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PROGRAMS FOR TEACHING OF OPTIMIZATION METHODS

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The paper presents two programs for teaching methods of non-linear programming. The model example is a chemical reactor in which a consecutive or reversible reaction takes place. The student's task consists in finding the optimum regime for the reactor, where according to the algorithm of search of the chosen method the independent variable is introduced and the program computes the gradually stabilizing regulated quantity, i.e. the dependent variable. The individual variables are loaded with generated random error, which brings the model closer to real situations.

Introduction

The methods of non-linear programming used for finding the optimum of functions are quite common at present [1,2], thanks especially to wide application

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of computer technology. That is why they are also included into various teaching programs. The principles of these methods, as usually described both in teaching and in available literature [3], are characterised by complicated mathematical relationships inclusive of a scheme of calculation procedure. Although these mathematical formulations are exact, their information ability is relatively small from the standpoint of elucidation of functional principle of the given optimization method. Therefore, programs OPTIM1 and OPTIM2 have been created for mono- and bi-dimensional optimization, respectively: the student introduces into these programs the manually calculated values of independent variable, and the programs calculate the corresponding value of dependent variable. The values of independent variable are calculated according to the principle of the chosen optimization method, and they are gradually refined until the minimum of purpose function is found with prescribed accuracy.

Principles of Programs

Two program systems – OPTIM1 and OPTIM2 – have been devised for modelling manufacturing processes; they enable a computer simulation of operation regime in a chemical flow reactor.

Program OPTIM1

The model used here is a consecutive chemical reaction A → B → C. This reaction can be described by the following mathematical relationship

$$x_B = \frac{\tau k_1}{(1 + \tau k_1)(1 + \tau k_2)} x_{A0} \tag{1}$$

where k_1, k_2 are the reaction rates according to the Arrhenius relatioship

$$k = A \exp\left(-\frac{E}{RT}\right) \tag{2}$$

τ is retention time of reaction mixture in reactor $\tau = V/Q$; x_{A0} – input concentration of substance A; A – frequency factor; E – activation energy; R – gas constant; T – reaction temperature; V – volume of reactor; Q – flow rate of mixture through the reactor.

Equation (1) expresses a one-parameter non-linear dependence of concentration of component B upon the temperature of reaction mixture in the reactor. In order to bring it closer to reality, equation (1) is loaded with a random error with

normal distribution. This program treatment simultaneously ensures differentiation of results and prevents the possibility of mutual sharing of experimental results among the students.

The given procedure then serves for simulation of obtaining the maximum concentration of substance B at the reactor outlet by means of temperature changes of reaction mixture, i.e. the optimum temperature of reaction mixture giving the maximum concentration of product is looked for.

The basic technological scheme is presented in Fig. 1.

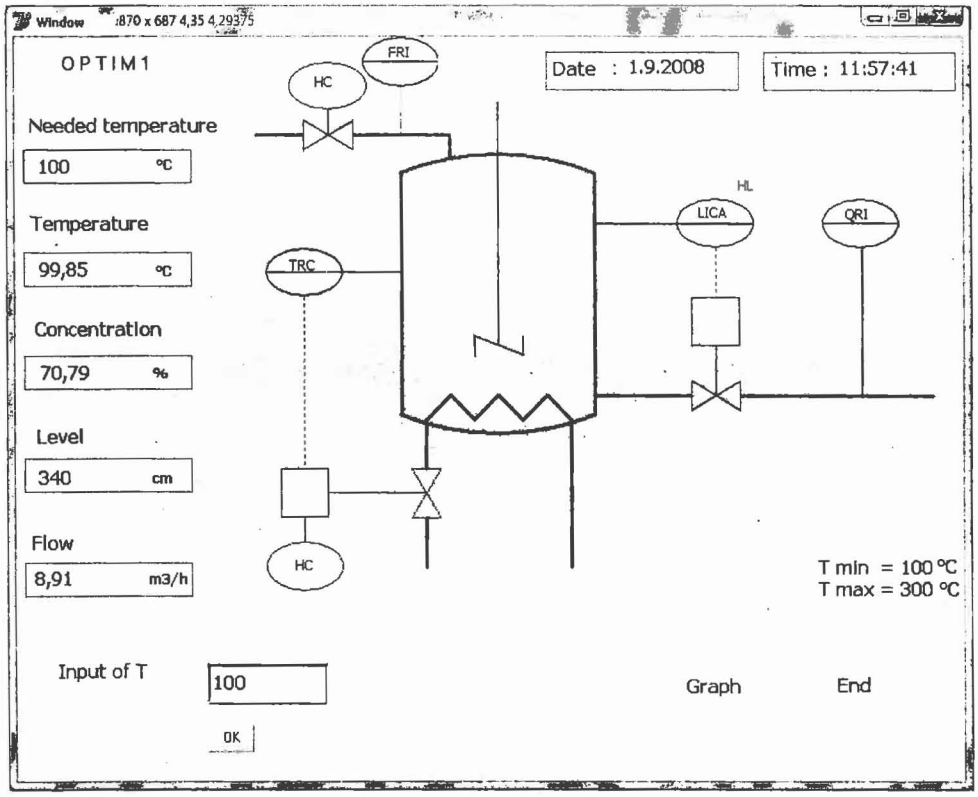

Fig. 1 Technological scheme used in program OPTIM1

The students' task is to verify – within an interactive regime – the properties and search procedure for the extreme value using the following methods of one-parameter optimization:

- reverse step
- bisection
- golden section
- Fibonacci's

Program OPTIM2

The model adopted here is a reversible chemical reaction A ⇄ B. The reaction course is described by an economic indicator in the following form

$$F = Q\left(x_A S_A + \tau S_R\right) \tag{3}$$

where $x_A = \dfrac{1 + \tau k_2}{1 + \tau k_1 + \tau k_2} x_{A0}$ (4)

S_A and S_R are the unit price of starting substance A and costs of the reactor volume unit, respectively.

Equation (3) represents a non-linear two-parameter dependence of production costs for manufacturing substance B upon the temperature and the retention time of reaction mixture in the reactor, when the production cost is the minimum one. Again, like in the case of Eq. (1), Eq. (3) is loaded with random error with normal distribution.

The basic technological scheme is presented in Fig. 2.

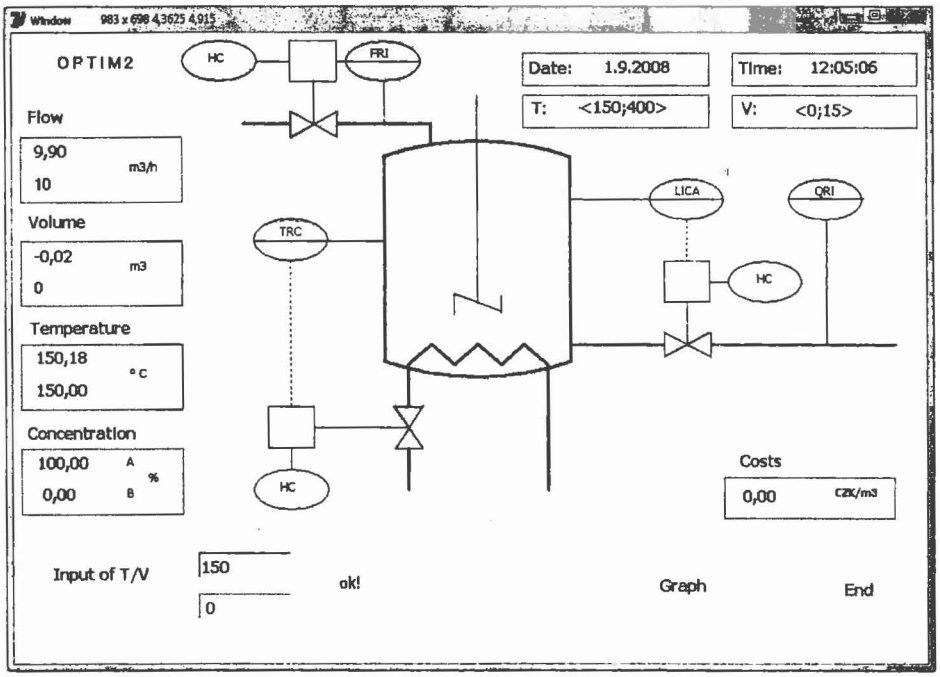

Fig. 2 Technological scheme used in program OPTIM2

In this program, the students' task is to find the optimum values of "operational" parameters in the chemical reactor making use of the following methods of multi-parameter optimisation:

- complete search (method of networks)
- Gauss–Seidel's method
- simplexes

The programs simulate the technological process regulated by an operator toward the optimum regime according to prescribed algorithm. The PC display unit shows a control panel with a scheme of the equipment and all the measured and controlled quantities. For the input starting conditions (temperature, flow rate) then the optimum values of remaining parameters are looked for. After completed optimization, it is possible to introduce new starting parameters and repeat the process.

An example of output from program OPTIM1 is presented in Fig. 3.

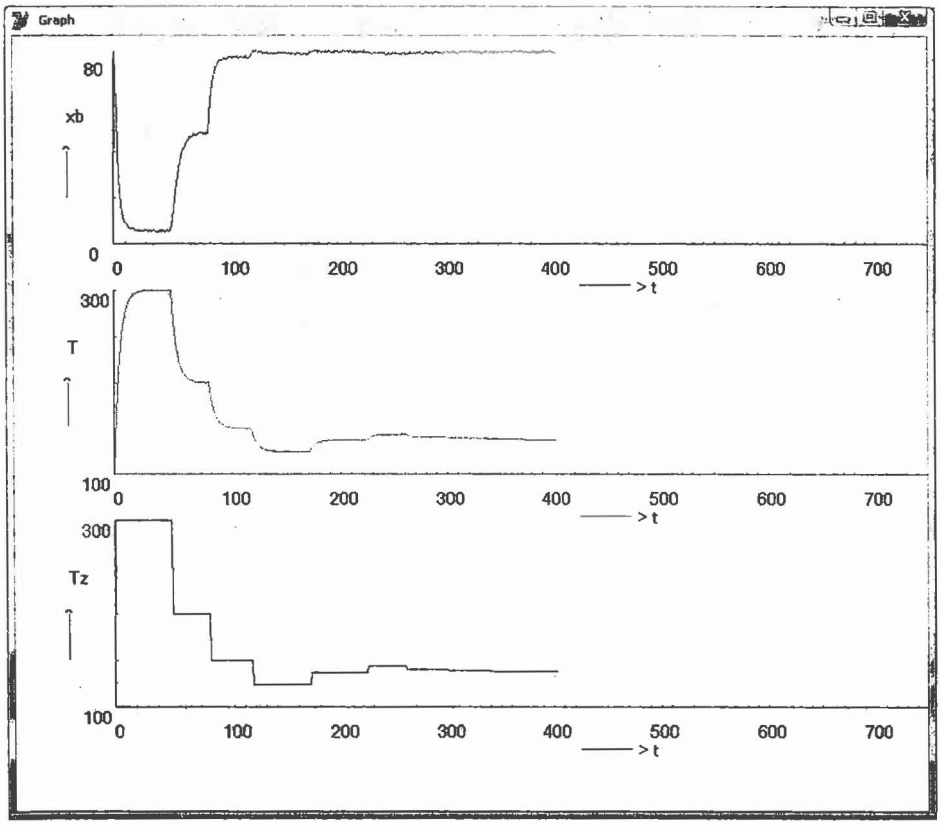

Fig. 3 Example of graphical output from program OPTIM1 (Method of halving of interval)

Description of Programs

The programs represent an innovation of earlier-used programs OPTIM1,2 [3], which were assembled in the program language Pascal 7.0 for the operation system MS DOS. Since the present versions of the Windows operation system commonly used do not support these programs, it was necessary to innovate them, i.e. transfer them into a more modern programming language — we chose the Delphi language — where, first of all, the display problems have been eliminated and, furthermore, also the operation of programs has been innovated, the input of data and program control being fully possible in display regime.

The students' task is to look for the optimum of the corresponding function, i.e. in the case of program OPTIM1 the concentration-temperature dependence, and in the case of program OPTIM2 the dependence of product cost upon the conditions in reactor (volume of reaction mixture and temperature). The user introduces the chosen values of independent variable, which he has calculated manually according to the algorithm of the respective optimization method. The program simulates a real manufacturing process by gradually approaching the changing variable to the prescribed value, i.e. it is gradually stabilized and then oscillates about the prescribed value within the framework of generated errors with normal distribution. The gradual stabilization of, e.g., the temperature is expressed in Eqs (5)-(7)

$$\mathrm{d}T_i = T_{inp} - T_0 \tag{5}$$

$$\mathrm{d}T = 0.819\,\mathrm{d}T + 0.181\,\mathrm{d}T_i \tag{6}$$

$$T = T_0 + \mathrm{d}T + (-0.5 + random)/2 \tag{7}$$

where T_0 is the original temperature value; T_{inp} – newly introduced temperature value; *random* – the function generating random error with normal distribution. Equations (6) and (7) are recursive ones, and the calculation according to them proceeds in a cycle until it is stopped by the user, who introduces a new temperature value.

Similarly in program OPTIM2, the gradually stabilising value of reaction mixture volume is calculated analogously; the only difference is in that Eq. (6) has the following form now

$$\mathrm{d}V = 0.7\,\mathrm{d}V + 0.3\,\mathrm{d}V_i \tag{8}$$

The generator of random numbers is used here in order to make the method as close as possible to real situation, and also to prevent sharing of the results among the students. However, due to the randomization of results it is impossible

to reach the precise value of the optimum, which is possible in the analytical approach: the values of resulting function oscillate within the framework of the chosen errors of "measurement" of the individual quantities – see Fig. 3. The optimum of function is then represented by the interval within which the optimized function does not change at the zero order of the value of dependent variable.

The programs provide besides a graphical output (Fig. 3) also two output files. The first one contains the entered data and individual input values of the independent variable with the computed value of the optimized function. The second file contains all the calculated values of both independent variable and dependent variable, i.e. the steps chosen and their gradual stabilization inclusive of the corresponding functional values. These files can further be exported, e.g., to Excel program in order to be additionally numerically processed. Examples of these output files are presented in Tables I and II.

Table I Example of the first output file from program OPTIM1

Method: Bisection		
Date: 18.9.2008		
Laboratory record – O P T I M I S A T I O N		
Students (names):		
1. Student 2. Student 3. Student		
Technological parameters:		
Frequency factor	$A1$	1777.8 s^{-1}
	$A2$	2222.2 s^{-1}
Activation energy	$E1$	46024.0 J mol^{-1}
	$E2$	62760.0 J mol^{-1}
Reactor volume	V	10.0 m^3
Reagent flow rate	Q	9.0 m^3 h^{-1}
Upper limit T_{max}		300.0 °C
Lower limit T_{min}		100.0 °C
Error of solution	*eps*	0.1 °C

Table I – continued

k	T_z, °C	T, °C	c, %	
1	300.00	300.01	5.40	
2	200.00	200.04	48.38	
3	150.00	150.26	80.62	Temperature is not stabilized
4	150.00	150.01	80.89	
5	125.00	125.10	82.33	
6	125.00	125.01	82.95	
7	137.50	137.51	83.66	
8	132.00	132.06	83.26	
9	143.00	142.99	82.61	

Table II Example of the second output file from program OPTIM1 (a part)

k	T_z, °C	T, °C	c, %
1	300.00	136.03	83.12
2	300.00	165.84	73.21
3	300.00	190.03	56.74
4	300.00	209.93	40.34
5	300.00	226.21	28.79
6	300.00	239.52	21.93
7	300.00	250.39	17.26
8	300.00	259.75	13.64
9	300.00	266.60	11.45
10	300.00	272.60	10.24
11	300.00	277.83	9.26
12	300.00	281.64	8.55
13	300.00	285.15	8.22
14	300.00	287.68	6.83
15	300.00	290.18	6.94

Table II — continued

k	T_z, °C	T, °C	c, %
16	300.00	291.90	6.49
17	300.00	293.53	6.61
18	300.00	294.32	6.74
19	300.00	295.68	6.33
20	300.00	296.38	5.77
21	300.00	296.87	6.04
22	300.00	297.36	5.71
23	300.00	297.97	5.56
24	300.00	298.46	5.95
25	300.00	298.42	5.31
26	300.00	298.83	5.85
27	300.00	299.09	5.51
28	300.00	299.07	5.30
29	300.00	299.24	5.78
30	300.00	299.38	5.47

Conclusion

The programs OPTIM1,2 have been designed for teaching purposes of optimization methods in various courses of MSc studies. They were successfully tested in the course "Optimization" at the Department of Process Control and are available for further use inclusive of the program manual.

Acknowledgements

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References

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