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Dias Nurmagambetov
Prairie View A&M University

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Dias Nurmagambetov

Department of Mathematics
Prairie View A&M University
Prairie View, TX 77446-0519
drdiaz@pvamu.edu

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Abstract

In this paper, we describe one of the solutions of a nonlinear optimal control problem for a chemical reactor. A solution on finding a chemical reactor's optimal temperature regime for having a maximum concentration of final product is presented. The optimal control has been found by immersion method for boundary value problem with a phase and control restrictions. This method is reducing the original boundary value problem to a special optimal control problem, using the general solution of the Fredholm integral equation of the first kind. With this method's solution had been created a software for the problem calculations. Analysis of the method is presented.

Keywords: Optimal control problem; Chemical reactor; Software; Boundary-value problem; Fredholm integral equation

AMS-MSC 2010 No.: 46N10, 90C99, 97A01

1. Introduction

The framework of ways to find a solution nonlinear problem of optimal control has been investigated by Andersson et al. (2019). As a result of his work, nowadays there is a software that is using block structure or general sparsity exploiting sequential quadratic programming (SQP) or interfaces to IPOPT/BONMIN, Block SQP, WORHP, KNITRO, and SNOPT successfully, but the main problem with the software is that there are too many machine resources needed to find a solution for real practical problem. The reason for it is that building a good programming became a priority, instead of providing a good theoretical optimal control research. For instance, Jafari et al. (2016) presented a comparison between iterative methods for solving nonlinear optimal control problems, and proved that modern methods are pretty much equivalent, which means that they use similar iterative formula to obtain the approximate/analytical solution. So, our research has gotten stuck somewhere. There is an objective need of a research with the principally new numerical method of solving a nonlinear

optimization problem. Observation of numerical methods of optimal control was presented by Körkel (2004).

A way of the problem' solution in this paper is based on the immersion method by Aisagaliev and Nurmagambetov (2001), where main idea is to reduce the original boundary value problem to a special optimal control problem by the general solutions of a Fredholm integral equation of the first kind. As we can see here this way provides a better accuracy and convergence rate, relative to previously used methods of finding the optimal regime of a chemical reactor. As an example, we were using task for chemical reactor by Staib (1965), which was formalized as a general optimal control problem. Fedorenko (1978) had presented different approaches to solve the problem.

Most interesting result is found in the work "Optimal control of a chemical reactor", where the original problem was converted into a sequence of linearly constrained quadratic programming problems, which we can find in the Cambridge University Press by Wong and Lock (2009).

2. Problem Statement

The following notations are used throughout the manuscript:

$t_0 = 0$ - time corresponding to the start of a chemical reaction;
T - contact reaction time (or the moment of completion of the reaction);
t - time elapsed since the start of the reaction;
$u(t)$ - value of the absolute temperature in the working area at a time;
$x_1(t)$ - concentration of the starting substance (raw material) at a time;
$x_2(t)$ - concentration of the intermediate product at a time;
$x_3(t)$ - concentration of the final product at a time; and
$K_i(u)$ $i = \overline{1,5}$, - intensities of the reactions, depending on the temperature (on the reaction scheme are indicated, K_1, K_2, K_3, K_4, K_5 respectively).

The kinetic constant reaction rates K_i, $i = \overline{1,5}$ is obeyed the law:

$$K_i = C_i e^{-\frac{E_i}{RT}},$$

where C_i, $i = \overline{1,5}$ are the frequency coefficients, E_i, $i = \overline{1,5}$ - activation energies, R - gas constant, and T - temperature. The $u_{\max}$ is a maximum possible temperature in the reactor, determined by the technological characteristics of the reactor, or the condition for the catalytic stability of the reaction.

Following system of differential equations describes the mathematical model of reactor:

$$\frac{dx_1}{dt} = -\left[K_1(u) + K_2(u) + K_3(u)\right] x_1,$$

$$\begin{aligned} \frac{dx_2}{dt} &= K_1(u)x_1 - K_4(u)x_2, \\ \frac{dx_3}{dt} &= K_4(u)x_2 - K_5(u)x_3, \quad 0 \le t \le T. \end{aligned} \tag{1}$$

The objective of controlling a chemical reactor is to find the optimum reaction's temperature and optimal contact time to give the greatest productivity of the chemical reactor. Therefore, we aim to find a maximum concentration of the final product. The cost function per unit time can be obtained by the expression:

$$-x_3(T) = \int_0^T \left[K_5\big(u(t)\big)x_3(t) - K_4\big(u(t)\big)x_2(t)\right]dt \to \inf . \tag{2}$$

3. The immersion method

By the immersion principle, the differential equations governing the system for (1) during the period $0 \le t \le T$ are described as follows:

$$\dot{y}_1 = \upsilon_1(t), \quad \dot{y}_2 = \upsilon_2(t), \quad \dot{y}_3 = \upsilon_3(t), \quad t \in I = [0,1], \tag{3}$$

$$y(0) = \begin{pmatrix} x_1(0) \\ x_2(0) \\ x_3(0) \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \qquad y(T) = \begin{pmatrix} x_1(T) \\ x_2(T) \\ x_3(T) \end{pmatrix} = \begin{pmatrix} x_{11} \\ x_{21} = \overline{X} \\ x_{31} \end{pmatrix}, \tag{4}$$

$$\upsilon_1(\cdot) \in L_2(I, R^1), \qquad \upsilon_2(\cdot) \in L_2(I, R^1), \qquad \upsilon_3(\cdot) \in L_2(I, R^1). \tag{5}$$

A solution we may represent as following expressions:

$$W(0,T) = \int_0^T \Phi(t_0, t)B(t)B^*(t)\Phi^*(t_0, t)dt = \int_0^T BB^* dt = \int_0^T I_3 dt = I_3 T = \begin{pmatrix} T & 0 & 0 \\ 0 & T & 0 \\ 0 & 0 & T \end{pmatrix},$$

$$\begin{aligned} \lambda_1(t, x_0, x_1) = C(t)a = B^*\Phi^*(t_0, t)W^{-1}(0,T)a = I_3 W^{-1}(0,T)a = \frac{1}{T} I_3 a \\ = \frac{1}{T}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} x_{11} - 1 \\ \overline{X}_2 \\ x_{31} \end{pmatrix} = \frac{1}{T}\begin{pmatrix} x_{11} - 1 \\ \overline{X}_2 \\ x_{31} \end{pmatrix}, \end{aligned}$$

and

$$N_1(t) = -C(t)\Phi(t_0, t_1) = -\frac{1}{T} I_3,$$

where

$$\Phi(t, \tau) = e^{At}e^{-A\tau} = I_3,$$

$$a = \Phi(t_0, t_1)\left[y_1 - \Phi(t_1, t_0)y_0\right] = y_1 - y_0 = \begin{pmatrix} -1 + x_{11} \\ \overline{X}_2 \\ x_{31} \end{pmatrix}, \qquad a = \begin{pmatrix} x_{11} - 1 \\ \overline{X}_2 \\ x_{31} \end{pmatrix}.$$

As we can see it above, the system (3) goes from the given initial condition into the final state. By implementing our immersion method, we modify the objective, so it becomes a task with the initial condition in a free ending state.

It is necessary and sufficient to be represented in the following form:

$$\upsilon(t) = v(t) + \lambda_1(t, x_0, x_1) + N_1(t)z(T)$$

$$= \begin{pmatrix} v_1(t) \\ v_2(t) \\ v_3(t) \end{pmatrix} + \frac{1}{T}\begin{pmatrix} x_{11} - 1 \\ \overline{X}_2 \\ x_{31} \end{pmatrix} - \frac{1}{T}\begin{pmatrix} z_1(T) \\ z_2(T) \\ z_3(T) \end{pmatrix} = \begin{pmatrix} v_1(t) + \frac{1}{T}(x_{11} - 1) - \frac{1}{T}z_1(T) \\ v_2(t) + \frac{1}{T}\overline{X}_2 - \frac{1}{T}z_2(T) \\ v_3(t) + \frac{1}{T}x_{31} - \frac{1}{T}z_3(T) \end{pmatrix},$$

or

$$\left.\begin{aligned} \upsilon_1(t) &= v_1(t) + \frac{1}{T}(x_{11} - 1) - \frac{1}{T}z_1(T), \\ \upsilon_2(t) &= v_2(t) + \frac{1}{T}\overline{X}_2 - \frac{1}{T}z_2(T), \\ \upsilon_3(t) &= v_3(t) + \frac{1}{T}x_{31} - \frac{1}{T}z_3(T). \end{aligned}\right\} \tag{6}$$

The vector v is an arbitrary vector function. The function

$$z(t) = \left(z_1(t), z_2(t), z_3(t)\right),\ t \in [0, T]$$

is a solution of the system of differential equations:

$$\dot{z}_1 = v_1(t),\ \dot{z}_2 = v_2(t),\ \dot{z}_3 = v_3(t),\ t \in [0, T],$$
$$z_1(0) = 0,\ z_2(0) = 0,\ z_3(0) = 0.$$

And if

$$\lambda_2(t, x_0, x_1) = W(t, T)W^{-1}(0, T)x_0 + W(0, t)W^{-1}(0, T)x_1,$$

a solution of the system (3) - (5) with control (6) we can find by the following expression:

$$y(t) = z(t) + \lambda_2(t, x_0, x_1) + N_2(t)z(T)$$
$$= \begin{pmatrix} z_1(t) + \frac{T-t}{T} + \frac{t}{T}x_{11} - \frac{t}{T}z_1(T) \\ z_2(t) + \frac{t}{T}\bar{X}_2 - \frac{t}{T}z_2(T) \\ z_3(t) + \frac{t}{T}x_{31} - \frac{t}{T}z_3(T) \end{pmatrix} = \begin{pmatrix} y_1(t) \\ y_2(t) \\ y_3(t) \end{pmatrix}.$$

4. An algorithm of the numerical solution

The optimization problem (2) - (5) can be written as

$$J = \int_0^T \left\{ \left[\nu_1(t) + \frac{1}{T}(x_{11}(t) - 1) - \frac{1}{T}z_1(T) + \left(K_1(u) + K_2(u) + K_3(u)\right) \times \left(z_1(t) + \frac{T-t}{T} + \frac{t}{T}x_{11}(t) - \frac{t}{T}z_1(T) \right) \right]^2 \right.$$
$$+ \left[\nu_2(t) + \frac{\overline{X_2}}{T} - \frac{1}{T}z_2(T) - K_1(u)\left(z_1(t) + \frac{T-t}{T} + \frac{t}{T}x_{11}(t) - \frac{t}{T}z_1(T) \right) \right.$$
$$\left. + K_4(u)\left(z_2(t) + 0.0437\frac{t}{T} - \frac{t}{T}z_1(T) \right) \right]^2 \quad (7)$$
$$+ \left[\nu_3(t) + \frac{1}{T}x_{31} - \frac{1}{T}z_3(T) - K_4(u)\left(z_2(t) + \overline{X_2}\frac{t}{T} - \frac{t}{T}z_2(T) \right) \right.$$
$$\left. + K_5(u)\left(z_3(t) + \frac{t}{T}x_{31} - \frac{t}{T}z_3(T) \right) \right]^2$$
$$\left. + \left[w - \left(z_3(t) + \tfrac{t}{T}x_{31} - \tfrac{t}{T}z_3(T) \right) \right]^2 \right\} dt \to inf.$$

If

$$\dot{z_1} = \nu_1(t),\ \dot{z}_2 = \nu_2(t),\ \dot{z}_3 = \nu_3(t), \quad (8)$$
$$z_1(0) = 0, z_2(0) = 0, z_3(0) = 0, \quad (9)$$
$$\nu_1(\cdot) \in L_2(I, R^1), \nu_2(\cdot) \in L_2(I, R^1), \nu_3(\cdot) \in L_2(I, R^1), \quad (10)$$
$$x_{11} \in R^1, x_{31} \in R^1, \quad (11)$$
$$w(\cdot) \in W = \{w(\cdot) \in L_2(I, R^1) | 0 \le w(t) \le 1\}, \quad (12)$$
$$u(\cdot) \in U = \{u(\cdot) \in L_2(I, R^1) | 0 \le u(t) \le 823\}, t \in [0, T]. \quad (13)$$

To find infimum of the functional (7) under conditions (8) - (13) we are using the project of gradient method. The Freshet derivative of functional are calculated by the following expressions:

$$J_1'(\xi)=\frac{\partial F_0}{\partial v_1}-\psi_1(t),\quad J_2'(\xi)=\frac{\partial F_0}{\partial v_2}-\psi_2(t),\quad J_3'(\xi)=\frac{\partial F_0}{\partial v_3}-\psi_3(t),$$
$$J_4'(\xi)=\frac{\partial F_0}{\partial w},\quad J_5'(\xi)=\frac{\partial F_0}{\partial u},\quad J_6'(\xi)=\int_0^T\frac{\partial F_0}{\partial x_{11}}dt\cdot$$

There is the solution of the adjoin system:

$$\dot\psi_1=\frac{\partial F_0}{\partial z_1},\quad \dot\psi_2=\frac{\partial F_0}{\partial z_2},\quad \dot\psi_3=\frac{\partial F_0}{\partial z_3},$$
$$\psi_1(T)=-\int_0^T\frac{\partial F_0}{\partial z_1(T)}dt,\quad \psi_2(T)=-\int_0^T\frac{\partial F_0}{\partial z_2(T)}dt,\quad \psi_3(T)=-\int_0^T\frac{\partial F_0}{\partial z_3(T)}dt\cdot$$

Minimizing sequences are constructed by the formulas:

$$v_1^{n+1}=v_1^n-\alpha_n J_1'(\xi_n),\qquad v_2^{n+1}=v_2^n-\alpha_n J_2'(\xi_n),\qquad v_3^{n+1}=v_3^n-\alpha_n J_3'(\xi_n),$$
$$w_{n+1}=P_W\left[w_n-\alpha_n J_4'(\xi_n)\right],\quad u_{n+1}=P_U\left[u_n-\alpha_n J_5'(\xi_n)\right],$$
$$x_{11}^{n+1}=x_{11}^n-\alpha_n J_6'(\xi_n),\qquad n=0,1,2,....$$

5. Numerical results and discussion

The initial conditions of the reaction intensities for model (2) - (5) are

$$K_1(u)=C_i e^{\frac{E_i}{R}\left[\frac{1}{658}-\frac{1}{u}\right]},\ i=\overline{1,5},$$

where the frequency coefficients C_i, $i=\overline{1,5}$. And activation energies $E_i, i=\overline{1,5}$ have following values:

$$C_1=1.02,\quad C_2=0.93,\quad C_3=0.386,\quad C_4=3.28,\quad C_5=0.084,$$
$$E_1=16000,\quad E_2=14000,\quad E_3=15000,\quad E_4=10000,\quad E_5=15000.$$

The universal gas constant is $R=1.9865$. The maximum possible temperature in the working area of the reactor is $u_{\max}=823$. We choose the value of the final moment in time as $T=1$. The initial control is $u_0(t)\equiv 673$, $t\in[0,1]$. There are the same conditions as well, as Fedorenko had made, so we may compare the effectiveness of calculation by the method via existed one.

The results of calculations we see on the Table 1. The concentration of the final product at the time $T=1$ has temperature: $x_3^0(1)=0.356775$. As we can see, the same temperature was chosen. We set the accuracy of calculating the lower value of the functional as $\varepsilon=10^{-5}$. The minimum values Δx_3 (the accuracy of calculating the maximum value of the final concentration of the final concentration $x_3(T)$) was $\Delta x_{3\min}=10^{-5}$. The grid step for the numerical solution of

differential equations was $h = 10^{-4}$. Hence, the numerical solution of the optimal control $u(t)$, $w(t)$, $v_i(t)$, $i = \overline{1,3}$ are calculated as grid functions.

Temperature regime function is showed on the Figure 1. The optimal control function is extremely high in the beginning of the process and goes down slowly by almost a half of the given time. Rest of the time the temperature remains very low. This approach is opposite to the constant temperature regime, which is being used by the industry. On the Figure 2, we may see a change in the concentration of the starting product over time at various temperature conditions. Changes of the concentration's intermediate product over time at various temperature conditions are showed on Figure 3.

To comparing results on Table 1 we can see final product concentration is 0.356775, but on Table 2 the final product concentration is 0.435515. Thus, the optimal temperature regime for the operation of the reactor was found to obtain the maximum yield of the final product, which gives a better productivity to the industry. This software may help to save many resources and give more of final product, using a better solution of optimal control of the temperature regime the chemical reactor.

Conclusion

As long as technical progress is developing, we are getting more complex problems of optimal control every day. In optimal control, the main problem is to find a global minimum for solving nonlinear problems. The existing methods do work, but for a guaranteed solution, many different conditions are imposed on the problem. So, the solution of optimal control is still open. This article is one of the approaches, according to the author, the most promising one. Because the condition of satisfying the Lipschitz inequality and the condition of piecewise continuity for the control function are imposed on the conditions of the problem. The effectiveness of this method has been proven in practice, which we see in this work. The resulting software for searching for the optimal temperature regime of a chemical reactor to obtain the maximum possible final product can be used in the chemical industry. This approach also effectively been applied by the author to solve other nonlinear optimal control problems in space aeronautics area research.

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APPENDICES

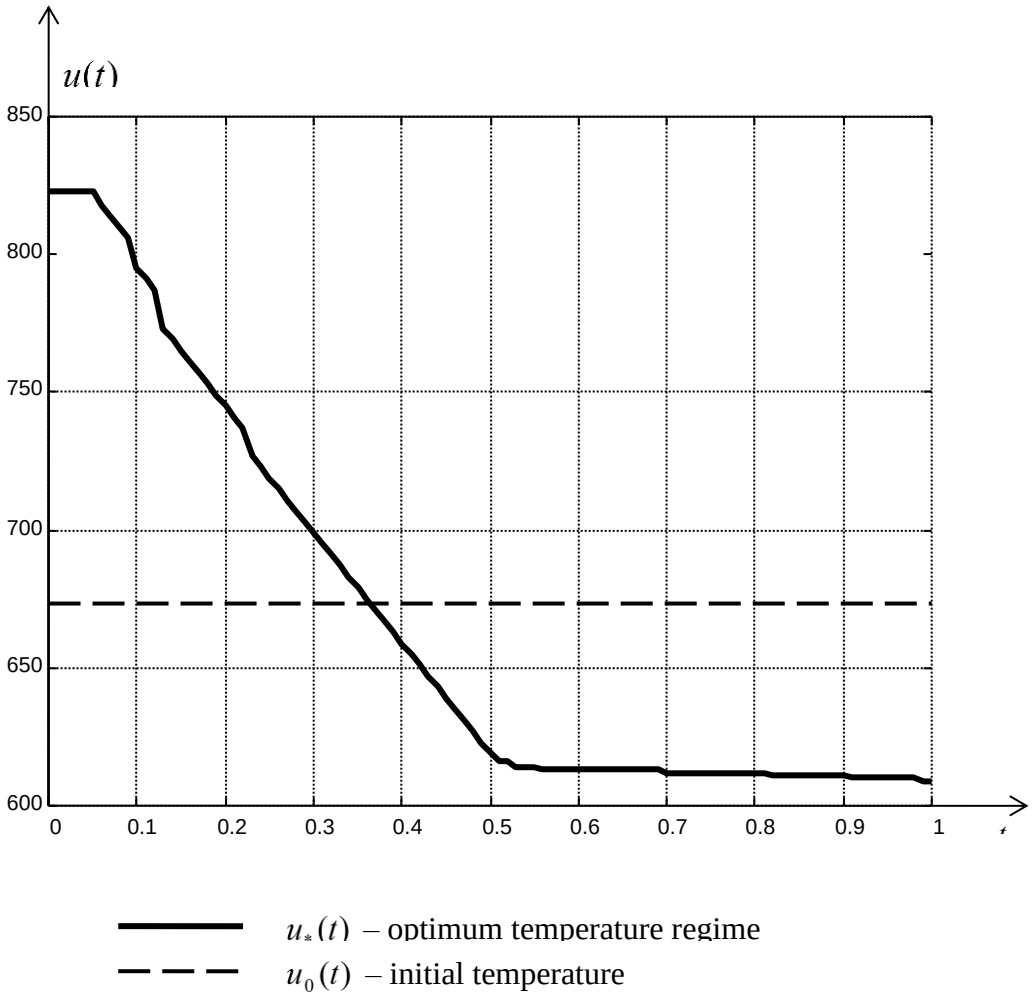

Figure 1. The function of optimal temperature regime

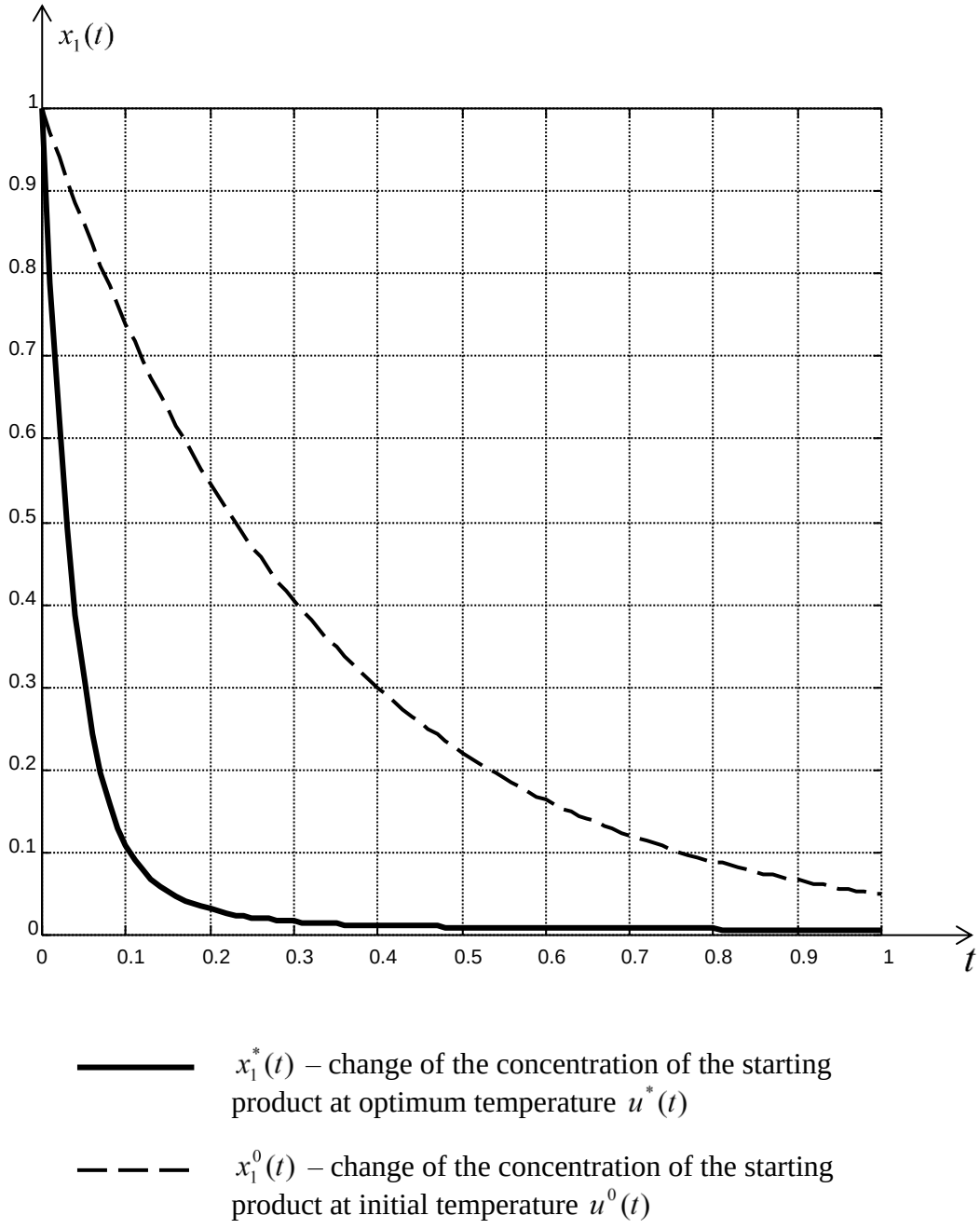

Figure 2. Concentration changes of the starting product over time

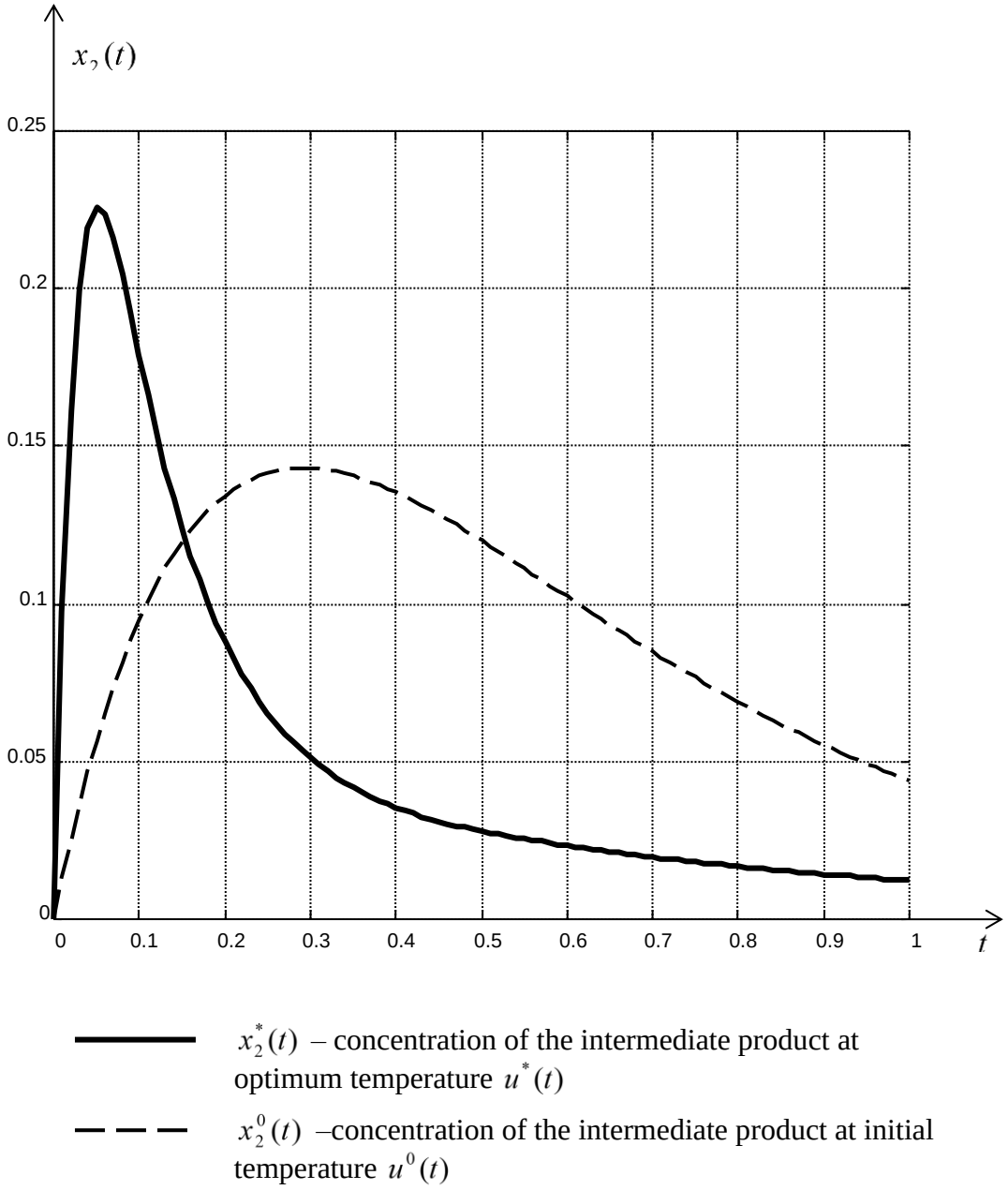

Figure 3. Concentrations changes of the intermediate product over time at various temperature conditions

Table 1. Characteristics of the reaction during time in the example

Time, t	Initial temperature, $u_0(t)$	Source Product Concentration, $x_1^0(t)$	The concentration of the intermediate product, $x_2^0(t)$	Final product concentration, $x_3^0(t)$
0.00	673.0	1.0	0.0	0.0
0.02	673.0	0.941410	0.025006	0.000994
0.04	673.0	0.886253	0.046677	0.003798
0.06	673.0	0.834328	0.065346	0.008161
0.08	673.0	0.785445	0.081319	0.013858
0.10	673.0	0.739425	0.094876	0.020687
0.12	673.0	0.696102	0.106268	0.028469
0.14	673.0	0.655318	0.115721	0.037045
0.16	673.0	0.616924	0.123446	0.046270
0.18	673.0	0.580779	0.129634	0.056012
0.20	673.0	0.546750	0.134458	0.066158
0.22	673.0	0.514716	0.138069	0.076609
0.24	673.0	0.484559	0.140606	0.087278
0.26	673.0	0.456170	0.142198	0.098084
0.28	673.0	0.429443	0.142963	0.108956
0.30	673.0	0.404282	0.143004	0.119834
0.32	673.0	0.380595	0.142412	0.130666
0.34	673.0	0.358296	0.141271	0.141409
0.36	673.0	0.337304	0.139656	0.152021
0.38	673.0	0.317542	0.137639	0.162468
0.40	673.0	0.298937	0.135280	0.172721
0.44	673.0	0.264934	0.129742	0.192556
0.46	673.0	0.249411	0.126656	0.202103
0.48	673.0	0.234799	0.123414	0.211382
0.52	673.0	0.208091	0.116593	0.229100
0.54	673.0	0.195899	0.113070	0.237527
0.56	673.0	0.184421	0.109506	0.245660
0.58	673.0	0.173616	0.105923	0.253498
0.60	673.0	0.163444	0.102337	0.261040
0.62	673.0	0.153868	0.098766	0.268287
0.64	673.0	0.144853	0.095221	0.275243
0.66	673.0	0.136366	0.091717	0.281909
0.68	673.0	0.128376	0.088263	0.288291
0.70	673.0	0.120855	0.084868	0.294392
0.72	673.0	0.113774	0.081538	0.300219
0.74	673.0	0.107108	0.078281	0.305777
0.76	673.0	0.100832	0.075101	0.311073
0.78	673.0	0.094925	0.072001	0.316114
0.80	673.0	0.089363	0.068987	0.320906
0.82	673.0	0.084127	0.066058	0.325457
0.84	673.0	0.079198	0.063218	0.329774
0.86	673.0	0.074558	0.060467	0.333864
0.88	673.0	0.070190	0.057806	0.337735
0.90	673.0	0.066077	0.055235	0.341395
0.92	673.0	0.062206	0.052754	0.344850
0.94	673.0	0.058561	0.050361	0.348109
0.96	673.0	0.055131	0.048056	0.351177
0.98	673.0	0.051901	0.045838	0.354064
1.00	673.0	0.048859	0.043706	0.356775

Table 2. Characteristics of the reaction with the optimal regime of temperature

Time, t	Initial temperature, $u_0(t)$	Source Product Concentration, $x_1^0(t)$	The concentration of the intermediate product, $x_2^0(t)$	Final product concentration, $x_3^0(t)$
0.00	823.0	1.0	0.0	0.0
0.02	823.0	0.623050	0.160951	0.027768
0.04	823.0	0.388187	0.219061	0.086412
0.06	818.8732	0.243568	0.223929	0.151995
0.08	810.7436	0.158743	0.204859	0.210584
0.10	795.6224	0.108733	0.179234	0.257830
0.12	787.8251	0.078504	0.154409	0.294279
0.14	769.3594	0.059592	0.133107	0.321770
0.16	761.9526	0.047192	0.115421	0.342659
0.18	753.0655	0.038211	0.100490	0.359244
0.20	745.3236	0.031602	0.087984	0.372413
0.22	737.9625	0.026635	0.077511	0.382924
0.24	723.3066	0.022971	0.068927	0.391184
0.26	715.4401	0.020275	0.061945	0.397655
0.28	707.2235	0.018168	0.056095	0.402900
0.30	699.8042	0.016476	0.051132	0.407218
0.32	691.3682	0.015116	0.046921	0.410780
0.34	683.9684	0.014011	0.043333	0.413741
0.36	675.2336	0.013106	0.040263	0.416220
0.38	667.0046	0.012361	0.037630	0.418307
0.40	659.1328	0.011747	0.035363	0.420076
0.42	651.2692	0.011237	0.033407	0.421582
0.44	643.9297	0.010814	0.031715	0.422873
0.46	635.3625	0.010460	0.030246	0.423986
0.48	627.4257	0.010167	0.028975	0.424948
0.50	619.9659	0.009925	0.027877	0.425778
0.52	616.2367	0.009711	0.026886	0.426524
0.54	614.2567	0.009510	0.025953	0.427218
0.56	613.9534	0.009314	0.025059	0.427873
0.58	613.5691	0.009127	0.024210	0.428488
0.60	613.5447	0.008946	0.023394	0.429068
0.62	613.3751	0.008768	0.022607	0.429618
0.64	613.3441	0.008593	0.021848	0.430138
0.66	613.3244	0.008422	0.021115	0.430631
0.68	613.0245	0.008254	0.020407	0.431095
0.70	612.9624	0.008092	0.019729	0.431532
0.72	612.5526	0.007935	0.019081	0.431941
0.74	612.2785	0.007785	0.018463	0.432323
0.76	612.2045	0.007639	0.017871	0.432681
0.78	612.1362	0.007496	0.017298	0.433018
0.80	612.0245	0.007355	0.016744	0.433335
0.82	611.6955	0.007217	0.016209	0.433631
0.84	611.5213	0.007084	0.015696	0.433908
0.86	611.4827	0.006954	0.015202	0.434166
0.88	611.3266	0.006826	0.014724	0.434406
0.90	611.2698	0.006700	0.014261	0.434630
0.92	610.6321	0.006578	0.013816	0.434837
0.94	610.5148	0.006458	0.013387	0.435029
0.96	610.3251	0.006342	0.012974	0.435205
0.98	610.0542	0.006228	0.012574	0.435367
1.00	609.7511	0.006117	0.012190	0.435515