

DYNAMIC OPTIMIZATION OF A HYBRID COUPLED TANKS SYSTEM

Tomáš Hirmajer — Miroslav Fikar *

In this paper we present dynamic optimization of a hybrid system — coupled tanks exhibiting hybrid dynamics. Dynamic optimization of this hybrid system is based on a control vector parameterization (CVP) approach which allows the computation of the optimal operating policies. The CVP approach transforms the original dynamic optimization into a non-linear programming (NLP) problem. Calculation of gradients for NLP solver is based on optimal control theory.

Several simulation studies including minimum time problems and quadratic performance criteria are presented and show usefulness of the proposed approach.

Key words: dynamic optimization, sequential approach, hybrid system

1 INTRODUCTION

Many units in process industries are described by multiple sets of differential and algebraic equations. As such they are difficult to control and optimize in transient regimes if switching between the sets is to be taken into account. The switches can involve different regimes of operation (occurrence multiphase phenomena, explosive areas in mixtures of gasses, *etc*) or external actions (addition of second unit when production increases, *etc*).

There are several approaches to solution of such dynamic optimization problems. If the process to be optimized can be described accurately enough by piece-wise linear and logic formulation, powerful algorithms in the area of explicit model predictive control exists [2].

If fully nonlinear processes are concerned, the original dynamic optimization problem has to be approximated by some simplified formulation. One approach is complete discretization of state and control variables — orthogonal collocation. Such a formulation can be found in [1,3,6,9]. Another possibility is to leave the states intact and approximate only the control variables as piece-wise constant, or with some higher order approximations. This approach is known as control vector parameterization. Here different formulations can be found, depending on how gradients of the resulting nonlinear programming problem (NLP) are calculated [12]. In [5,15] a system of sensitivity equations is formed and the gradients are calculated from its solution. The advantage of this method is easy formulation of the problem and forward integration of both states and sensitivity equations. The drawback of this method lies in a large system of differential equations as each optimized parameter generates a set of differential equations with the same dimension as the number of states of the optimized process.

Another possibility that is pursued in this work is to calculate the gradients of NLP via optimal control theory

using the so-called co-state, or adjoint equations [13,8]. The advantage is that the number of differential equations is not proportional to the number of optimized parameters, but to the number of constraints. On the other side, adjoint equations have to be solved in opposite direction of time, which makes the implementation more difficult. When dealing with processes comprised of a large number of state equations and only a small number of state-dependent constraints, this approach has favorable properties compared to calculation of sensitivities.

The main aim of this work is to show a possibility of solving optimal control problems for hybrid systems numerically using the adjoint variable approach. This method will be applied to an example of two tank level control that exhibits hybrid dynamics.

2 PROBLEM FORMULATION

We consider a process to be optimized described by sets of differential equations

$$\dot{\mathbf{x}} = \mathbf{f}_i(\mathbf{x}(t), \mathbf{u}, t), \quad t_{i-1} \leq t \leq t_i, \quad i = 1, \dots, P \quad (1)$$

with initial conditions ($t_0 = t_0(\mathbf{u})$, $\mathbf{x}^+(t_0) = \mathbf{x}_0(t_0, \mathbf{u})$). Here, P is the number of different system descriptions. We consider here the n -dimensional process state vector $\mathbf{x}(t)$ and a constant m -dimensional vector of optimized parameters \mathbf{u} . It is assumed that system states are governed by state equations $\mathbf{f}_i(\cdot)$ that are continuously differentiable.

The switching instant t_i at which one set of equations is replaced by another is determined by the switching conditions

$$\mathbf{g}_i(\mathbf{x}_i^-, t_i, \mathbf{u}) = \mathbf{0}, \quad i = 1, \dots, P. \quad (2)$$

We assume that the functions $\mathbf{g}_i(\cdot)$ are continuously differentiable with respect to all variables. At switching

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instants, the vector $\mathbf{x}(t)$ can have breaks defined by equations

$$\mathbf{x}_i^+ = \mathbf{x}_i^- + \mathbf{\Delta}_i(\mathbf{x}_i^-, t_i, \mathbf{u}), \quad i = 1, \dots, P-1 \quad (3)$$

where $\mathbf{\Delta}_i(\cdot)$ are also continuously differentiable vector functions and $\mathbf{x}_i^- = \mathbf{x}(t_i^-)$, $\mathbf{x}_i^+ = \mathbf{x}(t_i^+)$ are the values of the vector $\mathbf{x}(t)$ before and after the switching instant, respectively. In (3) we consider additive jumps that are superimposed on the continuous trajectory at points t_i (eg if $\mathbf{\Delta}_i = \mathbf{0}$, then $\mathbf{x}(t)$ is continuous at the point t_i).

In the next step we define the cost J to be optimized (or constraint to be satisfied) in a general Bolza form [4].

$$J(\mathbf{u}) = G(\mathbf{x}(t_P), \mathbf{u}, t_P) + \int_{t_0}^{t_P} F(\mathbf{x}(t), \mathbf{u}, t) dt \quad (4)$$

where J is the scalar performance index to be minimized (functional of the quality of the dynamic system), G defines the final time conditions and F the requirements along the time axis.

3 GRADIENT OF THE COST FUNCTION

For the purpose of NLP we need to derive the gradient of the cost function with respect to optimized parameters — \mathbf{u} . These will be obtained from the optimal control theory by the variational method.

Let us introduce the following simplifications:

$$\mathbf{f}(\mathbf{x}(t), \mathbf{u}, t) = \mathbf{f}(t), \quad F(\mathbf{x}(t), \mathbf{u}, t) = F(t), \quad (5)$$

$$G(\mathbf{x}(t_P), \mathbf{u}, t_P) = G(\cdot). \quad (6)$$

Optimality conditions for our problem differ slightly from the original approach by [11] and have been derived by [13]. First, the Hamiltonian $H(t)$ is defined as

$$H(\mathbf{x}, \mathbf{u}, \boldsymbol{\lambda}, t) = F(t) + \boldsymbol{\lambda}(t)^\top \mathbf{f}(t) \quad (7)$$

where the vector of the Lagrange multipliers $\boldsymbol{\lambda}$ is defined by the differential equation

$$\dot{\boldsymbol{\lambda}}(t) = -\frac{\partial H(t)}{\partial \mathbf{x}} \quad (8)$$

with the boundary value at point t_P and the switching condition of the Lagrange multipliers at switching instants

$$\boldsymbol{\lambda}^\top(t_P) = \frac{\partial G(\cdot)}{\partial \mathbf{x}(t_P)}, \quad (9)$$

$$\boldsymbol{\lambda}^\top(t_i^-) = \left\{ \boldsymbol{\lambda}^\top(t_i^+) \left[\mathbf{I} + \frac{\partial \mathbf{\Delta}_i}{\partial \mathbf{x}_i^-} + \left(\frac{\partial \mathbf{\Delta}_i}{\partial t_i} - \mathbf{f}_{i+1}(t_i^+) \right) \mathbf{a}_i \right] + (F(t_i^-) - F(t_i^+)) \mathbf{a}_i \right\} (\mathbf{I} - \mathbf{f}_i(t_i^-) \mathbf{a}_i)^{-1}. \quad (10)$$

The gradient of the cost function is then defined as

$$\frac{dJ}{d\mathbf{u}} = \frac{\partial G(\cdot)}{\partial \mathbf{u}} + \left[\boldsymbol{\lambda}^\top(t_0) \frac{\partial \mathbf{x}_0(t_0, \mathbf{u})}{\partial t_0} - H(t_0) \right] \frac{dt_0}{d\mathbf{u}}$$

$$\begin{aligned} & + \int_{t_0}^{t_P} \frac{\partial H(t)}{\partial \mathbf{u}} dt + \left[\frac{\partial G(\cdot)}{\partial t_P} + H(t_P) \right] \frac{dt_P}{d\mathbf{u}} \\ & + \boldsymbol{\lambda}^\top(t_0) \frac{\partial \mathbf{x}_0(t_0, \mathbf{u}_0)}{\partial \mathbf{u}} + \sum_{i=1}^{P-1} \left[\boldsymbol{\lambda}^\top(t_i^+) \left(\frac{\partial \mathbf{\Delta}_i(\cdot)}{\partial \mathbf{u}} \right) \right. \\ & \left. + \left[H(t_i^-) - H(t_i^+) + \boldsymbol{\lambda}^\top(t_i^+) \left(\frac{\partial \mathbf{\Delta}_i(\cdot)}{\partial t_i} \right) \right] \mathbf{b}_i \right] \quad (11) \end{aligned}$$

where coefficients \mathbf{a}_i , \mathbf{b}_i are defined as

$$\mathbf{a}_i = -\left(\frac{\partial \mathbf{g}_i(\mathbf{x}_i^-, t_i, \mathbf{u})}{\partial t_i} \right)^{-1} \left(\frac{\partial \mathbf{g}_i(\mathbf{x}_i^-, t_i, \mathbf{u})}{\partial \mathbf{x}_i(t_i^-)} \right), \quad (12)$$

$$\mathbf{b}_i = -\left(\frac{\partial \mathbf{g}_i(\mathbf{x}_i^-, t_i, \mathbf{u})}{\partial t_i} \right)^{-1} \left(\frac{\partial \mathbf{g}_i(\mathbf{x}_i^-, t_i, \mathbf{u})}{\partial \mathbf{u}} \right). \quad (13)$$

If $\mathbf{a}_i = \mathbf{0}$, the switching conditions are simplified considerably (if the value of the jump of state variables of the object $\mathbf{\Delta}_i$ does not depend on \mathbf{x}_i^- , then the multipliers are continuous):

$$\boldsymbol{\lambda}^\top(t_i^-) = \boldsymbol{\lambda}^\top(t_i^+) \left[\mathbf{I} + \left(\frac{\partial \mathbf{\Delta}_i}{\partial \mathbf{x}_i^-} \right) \right], \quad i = 1, \dots, P-1. \quad (14)$$

If state variables of the process are continuous at switching points ($\mathbf{\Delta}_i = \mathbf{0}$), then the integrand function F of the quality index is continuous, but the Lagrange multipliers contain discontinuity at the moment of switch

$$\boldsymbol{\lambda}^\top(t_i^-) = \boldsymbol{\lambda}^\top(t_i^+) \left[\mathbf{I} - \mathbf{f}_{i+1}(t_i^+) \mathbf{a}_i \right] (\mathbf{I} - \mathbf{f}_i(t_i^-) \mathbf{a}_i)^{-1}, \quad i = 1, \dots, P-1. \quad (15)$$

Finally, if the times of switch depend explicitly on control parameter ($t_i = t_i(\mathbf{u})$, $\mathbf{a}_i = \mathbf{0}$, and $\mathbf{b}_i = \frac{dt_i}{d\mathbf{u}}$), then the Lagrange multipliers are continuous.

4 PROCEDURE

4.1 Algorithm

We assume that the continuous control trajectory is piece-wise constant over P intervals. This makes it possible to convert the original problem of dynamic optimization into a nonlinear programming problem [7]. In this algorithm we assume that we have the functional J_0 and k constraints J_j , where $j = 1, \dots, k$. We further separate the optimized variables into times t_i and constant controls \mathbf{u} . For simplicity assume that the initial time t_0 and state $\mathbf{x}(t_0)$ are given and constant. Then we can write the following algorithm:

1. Integrate the system (1) and integral terms F_j together from $t = t_0$ to $t = t_P$. Restart integration with switching conditions (2), states can be discontinuous following equation (3).

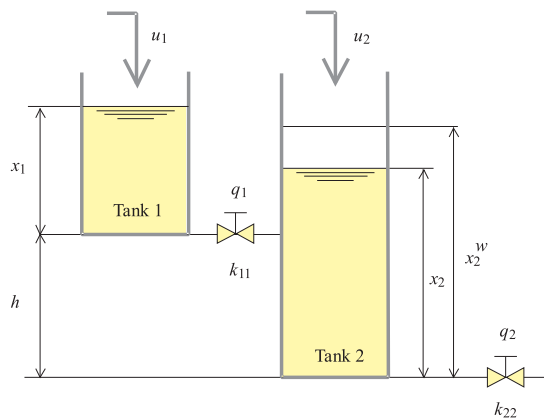


Fig. 1. Coupled tanks system.

2. For $j = 0, \dots, k$ repeat
 - (a) Initialize adjoint variables $\lambda_j^\top(t_P)$, according to equations (9).
 - (b) Initialize intermediate variables $\mathbf{J}_{D,j}$ as zero. These represent the integral part of the gradients.
 - (c) Integrate backwards from $t = t_P$ to $t = t_0$ the adjoint system (8) and intermediate variables. Allow for discontinuities of the adjoint equations as given in (14), restart integration at these points, and at the points of changes of dynamics

$$\dot{\lambda}_j = -\frac{\partial H_j}{\partial \mathbf{x}}, \quad (16)$$

$$\dot{\mathbf{J}}_{D,j} = \frac{\partial H_j}{\partial \mathbf{u}}. \quad (17)$$

- (d) Calculate the gradients of J_j with respect to times t_i and control \mathbf{u} , with help of (11).

$$\frac{\partial J_j}{\partial t_P} = H_j(t_P) + \frac{\partial G_j(\cdot)}{\partial t_P}, \quad (18)$$

$$\frac{\partial J_j}{\partial t_i} = \left[H_j(t_i^-) - H_j(t_i^+) + \lambda_j^\top(t_i^+) \left(\frac{\partial \Delta_i(\cdot)}{\partial t_i} \right) \right] \mathbf{b}_i, \quad (19)$$

$$i = 1, \dots, P - 1,$$

$$\frac{\partial J_j}{\partial \mathbf{u}_i} = \mathbf{J}_{D,j}(t_{i-1}) - \mathbf{J}_{D,j}(t_i) + \frac{\partial G_j(\cdot)}{\partial \mathbf{u}_i} + \lambda^\top(t_i^+) \left(\frac{\partial \Delta_i(\cdot)}{\partial \mathbf{u}} \right), \quad (20)$$

$$i = 1, \dots, P.$$

In this manner, the values of J_j are obtained in step 1 and the values of gradients in step 2d. This is all what is needed in NLP algorithm.

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

$$t_P = \sum_{i=1}^P \Delta t_i. \quad (21)$$

Therefore, the following holds for the derivatives

$$\frac{\partial J_j}{\partial \Delta t_i} = \sum_{r=1}^P \frac{\partial J_j}{\partial t_r} \frac{\partial t_r}{\partial \Delta t_i}. \quad (22)$$

4.2 Implementation of Algorithm

The algorithm was implemented in FORTRAN 77. The first part of this program contains a module for forward and backward integrations LSODAR [10] that is able to handle state events. The second module of the program computes gradients and calls the NLP solver NLPQL [14].

The user specifies initial conditions:

- $\mathbf{u}_0, \mathbf{x}_0$, lower and upper control bounds, number of time intervals,
- cost function, constraints,
- differential equations of the process.

4.3 Integration of Adjoint Equations

When the adjoint equations are integrated backwards in time, the knowledge of states $\mathbf{x}(t)$ is needed. In our case the program stores at first in the forward pass the states at a predefined grid points and interpolates them when adjoint equations are solved.

Two interpolations were implemented into the program: linear, and the approximations having continuous states and continuous first order derivatives across boundaries. All examples were simulated with the second one.

5 PROCESS

We assume a non-linear system of two tanks shown in Fig. 1 that is described by two sets of differential equations

$$\mathbf{f}_1 = \begin{pmatrix} \frac{u_1}{F_1} - \frac{k_{11}\sqrt{x_1}}{F_1} \\ \frac{u_2}{F_2} + \frac{k_{11}\sqrt{x_1}}{F_2} - \frac{k_{22}\sqrt{x_2}}{F_2} \end{pmatrix}, \quad (23)$$

$$\mathbf{f}_2 = \begin{pmatrix} \frac{u_1}{F_1} - \frac{k_{11}\sqrt{x_1 - (x_2 - h)}}{F_1} \\ \frac{u_2}{F_2} + \frac{k_{11}\sqrt{x_1 - (x_2 - h)}}{F_2} - \frac{k_{22}\sqrt{x_2}}{F_2} \end{pmatrix} \quad (24)$$

where F_1, F_2 [m²] are the cross-sectional areas of the tanks; k_{11}, k_{22} [l^{2.5} s⁻¹] — flow resistances; x_1, x_2 — state values — levels of liquid in the first and the second tank; u_1, u_2 [l s⁻¹] — control values — flow rates; h [m] — vertical distance between tanks.

The first dynamics with no interactions between the tanks takes place if the height h_2 in the second tank is smaller than h . In the opposite case, the tanks interact and are described by the dynamics \mathbf{f}_2 .

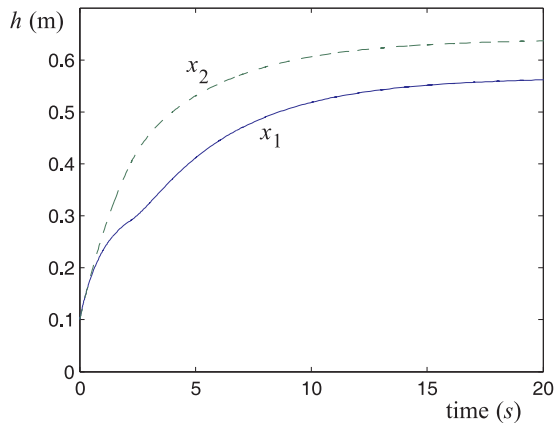


Fig. 2. Simulation of the hybrid system with constant control values.

Thus, the height h specifies the switching condition between dynamics \mathbf{f}_1 and \mathbf{f}_2 as

$$g_1 = h - x_2 \quad (25)$$

The concrete values of parameters are defined as: resistances $k_{11} = 1.75 \text{ l}^{2.5} \text{ s}^{-1}$, $k_{22} = 1.50 \text{ l}^{2.5} \text{ s}^{-1}$, surfaces $F_1 = 2.00 \text{ m}^2$, $F_2 = 4.00 \text{ m}^2$, vertical distance $h = 0.40 \text{ m}$, initial states $x_1(0) = x_2(0) = 0.10 \text{ m}$, desired state $x_2^w = 1.00 \text{ m}$.

The initial values of optimized parameters are $u_i = 1 \text{ l s}^{-1}$, $\Delta t_i = 1 \text{ s}$ with bounds defined as $u_i \in [0, 3]$ and $\Delta t_i \in [0.01, 10.00]$.

Fig. 2 shows the response of the plant to these initial optimized parameters with final time of simulation set to $t_P = 20.00 \text{ s}$. We can observe the change of dynamics at the switch time $t = 2.19 \text{ s}$.

5.1 Dynamic Optimization Problem Definitions

We consider two possible formulations for a change of steady-states. In both of them, it is assumed that the initial steady state is located in the region without interaction and the final one in the region with interaction. The controlled variable is the height of liquid in the second tank h_2 and control variables are inflows u_1, u_2 .

5.2 Minimum Time Problem

The aim of the optimal operation is in this case defined as to reach in a minimum time a new steady-state defined by a desired height in the second tank. Thus, the cost functional is defined as

$$\min_{t_P, u} J_0 = t_P \quad (26)$$

subject to the constraints:

$$J_1 = x_2(t_P) - x_2^w = 0, \quad (27)$$

$$J_2 = \frac{dx_1}{dt} = 0, \quad (28)$$

$$J_3 = \frac{dx_2}{dt} = 0 \quad (29)$$

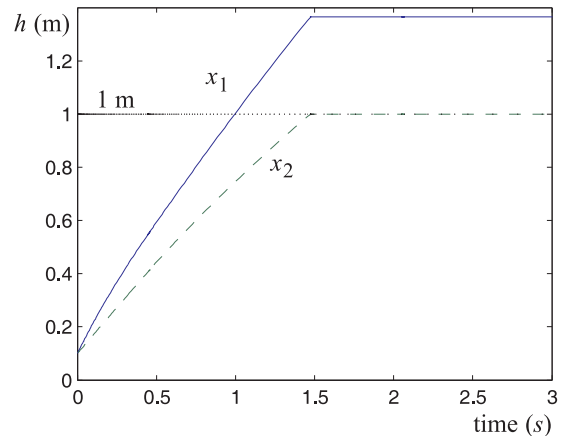


Fig. 3. Optimal state trajectories with multivariable time optimal control.

where x_2^w is the required level of the liquid in the second tank. Constraints J_2, J_3 represent the requirement of the new steady-state in the final time.

We consider that the control vector \mathbf{u} contains incoming flowrates u_1 and u_2 and that these are piece-wise constants. Then, we optimize the duration and value of piece-wise controls \mathbf{u} over specified number of time intervals.

2.3 LQ Cost Problem

Consider now a situation with a fixed terminal time t_P and the objective is to optimize a LQ cost functional

$$\min_u J_0 = \int_{t_0}^{t_P} ((x_2 - x_2^s)^2 + r(u_1 - u_1^s)^2) dt \quad (30)$$

where x_2^s, u_1^s are steady states of the values and r is a positive weight coefficient. Again, to achieve a new steady-state, constraints (27)–(29) have to be respected.

6 RESULTS AND DISCUSSION

6.1 Minimum Time Problems

6.1.1 Multivariable Time Optimal Control

In order to drive the process to the desired new steady-state as fast as possible, we consider both inflows to be optimized and set the number of optimized time intervals to two.

The optimization and integration tolerances were set as 10^{-6} and 10^{-10} , respectively. The minimum final time was obtained as $t_P = 1.47 \text{ s}$ after 8 NLP iterations. The optimal state variables can be found in Fig. 3 and the corresponding controls in Fig. 4. The control variables show typical bang-bang behavior that follows from the desired objective.

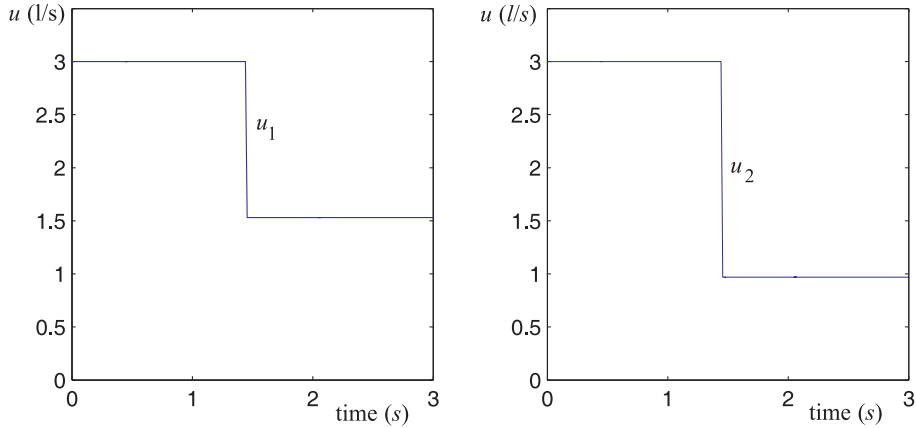


Fig. 4. Optimal control policy with multivariable time optimal control.

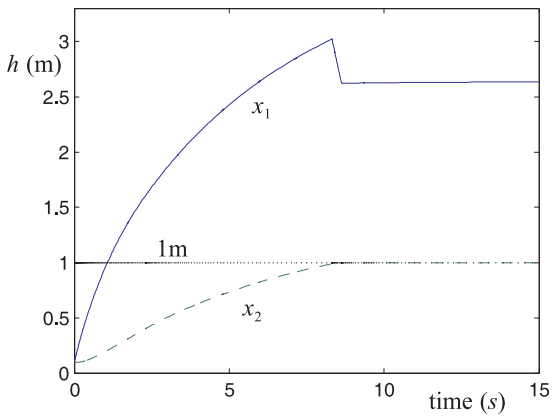


Fig. 5. Optimal state trajectories with singlevariable time optimal control.

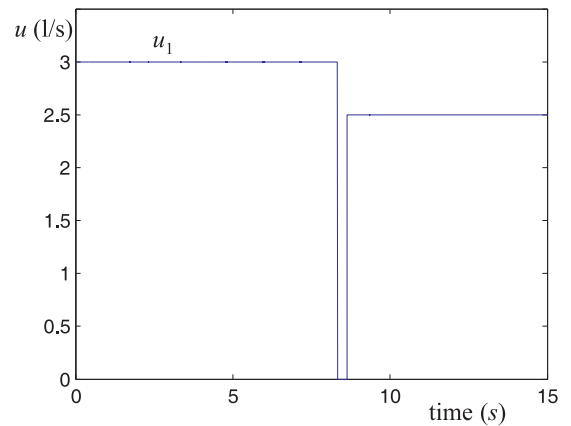


Fig. 6. Optimal control policy with singlevariable time optimal control.

6.1.2 Singlevariable Time Optimal Control

A more realistic example considers only one control variable — the inlet flowrate to the first tank. The number of time intervals was set to 8. Optimization and integration tolerances were set as 10^{-4} and 10^{-12} , respectively.

The optimal minimum time in this case was higher and was found as $t_P = 8.623$ s. The optimal state variables can be found in Fig. 5 and the corresponding controls in Fig. 6. Again, the control variables show a typical bang-bang behavior. Although 8 optimized intervals were chosen, only three would be enough — two for optimal control of the second order dynamics and the last one to achieve the desired steady-state.

6.2 LQ Cost Problem

In this case, we fix the number of time intervals to 15 and their duration to 1 s and optimize only the first control variable with the optimization and integration tolerances, which were set as 10^{-5} and 10^{-12} , respectively. Steady-state analysis gives the values of the new steady-state as $x_2^s = 1.00$ m, $u_1^s = 2.50$ $l s^{-1}$.

Various values of the penalization factor r have been considered, the optimal simulations in Fig. 7 (states) and Fig. 8 show three of them.

Decreasing the value of r leads to a behavior similar to that of time optimal control. On the other hand, its increase smoothes the control variable considerably with only a small loss of performance.

The optimal value of the cost function was 2.7517 with 7 NLP iterations if the weight coefficient $r = 1$ was obtained.

CONCLUSIONS

In this paper we have investigated the problem of dynamic optimization of systems described by multiple sets of differential equations. Control vector parameterization has been used and gradients for the nonlinear programming have been calculated based on the optimal control theory. This is in contrast to usual approaches where sensitivity equations are preferred due to simplicity of the implementation.

On the other hand, the adjoint variable approach has its advantage for systems described by a larger set dif-

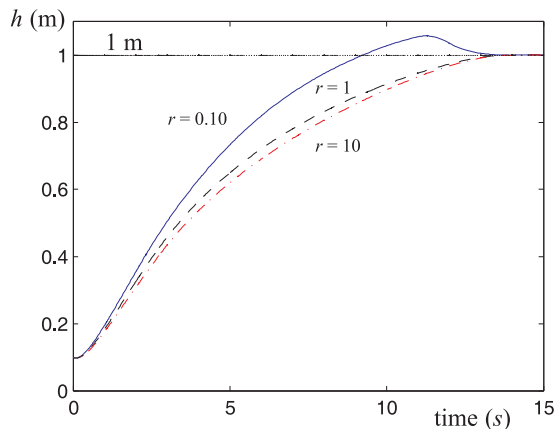


Fig. 7. Level of the liquid in the second tank for various choices of the coefficient r .

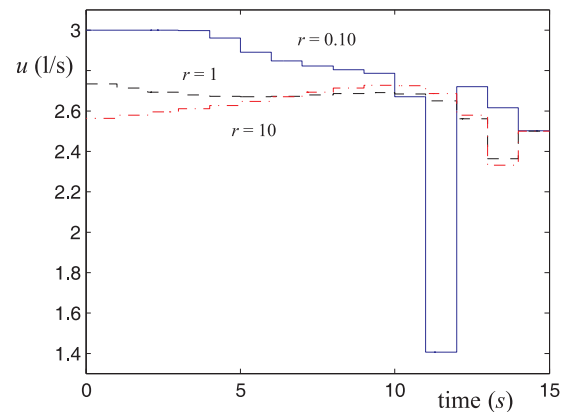


Fig. 8. Optimal LQ control policy.

ferential equations and it can reduce the computational time considerably.

Simulations with a simple chemical engineering example confirmed attractiveness of the proposed approach.

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