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A Two-Step Approach for Optimal Control of Kinetic Batch Reactor with electroneutrality condition

Abstract. *In the article a Multi-Step Solution Technique were used. This technique enables to translate a complex optimal control problem to easier nonlinear programming problems. Efficiency of the designed algorithm was verified on a real-live optimal control problem of a stiff and highly nonlinear differential-algebraic system with constraints. One of the algebraic state equations takes the form of an electroneutrality condition, which ensures failure-free run of the production process. The simulations were executed in MATLAB, which is a commonly known programming environment.*

Streszczenie. *W artykule wykorzystano technikę wieloetapowego poszukiwania rozwiązania. W ten sposób złożony problem sterowania optymalnego można traktować jako grupę prostszych problemów programowania nieliniowego. Działanie wykorzystanego w pracy algorytmu najlepiej widać na problemie doboru optymalnego sterownia dla złożonego układu opisanego za pomocą nieliniowych równań różniczkowo-algebraicznych z ograniczeniami. Jedno z algebraicznych równań stanu przybiera postać warunku elektronetralności zapewniającego bezawaryjny przebieg procesu. Symulacje zostały przeprowadzone w środowisku MATLAB. (Dwustopniowe podejście do sterowania optymalnego reaktorem wsadowym z warunkiem elektroobojętności)*

Keywords: optimal control, sequential quadratic programming, DAE systems, multiple shooting method
Słowa kluczowe: sterowanie optymalne, sekwencyjne programowanie kwadratowe, układy równań różniczkowo-algebraicznych, metoda wielopunktowych strzałów

Introduction

The optimal control problems are understood as a searching for optimal control trajectory, which minimizes a cost function for specified class of dynamical system. Expression ¨dynamic systems¨ one can found as structures, which can be described as a system of ordinary differential equations (ODEs). Another kind of dynamic systems are hybrid systems [1] [2]. There are ODEs, which contain switching instants. Specified type of optimal control problems was introduced together with using of periodic control [3]. When the article ¨Differential/algebraic equation's are not ODEs¨ [4] was published, many scientists around the world concentrated their attention in the new class of systems.

Differential-algebraic systems consist of two parts. There are differential equations in the first part, and algebraic equations in the second part. Typical problems, which can be expressed as DAEs, are Constrained Variational Problems, Network Modeling and Discretization of PDEs. The authors of one of most important books about Differential-Algebraic Equations ended their publication with the words ¨Applications such as mechanical systems, electrical networks, trajectory prescribed path control and method of lines solution of partial differential equations have had an enormous impact on the development of both the numerical analysis and mathematical software for DAE systems, and will undoubtedly continue to influence the future developments in this area¨. [5]

One of the advanced problem in chemical engineering is optimal control of Kinetic Batch Reactor. Kinetic Batch Reactor is described as an nonlinear and stiff DAE system [6, 7].This problem illustrates the interference of dynamic equilibrium conditions with various physical meaning. For example electrical charges and chemical phases. Difficulties associated with the searching for a solution led to the development of a new algorithm. To solve this problem a Two-Step Solution Technique was used. This method enables to solve this problems without using highly specialized codes, but only using popular, coupled to the MATLAB R2010b environment, solvers.

Optimal control of DAE systems

In the paper the following DAE optimization problem was considered

$$\varphi(p) = \sum_{l=1}^{N_T} \Phi^l(y^l(t_l), z^l(t_l), p^l) \rightarrow min, \tag{1}$$

subject to

$$\frac{dy^l}{dt} = f^l(y^l(t), z^l(t), p^l) \tag{2}$$

with initial conditions

$$y^l(t_{l-1}) = y_0^l \tag{3}$$

and algebraic equations

$$g^l(y^l(t), z^l(t), p^l) = 0, t \in (t_{l-1}, t_l], l = 1, ..., N_T \tag{4}$$

with bounds

$$p_L^l \le p^l \le p_U^l, \tag{5}$$

$$y_L^l \le y^l \le y_U^l, \tag{6}$$

$$z_L^l \le z^l \le z_U^l \tag{7}$$

and constraints

$$h(p^1, ..., p^{N_T}, y_0^1, y^1(t_1), y_0^2, y^2(t_2), ..., y_0^{N_T}, y^{N_T}(t_{N_T})) = 0. \tag{8}$$

There are differential variables $y(t)$ and algebraic variables $z(t)$ in the DAE system in semiexplicit form. The assumption of invertibility of $g(-, z(t), -)$ permits an implicit elimination of the algebraic variables $z(t) = z[y(t), p]$. While there are N_T periods in DAE equations, time-dependent bounds or other path constraints on the state variables are no longer considered [8]. The control profiles are represented as parameterized functions with coefficients that determine the optimal profiles [9, 10]. The decision variables in DAE equations appear only in the time independent vector p^l. Algebraic constraints and terms in the objective function are applied only at the end of each period.

The problem 1-8 can be represented as the following nonlinear program

$$\phi(p) \rightarrow min \tag{9}$$

subject to

$$c_E(p) = 0, \tag{10}$$

$$c_I(p) \leq 0. \tag{11}$$

In the literature one can find a lot of methods solving above problem (see [6, 8, 11, 12, 13, 14]).

Sequential dynamic optimization strategy

A sketch of the sequential dynamic optimization strategy for problem (1)-(8) is presented on Fig. 1.

To understand the concept presented on Fig. 1 it would be helpfull to investigate, how an iteration is executed. At l-iteration, variables p^l are specified by NLP solver. In this situation, when vaules of p^l are known, one can treat DAE system as an initial value problem and integrate (2)-(4) forward in time for periods $l = 1, ..., N_T$. For these purposes solver $ode15s$ was used, which can solve index-1 DAE. Differential state profile, algebraic state profile and control function profile were obtained as results of this step. Next component evaluates the gradient of the objective and constraint functions with respect to p^l. Because function and gradient informations are passed to the NLP solver, then the decision variables can be updated. The convergence of problem (9)-(11) is depending on NLP solver. In [8] it is suggested, that SQP codes, as $NPSOL$, $NLPQP$ and $fmincon$ are generally well suited for this task, as they require relatively few iterations to converge. Because SQP-codes can suffer, when an initial point is far from a solution [15], one decided to design the Two-Stage Solution Technique.

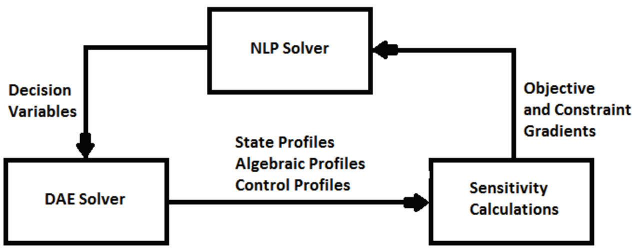

Fig. 1. Sequential dynamic optimization strategy.

Two-Stage Solution Technique and Multiple Shooting Method

The idea of using the Multi-Stage Solution Technique comes from premise, that a hard problem can be broken into a sequence of easier subproblems. The second motivation are results presented in the book [6]. The mentioned approach was used successfully for such problems as Optimal Lunar Swingby Trajectory and In-Flight Dynamic Optimization of Wing Trailing Egde Surface Positions. The first case consisted of four steps: (1) Three-Impulse, Conic Solution, (2) Three-Body Approximation to Conic Solution, (3) Optimal Three-Body Solution with Fixed Swingby Time and (4) Optimal Three-Body Solution. The second problem was solved in 3 steps: (1) Reference Trajectory Estimation, (2) Aerodynamic Drag Model Approximation and (3) Optimal Camber Prediction.

The main idea is to use results from $n-1$-step as an initial solution in n-step.

For optimal control of Kinetic Batch Reactor it was decided to design the Two-Stage Solution Technique. In the first stage an easier optimal control problem was investigated. The problem was solved with ¨classical¨single shooting method. The continuity conditions for state variables and control function are imposed explicite. Results obtained in this stage are going to be the initial conditions for the second stage. Because there are relatively few parameters in this step and a computation effort is acceptable , one can use $active-set$ approach [14]. As it was investigated, $active-set$ approach gave good results for wide range of problems and all iterations are feasible [16]. This step is aimed to obtain continuous state trajectory and continuous control tajectory as the solution. If it is possible, the most important constraints should be satisfied. The knowledge about the systems is necessery to constitute a model and then to design optimum batch process operating profiles. If ¨single shooting method/" does not give any results, there has to be used another method, ex. dichotomy approach [8].

Because in the second stage multiple shooting method was used, the NLP solver has to obtain a solution of more complex problem. One can hope, that initial conditions are close enough to the optimal solution. The optimization algorithm starts with initial conditions, which provide a feasible initial solution. The new cost function have to reflect this solution, so a new solution, which is not feasible can not be accepted. This step is aimed at the determination a solution satysiyng all the constraints. In other words, in this step the optimization algorithm starts with continuous state and control trajectories. Some constraints are satisfied as well. Now the algorithm searches for a new solution. This is enabled by adding optimization variables and new cost function. The first condition, which has to be satifiesd, is continuity of state trajectory. This approach is in opposition to solution presented in [6], where one of the obtained state trajectories has discontinuities. We allowed discontinuities only in control function, but the differences betwen control functions in grid points have to be minimized. Now it is expected, that obtained solution have high practical meaning. As NLP solver $fmincon$ in MATLAB R2010b with the option $Algorithm$ sqp [14] was proposed.

When the multiple shooting approach is used, the time domain is partitioned into smaller time periods and the DAE models are integrated separately in each element. To provide continuity of the states across elements, equality constraints are added to the nonlinear program. Inequality constraints for states and controls are then imposed directly at the grid points t_l. Path constraints on state trajectory may be violated between grid points [6, 8]. For optimal control problems with the multiple shooting approach, the following formulation was considered.

$$\phi(p) \rightarrow min, \tag{12}$$

subject to

$$y^{l-1}(t_{l-1}) - y_0^l = 0, l = 2, ...N_T, \tag{13}$$

$$y^{N_T}(t_{N_T}) - y_f = 0, y^l(0) = y_0^l, \tag{14}$$

$$p_L^l \leq p^l \leq p_U^l \tag{15}$$

$$z_L^l \leq z^l(t_l) \leq z_U^l \tag{16}$$

$$y_L^l \leq y^l(t_l) \leq y_U^l, l = 1, ..., N_T, \tag{17}$$

Table 1. Batch reactor dynamic variables.

	Description	
y_0	Differential state	$[HA]+[A^-]$
y_1	Differential state	$[BM]$
y_2	Differential state	$[HABM]+[ABM^-]$
y_3	Differential state	$[AB]$
y_4	Differential state	$[MBMH]+[MBM^-]$
y_5	Differential state	$[M^-]$
z_1	Algebraic state	$-log([H^+])$
z_2	Algebraic state	$[A^-]$
z_3	Algebraic state	$[ABM^-]$
z_4	Algebraic state	$[MBM^-]$
z_5	Reaction Temperature	

with the DAE system

$$\frac{dy^i}{dt}(t) = f^l(y^l(t), z^l(t), p^l), y^l(t_{l-1}) = y_0^l, \tag{18}$$

$$g^l(y^l(t), z^l(t), p^l), t \in (t_{l-1}, t_l], l = 1, ..., N_T. \tag{19}$$

Description of Kinetic Batch Reactor model

The Two-Stage Solution Technique was tested with the model of Kinetic Batch Reactor. There is a detailed description of the Kinetic Batch Reactor model in the book [6]. Here there are presented only these parts, which enables to write and to use the software and then to solve optimal control problem.

In the reactor the desired product AB is formed in the reaction

$$HA + 2BM \to AM + MBMH. \tag{20}$$

Here a kinteic model of the batch reactor system is presented in the same manner like in the book [6]. There are distinguished differential and algebraic states. Differential and algebraic variables are denoted as y_j and z_j, respectively. All of the species concentrations are given in mol per kg of the reaction mixture. There are batch reactor dynamic varibles in the table 1 and six differential mass balance equations in the model

$$\dot{y}_1 = -k_2 y_2 z_2, \tag{21}$$

$$\dot{y}_2 = -k_1 y_2 y_6 + k_{-1} z_4 - k_2 y_2 z_2, \tag{22}$$

$$\dot{y}_3 = k_2 y_2 z_2 + k_3 y_4 y_6 - k_{-3} z_3, \tag{23}$$

$$\dot{y}_4 = -k_3 y_4 y_6 + k_{-3} z_3, \tag{24}$$

$$\dot{y}_5 = k_1 y_2 y_6 - k_{-1} z_4, \tag{25}$$

$$\dot{y}_6 = -k_1 y_2 y_6 + k_{-1} z_4 - k_3 y_4 y_6 + k_{-3} z_3. \tag{26}$$

The electroneutrality condition

$$0 = p - y_6 + 10^{-z_1} - z_2 - z_3 - z_4, \tag{27}$$

There are three equilibrium condition

$$0 = z_2 - \frac{K_2 y_1}{K_2 + 10^{-z_1}}, \tag{28}$$

$$0 = z_3 - \frac{K_3 y_3}{K_3 + 10^{-z_1}}, \tag{29}$$

Table 2. Values of parameters

$\hat{k}_1 = 1.3708 \times 10^{12}$, $\hat{k}_{-1} = 1.6215 \times 10^{20}$,
$\hat{k}_2 = 5.2282 \times 10^{12}$,

$\beta_1 = 9.2984 \times 10^3$, $\beta_{-1} = 1.3108 \times 10^4$,
$\beta_2 = 9.5999 \times 10^3$,

$K_1 = 2.575 \times 10^{-16}$, $K_2 = 4.876 \times 10^{-14}$,
$K_3 = 1.7884 \times 10^{-16}$.

$$0 = z_4 - \frac{K_1 y_5}{K_1 + 10^{-z_1}}, \tag{30}$$

where

$$k_1 = \hat{k}_1 exp(-\beta_1/z_5), \tag{31}$$

$$k_{-1} = \hat{k}_{-1} exp(-\beta_{-1}/z_5), \tag{32}$$

$$k_2 = \hat{k}_2 exp(-\beta_2/z_5), \tag{33}$$

$$k_3 = k_1, \tag{34}$$

$$k_{-3} = \frac{1}{2} k_{-1}. \tag{35}$$

There are the values for the parameters $\hat{k}_j$ (kg / gmol / hr), β_j (K), and K_j (gmol / kg) in the table 2. As the control variable we treat the reaction temperature $T(K)$. For the duration of the process the control variable is limited to

$$293.15 \le z_5(t) \le 393.15. \tag{36}$$

One of the designed parameters is the initial catalyst concentration p(gmol / kg). This parameter is treated as an optimization variable and is restricted by the bounds

$$0 \le p \le 0.0262. \tag{37}$$

At the initail time $t = 0$ the initial catalyst concentration is realted to the corresponding state through the point constraint

$$= y_6(0) - p = 0. \tag{38}$$

From [6] it is known, that the remaining states are fixed by the boundary conditions

$$y_1(0) = 1.5776, \tag{39}$$

$$y_2(0) = 8.32, \tag{40}$$

$$y_3(0) = y_4(0) = y_5(0) = 0. \tag{41}$$

It is required, that at the free final time

$$y_4(t_F) \ge 1. \tag{42}$$

There is the nonlinear inequality path constraint in order to restrict the rate of product formation during the initial 25% of the process time. For $0 \le t \le (t_F/4)$

$$y_4(t) \ge at^2, \tag{43}$$

where $a = 2$(gmol / kg / hr · hr).

The desired objective function is to minimize the quantity

$$F = \gamma_1 t_F + \gamma_2 p, \tag{44}$$

where $\gamma_1 = 1$ and $\gamma_2 = 100$.

Results

To solve problem stated above, the Two-Stage Solution Technique was used. All calculations were performed on the processor Intel(R) Core(TM) i5 CPU 2.67 GHz.

In the first stage the single shooting method and linear control function were used. State variables and control function are continuous. We have to minimize augmented cost function, which were obtained as result of scalar product method with penalty function approach. Augmented cost function consists of added primary cost function F (44), final condition (42) and nonlinear inequality path constraint(43). To make the new cost function smooth, for last two terms the smoothing patrameter were used.

Three control functions were used.

(45) $$u_{5,1} = a_1 t + b_1$$

for the first stage,

(46) $$u_{5,2} = a_2 t + b_2$$

for the second stage and

(47) $$u_{5,3} = a_3 t + b_3$$

for the last stage. Because control function is continuous, parameters b_2 and b_3 can be obtained analytically. Vector p_1 was constituted as below

(48) $$p_1 = [a_1, b_1, a_2, a_3, p, t_f]^T.$$

Initial conditions

(49) $$p_1(0) = [1000, 293.15, 100, 100, 0.0262, 3.0]^T,$$

lower and upper bounds

(50) $$lb_1 = [-1000, 293.15, -100, -100, 0, 1.0]^T,$$

(51) $$ub_1 = [1000, 393.15, 100, 100, 0.0262, 3.0]^T.$$

The results, which were obtained after 537.3142 CPU time, are presented on the Fig. 2 - Fig. 7. There is the control function trajectory on the Fig. 8. State and control trajectories were denoted with the dotted line.

¨$Active-set$" with the options $options1$ was used as an optimization algorithm.

$options1 = optimset('TolFun', 1e-7, 'TolX', 1e-7, 'Algorithm', 'active-set', 'Hessian', 'fin-diff-grads', 'MaxFunEvals', 200000, 'Display', 'iter-detailed');$

In the second step the option sqp as $Algorithm$ was used. Results from previous step were used as initial condiotions. The obtained NLP problem is more complex, but now with good initial conditions, fast convergence can be expected.

Three control functions were used.

(52) $$U_{5,1} = A_1 t + B_1$$

for the first stage,

(53) $$U_{5,2} = A_2 t + B_2$$

for the second stage and

(54) $$U_{5,3} = A_3 t + B_3$$

for the last stage.

Because mulitple shooting method was used, control function is not continuous and parameters b_2 and b_3 will not be obtained analytically. Vector p_2 was constituted as below

(55) $$p_2 = [B_1, B_2, B_3, p, t_f, A_1, A_2, A_3]^T.$$

Initial conditions

(56) $$p_2(0) = [b_1, 393.15, 393.15, p, t_f, a_1, a_2, a_3]^T,$$

lower and upper bounds

(57)
$$lb_2 = [293.15, 293.15, 293.15, 0, 1.0, -1000, -100, -100]^T,$$

(58)
$$up_2 = [393.15, 393.15, 393.15, 0.0262, 3.0, 1000, 100, 100]^T.$$

The results were obtained after 7613.7 CPU time. They were denoted on the Fig. 2 - Fig. 7 and Fig. 8 with the solid line.

The optimization algorithm ¨sqp" with the options $options2$ was used

$options2 = optimset('TolFun', 1e-7, 'TolX', 1e-7, 'Algorithm', 'sqp', 'Hessian', 'fin-diff-grads', 'MaxFunEvals', 200000, 'Display', 'iter-detailed');$

In both stages solver $ode15s$ used Backward Differential Formula.

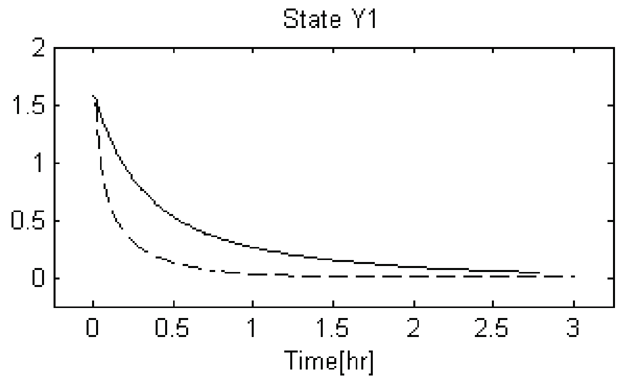

Fig. 2. Differential state Y1.

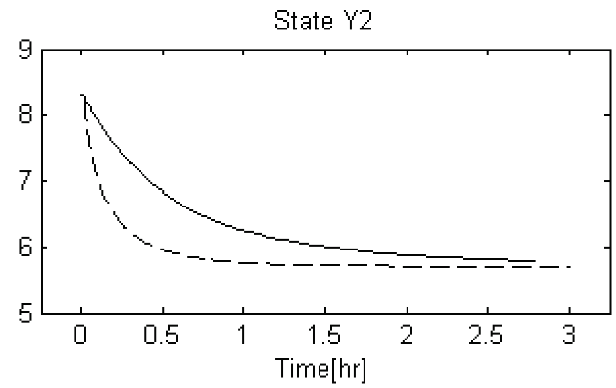

Fig. 3. Differential state Y2.

Conclusion

In the article a new approach for optimal control of a class of DAE systems were presented. The Two-Stage Solution Technique enables to use one of the general-purpose NLP solvers. Because the Matlab is commonly known among engineers, one can expect, that this approach will be useful

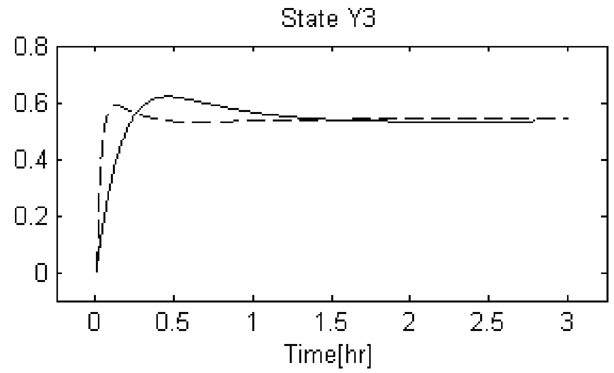

Fig. 4. Differential state Y3.

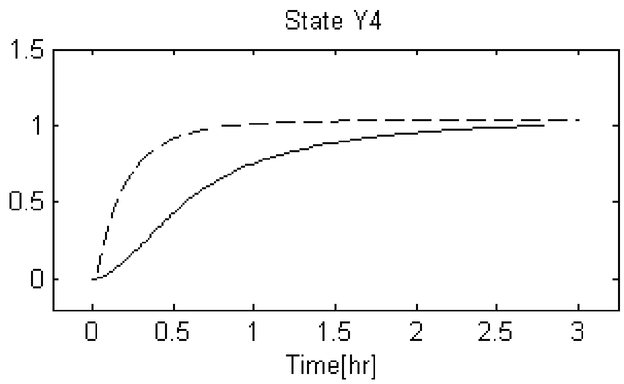

Fig. 5. Differential state Y4.

for finding solutions of the optimal control problems of real-life systems. The efficiency of this method was tested on the Kinetic Batch Reactor model as an example of the stiff and highly nonlinear DAE system. This model emphasizes the use of equilibrium constraints of various physical types, both electrical and chemical.

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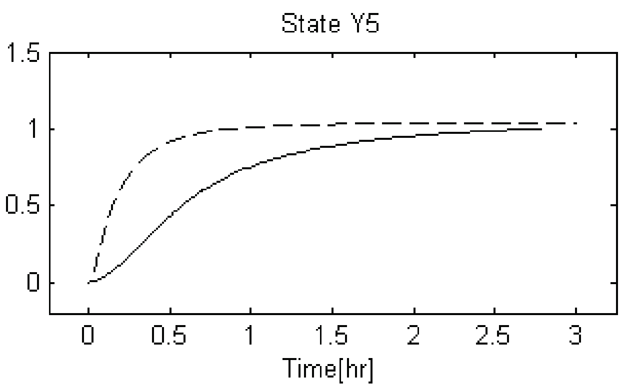

Fig. 6. Differential state Y5.

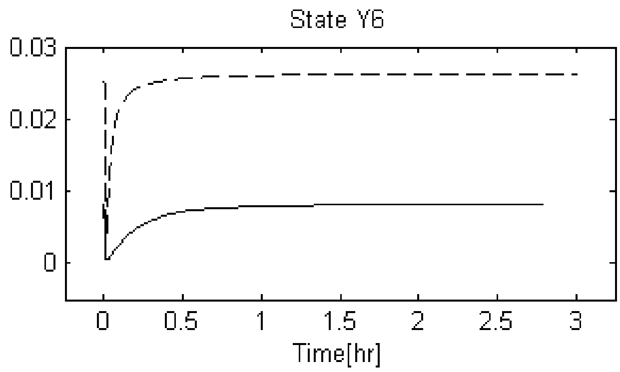

Fig. 7. Differential state Y6.

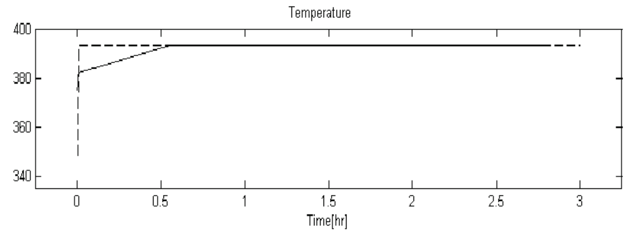

Fig. 8. Batch reactor control.

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