SCHOOL CHEMICAL EXPERIMENT OPTIMIZATION IN WOLFRAM MATHEMATICA ENVIRONMENT

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Abstract

An experiment is an integral part of natural sciences, especially chemistry. Therefore pupils and students should be in contact with it on regular bases during the process of learning chemistry. However, nowadays a major decrease of use of real chemical experiments is apparent in chemistry education. New or modified known experiments can help to reduce this trend. The proposed method of experiment optimization using Wolfram Research software Mathematica is one of the possible ways how to solve it. This method is based on sequential process of optimization and stochastic extreme value finding for functions of several variables. This problem has been solved at the Department of Chemistry and Chemistry Didactics as a part of a research project entitled "Teacher Profession in Changing Requirements on Education", executed by Faculty of Education. During the research a program was made that computes optimal values of experiment parameters from measured values. This was verified during teacher training courses at Charles University in Prague, Faculty of Education. This paper presents an example that shows the optimization procedure of a selected chemical reaction.
Key words: *chemical experiment, school experiment, optimization, chemist's clock, Wolfram Mathematica.*

Introduction

One of the teacher's key tasks by teaching chemistry and sciences in general is to lead the pupils to the interest in exploration of the world around them. (Abramenkova, 2007) In chemistry lessons experiments can be used very well to invoke the interest. It appears that the experiments done by pupils themselves have the best impact. However, nowadays a major decrease of use of real experiments is apparent in school education. Along with the strong development of ICT and their expansion into everyday life (Kubiatko, 2007) and into school practises (Rambousek, Bene , & Adamec, 2007) real experiments are being progressively substituted by reproduced or simulated ones. This trend makes chemistry problematic available to a broader group of interested people, e.g. by distant education. (Bóhmová & Šulcová, 2007) It can, however, lead to a general deflection from cultivation of manual dexterity of pupils and it decreases the motivation value of the exemplary experiment.

The complexity of the preparation is of one of the reasons of a lower portion of experiments in chemistry education. There is a great variety of instructions in literature, but a lot of them just reproduce old instructions, which may not correspond with the contemporary teacher´s intention. For many experiments the adjustment according to teacher´s requirements is very easy. However, for

some of them reaching the demanded changes means long experimentations. Experimental design and optimization also plays an important role in chemical research. Therefore it is good to include it into chemistry education (Bouzidi & Gozzi, 2008). Chemical kinetics is a large area of chemistry where the course of the experiment cannot be forseen, so it is vital to follow the instructions precisely so the results coud be achieved again. That is why this article is aimed at this area.

Model experiment for reaction rate

The teacher has to choose a well known reaction with predictable mechanism to be able to show the chosen principle of chemical kinetics to pupils (e.g. relation of the reaction rate and starting compound concentration, temperature...). Should the experiment be carried out by the pupils alone it is importantant that the it does not take long to complete and the consumption of the starting compound is not too high. There is big diference if the experimet is carried out by 20 students or the teacher alone. As said before common instructions are not very variable.

Therefore a mechanism was proposed which enables to adjust the initial conditions so they meet the chosen criteria (minimal compound consumption, achieving the needed time process of the experiment ....) (Bene , Reálné modelové experimenty ve výuce chemie, 1999).

Finding optimal conditions for an effective school chemical experiment which demonstrates the relation between the reaction rate and reactant concentration can be shown as an example of the proposed optimization. The motivation effect of the experiment is the gradual change of the reaction mixture from achromatic to intensive blue color under controlled temperature. This experiment is often called "the chemist´s clock". This experiment was published in 1973 (Trtílek, Hofmann, & Borovička, 1973) and the later sources reprint it unaltered.

Principle of the chosen chemical experiment:

An excess amount of potassium iodate is mixed with acidified water solution of sodium hydrogen sulfite and with amyl solution (iodine indicator). Three chemical reactions take place sequentially at different rates:

1. iodate ions react with hydrogen sulfite ions forming iodide ions (fast reaction) $IO_3^- + 3\ HSO_3^- \rightarrow I^- + 3\ HSO_3^-$
2. iodide ions react with iodate ions in presence of an acid forming iodine (slower reaction) $5\ I^- + IO_3^- + 6\ H^+ \rightarrow 3\ I_2 + 3\ H_2O$
3. excess of hydrogen sulfite ions reacts with already formed iodine (fast reaction) $5\ I^- + IO_3^- + 6\ H^+ \rightarrow 3\ I_2 + 3\ H_2O$

Had all the hydrogen sulfite contained in the solution reacted, the iodine formed in the reaction no. 2 is not consumed any more and its presence in the mixture is indicated by blue color of amyl.

Optimization algorithm

The optimization method is derived from the algorithm of sequential process of optimization and extreme value finding for functions of several variables. By this method an experiment is planned on the basis of former results. This is repeated until the optimization criterion adequately approaches the optimal value. The algorithm step can be described by following equation (Bene , Reálné modelové experimenty ve výuce chemie, 1999, p 88):

$$\vec{x}^{k+1} = \vec{x}^{k} + \rho^{k} \frac{\sum_{i=1}^{n} \left[f\left(x_1^k, \ldots, x_i^k + \alpha^k, \ldots, x_n^k\right) - f(\vec{x}^k) \right] \vec{e}_i}{\max_{i=1\ldots n} \left| f\left(x_1^k, \ldots, x_i^k + \alpha^k, \ldots, x_n^k\right) - f(\vec{x}^k) \right|}$$

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where: $\vec{x}^k \vec{x}^k$ estimation of the function maximum location in step *k*
ρ^k size of *k*-th step $\rho^k = 0{,}2(k+1)^{-1} \rho^k = 0{,}2(k+1)^{-1}$,
a^k size of *k*-th difference $a^k = 0{,}2(k+1)^{-0{,}4}\ a^k = 0{,}2(k+1)^{-0{,}4}$,
f chosen function which maximum is to be found,
$\vec{e}_i$ *i*-th unit vector,
n number of optimized variables.

Initial values of the optimized variables should be chosen near the center of the examined area $\vec{x}^0 = \left(\frac{1}{2}, \ldots, \frac{1}{2}\right)$. This method setup assumes the variable values x_i to be in range from 0 to 1. As shown later, these values have yet to be transformed should they be used with real physical quantities.

Optimization example on chosen reaction

By this reaction the optimization aim was to achieve the reaction duration of 30 s (from solutions mixing to the first major color change) and to minimize the consumption of reactants (compound concentration in mixed solutions). The algorithm is created to extreme value finding. The function value is given by the equations:

$$f(x_1, x_2) = x_1 + x_2 - (t - 30)^2$$

$$x_i = \frac{\log c_{max} - \log c_i}{\log c_{max} - \log c_{min}}$$

where: c_1 iodate concentration in solution A in mol dm^{-3},
c_2 hydrogen sulfite concentrations in solution B in mol dm^{-3},
c_{min} minimum considered concentration $10^{-2{,}4}$ mol dm^{-3},
c_{max} maximum considered concentration $10^{-1{,}6}$ mol dm^{-3},
t time to the first major color change of the solution in s.

In this experiment the iodate solution (A) and the acidified solution of hydrogen sulfite with amyl (10 mL H_2SO_4 and 4 g per 1L solution) (B) were at first diluted to needed concentrations and then mixed. By every couple of concentrations the time was measured three times from the moment they were mixed to the first major color change. Time was measured accurately in seconds. Each step has three phases (for two variables): three values are taken – value $f(x^k)$ at first then value $f(x_1+\alpha^k, x_2)$ and finally $f(x_1, x_2+\alpha^k)$. Value x^{k+1} is calculated from these values. The measured values are in Table 1.

Table 1. Optimization progress of the chosen reaction.

k	c_1 (mol dm^{-3})	c_2 (mol dm^{-3})	t (s)	$f(x^k)$
0	0,0093	0,0066	18	−142,74
	0,0064	0,0066	19	−119,54
	0,0093	0,0046	29	0,46
1	0,0064	0,0062	25	−23,50
	0,0049	0,0062	28	−2,35
	0,0064	0,0047	36	−34,35
2	0,0071	0,0052	31	0,55

The measured values show that the algorithm can be stopped after the second step, because we have reached the target time with 1s deviation. This can be considered sufficient. In this example it was necessary to calculate the optimization function value three times and use the conversion relation fourteen times to convert the concentrations. Repetitious calculations are used in this method so a computer program was created in the past (Beneš & Kukal, Optimalizace experimentu školním mikropočítačem, 1990).

Use of Wolfram Mathematica

This time existing computational software was used. Wolfram Mathematica was chosen because a multilicense of the software is available to students thanks to project "ICT support of science teacher training" supported by the Ministry of Education, Health and Sports. The advantage of work with Mathematica is the possibility to enter formulae in the way the mathematicians are used to. It is only necessary to enter the variables values and Mathematica calculates the results. The software also offers a possibility to create interactive calculations. The values are not entered directly as expressions but can be instead changed by moving slide-bars. This enables quick assessment of the influence the changes of values have on the results. These interactive calculations can be published in a format viewable by a freeware player.

Conclusion

The empirical cognitive processes, especially experiments, are essential part of chemistry education in every school. Until now school experiment were mostly realized on the basis of traditional approaches. Nowadays the requirements are changing. Apart of clearness, availability and safety new possibilities for time and chemicals savings are looked for. The goal is to find and recommend the best experiment variant using a suitable optimization criterion. An optimization method based on sequential process of extreme value finding for functions of several variables was chosen. Software Mathematica from Wolfram Research company was used for calculations. This procedure was verified by optimization of the experiment "the chemist's clock". This method was included in chemistry teacher training courses at Charles University in Prague, Faculty of Education, as a part of improving specific profession abilities of chemistry teachers.

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