Application of a dynamic optimization method to solve optimal control problems

Tomáš Hirmajer, Michal Čižniar, Miroslav Fikar

Abstract
The paper shows one possibility how to solve optimal control problems for nonlinear systems. These problems can be transformed into finite dimensional optimization problems, which can be solved by using a nonlinear programming (NLP). The numerical method with iterative approach is based on sequential quadratic programming (SQP) which needs information about gradients. These gradients are obtained by forward integration of the sensitivity equations, which are integrated simultaneously with the state equations. The detailed procedure of the application of the sensitivity approach is shown with application to batch and CSTR reactors. Results show that the sensitivity approach is an efficient gradient method with good results in comparison with other gradient methods.

Keywords: Dynamic optimization, control vector parameterization, sensitivity equations.

Introduction

There are many numerical methods able to solve nonlinear optimal control problems. Analytical methods represented by Bellman's optimal principle or Pontryagin's maximum principle that solve two-points boundary values problem (TPBP) are inappropriate in the case if a complicated nonlinear system is assumed. The same is true for the iterative methods represented by control vector iteration (CVI) or boundary condition iteration (BCI).

Another approach is to transform the optimal control problems into finite dimensional optimization problems using parametrization schemes.

One approach is a complete discretization of state and control variables – orthogonal collocation (OC). Such formulation can be found in [1, 3, 7, 13]. This approach is currently the most versatile and applicable also to mixed continuous/discrete cases [1]. However, the size of the resulting nonlinear programming problem (NLP) is very large.

Other possibility is to leave the states intact and approximate only the control variables as piecewise constants, or with some higher order approximations. This approach is known as control vector parameterization (CVP). With CVP, different formulations can be found, depending on how gradients of the resulting NLP are calculated [15].

There are three possible ways how the gradients can be solved. One of them is a total difference approach which is the easiest to implement. Main drawback of this method is the lowest accuracy in contrast to other gradient methods. The modified algorithm is possible to find in [18]. Another possibility is to use adjoint equations [9, 16, 17, 11] approach which is preferred for the system with a larger number of optimized parameters and smaller number of constraints. In a reverse case the sensitivity equations [4, 19, 8] are used due to its easy formulation of the problem and forward integration of both states and sensitivity equations. The drawback of this method is a generation of a large system of differential equations as each optimized parameter corresponds to a set of differential equations with the same dimension as the number of states of the optimized process.

The main aim of this paper is to show a derivation of sensitivity equations that are needed for the computation of gradients for CVP. The derivation accuracy is tested on some problems of chemical engineering. Next, the gradient methods are compared and their advantages and disadvantages are discussed.

1. Optimal Control Problem

1.1 System and Cost Description

Consider a dynamical system described by the vector of ordinary differential equations (ODEs) [5]

$$\dot{x} = f(t, x, u, p) \tag{1}$$

with given initial and terminal conditions

$$x(0) = x_0, \quad x(t_F) = x_F \tag{2}$$

where $x \in R^{n_x}$ is the vector of state variables, $u \in R^{n_u}$ is the vector of control variables, $p \in R^{n_p}$ is the vector of parameters and t_F is the final time of the process.

The optimal control problem is to find optimal control policy $u(t)$, vector of the parameters and the final time t_F (when minimum time problem is considered) that minimize the objective function in general Mayer form

$$\min_{t_F, u, p} J_0 = G_0(t_F, x_F, u, p) \tag{3}$$

with constraints defined in Mayer form as well

$$\min_{t_F, u, p} J_l = G_l(t_F, x_F, u, p), \quad l = \overline{1, m} \tag{4}$$

where m is the total number of constraints $m = m_e + m_i$ (m_e – equality constraints, m_i – inequality constraints).

It is assumed that the original continuous control trajectory can be approximated as piecewise constant on N time intervals

$$u(t) = u_i, \quad t_{i-1} \le t \le t_i, \quad i = \overline{1, N} \tag{5}$$

where $\Delta t_i = t_i - t_{i-1}$ is the interval length.

Next assumption is that the state variables are continuous at the boundaries

$$x(t_i^+) = x(t_i^-) \tag{6}$$

where t_i^- denotes the ending time of stage i and t_i^+ the beginning time of stage $i + 1$.

Further constraints are defined as lower and upper boundaries of optimized variables

$$\begin{aligned} &\Delta t_i \in [\Delta t_i^{\min}, \Delta t_i^{\max}] \\ &u_i \in [u_i^{\min}, u_i^{\max}] \\ &p_i \in [p_i^{\min}, p_i^{\max}] \end{aligned} \tag{7-9}$$

1.2 Optimized Parameters

The vector of optimized parameters $y \in R^{n_y}$ contains Δt_i – lengths of the time intervals, u_i – control variables, and p_i – parameters

$$y^T \in (\Delta t_1, ..., \Delta t_N, u_1^T, ..., u_N^T, p_1^T, ..., p_N^T) \tag{10}$$

2. Sensitivities

The sensitivities are defined as partial derivatives of state variables with respect to optimized parameters. Thus, the sensitivity coefficients $s_j(t)$ with initial conditions are defined as follows

$$s_j(t) = \frac{\partial x(t)}{\partial y_j}, \quad s_j(0) = 0, \quad j = \overline{1, n_y} \tag{11}$$

where n_y denotes number of optimized parameters.

Sensitivity coefficients contain information about the sensitivities of the state values to the optimized parameters. The partial differentiation of ODE (1) with respect to optimized parameters (10) gives

$$\frac{\partial \dot{x}}{\partial y_j} = \left(\frac{\partial f^T}{\partial x}\right)^T \frac{\partial x}{\partial y_j} + \left(\frac{\partial f^T}{\partial u}\right)^T \frac{\partial u_{i+1}}{\partial y_j} + \left(\frac{\partial f^T}{\partial p}\right)^T \frac{\partial p}{\partial y_j} \tag{12}$$

where $t_{i-1} \le t \le t_i$ and $i = \overline{0, (N-1)}$. The equation (12) can be rewritten using (11) as

$$\dot{s}_j(t) = \left(\frac{\partial f^T}{\partial x}\right)^T s_j(t) + \left(\frac{\partial f^T}{\partial u}\right)^T \frac{\partial u_{i+1}}{\partial y_j} + \left(\frac{\partial f^T}{\partial p}\right)^T \frac{\partial p}{\partial y_j} \tag{13}$$

The solution of state variable sensitivities with respect to optimized parameters can be obtained by forward integration of sensitivity equations (13).

When the sensitivity is computed with respect to time interval t_i the discontinuity must be taken into account. In our case the situation is considered when the state values are continuous (6) at the time interval boundaries. Thus, the total differential for a state variable gives

$$\begin{aligned} &\mathrm{d}x(t_i) = \delta x(t_i^+) + \dot{x}(t_i^+)\mathrm{d}t_i, \quad i = \overline{1, (N-1)} \\ &\mathrm{d}x(t_i) = \delta x(t_i^-) + \dot{x}(t_i^-)\mathrm{d}t_i \end{aligned} \tag{14}$$

as well as

$$\mathrm{d}x(t_i^+) = \mathrm{d}x(t_i^-) \tag{15}$$

which gives

$$\delta x(t_i^+) + \dot{x}(t_i^+)\mathrm{d}t_i = \delta x(t_i^-) + \dot{x}(t_i^-)\mathrm{d}t_i \tag{16}$$

Differentiating (16) with respect to optimized variables yields

$$\frac{\partial x(t_i^+)}{\partial y_i} + \dot{x}(t_i^+)\frac{\partial t_i}{\partial y_i} = \frac{\partial x(t_i^-)}{\partial y_i} + \dot{x}(t_i^-)\frac{\partial t_i}{\partial y_i} \tag{17}$$

$$\frac{\partial x(t_i^+)}{\partial y_i} = \frac{\partial x(t_i^-)}{\partial y_i} + [\dot{x}(t_i^-) - \dot{x}(t_i^+)]\frac{\partial t_i}{\partial y_i} \tag{18}$$

When the sensitivity coefficients (11) are used, formula (18) is simplified

$$s_j(t_i^+) = s_j(t_i^-) + [f(t, x, u_i, p) - f(t, x, u_{i+1}, p)]_{t_i} \frac{\partial t_i}{\partial y_i} \tag{19}$$

Next, the partial derivative of the cost function (3) or constraint (4) with respect to optimized variables gives the next formula

$$\frac{\partial J_l}{\partial y_i} = \left(\frac{\partial J_l}{\partial t_F}\right)\frac{\partial t_F}{\partial y_i} + \left(\frac{\partial J_l}{\partial x_F}\right)^T \frac{\partial x_F}{\partial y_i} + \left(\frac{\partial J_l}{\partial u}\right)^T \frac{\partial u}{\partial y_i} + \left(\frac{\partial J_l}{\partial p}\right)^T \frac{\partial p}{\partial y_i} \tag{20}$$

where it is considered that the variation of x_F following (14) gives

$$\frac{\partial x_F}{\partial y_i} = \left(\frac{\partial x_F}{\partial t_F}\right)\frac{\partial t_F}{\partial y_i} + \left(\frac{\partial x_F}{\partial x_F}\right)\frac{\partial x_F}{\partial y_i} = f(t_F, x_F, u_F, p)\frac{\partial t_F}{\partial y_i} + \frac{\partial x_F}{\partial y_i} \tag{21}$$

Taking into account the equation (20) and (21) the final equation is given as

$$\begin{aligned} \frac{\partial J_l}{\partial y_i} = &\left(\frac{\partial J_l}{\partial t_F}\right)\frac{\partial t_F}{\partial y_i} + \left(\frac{\partial J_l}{\partial u}\right)^T \frac{\partial u}{\partial y_i} + \left(\frac{\partial J_l}{\partial p}\right)^T \frac{\partial p}{\partial y_i} \\ &+ \left(\frac{\partial J_l}{\partial x_F}\right)^T \left[s_j(t_F) + f(t_F, x_F, u_F, p)\frac{\partial t_F}{\partial y_i} \right] \end{aligned} \tag{22}$$

3. Optimization Method Description

3.1 Static Optimization Problem

As the piecewise constant control trajectory is considered the problem of dynamic optimization is transformed into the problem of static optimization (NLP). Next, a suitable gradient method and algorithm of successive quadratic programming (SQP) type is needed. The solution of the problem with the SQP approach needs information about gradients. This information can be obtained with perturbation (finite difference), adjoint or sensitivity approach. The last one was used to solve the problem in our study.

3.2 Algorithm

(1) Initialization of the optimized variables $y = y_0$.
(2) Forward integration of the system (1) and sensitivity equations (13) ($x(t)$ and $s(t)$ are obtained).

(3) When the free time problem is investigated the sensitivities $s(t_i)$ ($i = \overline{1,(N-1)}$) have discontinuity following the equation (19).
(4) Calculation of the objective function (3), constraints (4), and gradients (22).
(5) Solution of the problem of dynamic optimization (SQP):
   (a) If the optimum is achieved the algorithm will stop $y = y_{optimal}$
   (b) else it is needed to repeat algorithm from 2 with new values of optimized parameters $y = y_{new}$.

3.2.1 Implementation of the Algorithm

The algorithm was developed and implemented into the MATLAB (The MathWorks Inc., Natick, Massachusetts) environment. It uses fmincon from Optimization Toolbox for NLP formulation and solution. Forward integration of the ODE and the sensitivity equations is assured by SUNDIALS Toolbox[1] that is able of simultaneous or staggered integration.

3.2.2 Gradients with Respect to Time

For numerical reasons, time increments Δt_i will be optimized rather than absolute time values t_i. Therefore, the gradients with respect to time have to be modified correspondingly. The relations between times and their increments are given as

$$t_F = \sum_{i=1}^{N} \Delta t_i \tag{23}$$

Therefore, the following holds for the derivatives

$$\frac{\partial J_l}{\partial \Delta t_i} = \sum_{r=1}^{N} \frac{\partial J_l}{\partial t_r} \frac{\partial t_r}{\partial \Delta t_i} \tag{24}$$

4. Examples

4.1 Batch Reactor

The simple batch reactor given in [6] was considered with following parameters: $k_{10} = 0.535\text{x}10^{11}$ min^{-1}, $k_{20} = 0.461\text{x}10^{8}$ min^{-1}, e_1 = 18000 cal mol^{-1}, e_2 = 30000 cal mol^{-1}, r = 2 cal mol^{-1} K^{-1}, β_1 = 0.53 mol l^{-1}, β_2 = 0.43 mol l^{-1}, $\alpha = \frac{e_2}{e_1}$, $c = \frac{k_{20}}{k_{10}^{\alpha}}$ and final time t_F = 8.0 min;

The system with initial conditions is described as follows

$$\dot{x}_1 = -ux_1, \quad x_1(0) = \beta_1 \tag{25}$$

$$\dot{x}_2 = ux_1 - cu^{\alpha}x_2, \quad x_2(0) = \beta_2 \tag{26}$$

with initial trajectory of control variable $u_i(0)$ = 0.5 ($i = \overline{1,N}$) and time intervals $\Delta t_i = \frac{N}{t_F}$.

The control variable u is related to the temperature T via the next formula

$$T = -\frac{e_1}{r \ln \frac{u}{k_{10}}} \tag{27}$$

The goal of the optimization is to maximize an amount of the product B at the final time $x_B(t_F)$

$$\min_{u_i} J_0 = -x_2(t_F) \tag{28}$$

subject to the piecewise constant control as assumed in the original article. The scenarios with fixed and free final time are considered.

4.1.1 Calculation of the Gradients

For simplicity and demonstrative purposes piecewise constant control variables (N = 3) were chosen. The dimension of the final system needed to be integrated is 8 ($n_x(n_y + 1)$). First a scenario with fixed time intervals was considered. The partial derivatives with respect to optimized variables (parametrized control variable) are defined as

$$\frac{\partial J_0}{\partial u_i} = -s_{2i}(t_F), \quad i = \overline{1,3} \tag{29}$$

To obtain necessary gradients (29) it is needed to integrate sensitivity equations over $t \in [t_0; t_F]$. The sensitivity coefficients for considered scenario are defined as

$$s_{1i} = \frac{\partial x_1}{\partial u_i}, \quad s_{2i} = \frac{\partial x_2}{\partial u_i}, \quad i = \overline{1,3} \tag{30}$$

together with sensitivity equations over $t \in [t_0; t_F]$

$$\begin{aligned}
\dot{s}_{11} &= -us_{11} - x_1R_1 \\
\dot{s}_{12} &= -us_{12} - x_1R_2 \\
\dot{s}_{13} &= -us_{13} - x_1R_3 \\
\dot{s}_{21} &= us_{11} - cu^{\alpha}s_{21} + (x_1 - \alpha cu^{\alpha-1}x_2)R_1 \\
\dot{s}_{22} &= us_{12} - cu^{\alpha}s_{22} + (x_1 - \alpha cu^{\alpha-1}x_2)R_2 \\
\dot{s}_{23} &= us_{13} - cu^{\alpha}s_{23} + (x_1 - \alpha cu^{\alpha-1}x_2)R_3
\end{aligned} \tag{31}$$

where R_i is equal to 1 or 0 depending on the time interval t_i and relevant control value. Note that not all equations need to be integrated in each time interval, because the optimized variable in the interval t_{i+1} does not affect on the interval t_i.

Consider now the scenario with free time intervals. In this case new sensitivities of dimension $n_x(N - 1)$ with respect to time are required

$$\begin{aligned}
\dot{s}_{14} &= -us_{14} \\
\dot{s}_{15} &= -us_{15}
\end{aligned} \tag{32}$$

$$\begin{aligned}
\dot{s}_{24} &= us_{14} - cu^{\alpha}s_{24} \\
\dot{s}_{25} &= us_{15} - cu^{\alpha}s_{25}
\end{aligned} \tag{33}$$

At the end of the time interval discontinuity of sensitivity equations (32), (33) is needed to compute from (19)

$$\begin{aligned}
\dot{s}_{14}(t_1^+) &= s_{14}(t_1^-) + [f_1(t,x,u_1,p) - f_1(t,x,u_2,p)]_{t_1} \\
\dot{s}_{15}(t_2^+) &= s_{15}(t_2^-) + [f_1(t,x,u_2,p) - f_1(t,x,u_3,p)]_{t_2} \\
\dot{s}_{24}(t_1^+) &= s_{24}(t_1^-) + [f_2(t,x,u_1,p) - f_2(t,x,u_2,p)]_{t_1} \\
\dot{s}_{25}(t_2^+) &= s_{25}(t_2^-) + [f_2(t,x,u_2,p) - f_2(t,x,u_3,p)]_{t_2}
\end{aligned} \tag{34}$$

Then the resulting gradients are derived from (22)

[1]homepage: http://www.llnl.gov/casc/sundials/

$$\frac{\partial J_0}{\partial t_1} = -s_{24}(t_F), \quad \frac{\partial J_0}{\partial t_2} = -s_{25}(t_F) \qquad (35)$$

The gradients with respect to final time are following (22) in this case equal to $-f_2$. Note that all time gradients were modified as was shown in Section 3.2.2. Detailed derivations of the sensitivity equations can be found in [11].

4.1.2 Results and Discussion

The simulations were performed with various values of tolerances for integration as well as optimization (see Table 1). The simulations with sensitivity approach were obtained with SUNDIALS Toolbox in MATLAB environment and with the adjoint approach were obtained with DYNO[2] package in Fortran environment.

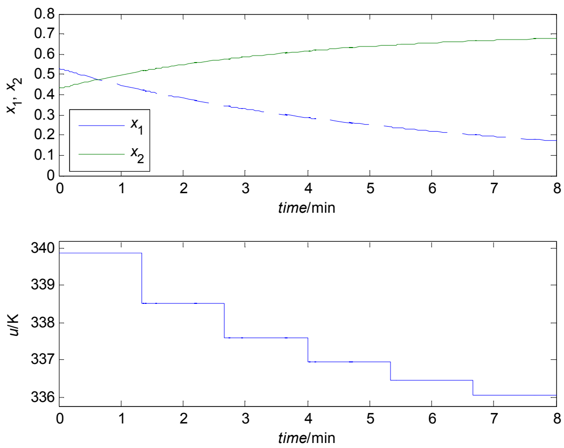

Fig.1 Optimal state trajectories with corresponding control, *N* = 6, T3

Fig. 1 shows optimal concentrations and control value obtained with sensitivity equations approach for 6 piecewise constant controls. The highest value of *N* smoothens the control trajectory considerably, following [6], where optimal continuous control trajectory was shown.

Level	Optimization	Integration
T1	10^{-3}	10^{-5}
T2	10^{-5}	10^{-7}
T3	10^{-7}	10^{-9}

Tab.1 Tolerance levels used in simulations

		T1		
N	***n*ODE**	***n*iter**	***J*0**	**CPU time[3]**
1	4	4	-0.678826	1.6
3	8	4	-0.679309	7.2
6	14	4	-0.679412	33.2
10	22	4	-0.679435	112.8
20	44	4	-0.679440	666.1
		T2		
1	4	5	-0.678825	2.3
3	8	6	-0.679341	15.2
6	14	5	-0.679411	61.9
10	22	5	-0.679428	216.1
20	44	5	-0.679435	1331.4
		T3		
1	4	6	-0.678825	2.9
3	8	6	-0.679341	21.7
6	14	6	-0.679411	109.3
10	22	6	-0.679428	392.9
20	44	6	-0.679435	2541.5

Tab.2 Results for the batch reactor with sensitivity equations approach

[2]homepage: http://www.kirp.chtf.stuba.sk/~fikar/dyno/

[3]Intel P4 2.4 GHz

		T1	
N	***n*ODE**	***n*iter**	***J*0**
1	5	5	-0.678617
3	5	3	-0.679136
6	5	4	-0.679305
10	5	5	-0.678988
20	5	4	-0.678876
		T2	
1	5	6	-0.678822
3	5	5	-0.679336
6	5	5	-0.679408
10	5	6	-0.679424
20	5	8	-0.679431
		T3	
1	5	7	-0.678825
3	5	7	-0.679341
6	5	6	-0.679411
10	5	7	-0.679428
20	5	11	-0.679435

Tab.3 Results for the batch reactor with adjoint equations approach

It can be seen from the results shown in Tables 2 and 3 that the obtained values of the cost functions for tolerance level T1 and T2 are better with sensitivity approach in comparison to adjoint approach with smaller or equal numbers of iterations except for one case. The values of the cost functions for tolerance level T3 are equal for both approaches, but the sensitivity equations need a smaller number of iterations. It shows that the accuracy of the gradients obtained with sensitivity equations is better mainly for the low value of the tolerance level.

The increasing numbers of piecewise constants change the total number of optimized variables too. Therefore, the number of equations needed to integrate changes considerably only for sensitivity approach, because each optimized variable generates a new set of differential equations. This change influences the total CPU time, as shown in the Table 2. Note that the computational effort for sensitivity approach can be considerably simplified using the second order of sensitivities following the article [20] and [2].

Finally, the adjoint equations approach (Table 3) with the low tolerance level has worse results, but when the tolerance level is growing the results are the same as in the sensitivity approach. Note that the increasing number of optimized variables does not affect the number of equations to be integrated.

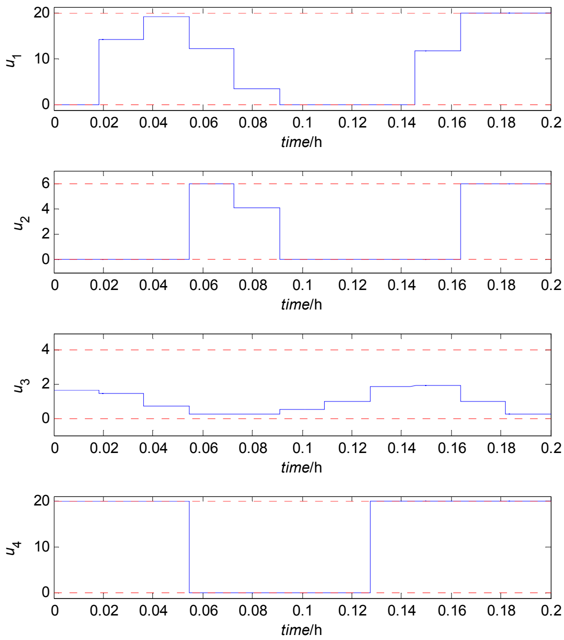

Fig.2 Optimal control profiles for nonlinear reactor (4 control variables) with corresponding upper and lower bounds (dotted red color), *N* = 11, T2

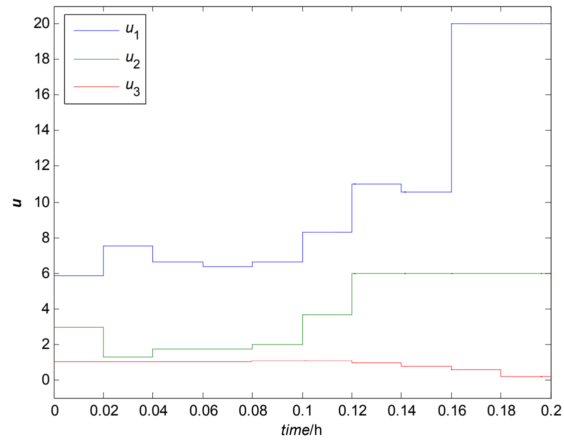

Fig.3 Optimal control profiles for nonlinear reactor (3 control variables), *N* = 10, T2

4.2 Nonlinear CSTR Reactor

Consider a problem given in [12, 14, 2]. In the isothermal continuous stirred tank reactor four simultaneous chemical reactions are taking place. The problem consists of determining four optimal control profiles to obtain a maximum economic benefit. The controls are the flowrates of three feed streams and an electrical energy input used to promote a photochemical reaction.

The system is described by the following set of differential equations

$$\dot{x}_1 = u_4 - qx_1 - 17.6x_1x_2 - 23x_1x_6u_3 \quad (36)$$

$$\dot{x}_2 = u_1 - qx_2 - 17.6x_1x_2 - 146x_2x_3 \quad (37)$$

$$\dot{x}_3 = u_2 - qx_3 - 73x_2x_3 \quad (38)$$

$$\dot{x}_4 = -qx_4 + 35.2x_1x_2 - 51.3x_4x_5 \quad (39)$$

$$\dot{x}_5 = -qx_5 + 219x_2x_3 - 51.3x_4x_5 \quad (40)$$

$$\dot{x}_6 = -qx_6 + 102.6x_4x_5 - 23x_1x_6u_3 \quad (41)$$

$$\dot{x}_7 = -qx_7 + 46x_1x_6u_3 \quad (42)$$

$$\begin{aligned}\dot{x}_8 &= 5.8(qx_1 - u_4) - 3.7u_1 - 4.1u_2 - 0.099 \\ &+ q(23x_4 + 11x_5 + 28x_6 + 35x_7) - 5u_3^2\end{aligned} \quad (43)$$

where $q = (u_1 + u_2 + u_4)$. The vector of process initial conditions is following

$$x(0) = [0.1883\ 0.2507\ 0.0467\ 0.0899\ \ 0.1804\ 0.1394\ 0.1046\ 0.000]^T \quad (44)$$

with the boundaries on control variables $u_1 \in [0;20]$, $u_2 \in [0;6]$, $u_3 \in [0;4]$ and $u_4 \in [0;20]$. The final time is fixed with the value $t_F = 0.2$.

The target of the optimization is to find optimal control profiles over the time t_F to maximize

$$\max_{u_i} J_0 = x_8(t_F) \quad (45)$$

Two scenarios with the tolerance level T2 were investigated:

- First one used 4 control variables with initial conditions $u(0) = [10\ 3\ 2\ 6]^T$ and 11 piecewise constants. Optimal solution (Fig. 2) acquired after 15 iterations with sensitivity equations approach is $J_0 = 21.7575$. The DYNO package finds after 165 iterations optimal value $J_0 = 21.7570$.
- Second one used 3 control variables (last one was constant on the value 6 over the time) with initial conditions $u(0) = [10\ 3\ 2]^T$ and 10 piecewise constants. Optimal solution (Fig. 3) with sensitivity equations approach acquired after 8 iterations is $J_0 = 20.0895$. The DYNO package is able to obtain value $J_0 = 20.0906$ after 61 iterations.

Conclusions

This paper presented one possibility for calculation of gradients for the method of control vector parametrization. Detailed derivations and the application of sensitivity equations approach to solve necessary gradients were described. The advantages and disadvantages of the presented method are compared to other gradient methods. The results show that this approach is able to solve optimal control problems of nonlinear systems with a high accuracy with a smaller number of iterations as compared to other gradient methods.

Acknowledgments

The authors are pleased to acknowledge the financial support of the Scientific Grant Agency of the Slovak Republic under grants No. 1/3081/06 and 1/4055/07 and within the framework of the European Social Fund (PhD Students for Modern Industrial Automation in SR, JPD 3 2005/NP1-047, No 13120200115).

References

[1] AVRAAM, M. P., SHAH, N., PANTELIDES, C. C.: Modelling and optimisation of general hybrid systems in the continuous time domain. Computers and Chemical Engineering, 22(1):S221–S228, 1998.

[2] CANTO, E. B., BANGA, J. R., ALONSO, A. A., VASSILIADIS, V. S.: Dynamic optimization of chemical and biochemical processes using restricted second-order information. Computers and Chemical Engineering, 25:539–546, 2001.

[3] BIEGLER, L. T., CERVANTES, A. M., WACHTER, A.: Advances in simultaneous strategies for dynamic process optimization. Chemical Engineering Science, 57(4):575–593, 2002.

[4] CARACOTSIOS, M., STEWART, W. E.: Sensitivity analysis of initial value problems with mixed odes and algebraic equations. Computers and Chemical Engineering, 9:359–365, 1985.

[5] CHMÚRNY, D., PROKOP, R., BAKOŠOVÁ, M.: Automatic control of technological processes, Alfa, Bratislava, 1988 (in Slovak).

[6] CRESCITELLI, S., NICOLETTI, S.: Near optimal control of batch reactors. Chemical Engineering Science, 28:463–471, 1973.

[7] CUTHRELL, J. E., BIEGLER, L. T.: On the optimization of differential-algebraic process systems. AIChE Journal, 33(8):1257–1270, 1987.

[8] GALÁN, S., BARTON, P. I.: Dynamic optimization of hybrid systems. Computers and Chemical Engineering, 22:183–190, 1998.

[9] GOH, C. J., TEO, K. L.: Control parameterization: A unified approach to optimal control problems with general constraints. Automatica, 24(1):3–18, 1988.

[10] HIRMAJER, T., FIKAR, M.: Optimal control of a two-stage reactor system. Chemical Papers, 60 (5):381–387, 2006.

[11] HIRMAJER, T., FIKAR, M.: Solution of dynamic optimization problems with sensitivity equations approach. Technical report, FCFT STU, Radlinského 9, 812 37 Bratislava, Slovakia, 2007.

[12] JENSEN, T..: Dynamic Control of Large Dimension Nonlinear Chemical Processes. PhD thesis, Princeton University, 1964.

[13] LOGSDON, J. S., BIEGLER, L. T.: Accurate solution of differential-algebraic optimization problem. Industrial and Engineering Chemistry Research, 28:1628–1639, 1989.

[14] LUUS, R.: Application of dynamic programming to high-dimensional non-linear optimal control problems. International Journal of Control, 52(1):239–250, 1990.

[15] ROSEN, O., LUUS, R.: Evaluation of gradients for piecewise constant optimal control. Computers and Chemical Engineering, 15(4):273–281, 1991.

[16] RUBAN, I.: Sensitivity coefficients for discontinuous dynamic systems. Computer and Systems Sciences International, 36:536–542, 1997.

[17] SCHLEGEL, M., MARQUARDT, W.: Direct sequential dynamic optimization with automatic switching structure detection. Cambridge, USA, 2004. DYCOPS 7.

[18] STØREN, S., HERTZBERG, T..: Obtaining sensitivity information in dynamic optimization problems solved by the sequential approach. Computers and Chemical Engineering, 23:807–819, 1999.

[19] VASSILIADIS, V. S., SARGENT, R. W. H., PANTELIDES, C. C.: Solution of a class of multistage dynamic optimization problems. 1. problems without path constraints, 2. problems with path constraints. Industrial and Engineering Chemistry Research, 33(9):2111–2122, 2123–2133, 1994.

[20] VASSILIADIS, V. S., CANTO, E. B., BANGA, J. R.: Second-order sensitivities of general dynamic systems with application to optimal control problems. Chemical Engineering Science, 54:3851–3860, 1999.

Ing. Tomáš Hirmajer, PhD.
Ing. Michal Čižniar
Doc. Dr. Ing. Miroslav Fikar

Slovenská technická univerzita v Bratislave
Fakulta chemickej a potravinárskej technológie
Ústav informatizácie, automatizácie a matematiky
Oddelenie informatizácie a riadenia procesov
Radlinského 9, 812 37 Bratislava
Tel.: 02/52 495 730
E-mail: tomas.hirmajer@stuba.sk