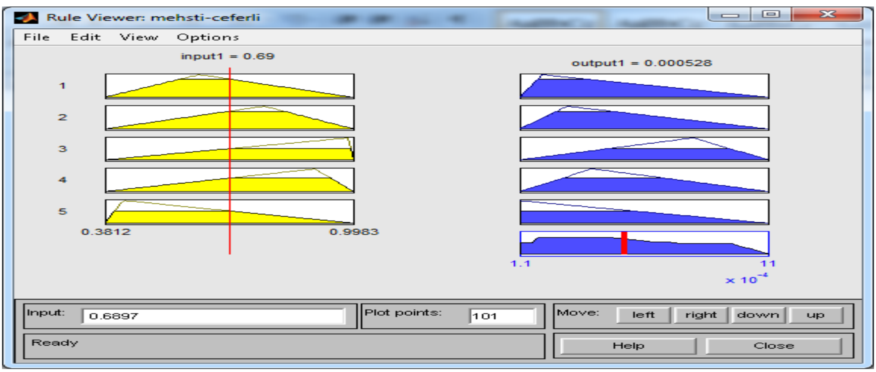

Figure 3. Computer simulation fragment (decayed concentration for c = 0.6897)

Test 2. IF Decayed concentration is 0.98 THEN rate constant is 0.000662(Figure 4.).

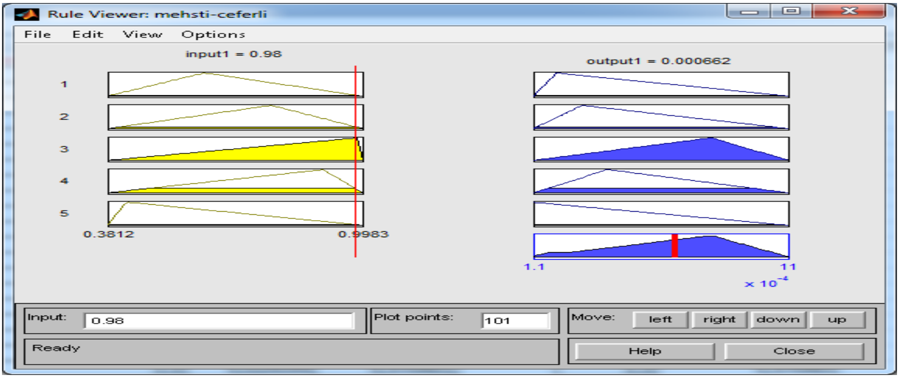

Figure 4. Computer simulation fragment (decayed concentration for c = 0.98)

Quality of the fuzzy model for determining isothermal reaction rate constant is characterized by some criteria.

The quality of the model closer to optimality is determined by the trade-off between criteria and requires solving the multicriterial decision problem.

Indexes of “Coverage”, “Transparency”, “Spesifity” are selected as quality criteria for fuzzy model. First of all, we consider the coverage index for the created rule base.

The Coverage index indicates that to what extend rules obtained from clustering cover data range intervals. Coverage index is calculated for the antecedent part of the rules.

In this case, a certain number of points are taken from the interval [0.3812 - 0.998] and values of membership degrees on the input points of the rules are obtained. The value of the membership degrees for each rule is determined by using formula.İf p_i is the domain of i-th input variable partitioned by membership functions $\{\mu_i^{(1)},...,\mu_i^{(p_i)}\}$, then coverage index is computed as

$$\mathrm{cov}_i = \frac{\int x_i \tilde{h}_i(x)dx}{N_i} \qquad (2)$$

where $\widetilde{h}_i(x)=\begin{cases} h_i(x), 0<h_i(x)<1 \\ \dfrac{p_i-h_i(x)}{p_i-1}, otherwise \end{cases}$ and $h_i(x)=\sum_{k=1}^{p_i}\mu_i^k(x)$

h_i – is the total MFs of *i-th* input variable with $N_i=\int_{X_i} dx$ for continuous domains.Coverage index is normalised as

$$.\overline{\text{cov}}=\sum_{i=1}^{r}\text{cov}_i/n_i$$

n_i - is the number of considered points r – is number of rules, cov_i -is the coverage degree calculated for input variables of the each rule. So, in our case coverage index on inputs of 5 rules equals:

$\overline{\text{cov}}$=0.545247117

Transparency index determines clearity and understandability of the rulebase for users. One of the most commonly used methods for detecting transparency factor is Nauck index detection. The Nauck index is equal to the production of complexity, coverage and partition coefficients. The Naucks index is defined by the following formula.

$$Nauck\ index = comp \times \overline{\text{cov}} \times \overline{part}$$

Complexity index measured as the number membership functions of output variables divided to the number of input variable in rules. Thus, we have 5 different membership functions in the output of the rules. The number of input variables is 1 for each rule.

$$comp = m/\sum_{i=1}^{r} n_i = \frac{5}{5} = 1,$$

where m- number of output variable, r-number of the rule, n_i - the number of input variables in i-th rules

Partition index is obtained as the inverse of the number of membership functions minus one for each input variable.

$$part_i = \frac{1}{p_i - 1}, \qquad \overline{part} = \sum_{i=1}^{r} \frac{part_i}{n_i}$$

where p_i -is total number of linguistical term for each input variable, $\overline{part}$ -denotes the average partition index for all input variables.
In our case $\overline{part}$ =0.25
So the Nauck index can be calculated as

$Nauck\ index = comp \times \overline{\text{cov}} \times \overline{part}$ =1 x 0.545247117x 0.25=0.136311779
Specifity index is computed as

$$Sp(A) = \int_0^{hgt(A)} \frac{1}{|A^{\mu}|} d\mu$$

The specifity index in our case for the inputs of 5 rules is:

$$Sp(A) = 0.491760052735662 \text{ s}$$

The overall result is as follows:
Complexity:1; Transparency: 0,545247117; Specifity:0,491760053; Partition :0,25; Nauck index:0,136311779.

These indexes allow us to analyze fuzzy models and to do decision about their suitability.

Here, a fuzzy model was analyzed to determine the rate of an isothermal chemical reaction. The values of indexes indicating the complexity, coverage, accuracy and transparency of the model were determined. The proposed approach allows researchers involved in fuzzy modeling to analyze models and correct decision parameters to achieve desirable quality of the model in the modeling process. For example, in fuzzy modeling, a high-quality model can be obtained by changing the choice at these stages, since the result depends on the number of membership functions, the chosen implication and inference method, as well as the above given indexes.

This chapter also addressed to the problem of reaction dynamics at the rate constant found on the basis of IF-THEN fuzzy model of isothermal chemical reaction. The behavior of the reaction is expressed by using fuzzy differential equation.

Assume that, isothermical reaction A→B is described by the following differential equation.

$$y''(s) = -Ny'(s) + RNy(s) - RN \qquad (3)$$

here $N = \frac{\vartheta L}{E_\alpha}$, $\mathrm{R} = \frac{\mathrm{kL}}{\vartheta}$.

E_a -an effective diffusion coefficient, k -reaction rate constant, L-is length of the tube in the reactor , ϑ axial velocity of species.

In this equation we denote

$$y = \frac{C_A}{C_{A0}}, \quad \mathrm{z} = \frac{x}{L}, \quad \mathrm{N} = \frac{\vartheta \mathrm{L}}{\mathrm{E}_a}, \quad \mathrm{R} = \frac{\mathrm{kL}}{\vartheta}$$

Initial condition is as the following form

$y(0) = 0,\ y'(0) = 0$

First we assume that N = 1 and R = 1 then equation (3) is transformed to $y''(s) = -y'(s) + y(s) - 1$.

$$y''(s) = -y'(s) + y(s) - 1$$

If uncertainty in initial conditions is taken into account,

$y(0) = \tilde{0},\ y'(0) = \tilde{0}$

then it can be written as differential equation.

$y''(s) = -y'(s) + y(s) - 1$

Here $y(s) \in E^1$ and E^1 are fuzzy subset of the real number R.

$\tilde{0}$ is fuzzy zero.

Taking into account this we get the following fuzzy initial condition problem .

$$y''(s) = -y'(s) + y(s) - 1$$
$$y(0) = \tilde{0},\ y'(0) = \tilde{0} \qquad (4)$$

Problem (4) by using α -cuts can described as follow:

$$y''(s,\alpha) = -y'(s,\alpha) + y(s,\alpha) - 1$$

$$y(0) = (0,\alpha) \;\; y'(0) = (0,\alpha)$$

This equation becomes interval type differential equation by using α-cut substitution as interval.

$$[y_l''(s,\alpha), y_r''(s,\alpha)] = [y_l(s,\alpha), y_r(s,\alpha)] - [y_l'(s,\alpha), y_r'(s,\alpha)] - 1$$

Thus, depending on the left and right boundaries we are getting below given equation.

$$y_l''(s,\alpha) = y_l(s,\alpha) - y_l'(s,\alpha) - 1 \tag{5}$$

$$y_r''(s,\alpha) = y_r(s,\alpha) - y_r'(s,\alpha) - 1 \tag{6}$$

If substituted $y_l(s,\alpha) = x_1$ and $y_l'(s,\alpha) = x_2$ then (5) equation becomes (7) system.

$$\begin{aligned} \dot{x}_1 &= x_2, \\ \dot{x}_2 &= x_1 - x_2 - 1 \end{aligned} \tag{7}$$

$$A_l = \begin{pmatrix} 0 & 1 \\ 1 & -1 \end{pmatrix}, \; X_l = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}, \; \dot{X}_l = \begin{pmatrix} \dot{x}_1 \\ \dot{x}_2 \end{pmatrix}, \; U_l = \begin{pmatrix} 0 \\ -1 \end{pmatrix}$$

matrix representation of the equation (6) using substitution can be as below:

$$\dot{X}_l = A_l * X_l + U_l.$$

Corresponding initial condition is as follow:

$$X_{0l} = \begin{pmatrix} -0.53 \\ 1.5 \end{pmatrix}$$

If substituted $y_r(s,\alpha) = x_3$ and $y_r'(s,\alpha) = x_4$ then equation (6) becomes to

$$\begin{aligned} \dot{x}_3 &= x_4, \\ \dot{x}_4 &= x_3 - x_4 - 1 \end{aligned}$$

$$A_r = \begin{pmatrix} 0 & 1 \\ 1 & -1 \end{pmatrix}, \; X_r = \begin{pmatrix} x_3 \\ x_4 \end{pmatrix}, \; \dot{X}_r = \begin{pmatrix} \dot{x}_3 \\ \dot{x}_4 \end{pmatrix}, \; U_r = \begin{pmatrix} 0 \\ -1 \end{pmatrix},$$

matrix representation of the equation (6) using substitution can be as below:

$$\dot{X}_r = A_r * X_r + U_r .$$

Corresponding initial condition is as follow:

$$X_{0r} = \begin{pmatrix} 0.53 \\ -0.2 \end{pmatrix}$$

α - cut approach is used to solve fuzzy diferential equation.

The behavior of the reaction depending on the rate constant , is considered in chapter 4.

In the fourth chapter we consider the fuzzy stability investigation problem of the isothermal chemical reaction. Fuzzy stability analysis of first order isothermal reaction was carried out.

To test the stability of the reaction given in chapter 3 as fuzzy differential equation, the values of rate constants obtained from IF-THEN fuzzy model are used.

α-cut approach and stability condition is used to test the stability of reaction described fuzzy differential equation which given in Chapter 3.

Initial condition problem for fuzzy differential equation is the following form:

$$\dot{x} = f(t,x),$$

$$x(t_0) = y_0 \in E^n, t \geq t_0, t_0 \in R_+ \qquad (8)$$

f function in $R_+ \times E^n$ is continuous and has continuous partial derivatives, that is $f \in C^1[R_+ \times E^n, E^n]$. Here, E^n is fuzzy subspace of R^n , R is real number axis. If f has continuous partial derivatives on x $\frac{\partial f}{\partial x}$ then Zadeh-Aliev stability criteria can describe as follow:

The solution $x(t, t_0, y_0)$ of the system (8) is fuzzy Lipschits stable to the solution $x(t,t_0,x_0)$ when for any solution $x(t,t_0,x_0)$, $t \geq t_0$ of the system (8) and $M = M(t_0) > 0$

$$\left\| x(t,t_0,y_0) -_h x(t,t_0,x_0) \right\|_{fH} \leq M(t_0) \left\| y_0 -_h x_0 \right\|_{fH} \qquad (9)$$

is satisfied.

Here $-_h$ Hukuhara difference of fuzzy numbers, $\|\cdot\|_{FH}$ - fuzzy Haustorf norm in E^n space.

If derivation $\dfrac{\partial f}{\partial x}$ is continuous in space $R_+ \times E^n$ then $F(t,t_0,\tilde{x}_0) = \dfrac{\partial x(t,t_0,\tilde{x}_0)}{\partial x_0}$ fundamental matrix solutions is bounded. In this case solution $x(t,t_0,y_0)$ of the system (8) is satisfies (9) condition.

α -cut of fundamental matrix solutions is form $F^\alpha = [F_l^\alpha, F_r^\alpha]$

When α =0 then $F^\alpha = [F_l, F_r]$.

$F^\alpha = [F_l, F_r]$ for considered system is:

*Fl=MatrixExp[Al*t]=*

$$\{\{\frac{1}{10}(5e^{\frac{1}{2}(-1-\sqrt{5})t} - \sqrt{5}e^{\frac{1}{2}(-1-\sqrt{5})t} + 5e^{\frac{1}{2}(-1+\sqrt{5})t} + \sqrt{5}e^{\frac{1}{2}(-1+\sqrt{5})t}),$$

$$-\frac{e^{\frac{1}{2}(-1-\sqrt{5})t} - e^{\frac{1}{2}(-1+\sqrt{5})t}}{\sqrt{5}}\}, \ \{-\frac{e^{\frac{1}{2}(-1-\sqrt{5})t} - e^{\frac{1}{2}(-1+\sqrt{5})t}}{\sqrt{5}},$$

$$\frac{1}{10}(5e^{\frac{1}{2}(-1-\sqrt{5})t} + \sqrt{5}e^{\frac{1}{2}(-1-\sqrt{5})t} + 5e^{\frac{1}{2}(-1+\sqrt{5})t} - \sqrt{5}e^{\frac{1}{2}(-1+\sqrt{5})t})\}\}$$

Fr=MatrixExp[Ar*t]=

$$\{\{\frac{1}{10}(5e^{\frac{1}{2}(-1-\sqrt{5})t}-\sqrt{5}e^{\frac{1}{2}(-1-\sqrt{5})t}+5e^{\frac{1}{2}(-1+\sqrt{5})t}+\sqrt{5}e^{\frac{1}{2}(-1+\sqrt{5})t}),$$

$$-\frac{e^{\frac{1}{2}(-1-\sqrt{5})t}-e^{\frac{1}{2}(-1+\sqrt{5})t}}{\sqrt{5}}\},\{-\frac{e^{\frac{1}{2}(-1-\sqrt{5})t}-e^{\frac{1}{2}(-1+\sqrt{5})t}}{\sqrt{5}},$$

$$\frac{1}{10}(5e^{\frac{1}{2}(-1-\sqrt{5})t}+\sqrt{5}e^{\frac{1}{2}(-1-\sqrt{5})t}+5e^{\frac{1}{2}(-1+\sqrt{5})t}-\sqrt{5}e^{\frac{1}{2}(-1+\sqrt{5})t})\}\}$$

Fls=MatrixExp[Al*s]/.s->t-s

$$\{\{\frac{1}{10}(5e^{\frac{1}{2}(-1-\sqrt{5})(-s+t)}-\sqrt{5}e^{\frac{1}{2}(-1-\sqrt{5})(-s+t)}+5e^{\frac{1}{2}(-1+\sqrt{5})(-s+t)}+\sqrt{5}e^{\frac{1}{2}(-1+\sqrt{5})(-s+t)}),$$

$$-\frac{e^{\frac{1}{2}(-1-\sqrt{5})(-s+t)}-e^{\frac{1}{2}(-1+\sqrt{5})(-s+t)}}{\sqrt{5}}\},\{-\frac{e^{\frac{1}{2}(-1-\sqrt{5})(-s+t)}-e^{\frac{1}{2}(-1+\sqrt{5})(-s+t)}}{\sqrt{5}},$$

$$\frac{1}{10}(5e^{\frac{1}{2}(-1-\sqrt{5})(-s+t)}+\sqrt{5}e^{\frac{1}{2}(-1-\sqrt{5})(-s+t)}+5e^{\frac{1}{2}(-1+\sqrt{5})(-s+t)}-\sqrt{5}e^{\frac{1}{2}(-1+\sqrt{5})(-s+t)})\}\}$$

Frs=MatrixExp[Ar*s]/.s->t-s

$$\{\{\frac{1}{10}(5e^{\frac{1}{2}(-1-\sqrt{5})(-s+t)}-\sqrt{5}e^{\frac{1}{2}(-1-\sqrt{5})(-s+t)}+5e^{\frac{1}{2}(-1+\sqrt{5})(-s+t)}+\sqrt{5}e^{\frac{1}{2}(-1+\sqrt{5})(-s+t)}),$$

$$-\frac{e^{\frac{1}{2}(-1-\sqrt{5})(-s+t)}-e^{\frac{1}{2}(-1+\sqrt{5})(-s+t)}}{\sqrt{5}}\},\{-\frac{e^{\frac{1}{2}(-1-\sqrt{5})(-s+t)}-e^{\frac{1}{2}(-1+\sqrt{5})(-s+t)}}{\sqrt{5}},$$

$$\frac{1}{10}(5e^{\frac{1}{2}(-1-\sqrt{5})(-s+t)}+\sqrt{5}e^{\frac{1}{2}(-1-\sqrt{5})(-s+t)}+5e^{\frac{1}{2}(-1+\sqrt{5})(-s+t)}-\sqrt{5}e^{\frac{1}{2}(-1+\sqrt{5})(-s+t)})\}\}$$

Sl=Fl.X0l+Integrate[Fls.Ul,{s,0,t}]=

$$\{\{1.-0.4362980073075309e^{\frac{1}{2}(-1+\sqrt{5})t}-1.093701992692469\mathrm{l}e^{-\frac{1}{2}(1+\sqrt{5})t}\},$$

$$\{e^{-\frac{1}{2}(1+\sqrt{5})t}(1.769646997739904-0.2696469977399039\mathrm{7}e^{\sqrt{5}t})\}\}$$

Sr=Fr.X0r+Integrate[Frs.Ur,{s,0,t}]=

$$\{\{0.9999999999999999 - 0.4295379140424817 6e^{\frac{1}{2}(-1+\sqrt{5})t} - 0.04046208595751829 6e^{-\frac{1}{2}(1+\sqrt{5})t}\},$$

$$\{e^{-\frac{1}{2}(1+\sqrt{5})t}(0.06546903033498441 - 0.2654690303349845e^{\sqrt{5}t})\}\}$$

$S^{\alpha} = [S_l, S_r]$ is the representation of the solution for fuzzy initial boundary problem using α -cut. In this case graphical representation of the solution can be as shown in Figure 5.

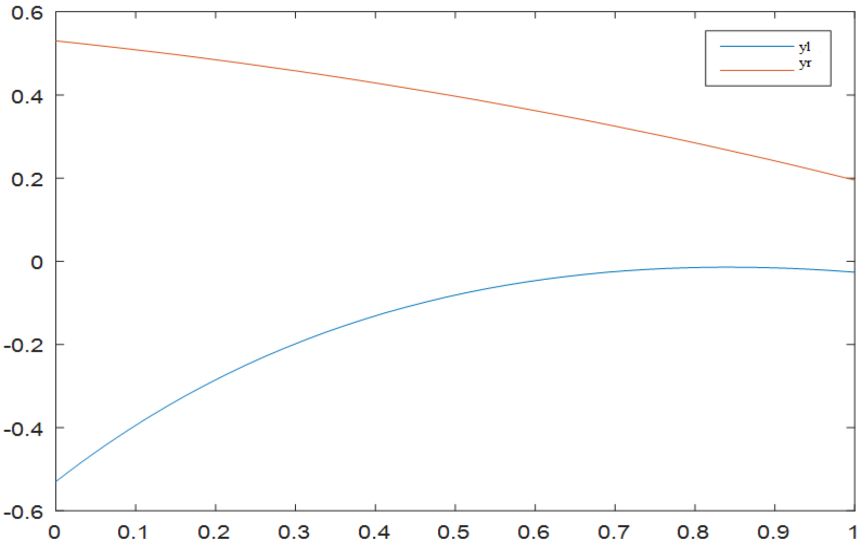

Figure 5. Representation of the chemical reaction dynamic described by fuzzy differential equation

In this case solution is Lipschitz stable.

Example. Unstable case. Let for equatin (3) N and R is as follow : R_l= 0.5, R_r=1.5, N_l= 0.5, N_r =1.5.

$$Al = \begin{pmatrix} 0 & 1 \\ Rl * Nl & -Nl \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 0.25 & -0.5 \end{pmatrix},$$

$$X_l = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix},\ \dot{X}_l = \begin{pmatrix} \dot{x}_1 \\ \dot{x}_2 \end{pmatrix},\ Ul = \begin{pmatrix} 0 \\ -Rl * Nl \end{pmatrix} = \begin{pmatrix} 0 \\ -0.25 \end{pmatrix},$$

$$\dot{X}_l = A_l * X_l + U_l$$

$$X0l = \begin{pmatrix} -0.53 \\ 1.5 \end{pmatrix};$$

$$Ar = \begin{pmatrix} 0 & 1 \\ Rr * Nr & -Nr \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 2.25 & -1.5 \end{pmatrix},\ X_r = \begin{pmatrix} x_3 \\ x_4 \end{pmatrix},$$

$$\dot{X}_r = \begin{pmatrix} \dot{x}_3 \\ \dot{x}_4 \end{pmatrix},\ Ur = \begin{pmatrix} 0 \\ -Rr * Nr \end{pmatrix} = \begin{pmatrix} 0 \\ -2.25 \end{pmatrix},$$

$$\dot{X}_r = A_r * X_r + U_r,$$

$$X0r = \begin{pmatrix} 0.53 \\ -0.2 \end{pmatrix}.$$

is obtained. Matrix of fundamental solutions is as follow:

$$Fl = MatrixExp[Al * t] =$$

$\{\{-0.777437524821136(0. - 0.3555182164812668e^{-0.8090169943749475t}) +$
$0.9554225632202383(0. + 0.7573683369074649e^{0.30901699437494745t}),$
$-0.777437524821136(0. + 1.1504811157728663e^{-0.8090169943749475t}) +$
$0.9554225632202383(0. + 0.9361587484235894e^{0.30901699437494745t})\},$
$\{0.628960169645094(0. - 0.3555182164812668e^{-0.8090169943749475t}) +$
$0.29524180884432627(0. + 0.7573683369074649e^{0.30901699437494745t}),$
$0.628960169645094(0. + 1.1504811157728663e^{-0.8090169943749475t}) +$
$0.29524180884432627(0. + 0.9361587484235894e^{0.30901699437494745t})\}\}$

$$Fr = MatrixExp[Ar * t] =$$

$$\{\{-0.38095372233513364(0.-0.7255296012224595e^{-2.4270509831248424t}) + 0.7333492283402898(0.+0.986715155325983e^{0.9270509831248424t}),$$
$$-0.38095372233513364(0.+0.782621036414731e^{-2.4270509831248424t}) + 0.7333492283402898(0.+0.40654900213739287e^{0.9270509831248424t})\},$$
$$\{0.9245941063185542(0.-0.7255296012224595e^{-2.4270509831248424t}) + 0.6798521231067103(0.+0.986715155325983e^{0.9270509831248424t}),$$
$$0.9245941063185542(0.+0.782621036414731e^{-2.4270509831248424t}) + 0.6798521231067103(0.+0.40654900213739287e^{0.9270509831248424t})\}\}$$

$$Fls = MatrixExp[Al * s] /. s \to t - s$$

$$\{\{-0.777437524821136(0.-0.3555182164812668e^{-0.8090169943749475(-s+t)}) + 0.9554225632202383(0.+0.7573683369074649e^{0.30901699437494745(-s+t)}),$$
$$-0.777437524821136(0.+1.1504811157728663e^{-0.8090169943749475(-s+t)}) + 0.9554225632202383(0.+0.9361587484235894e^{0.30901699437494745(-s+t)})\},$$
$$\{0.628960169645094(0.-0.3555182164812668e^{-0.8090169943749475(-s+t)}) + 0.29524180884432627(0.+0.7573683369074649e^{0.30901699437494745(-s+t)}),$$
$$0.628960169645094(0.+1.1504811157728663e^{-0.8090169943749475(-s+t)}) + 0.29524180884432627(0.+0.9361587484235894e^{0.30901699437494745(-s+t)})\}\}$$

$$Frs = MatrixExp[Ar * s] /. s \to t - s$$

$$\{\{-0.38095372233513364(0.-0.7255296012224595e^{-2.4270509831248424(-s+t)}) + 0.7333492283402898(0.+0.986715155325983e^{0.9270509831248424(-s+t)}),$$
$$-0.38095372233513364(0.+0.782621036414731e^{-2.4270509831248424(-s+t)}) + 0.7333492283402898(0.+0.40654900213739287e^{0.9270509831248424(-s+t)})\},$$
$$\{0.9245941063185542(0.-0.7255296012224595e^{-2.4270509831248424(-s+t)}) + 0.6798521231067103(0.+0.986715155325983e^{0.9270509831248424(-s+t)}),$$
$$0.9245941063185542(0.+0.782621036414731e^{-2.4270509831248424(-s+t)}) + 0.6798521231067103(0.+0.40654900213739287e^{0.9270509831248424(-s+t)})\}\}$$

$$Sl = Fl.X0l + Integrate[Fls.Ul,\{s,0,t\}]=$$

$$\{\{1.-1.7645223859424062e^{-0.8090169943749475t}+0.23452238594240615e^{0.30901699437494745t}\},$$
$$\{5.551115123125782\times10^{-17}+1.4275285971824365e^{-0.8090169943749475t}+$$
$$0.07247140281756381e^{0.30901699437494745t}\}\}$$

$$Sr = Fr.X0r + Integrate[Frs.Ur,\{s,0,t\}]=$$

$$\{\{0.9999999999999997-0.07027632565751546e^{-2.4270509831248424t}-$$
$$0.3997236743424843e^{0.9270509831248424t}\},$$
$$\{1.110223024625156\times10^{-16}+0.17056422527747434e^{-2.4270509831248424t}-$$
$$0.3705642252774744e^{0.9270509831248424t}\}\}$$

It shows that dynamics of the system is unstable.

Graphical representation of the solution of differential equation is given in Figure 6. Chemical reaction is unstable.

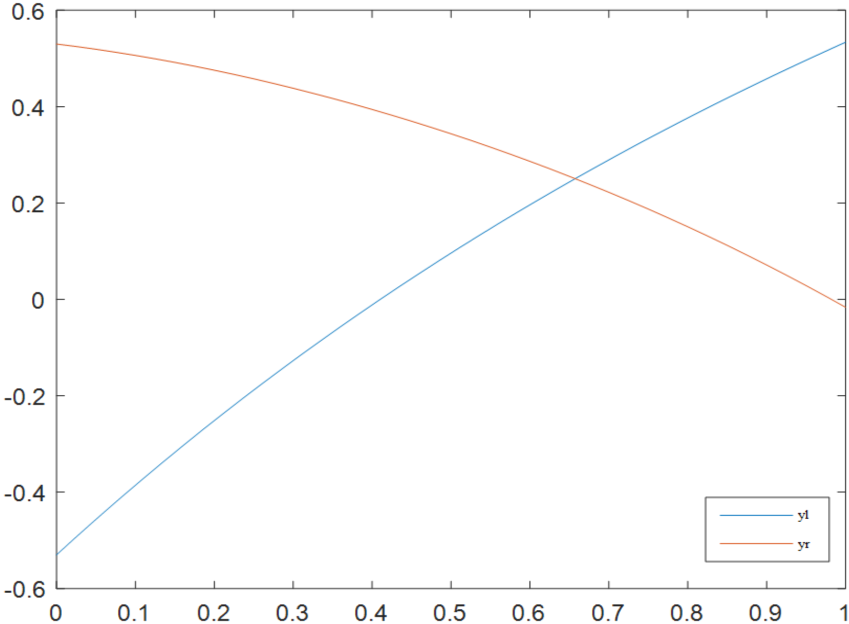

Figure 6. Unstable behavior of the reaction

The boundaries of unstability are given by points in Appendix.

Figure 6 illustrates unstable behavior of dynamics in considered isothermic reaction.

The sensitivity analysis for different values k was tested (Results are presented in the appendix). Fragments of the differential equation solution or behavioral values of the reaction are given in appendix.

The experimental investigation on fuzzy models of isothermal chemical reactions using computer simulation was considered in the **fifth chapter**. Results of experimental study based on computer simulation, decomposition of hydrogen-peroxide reaction, analysis of a fuzzy model of the alkylation reaction between propylene and benzene are given in current chapter.

Let us consider the problem determining the rate constant for decomposition reaction of hydrogen peroxide. Due to this decomposition reaction of hydrogen peroxide was simulated for 550 seconds.

Below given initial data was used for solving this problem :

$$k = [6.1, 6.9] \cdot 10^{-5} \cdot s^{-1} \qquad \Delta = \frac{[H_2O_2]_{t=550s}}{[H_2O_2]_0} = e^{-kt}$$

Δ is the ratio of decayed hydrogen peroxide in 550 seconds to the amount of it in initial moment.

$\delta = (100 - \Delta)\%$ illustrates the percentage of hydrogen peroxide decomposition during 550 seconds.

The relation between this indicator and the rate constant is obtained from computer simulation. The fragment is shown in Table 5.

Table 5

The relation between δ and k

Iterations		δ (%)	k($10^{-5}s^{-1}$)
1		3,299344	6,1
2		3,315298	6,13
3		3,33125	6,16
...	...	...	...
29		3,745071	6,94
30		3,760951	6,97

Clusters were extracted from above given initial data using FCM clustering approach and fuzzy model described in the relation between decomposition percentage of hydrogen-peroxide and k rate constant were created. Code book created for this reason is given in Table 6.

Table 6.

Fuzzy numbers for linguistical values of the input and output variables

Decayed concentration	Fuzzy umber (a,b,c)*10^{-5}	Rate constant	Fuzzy number (a,b,c)*10^{-5}
about 3.53	(3.30,3.53,3.75)	about 6.53	(6.12,6.53,6.75)
about 3.33	(3.30,3.33,3.75)	about 6.16	(6.12,6.16,6.75)
about 3.63	(3.30,3.63,3.75)	about 6.72	(6.12,6.72,6.75)
about 3.72	(3.30,3.72,3.75)	about 6.9	(6.12,6.9,6.75)

The input and output of the rule are represented by triangular fuzzy number Tr(a,b,c) as shown in Table 6.

Center of clusters were obtained as:

Cluster 1=(3.5272; 6.5289*10^{-5});
Cluster 2=(3.3336; 6.1645*10^{-5});
Cluster 3=(3.6265; 6.7161*10^{-5});
Cluster r 4=(3.7251; 6.9022*10^{-5}).

Using results of clustering the following fuzzy rule-base was created:

*If the percentage of hydrogen peroxide decomposition is about 3.53, Then the rate constant is about 6. 53 * 10^{-5};*
*If the percentage of hydrogen peroxide decomposition is about 3.33, Then the rate constant is about 6. 16 * 10^{-5};* (10)
*If the percentage of hydrogen peroxide decomposition is about 3.63, Then the rate constant is about 6. 72 * 10^{-5};*
*If the percentage of hydrogen peroxide decomposition is about 3.72, Then the rate constant is about 6. 9 * 10^{-5};*

Decomposition of hydrogen peroxide reaction was investigated by using Larcen inference algorithm in above given fuzzy model.

Rule- base (10) is fuzzy relation between and the rate constant. It can be described in matrix form.

Fuzzy relation matrixes are created by using Larcen implication(Table 7). Larcen implication is expressed as follow:

$$R_p = A \times B = \int_{X\times Y} \mu_{A(x)} \cdot \mu_{B(y)} /(x, y)$$

One of the relation matrix is given below:

Table 7

Fuzzy relation matrix for the first rule

	0,1	0,4	0,92	1	0,37	0,26	0,2
0	0	0	0	0	0	0	0
0,73	0,073	0,4	0,6716	0,73	0,2701	0,1898	0,146
0,91	0,091	0,4	0,8372	0,91	0,3367	0,2366	0,182
1	0,1	0,4	0,92	1	0,37	0,26	0,2
0,87	0,087	0,4	0,8004	0,87	0,3219	0,2262	0,174
0,08	0,008	0,08	0,0736	0,08	0,0296	0,0208	0,016
0,01	0,001	0,01	0,0092	0,01	0,0037	0,0026	0,002

Relation matrix was created for the each rule and combined fuzzy relation matrix is defined based on them. Using agregation operator combined fuzzy relation matrix is shown in Table 8.

Table 8

Combined fuzzy relation matrix

0,1	0,0102	0,1	0,1	0,1	0,1	0,1	0,06
0,2	0,073	0,2	0,2	0,2	0,2	0,2	0,146
0,34	0,091	0,34	0,34	0,34	0,34	0,34	0,219
1	0,1	0,67	0,92	1	0,92	0,67	0,3
0,43	0,087	0,43	0,43	0,43	0,43	0,43	0,219
0,08	0,0108	0,08	0,08	0,08	0,08	0,08	0,08
0,02	0,0039	0,02	0,02	0,02	0,02	0,02	0,0052
Y1	0,1	0,67	0,92	1	0,92	0,67	0,3

Here Y1 desribes the values of membership function of the obtained result.

Reaction rate constant of decomposition of hydrogene peroxide reaction on new input data are obtained from using computer simulation of reasoning mechanism.

Determined that, if percentage of hydrogen peroxide decomposition is approximately 3.45, then the reaction rate constant equals approximately $6.412*10^{-5.}$

The constructed model [8] can be used in the study of such reactions.

Let us consider the steps of creating a fuzzy model of the alkylation reaction between propylene and benzene. In this model, the main control parameter is the reaction rate.

Determining of the reaction rate constant for alkylation reaction between propylene and benzene depends on percentage rate C_0, C_1, C_2.

The volume of benzene, alkylbenzene and polymer is determined by the following mathematical expression.

$$C_0 = 100e^{-k_1 t}$$

$$C_1 = 100(6.67e^{0.85k_1 t} - 6.667e^{-k_1 t})$$

$$C_2 = 100(2.075e^{-0.28k_1 t} - 9.94e^{-0.85k_1 t} + 7.87e^{-k_1 t})$$

The dependence of the molar ratio of propylene-benzene from the reaction rate constant is described by the equation:

$$m = 4 - 1.125e^{-0.02k_1 t} - 1.913e^{-0.285k_1 t} - 3.473e^{-0.85k_1 t} + 2.110e^{-k_1 t}$$

The percentage rate of output at the reactor is determined by the following formulas:

$$C_0^{'}(t) = 100e^{-0.0055t}$$

$$C_1^{'}(t) = 100(6.67e^{-0.004675t} - 6.667e^{-0.0055t})$$

$$C_2^{'}(t) = 100(2.071e^{-0.00154t} - 9.941e^{-0.004675t} + 7.87e^{-0.0055t})$$

Construction of fuzzy model based on the data of benzene, alkylbenzene and polymer obtained from the given above equations, are based on the idea of extracting knowledge from data.Database contains 33 records. Each record describes the values of benzene (c0), alkylbenzene (c1) and polymers (c2), rate constant (k).

Table 9

Fragment values of the initial data

c0	c1	c2	k
99.59979	0.302643535	0.099999812	0.0045
99.59978	0.302737528	0.099999805	0.00466
99.59977	0.30283152	0.099999798	0.00482
99.59964	0.30442939	0.099999685	0.00754
99.59963	0.304523382	0.099999678	0.0077
99.59963	0.304617374	0.099999671	0.00786
99.59962	0.304711367	0.099999665	0.00802
…	…	…	…
99.59961	0.304805359	0.099999658	0.00818
99.59959	0.305087336	0.099999638	0.00866
99.59958	0.305181328	0.099999631	0.00882
99.59957	0.305369313	0.099999618	0.00914
99.59956	0.305463305	0.099999611	0.0093
99.59955	0.305580796	0.099999603	0.0095

The clusters obtained from the data by using Fuzzy C-means method are given in Table 10.

Table 10

Centers of clusters

c0	c1	c2	k
99.9996	0.3045	0.1	0.0076
99.9997	0.3041	0.1	0.0069
99.9997	0.3037	0.1	0.0063
99.9997	0.3041	0.1	0.0070
99.9996	0.3044	0.1	0.0074

Constructured fuzzy model consists of 5 rules:

If amount of benzene is norm and amount of alkylbenzene is very big and amount of polymer is average THEN rate constant is big;
If amount of benzene is high and amount of alkylbenzene is big and

amount of polymer is average THEN rate constant is small;
If amount of benzene is high and amount of alkylbenzene is norm and amount of polymer is average THEN rate constant is very small;
If amount of benzene is high and amount of alkylbenzene is big and amount of polymer is average THEN rate constant is small;
If amount of benzene is norm and amount of alkylbenzene is high and amount of polymer is average THEN rate constant is average;

The following linguistical terms are used in this model for representation of the relation between reaction rate constant and reagents, which are described trapezoidal fuzzy numbers:

Very small or less than A: $(0, I, A - Z, Z)$;
Big or about A: (Z, A, A, Z);
Very big or more than A: $(Z, A + Z, S, 0)$;
Average or neutral: $(Z, I + 2 * Z, I + 3 * Z, Z)$

I and S are minimum and maximum values of the universum, respectively, Z=(S-I)/5.

Result that obtained from using ESPLAN tool[1] is given below:

If amount of benzene is big and amount of alkylbenzene is very big and amount of polymer is average THEN define the reaction rate constant

Result:Rate constant is approximately 0.008.

RESULT

The main **scientific results** obtained in the dissertation are as follow :

1. Mathematical analysis of isothermal chemical reaction systems under uncertain conditions.
2. Fuzzy IF-THEN models have been developed to determine the rate constant of an isothermal reaction.
3. A multicriteria decision approach to quality estimation of suggested fuzzy models has been carried out.
4. The fuzzy stability of isothermal chemical reactions was

investigated for the first time.
5. Testing of stability on isothermal chemical reactions under uncertain conditions was performed and sensitivity analysis was carried out.
6. The obtained theoretical results were applied to two reactions.
7. The hydrogen peroxide decomposition reaction was investigated by using fuzzy model, the reaction rate constant was determined.
8. To determine reaction rate constant the fuzzy model of the alkylation reaction was rsuggested.

The proposed theoretical methods are universal and can be used to analyze various chemical isothermal reactions.

The main content of the dissertation work is published in the following works:

1. Babanlı, M.M. Application of fuzzy logic in molecular modelling(azeri) // XVII Scientific Conference of Masters, – Sumqayıt, – 11-12 May, – 2017, – s.261-262.
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[2] - problem statement and computer modeling.
[8] - investigation of the hydrogen peroxide decomposition reaction.

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