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Multiple shooting SQP-line search algorithm for optimal control of pressure-constrained batch reactor

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***Abstract*—In the article a new approach for control of a pressure-constrained batch reactor and a new multi-step optimization algorithm were presented. The considered batch reactor was described by both differential and algebraic equations. State constraints incorporate always difficulties into a mathematical model of the reactor, so a new algorithm based on a multiple shooting SQP-line search method was proposed and tested. The multiple shooting method was used not only to ensure a stability of the solution, but to divide a system into smaller subsystems, so a large-scale problem is considered. The considerations were made for a simultaneous approach, which allows to apply this algorithm to a wide class of differential-algebraic systems. The simulations were executed in Matlab environment using Wroclaw Centre for Networking and Supercomputing.**

***Index Terms*—optimal control, DAE systems, multiple shooting method, state constraints.**

I. Introduction

SEARCHING for controls that will result in a desired behavior of a system plays a key role in a process design [1], [2], [11]. To describe the system often only algebraic equations are enough. Especially, when changes in the state variables are slow and algebraic equations accurately reflects the behavior of the system. More complex processes are described by differential equations. Suitable numerical methods and optimization algorithms were proposed and implemented, so it is a group of well-known problems . It seems, that the most important feature of the differential systems is a existence of a solution for all initial conditions. Difficulties may, however, be caused by the instability of the equations and selection of the appropriate numerical methods for the equations [5].

Often, however, it happens that there are in the system simultaneously both algebraic and differential relations. Description with the system of equations, which can be easily divided in part consisting solely of differential equations and a group of algebraic equations is desirable for several reasons. (1) During the construction of the mathematical model one does not need to perform additional transformations to obtain allowed equations. (2) The variables in a model are known to have physical interpretation. When the equations are well scaled, then no other transformations are needed. Additionally, (3) one can explore the impact of different variables on the behavior of the model. But the searching for the solution of the initial value problem for differential-algebraic equations, which does not exist for all possible values of parameters, was always a challenge [3], [8], [9].

The main motivation of this paper is to present an algorithm, which can treat the large-scale optimal control problem. Every system with path constraints on state trajectory can be considered as an optimization problem with arbitrarily large number of variables [2]. Even systems with simple path constraints, but with large number of decision variables, may require a huge computational effort. The aim of this paper is to present a feasible-type algorithm that improves a feasible initial solution of a large-scale problem in a reasonable time. These features enable the use of this approach in the task of design and control of chemical processes.

The pressure-constrained batch reactor is usually described by the nonlinear differential-algebraic equations [6]. The control problem of the chemical reactor belongs to the group of tasks, the size of which is not clearly defined. Especially if the model takes into account constraints on the state variables. The statement that the size of the task is infinitely large does not help much in solving the problem. The practical approach leads to the use of the existing finite-dimensional methods.

To solve the control problem of the chemical reactor with the constraints on state variables, the new multi-step algorithm was designed. Its particular advantage is the possibility to take into account the large number of variables and to preserve the feasibility of all iterates, which start from the feasible initial conditions. The study was carried out on the large-scale task of about 4 000 variables and 3 000 differential equations [4]. The algorithm combines the multiple shooting method and the simultaneous approach.

The article is structured as follows. At the beginning the optimal control problem of DAE system was formulated. Then the simultaneous approach for the optimal control of differential algebraic systems and its relationship with the multiple shooting method is discussed. The Multi-step SQP-line search algorithm using the multiple shooting method is presented. The differential-algebraic model of the pressure constrained batch reactor is described and solved by the designed algorithm. Finally, the results of the large-scale simulations, which were performed using Wroclaw Centre for Networking and Supercomputing, were discussed.

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II. The simultaneous approach for multiple shooting optimal control of differential-algebraic systems

In the paper the following multiple shooting optimal control problem of differential-algebraic systems is considered

$$\min_{p} \phi(p) = \sum_{l=1}^{N_T} \Phi(z^l(t_l), y^l(t_l), p^l), \tag{1}$$

subject to

$$z^{l-1}(t_{l-1}) = z_0^l = 0; \qquad l = 2, \ldots, N_T, \tag{2}$$

$$z^{N_T}(t_{N_T}) - z_f = 0; \qquad z^l(0) = z_0^l, \tag{3}$$

$$p_L^l \leq p^l \leq p_U^l, \tag{4}$$

$$y_L^l \leq y^l(t_l) \leq y_U^l, \tag{5}$$

$$z_L^l \leq z^l(t_l) \leq z_U^l; \quad l = 1, \ldots, N_T, \tag{6}$$

with the DAE system

$$\frac{dz^l(t)}{dt} = f^l(z^l(t), y^l(t), p^l); \qquad z^l(t_{l-1}) = z_0^l, \tag{7}$$

$$g^l(z^l(t), y^l(t), p^l) = 0; t \in [t_{l-1}, t_l]; l = 1, \ldots, N_T. \tag{8}$$

In equations (1)-(8) $z(t)$ denotes the differential state trajectory and $y(t)$ denotes the algebraic state trajectory. The control profile is represented as a parametrized function with coefficients that determine the optimal profil [12], [13]. The decision variables on DAE equations appear only in the time independent vector p. The assumption on the invertibility of $g(-, y(t), -)$ permits an implicit elimination of the algebraic variables $y(t) = y[z(t), p]$ [3]. While there are N_T periods in DAE equations, the time dependent bounds and other path on the state variables are no longer considered. The algebraic constraints and terms in the objective function are applied only at the beginning of each period.

The mentioned optimal control problem of the reactor is an example of wide range control problems of systems described by differential-algebraic equations (eg. [11]). The instability of this type of equation resulted in development of shooting methods. The shooting method was adjusted for solving more difficult systems and is usually known as the multiple shooting method or the parallel shooting method. As a result of the application of the shooting methods, tested systems exhibit new properties, which could not be expected considering the general formulation of the optimal control problem of DAE systems. 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 the continuity of the states across elements, the equality constraints are added to the nonlinear program. The inequality constraints for states and controls are then imposed directly at the grid points t_l [1].

The aim of the simultaneous approach is searching for the optimal control trajectory, the differential and algebraic state trajectories in a special manner. A sketch of the sequential

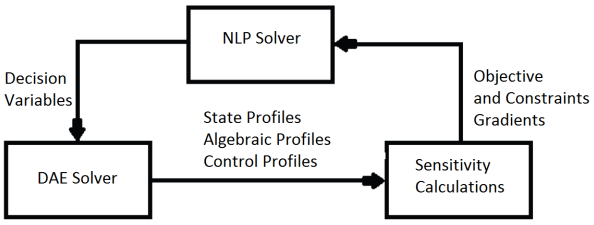

Fig. 1. Sequential dynamic optimization strategy.

dynamic optimization strategy for the problem (1)-(8) is presented on Fig. 1. At l-iteration, the variables p^l are specified by NLP solver. In this situation, when the values of p^l are known, one can treat DAE system as an initial value problem and integrate (2)-(4) forward in time for periods $l = 1, \ldots, N_T$. For these purposes Backward Differentiation Formula was used, which can solve index-1 DAEs. The Differential state profile, the algebraic state profile and the 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 information are passed to the NLP solver, then the decision variables can be updated [2].

III. Dynamic optimization of the pressure-constrained batch reactor

The reactions taking place in the reactor are

$$A \xrightarrow{k_1} 2B, \tag{9}$$

$$2B \xrightarrow{k_2} A, \tag{10}$$

$$A + B \xrightarrow{k_3} D. \tag{11}$$

The dynamic optimization problem is described as follows

$$\min_{F} J = C_D(t_f), \tag{12}$$

subject to

$$\dot{C}_A = -k_1 C_A + k_2 C_B C_B + \frac{F}{V} - k_3 C_A C_B, \tag{13}$$

$$\dot{C}_B = k_1 C_A - k_2 C_B C_B - k_3 C_A C_B, \tag{14}$$

$$\dot{C}_D = k_3 C_A C_B, \tag{15}$$

$$N = V(C_A + C_B + C_D), \tag{16}$$

$$PV = NRT, \tag{17}$$

$$P \leq 340000, \tag{18}$$

$$0 \leq F \leq 8.5, \tag{19}$$

$$[C_A(0), C_B(0), C_D(0)] = [100, 0, 0]. \tag{20}$$

The rate constants are $k_1 = 0.8$ per h, $k_2 = 0.02\ m^3/(mol \cdot h)$, $k_3 = 0.003\ m^3/(mol \cdot h)$, the volume $V = 1.0\ m^3$, the temperature $T = 400\ K$. There is one path constraint on the state variable P. The process duration is 2 hours.

The task is to find the optimal flow rate profile, which is treated as a control variable, to minimize the objective function (12). There are some possibilities of parametrization of the control variable. The most popular are piecewise constant, piecewise linear with continuity, piecewise linear without continuity, piecewise quadratic with continuity [12]. In [6] the simultaneous approach with piecewise linear parametrization with continuity was considered. It means, that for 11 time intervals the size of NLP was originally 42, and 35 by model decomposition method presented in this article. Because "the optimal control is highly nonlinear which makes this problem difficult for general control parametrization methods" [6], the new control algorithm for the simultaneous approach with constant parametrization of the control variables was proposed and tested. So, there are decision variables connected only with the control function and the state variables.

IV. The Multi-step SQP line search algorithm

The designed algorithm belongs to a group of the Sequential Quadratic Programming methods [10]. Its main part is as follows.

The equality constrained problem is considered

$$\min_p f(p), \tag{21}$$

subject to

$$c(p) = 0, \tag{22}$$

where the objective function $f : \mathcal{R}^n \to \mathcal{R}$ and the vector of equality constraints $c : \mathcal{R}^n \to \mathcal{R}^m$ are smooth functions. The idea behind the SQP approach is to model (21)-(22) at the current iterate p_k by a quadratic programming subproblem. Then the subproblem is minimized and the new iterate p_{k+1} is defined.

The Lagrangian function for this problem is

$$\mathcal{L}(p, \lambda) = f(p) - \lambda^T c(p). \tag{23}$$

The matrix $A(p)$ were used to denote the Jacobian matrix of the constraints

$$A(p) = [\nabla c_1(p), \nabla c_2(p), \ldots, \nabla c_m(p)]^T, \tag{24}$$

where $c_i(p)$ is the ith component of the vector $c(p)$.

The first order KKT conditions of the equality constrained problem (21)-(22) can be written as the system on $n + m$ equations and the $n + m$ unknowns p and λ,

$$\begin{bmatrix} \nabla f(p) - A(p)^T \lambda \\ c(p) \end{bmatrix} = 0. \tag{25}$$

Any solution (p^*, λ^*) of the equality constrained problem (21)-(22) for which $A(p^*)$ has full row rank satisfies (25). The nonlinear system (25) can be solved by the Newton method.

The Jacobian of (25) with respect to p and λ is given by

$$\begin{bmatrix} \nabla^2_{pp}\mathcal{L}(p, \lambda) & -A(p)^T \\ A(p) & 0 \end{bmatrix} = 0. \tag{26}$$

The Newton step from the iterate (p_k, λ_k) is given by

$$\begin{bmatrix} p_{k+1} \\ \lambda_{k+1} \end{bmatrix} = \begin{bmatrix} p_k \\ \lambda_k \end{bmatrix} + \begin{bmatrix} d_k \\ d_\lambda \end{bmatrix}, \tag{27}$$

where d_k and d_λ solve the Newton-KKT system

$$\begin{bmatrix} \nabla^2_{pp}\mathcal{L}(p, \lambda) & -A(p)^T \\ A(p) & 0 \end{bmatrix} = \begin{bmatrix} d_k \\ d_\lambda \end{bmatrix} + \tag{28}$$

$$+ \begin{bmatrix} -\nabla f(p) + A(p)^T \lambda \\ -c(p) \end{bmatrix},$$

The Newton step is well defined when KKT matrix in (26) is nonsingular. This is satisfied, when the following assumptions hold [10]

Assumption 1: The Jacobian of the constraints $A(p)$ has full row rank.

Assumption 2: The matrix $\nabla^2_{pp}\mathcal{L}(p, \lambda)$ is positive definite on the tangent space of the constraints, that is, $d^T \nabla^2_{pp}\mathcal{L}(p, \lambda)d > 0$ for all $d \neq 0$ such that $A(p)d = 0$.

Suppose that at the iterate (p_k, λ_k) the problem (21)-(22) is modeled by the quadratic program

$$\min_p f_k + \nabla f_k^T p + \frac{1}{2}\nabla^2_{pp}\mathcal{L}_k p, \tag{29}$$

subject to

$$A_k(p) + c_k = 0. \tag{30}$$

If Assumptions 1 and 2 hold, then this problem has the unique solution (d_k, l_k) that satisfies

$$\nabla^2_{pp}\mathcal{L}_k d_k + \nabla f_k - A_k^T l_k = 0, \tag{31}$$

$$A_k d_k + c_k = 0. \tag{32}$$

The vectors d_k and l_k can be identified with the solution of the Newton equation (28).

ALGORITHM 1. Local SQP Algorithm for solving the equality constrained problem

Choose an initial par (p_0, λ_0);
  (if p_0 is given, then λ_0 is given by eq. (25))
Set $k \leftarrow 0$;
REPEAT UNTIL convergence test is satisfied
  evaluate f_k, ∇f_k, $\nabla^2_{pp}\mathcal{L}_k$, c_k, A_k;
  solve (29)-(30) to obtain d_k and l_k;
  set $p_{k+1} \leftarrow p_k + d_k$; $\lambda_{k+1} \leftarrow l_k$;
END (REPEAT)

On this basis, the new algorithm was designed.

ALGORITHM 2. The line search SQP algorithm

choose parameters $\eta \in (0, 0.5)$, $\tau \in (0, 1)$
and an initial pair (p_0, λ_0);
evaluate $f(p_0)$, $\nabla f(p_0)$, $c_i(p_0)$,
$A_0 = [\nabla c_1(p_0), \nabla c_2(p_0), \ldots, \nabla c_m(p_0)]^T$;
if a quasi-Newton approximation is used, choose
an initial $n \times n$ symmetric positive definite Hessian
approximation B_0, otherwise compute $\nabla^2_{pp}\mathcal{L}_0$;
WHILE convergence test is not satisfied DO
  compute d_k by solving (28), let λ be
  the corresponding multiplier;
  $d_\lambda \leftarrow \hat{\lambda} - \lambda_k$;
  choose μ_k to satisfy eq. (33) with $\sigma = 1$;
  set $\alpha_k \leftarrow 1$;
  WHILE $\Phi_1(p + \alpha_k d_k; \mu_k) >$
    $\Phi_1(p_k; \mu_k) + \eta\alpha_k D_1(f(p_k; \mu_k); d_k)$ DO
    reset $\alpha_k \leftarrow \tau_\alpha \alpha_k$ for some $\tau_\alpha \in (0, \tau]$;
  END (WHILE)
  set $p_{k+1} \leftarrow p_k + \alpha_k d_k$ and $\lambda_{k+1} \leftarrow \lambda_k + \alpha_\lambda d_\lambda$;
  IF a quasi-Newton approximation is used THEN
    set $s_k \leftarrow \alpha_k d_k$;
    set $\hat{y}_k \leftarrow \nabla_p \mathcal{L}(p_{k+1}, \lambda_{k+1}) - \nabla_p \mathcal{L}(p_k, \lambda_{k+1})$;
    obtain B_{k+1} by updating B_k using
    a quasi-Newton formula
    $B_{k+1} = B_k + \frac{(\hat{y}_k - B_k s_k)(\hat{y}_k - B_k s_k)^T}{(\hat{y}_k - B_k s_k)^T s_k}$
  END (IF)
END (WHILE)

The strategy for choosing μ in the Algorithm 2 considers the effect of the step on a model of the merit function, so μ has to satisfy the inequality

$$\mu \geq \frac{\nabla f_k^T d_k + \frac{\sigma}{2} d_k^T \nabla^2_{pp}\mathcal{L}_k d_k}{(1-\rho)\|c_k\|_1}. \tag{33}$$

If the value of μ from the previous iteration of the SQP method satisfies eq. (33), it is left unchanged. Otherwise, μ is increased, so that satisfies this inequality with some margin. The constant σ is used to handle the case in which Hessian $\nabla^2_{pp}\mathcal{L}_k$ is not positive definite. We define $\sigma = 1$ if $d_k^T \nabla^2_{pp}\mathcal{L}_k d_k > 0$, and $\sigma = 1$ otherwise.

The l_1 merit function for the problem (21)-(22) takes the form

$$\Phi_1(p; \mu) = f(p) + \mu\|c_k\|_1. \tag{34}$$

The directional derivative of Φ_1 in the direction d_k satisfies

$$D(\Phi_1(p_k; \mu); d_k) = \nabla f_k^T d_k - \mu\|c_k\|_1. \tag{35}$$

ALGORITHM 3. The SQP-line search algorithm for solving the equality constrained problem

BEGIN
  define a vector of decision variables $\tilde{p}$
    and its initial conditions;
  choose from vector $\tilde{p}$ a subvector p,
    which describes a subsystem
    $S = f(p)$
  solve problem (36) using Algorithm 2;
  update values of vector $\tilde{p}$ using results
    from the previous step;
END

As one can see, the Algorithm 2 can be thought as an inner loop in Algorithm 3. The last question is, what is the rate of convergence of the considered algorithm.

Assumption 3: The point p^* is a local solution of the problem (21)-(22) at which the following conditions hold.

a) The functions f and c are twice differentiable in a neighborhood of p^* with Lipschitz continuous second derivatives.

b) The linear independence constraint qualification holds at p^*.

c)The second order sufficient conditions hold at (p^*, λ^*).

Now one can call the theorem, which justifies the correctness of the presented algorithm.

Theorem ([10]): Suppose, that Assumption 3 holds and that the iterates p_k generated by Algorithm 1 with guasi-Newton approximate Hessian B_k, converge to p^*. Then p_k converges superlinearly if and only if the Hessian approximation satisfies

$$\lim_{k\to\infty} \frac{\|(B_k - \nabla^2_{pp}\mathcal{L}_*)(p_{k+1} - p_k)\|}{\|p_{k+1} - p_k\|} = 0. \tag{36}$$

Lemma 4: Algorithm 3 generates a sequence of the feasible solutions with decreasing values of the goal function. In this bounded sequence one can distinguish a subsequence, which is superlinearly convergent to the locally optimal solution p^*.

V. Numerical results

Simulations were executed on the large-scale model of the pressure-constrained batch reactor.

When the model was divided into 1 000 submodels, then for solving the KKT system more than 24 hours was needed. So, the reactor was divided into 100 parts and the solution was obtained in 12 hours. At this step the vector of decision variables was stated as follows

$$p = [u_1 \cdots u_{100}, C_{A0,2} \cdots C_{A0,100}, \tag{37}$$
$$C_{B0,2} \cdots C_{B0,100}, C_{D0,2} \cdots C_{D0,100}].$$

Solution of this model was used as the initial conditions in the further work.

The question is, how to choose the vector of decision variables, to obtain in a reasonable time a possibly greatest improvement of the solution.

Then the reactor was divide into 1 000 parts. There are 3 997 decision variables in the system (1 000 piecewise

TABLE I
RESULTS OF THE SIMULATIONS IN CASE 1.

Size of subvector p	Number of iterations	$\bar{d}$
10	37	$8.6448e-004$
20	17	$8.4317e-004$
50	6	$9.3396e-004$
100	3	$9.3396e-004$

TABLE II
RESULTS OF THE SIMULATIONS IN CASE 2.

Size of subvector p	Number of iterations	$\bar{d}$
10	130	$7.5896e-004$
20	82	$7.6063e-004$
50	40	$7.6116e-004$
100	19	$7.6136e-004$

constant control functions and 2 997 variables treated as initial conditions for differential state trajectories).

$$\widetilde{p} = [u_1 \cdots u_{1000}, C_{A0,2} \cdots C_{A0,1000}, \quad (38)$$
$$C_{B0,2} \cdots C_{B0,1000}, C_{D0,2} \cdots C_{D0,1000}].$$

The simulations were executed for 4 different possible number of variables in the subvector $\widetilde{p}$: 10, 20, 50 and 100. As decision variables only control function, especially in the initial phases of the process, were considered. This enables increase the accuracy of the calculation, when the reactions proceed quickly. The initial average discontinuity in the state variables was $\bar{d} = 1.1e-3$ and $C_D(t_f) = 10.7240\ mol/m^3$. The final value of $C_D(t_f)$ is about 8.7% better then result presented in [6].

In the simulations two different stop criteria in Algorithm 2 were used. In the implementation convergence is declared when $TolFun < \epsilon_1$ and $TolCon < \epsilon_2$. $TolFun$ denotes termination tolerance on the function value, and $TolCon$ denotes tolerance on the constraint violation.

1) Case 1: In the first case the local optimization processes were performed more precisely. So, $TolFun < 1e-6$ and $TolCon < 1e-6$.

2) Case 2: In the second case stop criterion in local optimization were no so rigorous: $TolFun < 1e-3$ and $TolCon < 1e-3$.

The main stop criterion was the performance time. When computing time exceeded 12 hours, then optimization process was stopped.

In both cases the augmented objective function was considered

$$f(p) = C_D(t_f) + \rho \sum_{l=1}^{N_T} (z_0^{l+1} - \hat{z}_l)^2, \quad (39)$$

where penalty parameter $\rho = 10^6$.

Equation (39) shows the balance in the quest to minimize the concentration of component D and to meet the continuity constraints in differential-algebraic equations.

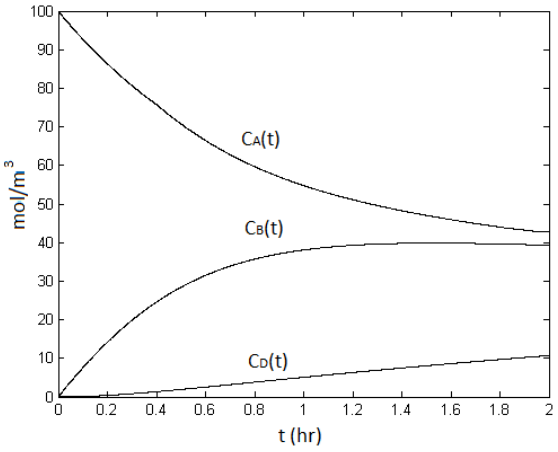

Fig. 2. Differential state trajectories. Results for size of subvector p=10. Stop criteria like in case 2.

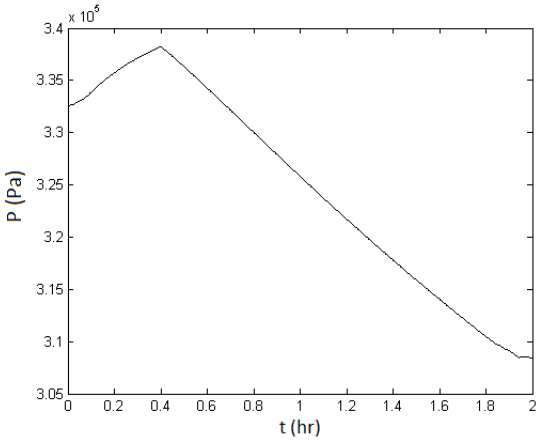

Fig. 3. The optimal pressure trajectory.

Results presented in the Table 1 and Table 2 show, that the inexact algorithm with the weak stop criteria, can obtain a better improvement of the initial solution.

As it was mentioned, in the considered problem two opposite tasks were considered. The minimization of the component D stands in opposition to fulfilment the constraints. As a result, the final concentration was improved and the obtained solution meets the constraints with high accuracy, so this method can be applied in real-life chemical processes.

The solutions obtained for size of the subvector $p = 10$ and stop criteria like in case 2 were presented on the figures 2-4. There are the differential state trajectories in the figure 2, the optimal pressure trajectory in the fig. 3 and the optimal flowrate profile in the fig. 4

VI. CONCLUSION

In the article the task of control of the pressure-constrained batch reactor was considered. The complex model of the reactor was designed using the simultaneous approach. The

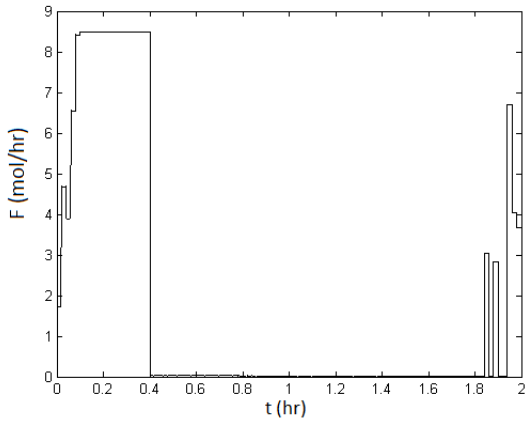

Fig. 4. Control variable - the optimal flowrate profile.

new SQP-line search algorithm was designed and tested. The algorithm, which takes in each iteration only a few number of decision variables into account, can do new iterations and improve the initial solution. But in both approaches a large number of variables were considered.

Because in the pure form, SQP algorithm is convergent to the locally solution, line search was used as a globalization approach to construct a sequence of feasible solutions with decreasing values of the objective function.

This type of algorithms can be successfully applied to the large systems, when Jacobian and Hessian matrices are dense and structure of these matrices can not be effectively used.

As the conclusion we want to pay attention to need for solver for the large-scale optimization and optimal control problems. Second order information, which can be approximated using BFGS method, can be unavailable when Jacobian matrix is difficult to calculate. This situation one can be met very often, when simultaneous approach is used. Multistep algorithms, which need feasible initial conditions, can improve the solution in considerable short time. At the end we want to emphasize the need for Jacobian-free optimization algorithm, which could solve the large-scale optimization tasks [7].

VII. Nomenclature

C	concentration (mol/m^3)
$\bar{d}$	average discontinuity in the state variables
F	flowrate (mol/hr)
f	objective function in optimization problem
g	function of algebraic constraints
k_1, k_2, k_3	rate constants
N_T	number of shots
n, m	dimensions of the space
p	vector of decision variables
S	function describing subproblem
t	time (hr)
z	state variables
y	algebraic variables
$\mathcal{L}$	Lagrangian function
$\mathcal{R}$	real numbers

Greek symbols

Φ	function describing optimization problem
ϕ	function describing system
λ	Lagrangian multipliers
ρ	penalty parameter
ϵ	tolerance

Superscripts

T	transposition of the matrix

Subscripts

A, B, D	components of the reaction
L	lower bound
U	upper bound
l	number of a shot

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