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Optimal Control of a Fedbatch Fermentation Process: Numerical Methods, Sufficient Conditions and Sensitivity Analysis

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Abstract— **Bang-bang and singular optimal controls in a fedbatch fermentation process are computed for a range of time horizons. Numerical algorithms for determining the optimal control structure and computing the switching times are presented. Second order sufficient optimality conditions and sensitivity of optimal solutions are discussed.**

I. INTRODUCTION

Optimal control of fedbatch reactors is a problem of high technical importance (see Henson [7] and the references therein). Solutions often exhibit features interesting from the mathematical point of view, including control structures with singular arcs. The typical computational algorithms used for solving such problems, both direct and indirect, have one flaw in common: they do not find the optimal control structure in an automatic way, without 'try-and-error' participation of the user. In this work we study optimal control of a fedbatch fermentation process. An analytic expression for singular control is derived in a state feedback form. Two direct optimization algorithms, that of *Monotone Structural Evolution* (MSE, Szymkat et al. [14], [15], [16]) and the code NUDOCCCS (Büskens [2], [4]) are used for optimal control computations. A new feature of the MSE is that it automatically produces the structure of extremal controls, i.e., those satisfying the optimality conditions of the Maximum Principle. Second order sufficient optimality conditions are checked for the induced optimization problems with respect to switching times and, in the bang-bang case, for the original problem. Sensitivity analysis of parametric optimal solutions is discussed.

In the considered problem the Hamiltonian is affine w.r.t. control, which is constrained to a compact interval. In such problems, trajectories arbitrarily close to singular may be obtained with purely bang-bang controls; often only few switchings are sufficient for a good approximation. Still, calculation of singular control has practical value. Firstly, quality of approximation can be best evaluated, if the approximated object is known. Secondly, more exact bang-bang approximations require many frequent switchings, difficult to realize and harmful for the actuators. Such switchings are also disadvantageous for optimization, since the problem becomes higher dimensional and ill conditioned. Finally, the knowledge of optimal control structure allows approximation of singular arcs with parametric, explicit functions of time and is helpful in adaptive control [7], [13].

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II. PROBLEM FORMULATION

Optimal control of a fedbatch process of alcoholic fermentation will be considered. The process consists in biological degradation of the substrate (glucose) into the metabolite (alcohol) resulting from the action of microorganisms (yeast). We use the mathematical model due to Ghose and Tyagi, after Queinnec and Dahhou who employ it in [12] to describe their experimental setup. The model involves four state variables: biomass concentration X [g/l], substrate concentration S [g/l], product concentration P [g/l] and working volume V [l]. The feeding rate u [l/h] of nutrient substrate solution is the control variable. Denote the concentration of substrate in the solution fed into the process by S_{in} [g/l]. The dynamics of the fermentation process is described by four state equations

$$\begin{aligned} \dot{X} &= MX\left(1-\frac{P}{P_m}\right)-\frac{u}{V}X\,, &(1)\\ \dot{S} &= -NX-\frac{u}{V}(S-S_{\text{in}})\,, &(2)\\ \dot{P} &= y_pNX-\frac{u}{V}P\,, &(3)\\ \dot{V} &= u\,, &(4)\end{aligned}$$

where the time variable t is expressed in hours, and

$$M=\frac{\mu S}{K_s+S+S^2/K_i}\,,\quad N=\frac{\nu S}{K_s'+S+S^2/K_i'}\,. \quad (5)$$

The values of the constants are as follows: $y_p = 0.43$, $\mu = 0.54$ [h^{-1}], $K_s = 5$ [g/l], $K_i = 201$ [g/l], $\nu = 2.1/0.43$ [h^{-1}], $K_s' = 9$ [g/l], $K_i' = 297$ [g/l]. The constant P_m, not specified in [12], is a parameter taking values in the range $[100,\ 150]$ [g/l]. It denotes the concentration of alcohol above which the microorganisms suffer intensive atrophy and the model is no longer valid.

A simple observation allows us to reduce the number of state equations to three. It follows from equations (2) – (4) that for an arbitrary time moment t the mass of substrate m_s consumed for alcohol production is related to the mass of the product m_p by the equality $m_p(t) = y_p m_s(t)$. Putting $T = S_{\text{in}} - S$ we obtain from the mass balance

$$P = y_pT + \frac{c_0}{V}\,, \quad (6)$$

where $c_0 = V(0)\,(P(0) - y_p T(0))$. For shortness, denote $R = 1 - P/P_m$, $y = y_p/P_m$ and $c = c_0/P_m = V(1 - R - yT)$. The new state equations read

$$\dot{X} = \left(MR - \frac{u}{V}\right) X\,, \tag{7}$$

$$\dot{S} = -NX + \frac{uT}{V}\,, \tag{8}$$

$$\dot{V} = u\,. \tag{9}$$

The initial state is fixed and the terminal state is free. The product concentration is determined from (6). The optimal control problem is to minimize a cost functional being a weighted difference of the final masses of substrate and product

$$J_0(u) = (a_0 S(t_f) - b_0 P(t_f))\,V(t_f)$$

where t_f is a fixed termination time, and a_0 and b_0 are nonnegative constants. Putting $J_0 = J - a_0 c_0$, $a = a_0 + b_0 y_p$, $b = b_0 y_p S_{\rm in}$ we obtain a simpler, equivalent form of the cost

$$J(u) = (aS(t_f) - b)\,V(t_f). \tag{10}$$

The control is subject to the simple bounds $0 \le u \le u_{\max}$.

III. MAXIMUM PRINCIPLE

In order to apply the Maximum Principle, we define the Hamiltonian

$$H = \psi_1 \left(MR - \frac{u}{V}\right) X + \psi_2 \left(-NX + \frac{uT}{V}\right) + \psi_3 u\,.$$

The adjoint variables ψ_1, ψ_2 and ψ_3 satisfy the adjoint set of differential equations

$$\dot{\psi}_1 = -\frac{\partial H}{\partial X} = -\psi_1 \left(MR - \frac{u}{V}\right) + \psi_2 N\,, \tag{11}$$

$$\dot{\psi}_2 = -\frac{\partial H}{\partial S} = -\psi_1 X (RM' + yM) + \psi_2 \left(XN' + \frac{u}{V}\right)\,, \tag{12}$$

$$\dot{\psi}_3 = -\frac{\partial H}{\partial V} = \frac{-\psi_1 X (cM + u) + \psi_2 u T}{V^2} \tag{13}$$

with the terminal conditions

$$\psi_1(t_f) = 0, \quad \psi_2(t_f) = -aV(t_f), \quad \psi_3(t_f) = -aS(t_f) + b.$$

The derivatives of M and N w.r.t. S are denoted by primes. From (5),

$$M' = \frac{M^2 (K_s/S - S/K_i)}{\mu S}\,, \quad N' = \frac{N^2 (K_s'/S - S/K_i')}{\nu S}\,.$$

The Hamiltonian is an affine function of the control u, of the form $H = H_0 + H_1 u$ with

$$\begin{aligned} H_0 &= (\psi_1 MR - \psi_2 N) X\,, \\ H_1 &= H_1(X, S, V, \psi_1, \psi_2, \psi_3) = \\ &= \frac{1}{V}(-\psi_1 X + \psi_2 (S_{\rm in} - S)) + \psi_3\,. \end{aligned} \tag{14}$$

The function H_1 is called the *switching function*; its values along a state and adjoint trajectory are denoted by $H_1[t]$. The optimal control maximizes the Hamiltonian for a.a. $t \in [0, t_f[$, and hence satisfies the relation

$$u(t) = \begin{cases} 0, & \text{if} \quad H_1[t] < 0 \\ u_{\max}, & \text{if} \quad H_1[t] > 0 \\ \text{undetermined}, & \text{if} \quad H_1[t] = 0 \end{cases} \tag{15}$$

IV. SINGULAR CONTROL

Notice in view of (15) that for $H_1[t] = 0$ the maximization of the Hamiltonian does not provide any value of the control $u(t)$. As long as the switching function vanishes only at isolated points of time (or, more generally, on a set of zero measure), this has no consequences for the determination of optimal control. The situation is different if the function $H_1[t]$ is identically zero in a certain time interval. Such a case, called *singular control*, requires further analysis. In every interval of singularity the following identity holds

$$VH_1 = -\psi_1 X + \psi_2 T + \psi_3 V \equiv 0.$$

Differentiating this, we obtain a new identity

$$H_1 u + XH_2 \equiv 0 \quad \text{or} \quad H_2 \equiv 0\,, \tag{16}$$

where

$$H_2 = -\rho\psi_1 + TN'\psi_2\,, \quad \rho = RTM' + (1 - R)M. \tag{17}$$

The differentiation of (16) with respect to time gives another identity

$$H_3 \frac{Tu}{V} + H_4 \equiv 0\,, \tag{18}$$

where

$$H_3 = -\left(RTM'' + 2(1 - R)M'\right)\ \psi_1 + N'' T \psi_2\,, \tag{19}$$

$$H_4 = H_{41}\psi_1 + H_{42}\psi_2\,, \tag{20}$$

$$H_{41} = \rho RM - (RM' + yM) N' TX + \left(RTM'' + (1 - 2R)M' + y(TM' - M)\right) NX, \tag{21}$$

$$H_{42} = TXN'^2 - N\left((TN'' - N')X + \rho\right). \tag{22}$$

The second derivatives in the right-hand sides are given by

$$M'' = \frac{2M\left(M'(K_s/S - S/K_i) - MK_s/S^2\right)}{\mu S}\,,$$

$$N'' = \frac{2N\left(N'(K_s'/S - S/K_i') - NK_s'/S^2\right)}{\nu S}\,.$$

It follows from (16) and (17) that

$$\psi_2 = \frac{\rho\psi_1}{TN'}\,.$$

Substituting this in (19) and (20), compute H_3 and H_4

$$H_3 = H_{30}\psi_1, \quad H_4 = H_{40}\psi_1\,, \tag{23}$$

where

$$H_{30} = -RTM'' - 2(1 - R)M' + \rho\frac{N''}{N'}\,, \tag{24}$$

$$H_{40} = \rho RM + \frac{cXM}{V}\left(N' + \frac{N}{T}\right) - \left(H_{30} + \frac{cM'}{V}\right) XN - \frac{\rho^2 N}{TN'}\,. \tag{25}$$

The substitution of (23) – (25) in the identity (18) yields a formula for the singular optimal control

$$u_s = u_s(X,S,V) = -\frac{VH_{40}}{TH_{30}} \ . \quad (26)$$

Note that the knowledge of adjoint variables in the interval of singularity is not needed for the determination of optimal control.

V. ADJOINT EQUATIONS IN CANDIDATE SINGULAR INTERVALS

In order to compute derivatives of the cost with respect to the ends of candidate singular intervals (CSI), where the expression for singular control u_s (26) is substituted in the right-hand sides of the state equations (7) – (9), we need the appropriate adjoint equations. Of course, outside the CSIs the state and adjoint equations remain unchanged. We assume that $u_s \in \,]0, u_{\max}[$. The Hamiltonian in a CSI is given by

$$H = \psi_1\left(MR - \frac{u_s}{V}\right)X + \psi_2\left(-NX + \frac{u_s}{V}T\right) + \psi_3 u_s.$$

The adjoint equations there read

$$\dot{\psi}_1 = -\psi_1\left(MR - \frac{u_s}{V}\right) + \psi_2 N - H_1\frac{\partial u_s}{\partial X} \ , \quad (27)$$

$$\dot{\psi}_2 = -\psi_1 X(RM' + yM) + \psi_2\left(XN' + \frac{u_s}{V}\right) - H_1\frac{\partial u_s}{\partial S} \ , \quad (28)$$

$$\dot{\psi}_3 = \frac{-\psi_1 X(cM + u_s) + \psi_2 u_s T}{V^2} - H_1\frac{\partial u_s}{\partial V} \ . \quad (29)$$

Note that in the optimal solution the CSIs coincide with the singular intervals and then the coefficient H_1 becomes identically zero. The derivatives of u_s are as follows

$$\begin{aligned}
\frac{\partial u_s}{\partial X} &= \frac{u_s}{H_{40}}\frac{\partial H_{40}}{\partial X} \ , \\
\frac{\partial u_s}{\partial S} &= u_s\left(\frac{1}{H_{40}}\frac{\partial H_{40}}{\partial S} - \frac{1}{H_{30}}\frac{\partial H_{30}}{\partial S} + \frac{1}{T}\right) , \\
\frac{\partial u_s}{\partial V} &= u_s\left(\frac{1}{H_{40}}\frac{\partial H_{40}}{\partial V} - \frac{1}{H_{30}}\frac{\partial H_{30}}{\partial V} + \frac{1}{V}\right) ,
\end{aligned}$$

where

$$\begin{aligned}
\frac{\partial H_{40}}{\partial X} &= cM\frac{N' + N/T}{V} - \left(H_{30} + c\frac{M'}{V}\right)N \ , \\
\frac{\partial H_{30}}{\partial S} &= 2yM' - (2 + yT - 3R)M'' - RTM''' + \\
&\quad + \frac{\rho' N'' - \rho(N''^2/N' - N''')}{N'} \ , \\
\frac{\partial H_{40}}{\partial S} &= \rho' RM + \rho(yM + RM') + \\
&\quad + \frac{cX}{V}\left(MN'' + \frac{M'N + MN'}{T} + \frac{MN}{T^2}\right) - \\
&\quad - \left(\left(\frac{\partial H_{30}}{\partial S} + c\frac{M''}{V}\right)N + H_{30}N'\right)X - \\
&\quad - \frac{\rho N}{TN'}\left(2\rho' + \frac{\rho}{T} - \frac{\rho N''}{N'}\right) - \frac{\rho^2}{T} \ , \\
\frac{\partial H_{30}}{\partial V} &= c\frac{2M' - TM'' + (TM' - M)N''/N'}{V^2} \ , \\
\frac{\partial H_{40}}{\partial V} &= \frac{c}{V^2}M\left((TM' - M)R + \rho - X\left(N' + \frac{N}{T}\right)\right) + \\
&\quad + \frac{c}{V^2}N\left(M'X - 2\rho\frac{TM' - M}{TN'}\right) - \frac{\partial H_{30}}{\partial V}XN \ , \\
M''' &= -3M\frac{2M'/K_i + M''\ (1 + 2S/K_i)}{\mu S} \ , \\
N''' &= -3N\frac{2N'/K_i' + N''\ (1 + 2S/K_i')}{\nu S} \ , \\
\rho' &= (yT - 2R + 1)M' + RTM'' - yM \ .
\end{aligned}$$

VI. NUMERICAL EXAMPLE

Assume the following values of the parameters: $P_m = 150$, $S_{\text{in}} = 200$, $u_{\max} = 1$, $X(0) = 3$, $S(0) = 40$, $P(0) = 0$, $V(0) = 4$, $a_0 = 1$, $b_0 = 1$. Hence, we have $a = 1.43$ and $b = 86$ in the cost functional (10). The structure of the optimal control, i.e., the sequence of bang-bang and singular arcs, depends crucially on the choice of the final time t_f; cf. the survey of results in Fig. 5. Let us now discuss in greater detail three typical control structures arising from the final times $t_f = 6$, $t_f = 7.5$ and $t_f = 12$.

A. *Final time $t_f = 6$: bang-bang and singular arcs*

A first approximation of the optimal control is calculated with the use of the MSE [14], [16] with only bang-bang controls admitted. The state equations (7) – (9) and adjoint equations (11) – (13) are solved by the RK4 method. The derivative of the cost (10) with respect to a switching time t_i is equal to the jump of the Hamiltonian

$$\nabla_{t_i} J = H[t_i+] - H[t_i-] \ . \quad (30)$$

A BFGS gradient optimization scheme is employed. After 150 iterations (gradient computations) the results depicted in Figures 1 and 2 are obtained, with 94 switchings and the cost equal to -629.1974099. This should be compared with -629.1975893, the optimal value with ten digit accuracy. It is worth noting that the optimal result for bang-bang controls with only four switchings is -629.0822, which shows that the singular control arc in this case is more of theoretical than practical interest. These results suggest the following structure of optimal control

$$u(t) = \begin{cases} 0 & \text{for} \quad 0 \le t < t_1 \\ u_s(X(t), S(t), V(t)) & \text{for} \quad t_1 \le t < t_2 \\ 1 & \text{for} \quad t_2 \le t < t_3 \\ 0 & \text{for} \quad t_3 \le t \le t_f \end{cases} \quad (31)$$

where $0 < t_1 < t_2 < t_3 < t_f$. The control is singular in the interval $[t_1, t_2[$, and is determined by the feedback expression (26). Precise values of the switching times t_1, t_2 and t_3, the optimal control in the singularity interval and the final approximation of the optimal state and adjoint trajectories can be determined by the following two approaches.

MSE method [14], [15], [16]. We admit arcs that are either boundary or candidate singular (interior). The adjoint equations for candidate singular arcs are given by (27)–(29),

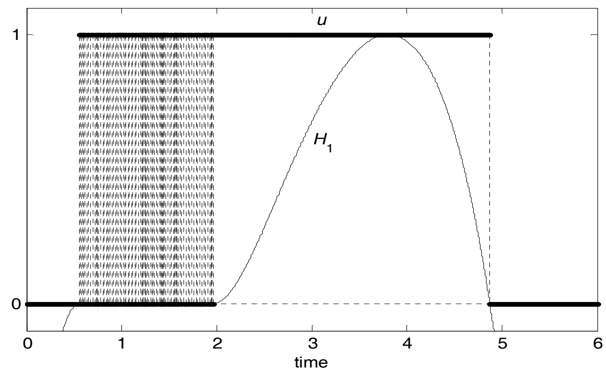

Fig. 1. Approximation of optimal solution: control u and normalized switching function H_1

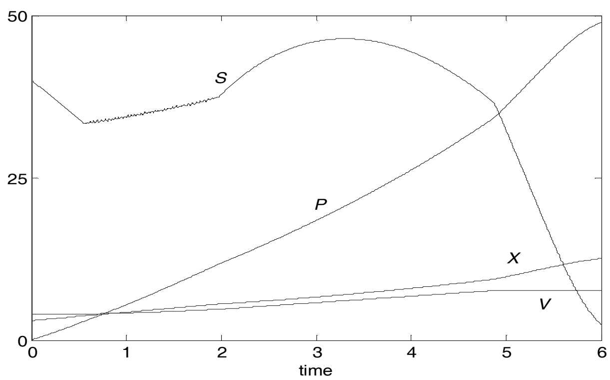

Fig. 2. Approximation of optimal solution: state variables

and by (11) – (13) elsewhere. The derivative of the cost (10) with respect to a control discontinuity point is computed again from (30) with the respective adjoint solution used in the Hamiltonian.

In this application, only spike and saturation generations are used. A spike generation consists in adding two nodes at the same point $\tau \in]0, t_f[$, or one node at $\tau = 0$ or $\tau = t_f$. A seed of a new arc is thus planted into the structure. The procedure for control calculation in the new spike is selected as follows. The arc is candidate singular, if

$H_1[\tau] > 0$ and $u(\tau) < u_s[\tau] < 1$ or

$H_1[\tau] < 0$ and $0 < u_s[\tau] < u(\tau)$.

If neither of these occurs, the upper control bound is taken when $H_1[\tau] > 0$ and $u(\tau) < 1$, and the lower bound when $H_1[\tau] < 0$ and $u(\tau) > 0$. Besides, the rules of Section 3.4 in [14] are applied. The nodes coinciding with discontinuity points are the only decision variables. For a more detailed description of the MSE generations, see [16].

The optimization is started with a bang-bang control that switches from 0 to 1 at $t = 3$. During the optimization the control structure evolves in a number of generations and reductions. The first spike generation from the upper to lower bound is shown on the right of the first plot of Fig. 3. After a few iterations in a constant decision space, two other generations to u_s occur (second plot). Further optimization leads to an expansion of the new interior arcs (third plot). Finally, after two reductions and combining two interior arcs into one, we obtain the optimal control shown in the last plot of Fig. 3. The 10 digit optimal value of the cost -629.1975893 is attained in 33 iterations. The dimension of decision space varies from 1 to 6, to reach the final value of 3 in the 28th iteration when the optimal structure of control is obtained. The optimal switching times are: $t_1 = 0.5536278$, $t_2 = 1.969518$, $t_3 = 4.874455$.

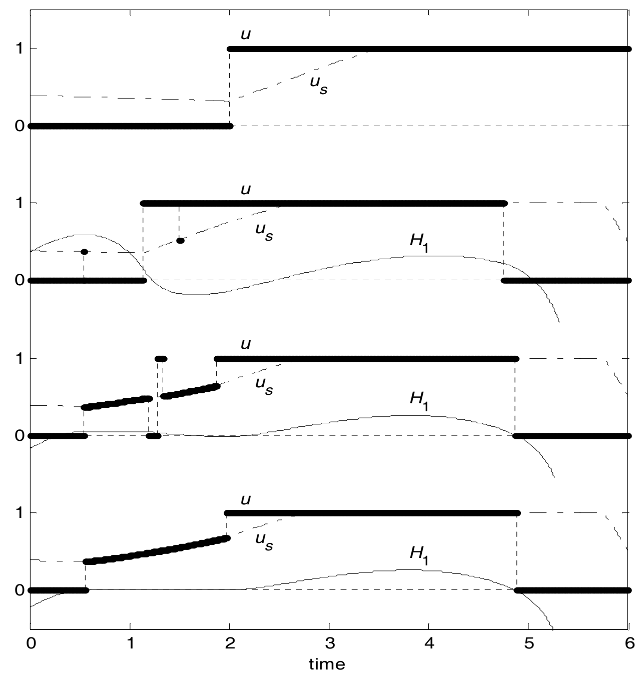

Fig. 3. Control structure evolution

Arc-parameterization method [9], [17], [18], sufficient conditions and sensitivity analysis. After assuming the control structure (31) with the singular feedback control $u_s(X, S, V)$, the optimal control problem is equivalent to a nonlinear programming problem, where the switching times t_1, t_2, t_3 are the sole decision variables. This problem can be solved very fast. The arc-parameterization in [9] was originally designed to optimize switching times for purely bang-bang controls. It is straightforward to extend this method to control functions that are given in feedback form on some intervals. Rather than optimizing the switching times t_i, it is more convenient to optimize the vector $z := (\xi_1, \xi_2, \xi_3)$ of *arclengths* defined by

$$\xi_1 = t_1,\ \xi_2 = t_2 - t_1,\ \xi_3 = t_3 - t_2\,.$$

The terminal arclength then is given by $\xi_4 = t_f - \xi_1 - \xi_2 - \xi_3$. The arc-parameterization method can be efficiently implemented using the code NUDOCCCS developed by Büskens [2], [3], [4]. This code was originally designed to solve nonlinear programming problems arising from discretizations of optimal control problems.

The integration steps in the arc-parameterization method are either performed with a high-order Runge-Kutta method or the routine RADAU5 [6] using a local error tolerance of 10^{-14}. The computed arclengths and switching times differ very little from those obtained by the MSE method:

$$\begin{array}{ll} \xi_1 = 0.5536212, & t_1 = 0.5536212, \\ \xi_2 = 1.415916, & t_2 = 1.969538, \\ \xi_3 = 2.904918, & t_3 = 4.874456, \\ \xi_4 = 1.125545, & t_f = 6.000000. \end{array}$$

The cost value $J(u) = -629.1975893$ is identical with that obtained by the MSE method. The computed initial values of the adjoint variables are $\psi_1(0) = 111.2389$, $\psi_2(0) = -5.751498$, $\psi_3(0) = 104.1716$. Thus, we can show that all *necessary* optimality conditions are satisfied with high precision.

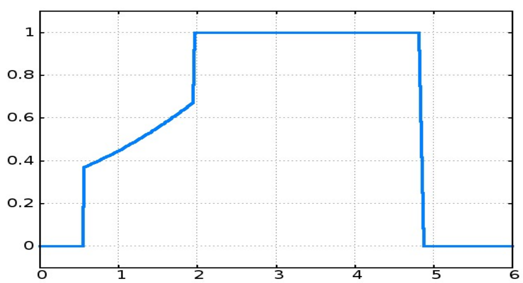

Fig. 4. Final time $t_f = 6$: optimal control by NUDOCCCS

Up to now, we were not able to show that some kind of *sufficient optimality conditions* hold for the computed extremal solution. The example seems to be too complex to apply *synthesis analysis* along the lines of Piccoli, Sussmann [11], Ledzewicz, Schättler [8]. So far, a suitable extension of the second-order sufficient conditions for *purely* bang-bang controls [1], [10] to bang–singular controls has not yet been reported in the literature.

However, we can at least verify that second-order sufficient conditions are satisfied for the induced optimization problem with respect to the vector $z = (\xi_1, \xi_2, \xi_3)$ of arclengths. The numerical test of second-order condtions is an additional option provided by the code NUDOCCCS [2], [3], [4]. The cost functional $J(u)$ in (10) reduces to the function $\mathcal{J}(z)$ of the arclengths z. The Hessian of $\mathcal{J}(z)$ is computed as

$$\mathcal{J}_{zz} = \begin{pmatrix} 58.0555 & 5.22847 & -11.0766 \\ 5.22847 & 104.031 & 145.445 \\ -11.0766 & 145.445 & 211.266 \end{pmatrix}$$

The Hessian is positive definite, since its smallest eigenvalue is 0.6648. Thus we conclude that switching times provide a local minimum for the given control structure (31).

This second-order condition has an important consequence for the stability and sensitivity of solutions depending on a parameter in the control system. Suppose that p is any parameter or perturbation vector which can vary in a certain range around its nominal value p^0. It follows from the Implicit Function Theorem that the perturbed switching times $t_i(p)$ or arclengths $\xi_i(p) (i = 1, 2, 3)$ exist in a small neighborhood of p^0 and are C^1–functions with respect to p. Moreover, the singular control (26) can be computed as a parametric feedback expression $u_s(X, S, V, p)$. Then the perturbed optimal control $u(t, p)$ has the same structure as in (31) with switching times $t_i(p)$, $i = 1, 2, 3$.

An easily implementable real-time control approximation of the perturbed optimal control is based on the computation of the first order parametric sensitivity derivatives $d\xi_i/dp, i = 1, 2, 3$, resp., $dt_i/dp\,(i = 1, 2, 3)$ or uses higher order derivatives. These quantities can be computed *off-line* via a well known sensitivity formula as a byproduct of the optimization process; cf., [5], [2], [3]. For the simplest *on-line approximations*, we approximate the exact switching times by their first order Taylor expansions

$$t_i(p) = t_i(p^0) + \frac{dt_i}{dp}(p^0)(p - p^0), \quad i = 1, 2, 3.$$

It is important to note that an approximation for the perturbed singular control is *not* needed, since its values are determined by the parametric feedback expression. For purpose of demonstration, let us choose the parameters $p = \mu$, $p = S_{\rm in}$, $p = y_p$ with nominal values $\mu^0 = 0.54$, $S^0_{\rm in} = 200$, $y^0_p = 0.43$. The sensitivity derivatives of arclengths provided by NUDOCCCS are given in Table I.

TABLE I

SENSITIVITY DERIVATIVES FOR PARAMETERS $\mu, S_{\rm in}, y_p$.

i	$d\xi_i/d\mu$	$d\xi_i/dS_{\rm in}$	$d\xi_i/dy_p$
1	$0.38725\,e+0$	$-0.54116\,e-2$	$-0.21448\,e+1$
2	$-0.12479\,e+2$	$0.52475\,e-1$	$0.86715\,e+1$
3	$0.19209\,e+2$	$-0.64572\,e-1$	$-0.12633\,e+2$

B. Final time $t_f = 7.5$: three bang-bang arcs

For the final time $t_f = 7.5$, both the MSE method and the code NUDOCCCS provide the following control structure with three bang-bang arcs:

$$u(t) = \begin{cases} 0 & \text{for} \quad 0 \le t < t_1 \\ 1 & \text{for} \quad t_1 \le t < t_2 \\ 0 & \text{for} \quad t_2 \le t \le t_f \end{cases} \qquad (32)$$

The switching times t_1, t_2, resp., arclenghts $\xi_1 = t_1$, $\xi_2 = t_2 - t_1$, $\xi_3 = t_f - \xi_1 - \xi_2$ are determined as

$$t_1 = \xi_1 = 0.47660075,\ \xi_2 = 6.5127971,\ t_2 = 6.9893979\,.$$

The cost is $\mathcal{J}(\xi_1, \xi_2) = -874.575953$. The initial values of adjoint variables are found as $\psi_1(0) = 139.4264$, $\psi_2(0) = -0.4950444$, $\psi_3(0) = 121.9677$. The Hessian of $\mathcal{J}(z)$ is computed as

$$\mathcal{J}_{zz} = \begin{pmatrix} 151.96 & 62.966 \\ 62.966 & 231.15 \end{pmatrix}$$

which is obviously positive definite. Hence, we conclude that the computed arclengths, resp., switching times provide a strict local minimum for the control structure (32). Moreover, in the bang-bang case we can apply the second-order sufficient conditions in [1], [10] to show that the computed control provides indeed a *strict strong minimum* for the optimal control problem. It suffices to check here that the switching function $H_1[t] = (-\psi_1(t)X(t) + \psi_2(t)(S_{\rm in} - S(t)))/V(t) + \psi_3(t)$ satisfies the *strict bang-bang property*

$$H_1[t] \neq 0 \quad \forall\, t \neq t_1, t_2\,, \quad \frac{dH_1}{dt}[t_1] > 0,\ \frac{dH_1}{dt}[t_2] < 0.$$

This property is a consequence of the numerical results for the state and adjoint variables. Note that sensitivity analysis and real-time approximations of perturbed control functions can be carried out in the same way as for the final time $t_f = 6$.

C. Final time $t_f = 12$: two bang-bang arcs

For larger final times t_f, the first bang-bang arc in (32) disappears. Therefore, the control has only one switch at t_1,

$$u(t) = \begin{cases} 1 & \text{for} \quad 0 \le t < t_1 \\ 0 & \text{for} \quad t_1 \le t \le t_f \end{cases}$$

The MSE and arc-parameterization methods yield the values $t_1 = 11.8151803$, $\mathcal{J}(t_1) = -1348.87986$. NUDOCCCS provides the second derivative $d^2\mathcal{J}/dt_1^2 = 625.72$. The initial values of adjoint variables are given by $\psi_1(0) = 1.568899$, $\psi_2(0) = 0.05192783$, $\psi_3(0) = 84.61079$. One verifies herewith that the *strict bang-bang property* holds: $H_1[t] \neq 0\ \forall\ t \neq t_1$, $\frac{dH_1}{dt}[t_1] < 0$. Hence, the computed control provides a strict strong minimum for the control problem.

Along these lines, optimal control structures can be analyzed for abitrary values of the time horizon t_f. The results are presented in Fig. 5.

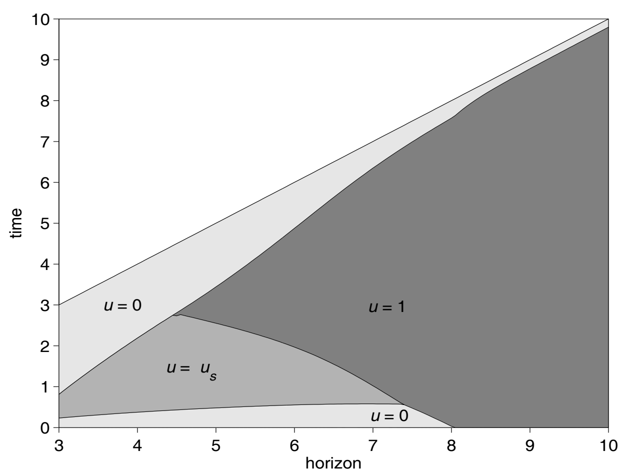

Fig. 5. Dependence of optimal control structure on time horizon t_f

VII. CONCLUSIONS

A dynamic optimization problem for a fedbatch fermentation process has been studied. It was shown that the structure of the optimal control with bang-bang and singular arcs depends crucially on the time horizon. An analytic expression for the singular optimal control has been derived in a state feedback form. The adjoint equations have been evaluated inserting the candidate singular control in the right-hand side of the state equations. These results enhance the efficiency of optimal control computations. The method of monotone structural evolution (MSE) has been applied which automatically generates the structure of the optimal control. A second method, based on arc-parameterization and using the code NUDOCCCS, confirmed the results and produced data for the sensitivity analysis of optimal solutions under parameter perturbations. Second order sufficient optimality conditions have been checked for the induced optimization problem wih respect to switching times and, in the bang-bang case, for the original control problem.

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