Mathematical Modelling of the Effect of Temperature on the Rate of a Chemical Reaction

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Abstract

Mathematical modelling is quite frequent in chemical kinetics which studies the rates of chemical reactions of physical and/or chemical processes. The rate of chemical reactions and the determination of their order are described in this paper via mathematical equations based on derivatives and integrals. The temperature and the reaction rate constant are just some of the factors that have an effect on the reaction rate, and that effect was illustrated using linear, exponential and logarithmic functions. Data obtained through experiments was processed with the help of a computer, more specifically using the GeoGebra software package.

Key words: *computer-based learning, fitting, function, integral, mathematical model.*

Introduction

Modelling

One of the important roles of mathematics is to describe and explain phenomena from the real world, explore key questions about the observed world and test specific ideas by means of mathematical modelling. The model is then used to make predictions about the behaviour of the given phenomenon under given conditions (Tall, 1977). The process of developing a mathematical model is called mathematical modelling.

The hypotheses that involve functioning of the world are translated into the language of mathematics. This has multiple advantages. Firstly, mathematical language is precise, which helps in the formulation of ideas and identification of basic postulates. Secondly, mathematical language is concise, having strictly defined regulations for performing specific operations. Thirdly, all results previously proven by mathematicians are at

our disposal. Lastly, computers can be used for the display of graphical forms and numerical calculations.

Because the real world implies areas such as the economy, ecology, chemistry, engineering, mathematical modelling can be regarded as activities which enable a mathematician to become an economist, an ecologist, a chemist. Instead of performing real-world experiments, he or she can perform experiments from a mathematical aspect of the world. The challenge in such modelling is 'not to obtain the most extensive descriptive model, but to produce the simplest model possible which includes the main features of the observed phenomenon' (Howard Emmons) (De Vries, 2001).

Certain limitations exist in the process of mathematical modelling. The fact that the model, by its very nature, focuses on specific aspects of the situation, disregarding others, can present a problem. Such process of simplification can probably predict with great accuracy certain aspects on which it focuses, while being partially imprecise regarding others. The existence of a model is not sufficient on its own; it requires focusing on the most important parts of the observed situation and understanding its limitations and conditions under which it should be treated (Tall, 1977). Further on, mathematics has the potential to prove general results, but these results can depend on the form of the equations used. Small changes in the equation structure can produce great changes in the mathematical methods. The use of computers in modelling does not always give rise to elegant solutions; nevertheless it provides reliability in respect to other alternative procedures.

The process of mathematical modelling can be presented by the following scheme: (Kraljević & Čižmešija, 2009).
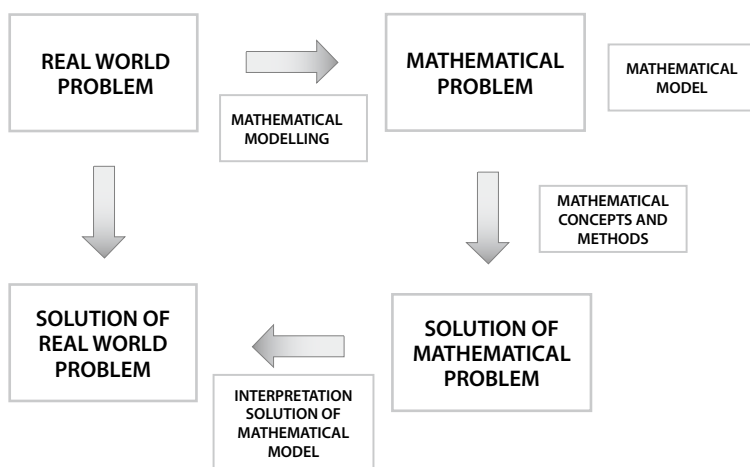
Figure 1. *The mathematical modelling scheme*

GeoGebra Software

Visualising the correlation of the chosen contents in the modelling process carries specific importance. In this paper, free educational software GeoGebra 3.2 and the advanced version, GeoGebra Beta 4.0, which include needed didactical principles, were used.

GeoGebra is a computer tool which encompasses geometry, algebra and calculus, connecting the iconic and symbolic form of presentation, thus offering numerous advantages. The iconic presentation serves at the transitional level between literal, realistic presentation and symbolic, absolutely abstract presentation. The iconic presentation keeps the basic elements and reality contours, while in the case of symbolic presentation, the link with reality is purely conventional. GeoGebra offers both iconic and symbolic presentations of objects in the geometric and algebraic window at the same time. The parallel presentation of geometry and algebra is frequently found in the theory of electronic learning as well as in the didactics of natural sciences.

The acquired knowledge is here manifested as active - through activity, processing and work; as iconic - through images; symbolic - through symbols and language.

The possibility of interactive manipulation of objects is the greatest and key advantage of new media, contrasted with traditional learning. Students can discover new abilities on their own; the presumed ones can be tested, proven, and if needed, corrected. The principle of active learning becomes expressed through the active component of learning.

Knowledge which is acquired by means of various presentations is more permanent. The ability to transport knowledge into other shapes increases flexibility and success while solving problems. This is also the basic didactical idea behind GeoGebra. A student that relates different presentations of a single concept is therefore able to recognize more situations where that concept plays a role (Herceg, D. & Herceg, Đ., 2007).

The Correlation of Mathematical and Chemical Concepts

Mathematical analysis is a field of mathematics that studies limits, derivatives and integrals, among others. This field is also known as calculus. According to the validated learning plan and program for the science department in the Secondary Grammar School (Gymnasium), students are first taught the concept of the exponential function, and then the logarithmic function as its inverse pair and in the fourth grade derivatives and integrals are explored. However, that order can be changed without losing out on any didactical and methodical principles, thus offering better quality knowledge.

Once the students adopt specific knowledge about functions, derivatives and integrals, the last step can be achieved through a scientific student debate on the matter of correlation of the mentioned concepts. The motivation for a student to make judgments about the connections that govern between them is in every aspect more efficient than exploring these concepts individually.

After learning the properties of the definite integral, the teacher could point out the following to students:

If a real interval *I* is given, *a* being the fixed element of the interval *I*, *x* being the arbitrary element of the interval *I*, and if *f* is an integrable function on *I*, we can define a function *F* in the following manner:

$$F(x)=\int_a^x f(t)dt$$

This way, with the aid of integrals, it is possible to define the logarithmic function:

$$\ln(x)=\int_1^x \frac{1}{t}dt$$

and then define the exponential as its inverse function:

$$\forall x \in R, \forall y \in (0,\infty): y = e^x \Leftrightarrow \ln(y) = x \quad \text{(Tall, 1975).}$$

Knowledge about these concepts can be of better quality and permanence if it is related with the respectful concepts of another field of science. The example of correspondence of these concepts with the concepts of chemistry, precisely chemical kinetics is presented in the paper.

Chemical kinetics is a field of chemistry that is based on the study of rates of chemical reactions, further introducing the concept of reaction order. The modelling of the chemical reaction rate and reaction order is done via derivatives and integrals. When determining the reaction order the link between the definite integral and the logarithmic function is seen. Furthermore, the reaction rate and order are in relation with temperature at which a reaction occurs. The modelling of this dependence is done with the help of the exponential function, but also some properties of logarithms are used. Graphically, the equivalence and correlation of these concepts can be presented as follows:
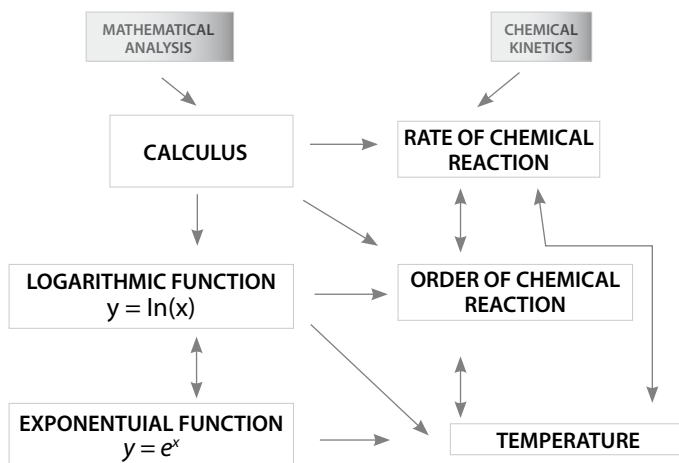

Figure 2. *Links between mathematical and chemical concepts*

An Overview of the Previous Major Studies

Mathematics and other natural sciences teaching methodology developed plenty of material about mathematical modelling. Here, we concentrate on studies concerning the secondary school level.

In the framework of the PAM project, Carr (1987) and Galbraith (1991) have presented examples of models in lectures marked as lower-middle level with great detail, encompassing a wide range of extra- and intra-mathematical topics.

In his books, Lowe (1988, 1991) offers detailed examples for classes 7-12, in which he stresses computers as the key tool in modelling.

One of the more important elements in teaching is the method of assessment of teaching programs oriented towards modelling, as shown by Clatworthy and Galbraith (1991).

The Freudenthal Institute in Utrecht has developed various materials, including textbooks, for all school grades. In these studies, accent is given to structures nearing mathematical topics, and examples of modelling are designed as support in learning mathematics.

The comprehensive mathematical course of the Centre for Innovation in Mathematics Teaching at Mathematics of the University of Exeter focuses on the application of models in teaching. Both Shell and CIMT materials accent the structures having to do with real-world problems, less with mathematics, with the goal of prompting student activity.

Spode Group (1992) presents detailed examples adapted for direct use of models in the classroom.

Garfunkel and Steen (1991) assert the importance of the application of mathematics in practice, especially when computers are concerned, pointing out the activity of students while modelling this way. Such an approach provided the basis for the authors of this study.

Boer (1990) and Jannack (1992) have shown several detailed global teaching units, where they hold the development of the ability of students to act competent in real life situations as the main goal of modelling.

Kaiser-Messmer (1991) asserts the importance of applying teaching plans and programs oriented towards knowledge application at all levels of education.

The work of Blum (1995) must also be mentioned, as he has given great contributions in studying modelling. In his papers, several arguments explained in-depth can be found, which go in favour of applying models in teaching. As the most important, he lists: motivation, understanding of the role of mathematics in society, its application in different science disciplines, the development of the ability to explore and easier learning.

In the papers of Niss and Jensen (2007), modelling in class is stressed as one of the key mathematical competences of students. Blomhøj (2003, 2007) also develops the approach in which the student takes the central part in the process of teaching, hence also in his competence.

The didactical and methodical importance of the application of GeoGebra in teaching modelling is emphasized by Karadag and McDougall (2009).

The Methodological Framework of the Conducted Study

The idea of this study was to pave the way for a more significant introduction of modelling to secondary school (gymnasium) teaching, having in mind the fact that modelling can be very successfully carried out in a computer environment.

- *The studied problem* was defined as following: How much do mathematical modelling and the application of computers help in the teaching of natural science concepts in class; and is that way of studying more useful for students and teachers in contrast to the traditional teaching approach?
- *The subject of study.* Here we take into account the realization of the contemporary didactical model of teaching, aimed at goals of chemistry teaching; more precisely, chemical kinetics, with the application of the GeoGebra educational software.
- *The goal of the study.* The real goal is to examine whether it is possible to enhance the level of quality of teaching when applying modelling in chemistry and using computers in class. The secondary goal was formulated as investigating the possibility of easier and more durable acquisition of knowledge when using modelling and computers instead of traditional methods.
- *The tasks of the study.* With respect to the previously formulated criteria variables and goals of the study, the following tasks can be defined: 1) to discover the indicators which mean that mathematical modelling in chemistry increases the quality of teaching; 2) to discover that this approach increases student motivation; 3) to discover that modelling contributes to a better understanding of new learning content of chemical kinetics; 4) to find out the rate at which modelling affects durability and applicability of formerly acquired knowledge of mathematics; 5) to affirm that students can apply mathematical knowledge even on other teaching contents.
- *The hypothesis of the study*: With the application of modelling with the aid of computers during the study of concepts of chemical kinetics, it is possible to obtain significant statistical data which will indicate an enhancement of the quality of teaching in contrast to traditional teaching.
- *Methods of the study.* The descriptive method is applied when gathering, processing and interpreting data, and in understanding and establishing the basic theoretical postulates, practical solutions of the subject of the study and the obtained results of the experimental study. The experimental method with parallel groups is used in the part of the study focusing on comparing the effects of teaching through modelling and the traditional teaching approach.
- *Techniques of the study.* The study is carried out using the testing technique. A

test will show the mutual relationship of the results in the experimental and control group.
- *The population and sample of the study.* The study was conducted with the fourth year students of the science department of the secondary school (Gymnasium) 'Isidora Sekulić' in Novi Sad, during the school year 2010/2011. It encompassed 59 students: 30 students in the control group (C) and 29 students in the experimental group (E).

Working with the Control Group

The work with the control group was realized using the method of oral presentation by the teacher, and frontal teaching, which is a characteristic of the traditional teaching approach. The intention was that students were to acquire new knowledge from the field of chemical kinetics, which concerns the concepts of reaction rate and order, the effect of temperature on a chemical reaction, the energy of activation and preexponential factor. The teacher's lecture is presented here in a concise form.

General Kinetics of Chemical Reactions

Every chemical reaction possesses its reaction rate, defined as the absolute change in concentration of a reactant or a product in the unit of time (House, 2007). It has been shown that there are different ways to express a reaction rate (Milanović & Raičević, 2011). The instantaneous reaction rate is computed as:

$$v_t = \lim_{\Delta t \to 0} \frac{c_{t+\Delta t} - c_t}{\Delta t} = \frac{dc}{dt} \tag{1}$$

where the expression is positive if the concentration of a product is taken into consideration or negative if the concentration of a reactant is taken into consideration. According to the collision theory, for a reaction whose rate depends on only one reactant, the rate law is:

$$v = k[A]^m \tag{2}$$

where k is the reaction rate constant, $[A]$ the concentration of the reactant A, while m presents the specific exponent which, in this case, also presents the reaction order.

In order to explore how the concentration varies through time in reactions of different orders, equations (1) and (2) are equated and solved for zeroth, first and second order ($m = 0, 1, 2$):

$$-\frac{d[A]}{dt} = k\,[A]^m \tag{3}$$

For $m = 1$, equation (3) becomes:

$$\ln[A] = -kt + \ln[A]_0 \tag{4}$$

For $m = 2$, equation (3) takes the form of:

$$\frac{1}{[A]} = kt + \frac{1}{[A]_0} \tag{5}$$

Lastly, for $m = 0$, equation (3) is:

$$[A] = [A]_0 - kt \qquad (6)$$

The obtained equations (4), (5) and (6) are presented in form of linear functions, so that it can be possible to determine the value of the ordinate of the graph which shows a linear function after plotting experimental data regarding the change of concentration over time. They show the change of concentration $[A]$ of a reactant A with initial concentration $[A]_0$ through a time interval of t in a reaction that can either be first, second or zeroth order with the reaction rate of k. Taking into account graph on which the obtained function is linear (graphs with $[A]$, $\ln[A]$ or $1/[A]$ ordinates), the order of the chemical reaction can be determined easily. Seeing that the slopes of these functions are respectfully $-k$, k and $-k$, the chemical reaction rate constant can be determined as the slope of the function (Milanović & Raičević, 2011).

The Effect of Temperature on the Rate of a Chemical Reaction

The Arrhenius Equation

As seen in the previously examined way of quantifying the chemical reaction rate using the collision theory, the rate of a chemical reaction increases if the concentrations of the reactants increase. However, a single system with constant conditions has been taken into consideration, in order for the rate constant to stay the same so it can be evaluated for those conditions. On the other hand, the rate constant is a value that depends on the nature of the reactants, presence of a catalyst and temperature. Different reactions with different natures of their reactants possess different reaction constants. If a catalyst is presented to the system, the chemical reaction rate increases, regarding the catalyst. Lastly, a significant effect of temperature on the chemical reaction rate has been observed.

For example, magnesium in a system with cold water reacts very slowly (Atkins *et al.*, 2006). If magnesium is introduced to hot water, the reaction of forming magnesium hydroxide and hydrogen is evidently faster. Therefore, with the increase of temperature an increase of the reaction rate is observed. Although such a trend was realized, it was necessary to determine in what way the reaction rate increases with temperature. Using a mathematical model presented by a function it is possible to describe the relation between the reaction rate and temperature.

Although not all reactions abide this law, Svante August Arrhenius in the late 19th century suggested that the rate constant varies with temperature in such a way: (House, 2007)

$$k = Ae^{\frac{-Ea}{RT}} \qquad (7)$$

The previous equation is also known as the Arrhenius equation.

The chemical reaction rate constant is presented by k, A is the frequency factor (or pre-exponential factor) which is dependent on the frequency of collisions of molecules

during a chemical reaction, R is the universal gas constant (8.314 J K^{-1} mol^{-1}), T presents temperature and E_a the energy of activation.

The energy of activation presents the amount of energy needed to be handed over to the molecules in order for the chemical reaction to occur and it is characteristic to each reaction. It measures the difference between the extreme values, the maximal and minimal energy in the reaction system during time.

The physical sense of the Arrhenius equation is understood when we take into consideration that molecules on higher temperatures move faster, therefore increasing the frequency of collisions of the molecules of the reactants.

Energy of Activation and Frequency Factor

The effect of the parameters of the Arrhenius equation on the rate constant has been mentioned. Further on, a way for determining these parameters, the energy of activation and frequency factor, will be shown using experimental measurements of reactant concentrations on various temperatures.

If we take the natural logarithm of both sides of the Arrhenius equation:

$$\ln k = -\frac{E_a}{R}\frac{1}{T} + \ln A \tag{8}$$

it can be seen that the graph showing a linear dependence of the rate constant and temperature has the abscissa $1/T$ and ordinate $\ln k$, as well as a slope of - E_a/R.

Working with the Experimental Group

After the oral presentation of the lecture by the teacher (in the same way as with the control group), mathematical modelling with the help of a computer was approached. The basis of the model was a problem of determining the energy of activation and the preexponential factor.

Problem: a) Determine the chemical reaction rate if the experimental measurements have been obtained (presented in Table 1) (House, 2007):

Table 1. *Experimental data*

	[A], M				
t, min	T = 25 °C	T = 30 °C	T = 35 °C	T = 40 °C	T = 45 °C
0	0.750	0.750	0.750	0.750	0.750
15	0.648	0.622	0.590	0.556	0.520
30	0.562	0.530	0.490	0.440	0.400
45	0.514	0.467	0.410	0.365	0.324
60	0.460	0.410	0.365	0.315	0.270
75	0.414	0.378	0.315	0.275	0.235
90	0.385	0.336	0.290	0.243	0.205

Solution: Very often, when the graph of some of the mentioned dependencies of time is drawn, it is clear at first if it is linear or not. However, it should be noted that the data obtained through an experimental method always contains an experimental

error. In some cases, by using the visual method it is difficult to determine whether it is linear or not.

In this case, the software package GeoGebra with the possibility of determining the "success" of fitting the entered points was used.

In a more advanced version of GeoGebra, the GeoGebra 4.0 Beta, it was possible to use the command *RSquare*. *RSquare* is a type of statistical test that checks how much a given point corresponds to the function graph by calculating the coefficient of determination (R^2), which ranges from 0 to 1. The more the points correspond to the type of dependency, the closer the value is to 1 (House, 2007).

Since the reaction order does not vary with temperature, it can be determined on any temperature. In the testing that will follow, the values for time and concentrations have been taken for the temperature T = 25 ˚C.

Test 1.
- A Spreadsheet View is used; the table values are entered for the time *t* and concentration [*A*] in order to check whether the reaction is zeroth order.
- Then, using this data, a List of Points was made with the command *Create List of Points*.
- A List of Points is then assigned to the graphical display, where the value of time is on the abscissa, and values of concentration are on the ordinate.
- Then fitting was initiated using the command *FitLinear*.
- By visual method, it was determined that the obtained graph is not the graph of a linear function, but the advanced version of GeoGebra also determined the coefficient of determination $R^2 = 0.962$.
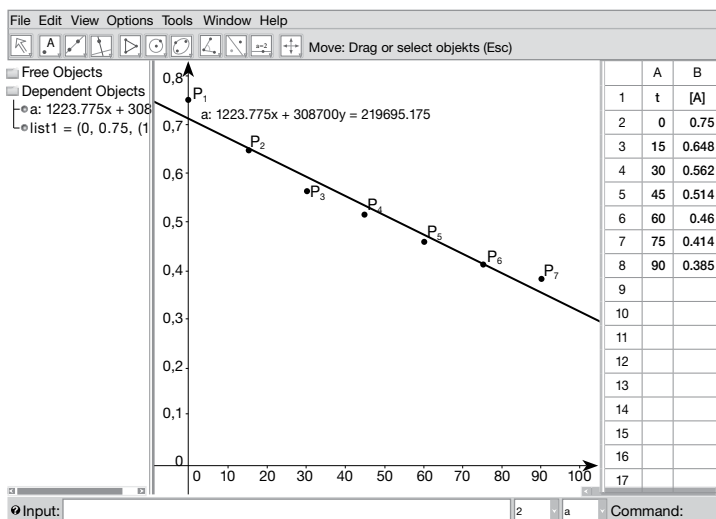

Figure 3. *The interface of the program GeoGebra during the first test*

Test 2.

- A Spreadsheet View is used; the table values are entered for the time t and for the natural logarithm of concentration, ln[A], in order to check whether this is a first order reaction.
- Then, using this data, a List of Points was made with the command Create List of Points.
- A List of Points is then assigned to the graphical display, where the value of time t is on the abscissa and the values of ln[A] are on the ordinate.
- Then the fitting was initiated using the command FitLinear.
- The visual method was slightly less obvious in determining that it is not a linear graph of the function. The coefficient of determination $R^2 = 0.990$ was calculated.
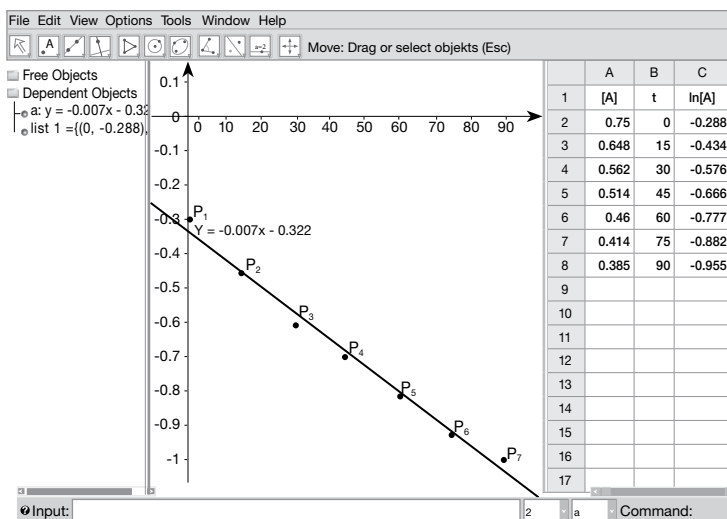

Figure 4. *The interface of the program GeoGebra during the second test*

Test 3.

- A Spreadsheet View is used, the table values are entered for the time t and for the reciprocal of the concentration, 1/[A] in order to check whether the reaction is second order.
- Then, using this data, a List of Points was made with the command Create List of Points.
- A List of Points is then assigned to the graphical display, where the value of time t is on the abscissa and the value of 1/[A] is on the vertical axis.
- Then the fitting was initiated using the command FitLinear.
- It is obvious that this is a graph of a linear function, which was confirmed by the coefficient of determination, which amounted to R2 =0.999 (higher than in the previous two cases, which certainly removes any doubt).
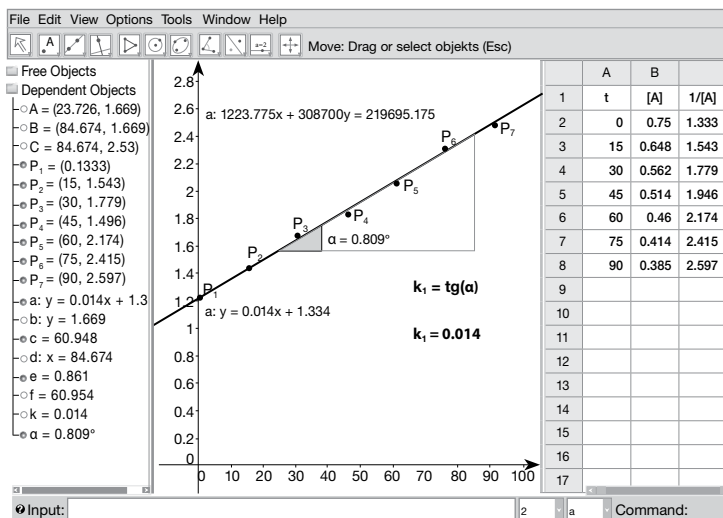
Figure 5. *The interface of the program GeoGebra during the third test*

- Based on the results obtained in all tests, it was found that the reaction whose experimental data was treated was second order.
- The reaction rate coefficient corresponds to the slope obtained in Test 3, and using the command Angle a value $\alpha = 0.809°$ is obtained (the angle that the line forms with the positive part of the x-axis).
- Using the command Tan(α) the value k1=tg(α)=0.014 is obtained.
- Given that it is a second-order reaction and that the time is measured in minutes, the reaction rate constant is 0.014 dm^3/(mol min).

Problem: b) Determine the activation energy and frequency factor of the given chemical reaction using the experimental data from Table 1.

Solution: It has been concluded that the reaction is of second order. It is necessary to repeat Test 3 for t time values and concentration values of 1/[A], this time on different temperatures. That way, the values of k_i are obtained for i=1, 2, 3, 4, 5. For further calculations, the temperature values have been converted into Kelvins and the reaction rate constants into $dm^3/(mol \cdot s)$. The results are presented in Table 2.

Table 2. *The values of the rate constant k on different temperatures*

Measurement number	Temperature T (K)	Rate constant k (dm³/(mol s))
1.	298.15	0.000233
2.	303.15	0.000300
3.	308.15	0.000400
4.	313.15	0.000516
5.	318.15	0.000650

Test 4.

• A Spreadsheet View is used; the table values are entered for the reciprocal of the temperature ($1/T$) and for the natural logarithm of the reaction rate constant ($\ln(k)$).

• Then, on the basis of this data a List of Points was made, using the command *Create List of Points.*

• A List of Points is then assigned to the graphical display, where the value of $1/T$ is on the abscissa and the value of $\ln(k)$ is on the ordinate.

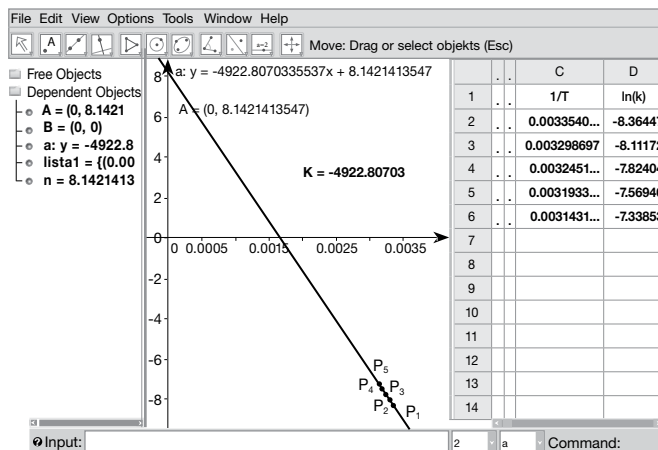• Then the fitting was initiated using the command *FitLinear*.

Figure 6. *The interface of the program GeoGebra during the fourth test*

Considering the results obtained in Test 4, it can be concluded that the y-intercept of the linear function ($1/T$ vs. $\ln(k)$) is 8.142141, the slope being 4922.80703, and seeing that its form is $\ln k = -\frac{E_a}{R}\frac{1}{T} + \ln A$, we find $\ln A = 8.142141$, $-E_a/R = -4922.80703$, from where it is obvious that $A = 3436.267$ dm³/(mol·s) and $E_a = 40928.217$ J, which was needed to be found.
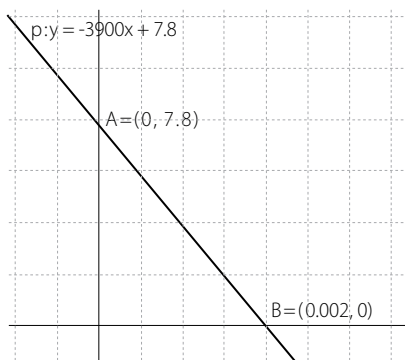
Results of the Study

After the complete process of modelling was performed, the students of both groups were tested. A combined type didactical test was used, which included gap filling questions and multiple choice questions. The testing lasted for 45 minutes.

Test

1. Write down the equation expressing the instantaneous chemical reaction rate.

_____

2. Rate of the chemical reaction depends on (circle the correct answer):
  a) reactant concentration, reactant nature and temperature
  b) reactant concentration
  c) temperature.

3. What is the chemical reaction order? _____

4. Concentration of a reactant being decomposed in a zero-order reaction:
(circle the correct answer)
a) increases linearly with time
b) decreases exponentially with time
c) decreases linearly with time

5. Write down the equation describing the change of concentration of a reactant over time in a second-order reaction. _____

6. The equation $-3196.03x + 13310y = 10728.72$ describes the dependence of concentration of a reactant over time. What is the rate constant of this reaction?

_____

7. Chemical reaction rate (circle the correct answer):
a) is not dependent of temperature
b) is dependent of temperature
c) is dependent of temperature on a case-to-case basis.

8. The chemical reaction rate constant, with the increase of temperature (circle the correct answer):
a) linearly decreases
b) exponentially decreases
c) exponentially increases.

9. At a given temperature, with the increase of the preexponential factor, the chemical reaction rate (circle the correct answer):
a) increases
b) decreases
c) the chemical reaction rate is not dependent of the preexponential factor.

10. The picture below shows a graph of a function that describes the chemical reaction rate constant change under different temperatures.

p: $y = -3900x + 7.8$
A = (0, 7.8)
B = (0.002, 0)

On the basis of the given data, determine:
1) What is the frequency factor of this reaction? _____
2) What is the activation energy of this reaction? _____

Discussion

The analysis of the results of the testing (presented in Table 3 and Figure 7) suggests that it can be concluded that students of the experimental group achieved significantly better results in contrast to the control group students. A lower difference can be seen when comparing questions that included plain reproduction of the teaching content. A more significant difference stands out in questions that included a certain degree of logical thought and reasoning.

It can thus be concluded that the hypothesis of the study is proven. The application of mathematical modelling with the help of computers in teaching chemistry positively affects the quality of teaching and the quality and permanence of acquired student knowledge.

Table 3. *Tabular representation of the results*

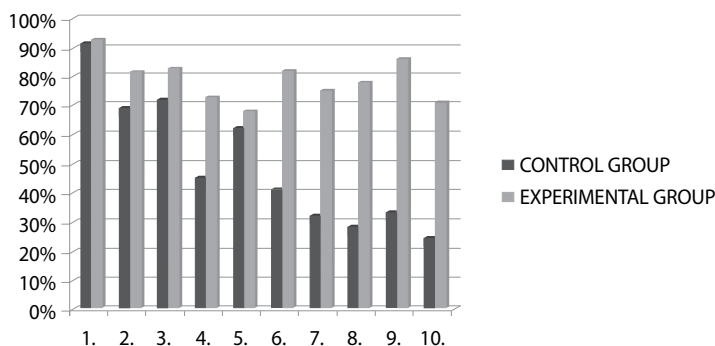| Question number	Control group	Experimental group	Question number	Control group	Experimental group
1.	91%	92%	6.	41%	82%
2.	69%	82%	7.	32%	75%
3.	72%	83%	8.	28%	78%
4.	45%	73%	9.	33%	86%
5.	62%	68%	10.	24%	71%

Figure 7. *Graphical representation of the results*

Conclusion

The approach described in this paper can be contrasted with the traditional method of teaching mathematics and other natural sciences. The basis is presented by studying theory and solving problems from particular subject area, chemistry, with the aid of mathematical modelling. At the same time, students adopt chemical concepts and

practice mathematical concepts. A sensible and obvious bond is formed between real world concepts and mathematics, which implies the same for the bond between theory and practice. The knowledge that students obtain this way becomes permanent, functional and applicable.

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Matematičko modeliranje utjecaja temperature na brzinu kemijske reakcije

Sažetak

Matematičko modeliranje je učestala metoda u kemijskoj kinetici koja proučava brzinu kemijskih i fizikalno-kemijskih procesa. U ovome su radu brzina kemijskih reakcija, kao i određivanje njihovog reda opisani matematičkim formulama temeljenima na derivacijama i integralima. Temperatura i konstanta brzine reakcije su samo neki od čimbenika koji utječu na brzinu reakcije, a taj je utjecaj prikazan uporabom linearnih, eksponencijalnih i logaritamskih funkcija. Podatci prikupljeni tijekom eksperimenta su obrađeni uporabom računala, točnije uporabom računalnog programskog paketa GeoGebra.

Ključne riječi: *učenje pomoću računala (computer-based learning), prilagođavanje (fitting), funkcija, integral, matematički model.*

Uvod

Modeliranje

Jedna od važnih uloga matematike je opisati i objasniti pojave iz stvarnog svijeta, istražiti ključna pitanja o promatranom svijetu i testirati određene ideje posredstvom matematičkog modeliranja. Model se potom koristi za predviđanja ponašanja promatrane pojave u zadanim uvjetima (Tall, 1977). Proces formiranja matematičkog modela naziva se matematičko modeliranje.

Hipoteze koje uključuju i funkcioniranje svijeta prevode se u matematički jezik. To ima višestruke prednosti. Prvo, matematički jezik je precizan, što pomaže pri formulaciji ideja i identificiranju temeljnih postulata. Drugo, matematički jezik je koncizan, imajući strogo određena pravila za izvođenje određenih operacija. Treće, na raspolaganja nam stoje svi prethodni rezultati koje su dokazali drugi matematičari. Na kraju, uporabom računala možemo prikazati grafikone i numeričke izračune.

S obzirom na to da stvarni svijet implicira područja poput ekonomije, ekologije, kemije, inženjerstva, prema matematičkome modeliranju možemo se odnositi kao prema aktivnosti koja matematičarima omogućava da postanu ekonomist, ekolog ili kemičar. Umjesto provođenja pravih eksperimenata, matematičar može izvesti eksperimente na matematičkom modelu svijeta. Izazov takvog modeliranja nije u "stvaranju najopsežnijeg deskriptivnog modela, već stvoriti najjednostavniji mogući model koji sadrži glavne osobine promatrane pojave" (Howard Emmons) (De Vries, 2001).

U procesu matematičkog modeliranja postoje i određena ograničenja. Činjenica da se model, po svojoj prirodi, usredotočuje na određeni aspekt dane situacije, zanemarujući sve ostale, može predstavljati problem. Takav proces pojednostavljivanja, vjerojatno s velikom točnošću može predvidjeti određene aspekte na koje je usmjeren, istovremeno bivajući djelomično neprecizan s obzirom na ostale. Postojanje modela nije samodostatno; zahtjeva fokusiranje na najvažnije dijelove promatrane situacije i razumijevanje ograničenja i uvjeta u kojima treba biti tretiran (Tall, 1977). Nadalje matematika ima potencijal dokazivanja općih rezultata, ali ti rezultati mogu ovisiti o obliku korištene formule. Sitne promijene u strukturi formule mogu rezultirati ogromnih promjenama u matematičkim metodama. Uporaba računala ne rezultira uvijek elegantnim rješenjima; svejedno pruža pouzdanost s obzirom na druge alternativne postupke.

Proces matematičkog modeliranja može biti predstavljen prikazanom shemom: (Kraljević & Čižmešija, 2009).

Slika 1.

GeoGebra – računalni programski paket

U procesu modeliranja značajno mjesto zauzima vizualizacija korelacija odabranih sadržaja. U ovome radu su korišteni besplatni obrazovni računalni programi GeoGebra 3.2 i unaprijeđena inačica, GeoGebra Beta 4.0, a u kojima su sadržana i potrebna didaktička načela.

Usvojeno znanje ovdje se očituje kao aktivno – kroz aktivnost, obradu i rad; kao ikonografsko – kroz slike; simboličko – kroz simbole i jezik.

Mogućnost interaktivnog rukovanja objektima je najveća i ključna prednost novih medija, u usporedbi s tradicionalnim učenjem. Učenici mogu samostalno otkrivati nove mogućnosti; pretpostavke se mogu provjeravati, dokazivati i prema potrebi korigirati. Princip aktivnog učenja biva izražen upravo kroz aktivnu komponentu učenja.

Znanje usvojeno putem različitih prezentacija je trajnije. Sposobnost prenošenja znanja u druge oblike povećava fleksibilnost i uspješnost pri rješavanju problema. To je ujedno i temeljna didaktička ideja na kojoj se GeoGebra temelji. Učenik koji u suodnos dovodi različite prikaze jednog koncepta, moći će prepoznati više situacija kojih je taj koncept sastavni dio (Herceg, D. & Herceg, Đ., 2007).

Korelacija matematičkih i kemijskih koncepata

Matematička analiza je grana matematike koja, između ostalog, proučava granične vrijednosti, derivacije i integrale. Ta grana matematike je još poznata i kao infinitezimalni račun ili kalkulus. Prema trenutno važećem Nastavnom planu i programu za prirodno-matematički smjer u gimnaziji učenici prvo uče koncept eksponencijalne funkcije, zatim logaritamske funkcije kao njenog inverznog para i u četvrtom razredu proučavaju derivacije i integrale. Međutim, taj redoslijed je moguće promijeniti bez da se izgube bilo koji od didaktičkih i metodičkih načela, istovremeno nudeći bolju kakvoću znanja.

Jednom kad učenik usvoji određena znanja o funkcijama, derivacijama i integralima, posljednji korak se može postići kroz znanstvenu raspravu među učenicima na temu korelacije navedenih koncepata. Učenička motivacija o prosuđivanju veza koje vladaju među navedenim konceptima je u tom slučaju daleko veća nego da se svaki od tih koncepata proučava zasebno.

S obzirom na poznate osobine određenog integrala, nastavnik učenicima može skrenuti pozornost na sljedeće:

Ako je zadan interval I na skupu realnih brojeva, gdje je a fiksni element intervala I, x je proizvoljni element intervala I, i f je integrabilna funkcija na I, funkciju F možemo definirati na sljedeći način:

$$F(x) = \int_a^x f(t)dt$$

Na ovaj način, pomoću integrala, moguće je definirati logaritamsku funkciju:

$$\ln(x) = \int_1^x \frac{1}{t}dt$$

i tada definirati eksponencijalnu kao njenu inverznu funkciju:

$$\forall x \in R, \forall y \in (0,\infty): y = e^x \Leftrightarrow \ln(y) = x \quad \text{(Tall, 1975)}.$$

Znanje o tim konceptima može biti kvalitetnije i trajnije ako se poveže s odgovarajućim konceptima drugih znanstvenih područja. U ovome radu su opisani primjeri mogućeg odnosa tih koncepata s konceptima u kemiji, točnije kemijskoj kinetici.

Kemijska kinetika je područje kemije temeljeno na proučavanju brzine kemijskih reakcija, koje dalje utječu na red reakcije. Pri modeliranju brzine kemijske reakcije kao i njenog reda koristimo derivacije i integrale. Prilikom određivanja reda reakcije vidljiva je veza između određenog integrala i logaritamske funkcije. Nadalje, brzina i red reakcije je u vezi s temperaturom pri kojoj se reakcija odvija. Modeliranje te veze je moguće uz pomoć eksponencijalne funkcije, no koriste se i neka svojstva logaritama. Grafički se ekvivalencija i korelacija ovih koncepata može prikazati na sljedeći način:

Slika 2.

Pregled dosadašnjih važnijih istraživanja

Metodika poučavanja matematike i drugih prirodnih znanosti razvila je mnoštvo materijala o matematičkom modeliranju. Ovdje ćemo se koncentrirati na istraživanja koja su se bavila srednjoškolskom razinom.

Carr (1987) i Galbraith (1991) su u okviru PAM projekta predstavili detaljne primjere modela u nastavi označene kao niža-srednja razina, pridružujući im široki spektar ekstra- i intra-matematičkih tema.

U svojoj knjizi Lowe (1988, 1991) nudi detaljan prikaz za 7-12 razred, u kojem naglašava uporabu računala kao ključnog alata u modeliranju.

Jedan od važnijih elemenata u poučavanju je metoda vrednovanja nastavnih programa orijentiranih prema modeliranju, kao što su prikazali Clatworthy and Galbraith (1991).

Freundthal institut u Utrechtu je razvio raznolike materijale, uključujući i udžbenike za sve razrede u školi. U tim istraživanjima, naglasak je na strukturama koje se dotiču matematičkih tema, a primjeri modeliranja su napravljeni kao potpora učenju matematike.

Opći matematički smjer Centra za inovacije, Matematičkog odsjeka Sveučilišta u Exeteru usmjeren je primjeni modela u poučavanju. Materijali koje su razvili Shell i CIMT više naglašavaju važnost koju strukture imaju u problemima stvarnog svijeta, a manje u matematici, s ciljem poticanja aktivnosti učenika.

Skupina Spode (1992) je predstavila detaljne primjere prilagođene izravnoj uporabi modela u učionici.

Garfunkel i Steen (1991) ističu značaj primjene matematike u praksi, posebice kad su u pitanju računala, ukazujući na aktivnosti studenata prilikom modeliranja. Takav pristup je pružio temelje za istraživanje autorima ovog rada.

Boer (1990) i Jannack (1992) su predstavili nekoliko globalnih nastavih jedinica za koje tvrde da je glavni cilj modeliranja razvoj sposobnosti studenata da djeluju kompetentno u stvarnim životnim situacijama.

Kaiser-Messmer (1991) ističe značaj primjene nastavnih planova i programa orijentiranih prema primijenjenom znanju na svim razinama obrazovanja.

Moramo spomenuti i Blumov (1995) rad s obzirom na veliki doprinos u proučavanju modeliranja. U njegovim radovima se mogu pronaći detaljno objašnjeni argumenti koji podržavaju primjenu modela u nastavi. Kao najvažnije navodi: motivaciju, razumijevanje uloge matematike u društvu, njenu primjenu u različitim znanstvenim disciplinama, razvoj sposobnosti istraživanja i lakše učenje.

U radovima Nissa i Jensena (2007), modeliranje u nastavi je naglašeno kao jedna od ključnih matematičkih kompetencija studenata. Blomhøj (2003, 2007) je također razvio pristup u kojem studenti imaju glavnu ulogu u procesu poučavanja, samim time i njihove kompetencije.

Karadag i McDougall (2009) naglašavaju didaktičku i metodičku važnost primjene GeoGebre u poučavanju modeliranja.

Metodolški okvir provedenog istraživanja

Ideja ovog istraživanja bila je utrti put značajnijem uvođenju poučavanja modeliranja u srednje škole (gimnazije), imajući na umu činjenicu da se modeliranje može vrlo uspješno provesti u računalnom okruženju.

- *Problem istraživanja je definiran na sljedeći način:* U kojoj mjeri matematičko modeliranje i primjena računala pomažu u poučavanju pojmova iz prirodnih znanosti; i je li takav način učenja korisniji učenicima i nastavnicima u usporedbi s tradicionalnim pristupom poučavanju.

- *Predmet istraživanja.* Ovdje uzimamo u obzir realizaciju suvremenih didaktičkih modela poučavanja, usmjerenih ka cilju poučavanja kemije; točnije kemijske kinetike, s primjenom obrazovnog softvera GeoGebra.

- *Cilj istraživanja.* Pravi cilj je bio istražiti postoji li mogućnost unaprijediti razinu kakvoće poučavanja primjenom modeliranja u kemiji i uporabom računala u nastavi. Drugi cilj je formuliran kao istraživanje mogućnosti lakšeg i trajnijeg stjecanja znanja uporabom modeliranja i računala umjesto tradicionalnih metoda.

- *Zadaća istraživanja.* S obzirom na prethodno formuliranje kriterijske varijable i ciljeve istraživanja mogu se odrediti i njegovi zadaci: 1) otkriti pokazatelje koji znače da se primjenom matematičkih modela u kemiji povećava kakvoća poučavanja; 2) otkriti da takav pristup povećava motivaciju studenata; 3) otkriti da modeliranje pridonosi boljem razumijevanju novih nastavnih sadržaja iz kemijske kinetike; 4) utvrditi u kojoj mjeri modeliranje utječe na trajnost i primjenjivost ranije usvojenih znanja iz matematike; 5) potvrditi da studenti mogu matematičko znanje upotrijebiti i na drugim nastavim sadržajima.

- *Hipoteza istraživanja:* S primjenom modeliranja uz potporu računala tijekom istraživanja koncepata kemijske kinetike, moguće je prikupiti značajne statističke podatke koji će ukazati na unaprjeđenje kakvoće poučavanja u usporedbi s tradicionalnim načinima.

- *Metode istraživanja.* Deskriptivna metoda će se upotrijebiti prilikom prikupljanja, obrade i interpretacije podataka, kao i u razumijevanju i postavljanju temeljnih teoretskih postulata, praktičnih rješenja za predmet istraživanja i za prikupljene rezultate eksperimentalnog istraživanja. Eksperimentalna metoda s paralelnim skupinama je korištena u dijelu istraživanja usmjeravajući se na usporedbu učinaka poučavanja uporabom modeliranja i tradicionalnih pristupa poučavanju.

- *Tehnike istraživanja.* Istraživanje je provedeno uporabom tehnike testiranja. Test će pokazati međusobni odnos rezultata eksperimentalne i kontrolne skupine.

- *Populacija i uzorak istraživanja.* Istraživanje je provedeno sa učenicima četvrte godine znanstvenog odsjeka srednje škole (gimnazije) "Isidora Sekulić" u Novom Sadu, tijekom školske godine 2010/2011. Obuhvatilo je 59 studenata: 30 studenata u kontrolnoj skupini (C) i 29 studenata u eksperimentalnoj skupini (E).

Rad s kontrolnom skupinom

S kontrolnom skupinom su korištene metode usmenog izlaganja nastavnika i frontalna nastava, što su metode svojstvene tradicionalnom pristupu počavanju. Cilj je bio da učenici usvoje novo znanje iz područja kemijske kinetike, koje se tiče pojmova brzine i reda reakcije, utjecaja temperature na kemijsku reakciju, energiju aktivacije i preeksponencijalni faktor. Ovdje prikazujemo održano predavanje u sažetom obliku.

Opća kinetika kemijskih reakcija

Svakoj kemijskoj reakciji svojstvena je brzina reakcije, određena kao apsolutna promjena u koncentraciji reakatanta ili proizvoda u jedinici vremena (House, 2007). Pokazano je da postoje različiti načini iskazivanja brzine reakcije (Milanović & Raičević, 2011). Trenutna brzina kemijske reakcije se prikazuje kao:

$$v_t = \lim_{\Delta t \to 0} \frac{c_{t+\Delta t} - c_t}{\Delta t} = \frac{dc}{dt} \qquad (1)$$

gdje je vrijednost pozitivna ako se u obzir uzima koncentracija proizvoda ili negativna ako se u obzir uzima koncentracija reaktanta. Prema teoriji sudara, za reakciju čija brzina ovisi o samo jednom reaktantu, trenutna brzina kemijske reakcije iznosi:

$$v = k[A]^m \qquad (2)$$

gdje je k konstanta brzine kemijske reakcije, $[A]$ koncentracija reaktanta A, dok je m odgovarajući eksponent koji istovremeno predstavlja i red kemijske reakcije.

S ciljem istraživanja kako se koncentracija reaktanta mijenja kroz vrijeme u reakcijama različitih redova izjednačene su jednadžbe (1) i (2) i riješene su za reakcije nultog, prvog i drugog reda (m = 0, 1, 2):

$$-\frac{d[A]}{dt} = k\,[A]^m \qquad (3)$$

Za m = 1, jednadžba (3) glasi:

$$\ln[A] = -kt + \ln[A]_0 \qquad (4)$$

Za m = 2, jednadžba (3) ima oblik:

$$\frac{1}{[A]} = kt + \frac{1}{[A]_0} \qquad (5)$$

Konačno, za m = 0, jednadžba (3) je:

$$[A] = [A]_0 - kt \qquad (6)$$

Dobivene jednadžbe (4), (5) i (6) su prikazane u obliku linearnih funkcija, da bi se obradom eksperimentalnih podataka o promijeni koncentracije u vremenu dobio podatak o tome kakva treba biti ordinata grafa na kome je promjena koncentracije u vremenu linearna. One pokazuju funkciju promjene koncentracije $[A]$ reaktanta A s

početnom koncentracijom $[A]_0$ tijekom vremena t u reakciji konstantne brzine k koja je nultog, prvog, odnosno drugog reda. Ovisno o tome na kojem je grafu dobivena linearna funkcija (graf s ordinatom $[A]$ ln$[A]$ ili $1/[A]$), lako se može odrediti red kemijske reakcije. S obzirom na to da su koeficijenti pravca tih funkcija redom –k, k i –k, konstanta brzine kemijske reakcije može se odrediti kao koeficijent pravca (Milanović & Raičević, 2011).

Utjecaj temperature na brzinu kemijske reakcije

Arrheniusova jednadžba

Kao što smo prethodno prikazali kvantifikaciju brzine kemijske reakcije uporabom teorije sudara, brzina kemijske reakcije se povećava povećanjem koncentracije reaktanata. Međutim, promatran je jedan sustav s konstantnim uvjetima, kako bi brzina reakcije bila konstantna da bi se mogla vrednovati za određenu reakciju pri tim uvjetima. S druge pak strane, konstanta brzine je vrijednost koja ovisi o prirodi reaktanata, prisutnosti katalizatora i temperaturi. Različite reakcije, s reaktantima različite prirode, posjeduju i različite konstante reakcija. Ako se u sustav uvede katalizator, brzina kemijske reakcije se povećava, ovisno o katalizatoru. Konačno, primijećen je značajan utjecaj temperature na brzinu kemijske reakcije.

Primjerice, magnezij u sustavu s hladnom vodom reagira iznimno sporo (Atkins i sur., 2006). Ako se magnezij uroni u vruću vodu, reakcija stvaranja magnezij-hidroksida i hidrogena je zamjetno brža. Stoga primjećujemo da se povećanjem temperature povećava i brzina reakcije. Unatoč tomu, bilo je potrebno odrediti na koji se način brzina reakcije povećava s s povećanjem temperature. Uporabom matematičkog modela predstavljenog funkcijom moguće je opisati odnos između brzine reakcije i temperature.

Iako nisu sve reakcije u skladu s tim zakonom, Svante August Arrhenius krajem 19. stoljeća predlaže da se konstanta brzine u odnosu na temperaturu mijenja na sljedeći način: (House, 2007).

$$k = Ae \frac{-Ea}{RT} \qquad (7)$$

Navedena jednadžba je još poznata i kao Arrheniusova jednadžba.

Konstanta brzine kemijske reakcije je predstavljena slovom k, A je faktor frekvencije (ili pre-eksponencijalni faktor) koji je ovisan o frekvenciji sudara molekula tijekom kemijske reakcije, R je plinska univerzalna konstanta (8.314 J K^{-1} mol^{-1}), T predstavlja temperaturu i Ea energiju aktivacije.

Energija aktivacije predstavlja količinu energije koju je potrebno prenijeti molekuli da bi se potaknula kemijska reakcija i svojstvena je svakoj reakciji ponaosob. Ona mjeri razliku između krajnjih vrijednosti, maksimalnu i minimalnu energiju u sustavu reakcije tijekom vremena.

Fizički smisao Arrheniuseve jednadžbe je shvaćen kad se uzme u obzir da se molekule na višoj temperaturi gibaju brže i stoga se povećava učestalost sudaranja molekula reaktanata.

Energija aktivacije i faktor frekvencije

Spomenuli smo učinak parametara Arrheniusove jednadžbe na ovisnost brzine kemijske reakcije o temperaturi. Kasnije ćemo pokazati način za utvrđivanje tih parametara, energije aktivacije i faktora frekvencije, pomoću eksperimentalnih mjerenja koncentracija na različitim temperaturama.

Ako logaritmiramo obje strane Arrheniusove jednadžbe, dobit ćemo:

$$\ln k = -\frac{E_a}{R}\frac{1}{T} + \ln A \tag{8}$$

vidimo da prikaz grafa linearne zavisnost konstante brzine sa temperaturom ima apscisu $1/T$ i ordinatu lnk, kao i koeficijent pravca *-Ea/R.*

Rad s eksperimentalnom skupinom

Nakon usmenog izlaganja nastavnika (na isti način kao i kod kontrolne skupine), pristupilo se matematičkom modeliranju potpomognutom računalom. Temelj modela bio je problem određivanja energije aktivacije i preeksponencijalnog faktora.

Problem: a) Odrediti brzinu kemijske reakcije ako su pribavljeni eksperimentalni podaci (Tablica 1) (House, 2007):

Tablica 1.

Rješenje: Vrlo često kad se nacrta graf neke od spomenutih funkcija zavisnosti s vremenom, jasno je na prvi pogleda radi li se o linearnoj zavisnosti ili ne. Unatoč tomu, potrebno je napomenuti da podaci dobiveni eksperimentalnom metodom uvijek sadrže i eksperimentalnu grešku. U nekim slučajevima je iznimno teško vizualnom metodom odrediti postojanje linearnosti.

U ovom slučaju je korišten programski paket GeoGebra s mogućnošću određivanja "uspješnosti" pripasivanja unesenih točaka.

U naprednijoj inačici GeoGebre, GeoGebra 4.0 Beta, moguće je koristiti naredbu *Rsquare*. Rsquare je vrsta statističkog testa koji provjerava u kojoj mjeri dana točka odgovara funkciji grafa, računajući koeficijent determinacije (R^2), koji ima raspon od 0 do 1. Što točka više odgovara vrsti zavisnosti, to je vrijednost bliža 1 (House, 2007).

S obzirom da se red reakcije ne mijenja s promjenom temperature, može se utvrditi pri bilo kojoj temperaturi. U testiranju koje slijedi, vrijednosti vremena i koncentracije su uzete za temperaturu T = 25 ˚C.

Test 1.

- koristi se tablični prikaz, u tablicu su unesene vrijednosti vremena i koncentracije [*A*] radi provjere je li reakcija nultog reda.
- Zatim je temeljem tim podataka napravljena lista točaka uporabom naredbe *IzradiListu*.
- Listi točaka je dodan grafički prikaz, vrijednosti vremena su na apscisi, a vrijednosti koncentracije su na ordinati.

- Potom se pristupilo pripasivanju uporabom naredbe *PrilagodbaLinearna*.
- Vizualnom metodom je utvrđeno da točke ne pripadaju grafu linearne funkcije, također je u naprednijoj inačici GeoGebre izračunat koeficijent determinacije $R^2 = 0.962$.

Slika 3.

Test 2.

- Koristi se tablični prikaz, u tablicu su unesene vrijednosti vremena t i vrijednosti prirodnog logaritma koncentracije ln[A], da bismo provjerili je li reakcija prvog reda.
- Zatim je temeljem tih podataka napravljena lista točaka odabirom naredbe *IzradiListu*.
- Listi točaka je dodijeljen grafički prikaz, vrijednosti t su na apscisi, a vrijednosti ln[A] su na ordinati.
- Potom se pristupilo pripasivanju naredbom *PrilagodbaLinearna*.
- Vizualnom metodom je utvrđeno da točke ne pripadaju grafu linearne funkcije, također je u naprednijoj inačici GeoGebre izračunat koeficijent determinacije R2 = 0.990.

Slika 4.

Test 3.

- Koristi se tablični prikaz, u tablicu su upisane vrijednosti vremena t i recipročne vrijednosti koncentracije 1/[A], da bismo provjerili je li reakcija drugog reda.
- Zatim je temeljem tih podataka napravljena lista točaka odabirom naredbe *IzradiListu*.
- Listi točaka je dodan grafički prikaz, vrijednosti t su na apscisi, a vrijednosti 1/[A] su na ordinati.
- Potom se pristupilo pripasivanju naredbom *PrilagodbaLinearna*.
- Očito je da dobivene točke pripadaju grafu linearne funkcije, što je potvrđeno i računanjem koeficijenta determinacije koji ovdje iznosi R2 =0.999 (najbliži 1 u odnosu na sva tri testa).

Slika 5.

- Temeljem rezultata sva tri testa, utvrđeno je da je reakcija čiji su eksperimentalni podaci obrađeni reakcija drugog reda.
- Koeficijentu brzine odgovara koeficijent pravca dobiven u testu 3, pa naredbom *Kut* dobije se vrijednost α=0.809° (kut koji pravac zatvara s pozitivnim dijelom x-osi).
- Naredbom *Tan(α)* izračunata je vrijednost $k_1=tg(α)=0.014$.
- Imajući na umu da je u pitanju reakcija drugog reda, te da je vrijeme mjereno u minutama, konstanta kemijske reakcije je 0.014 *dm³/(mol min)*.

Problem: b) Odrediti energiju aktivacije i faktor frekvencije dane kemijske reakcije, koristeći eksperimentalne podatke iz tablice 1.

Rješenje: Utvrđeno je da je reakcija drugog reda. Test 3 je potrebno ponoviti sa vrijednostima za vrijeme t i koncentraciju 1/[*A*],a na različitim temperaturama. Slijede vrijednosti za k_i za *i*=1, 2, 3, 4, 5. Zbog daljnjih računanja temperature su pretvorene u Kelvine a konstante brzine u dm³/(mol·s). Dobiveni rezultati su predstavljeni u tablici 2.

Tablica 2.

Test 4.

- Koristi se tablični prikaz, u tablicu su upisane recipročne vrijednosti temperature (1/*T*) i vrijednosti prirodnog logaritma koeficijenta brzine (ln(*k*)).
- Zatim je temeljem tih podataka napravljena lista točaka naredbom *IzradiListu.*
- Listi točaka je dodijeljen grafički prikaz, vrijednosti 1/*T* su na apscisi, a ln(*k*) vrijednosti su na ordinati.
- Potom se pristupilo pripasivanju naredbom *PrilagodbaLinearna*.

Slika 6.

Temeljem rezultata u testu 4 možemo zaključiti da odsječak pravca koji predstavlja linearnu zavisnost 1/T i ln(*k*)) na y-osi iznosi 8.142141, koeficijent pravca iznosi -4922.80703, a kako joj odgovara oblik ln*k*=-E_a/(RT)+ln*A*, proizlazi da je ln*A* = 8.142141, -E*a*R = -4922.80703, iz čega proizlaze tražene vrijednosti A=3436.267 dm³/ (mol·s) odnosno E_a=40928.217 J.

Rezultati istraživanja

Nakon što je završen proces modeliranja, testirane su obje skupine studenata. Korišten je didaktički test kombiniranog tipa, s pitanjima za popunjavanje i pitanjima s višestrukim izborom. Provjera je trajala 45 minuta.

Test

1. Napisati izraz koji opisuje trenutnu brzinu kemijske reakcije

_____

2. Brzina kemijske reakcije zavisi od (zaokružiti točan odgovor):
a) koncentracije, prirode reaktanta i temperature
b) koncentracije
c) temperature

3. Što je red kemijske reakcije? _____

4. Koncentracija reaktanta koji se raspada po reakciji nultog reda (zaokružiti točan odgovor):
a) raste linearno s vremenom
b) opada eksponencijalno s vremenom
c) opada linearno s vremenom

5. Napišite jednadžbu koja opisuje promjenu koncentracije reaktanta u vremenu pri reakciji drugog reda. _____

6. Jednadžba $-3196.03x + 13310y = 10728.72$ opisuje zavisnost koncentracije reaktanta sa vremenom. Kolika je konstanta brzine ove kemijske reakcije?

_____

7. Red kemijske reakcije (zaokružiti točan odgovor):

a) ne ovisi o temperaturi

b) ovisi o temperaturi

c) kod nekih ovisi o temperaturi a kod nekih ne

8. Konstanta brzine kemijske reakcije se s povećanjem temperature (zaokružiti točan odgovor):

a) Linearno smanjuje

b) Eksponencijalno smanjuje

c) Eksponencijalno povećava

9. Pri zadanoj temperaturi, s povećanjem preeksponencijalnog faktora, brzina kemijske reakcije se (zaokružiti točan odgovor):

a) povećava

b) smanjuje

c) brzina kemijske reakcije nije ovisna o preeksponencijalnom faktoru

10. Na slici je prikazan graf funkcije koja opisuje promjenu konstante brzine kemijske reakcije na različitim temperaturama.
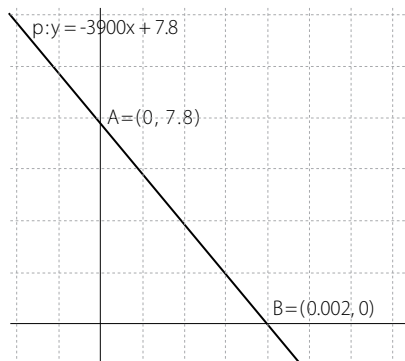
Na temelju dostupnih podataka potrebno je odrediti:

1. Koliko iznosi faktor frekvencije ove reakcije? _____

2. Koliko iznosi energija aktivacije ove reakcije? _____

Rasprava

Analizirajući rezultate testiranja (prikazani u tablici 3 i slici 7) moguće je uočiti da su učenici eksperimentalne skupine postigli znatno bolje rezultate u odnosu na učenike kontrolne skupine. Manja razlika je uočena kod pitanja koja su podrazumijevala

reprodukciju nastavnog sadržaja. Značajna razlika u rezultatima je uočljiva kod pitanja koja su uključivala i određen stupanj logičkog razmišljanja i zaključivanja učenika.

Temeljem toga možemo zaključiti da je postavljena hipoteza istraživanja dokazana. Primjena matematičkog modeliranja uz pomoć računala u nastavi kemije pozitivno utječe na kakvoću nastave i trajnost znanja učenika.

Tablica 3.

Slika 7.

Zaključak

U odnosu na tradicionalnu nastavu matematike i drugih prirodnih znanosti, u radu je prikazan jedan drugačiji pristup. Temelj je u proučavanju teorije i rješavanju problema iz jednog predmeta, kemije, uporabom matematičkog modeliranja. Istodobno se usvajanju znanja iz kemije i utvrđuju i uvježbavaju matematički sadržaji. Stvara se svjesna i očita veza između pojmova iz stvarnog svijeta i matematike te veza između teorije i prakse. Učenička znanja stečena na takav način, postaju trajna, funkcionalna i primjenjiva.