Proceedings of the 16th Conference on Computer Science and Intelligence Systems pp. 211–215
DOI: 10.15439/2021F47
ISSN 2300-5963 ACSIS, Vol. 25

A shortened time horizon approach for optimization with differential-algebraic constraints

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***Abstract*—In this work a new numerical optimization scheme based on a shortened time horizon approach was designed. The shortened time horizon strategy has never been presented or tested numerically. The new methodology was applied for a single objective optimization task subject to a system of nonlinear differential-algebraic constraints, which can take a form of differential-algebraic equations (DAEs). Moreover, it was assumed, that an application of a cooperated multiple shooting with direct solution method, like direct shooting approach, does not enable us to solve the DAE system, even on relatively small subintervals. Therefore, the new solution procedure is based on two main parts: i) designing of an alternative differential-algebraic constraints, ii) parametrization of a new constraints system by the multiple shooting approach and further simulation of the alternative system independently on small subintervals. Then, the simulation interval can be modified by the shortened time horizon approach. The presented algorithm was used to solve a highly nonlinear optimization task of a fed-batch reactor operation.**

***Index Terms*—numerical optimization, differential-algebraic constraints, shortened time horizon, multiple shooting method**

I. Introduction

The appropriate treatment of the nonlinear constraints can enable us to implement new numerical procedures, helpful in the model-based simulations [3], [4], [9]. In this work, the attention is paid on an optimization task with differential-algebraic constraints, which can take a form of differential-algebraic equations (DAEs). Classically, the systems of the nonlinear DAE constraints can be solved with the multiple shooting approach [6], [7], [11]. Unfortunately, even the multiple shooting methods can fail, when initial conditions are far from the solution trajectory [1], [2], [5]. Therefore, a shortened time horizon (STH) approach was considered as a tool to influence a difficulty of a nonlinear optimization task. The combination of the multiple shooing method with the STH approach can be treated as a base to design a new efficient optimization method subject to the nonlinear differential-algebraic constraints.

This article is constructed as follows. In Section 2 the shortened time horizon approach for DAE constraints is introduced. Then, in Section 3, the new solution procedure is presented. The results of numerical computations are discussed in Section 4. Finally, the presented considerations are summarized in Section 5.

This research was funded by the Department of Control Systems and Mechatronics at Wrocław University of Science and Technology.

II. The shortened time horizon for differential-algebraic constraints

In this work, a system of the nonlinear differential-algebraic constraints is considered

$$(DAE) \quad \left\{ \begin{array}{rcl} \dot{y}(t) & = & f(y(t), z(t), u(t), p, t) \\ 0 & = & g(y(t), z(t), u(t), p, t) \\ t & \in & [t_0 \quad t_f] \\ y(t_0) & = & y_0 \\ z(t_0) & = & z_0 \end{array} \right. \tag{1}$$

where the state of the DAE constraints (1) is represented by a vector of differential variables $y(t) \in \mathcal{R}^{n_y}$ and a vector of algebraic variables $z(t) \in \mathcal{R}^{n_z}$ with $\dot{y}(t) = \frac{dy(t)}{dt}$. Moreover, $u(t) \in \mathcal{R}^{n_u}$ denotes a vector of input functions. A vector of model parameters constant in time is represented by $p \in \mathcal{R}^{n_p}$, $t \in \mathcal{R}$ is an independent variable and a range of t is known *a priori*. The functions f and g are of C^2 class and

$$\begin{array}{ll} f: & \mathcal{R}^{n_y} \times \mathcal{R}^{n_z} \times \mathcal{R}^{n_u} \times \mathcal{R}^{n_p} \times \mathcal{R} \to \mathcal{R}^{n_y} \\ g: & \mathcal{R}^{n_y} \times \mathcal{R}^{n_z} \times \mathcal{R}^{n_u} \times \mathcal{R}^{n_p} \times \mathcal{R} \to \mathcal{R}^{n_z} \end{array} \tag{2}$$

The shortened horizon approach is based on an appropriate modification of a considered range of the assumed independent variable. The name of this method reflects, that in many cases *time* is considered as the natural independent variable. The shortened time approach is motivated, that the number of shooting intervals does not have to be known *a priori*. Therefore, the range of the independent variable is shortened according to the computational algorithms capabilities. Then, with a known solution obtained for a shortened range, the calculation can be continued iteratively for wider ranges of the independent variable.

Assumption 1. The range of the independent variable $t \in [t_0 \quad t_f]$ can be modified and parametrized by $q \in [0 \quad 1]$ in the shortened horizon approach as $t \in [q \cdot t_0 \quad q \cdot t_f]$.

Therefore, the formulation of the considered constraints (1) in the context of the shortened time horizon method takes a new form

$$\Big(DAE(q)\Big) \quad \left\{ \begin{array}{rcl} \dot{y}(t) & = & f(y(t), z(t), u(t), p, t) \\ 0 & = & g(y(t), z(t), u(t), p, t) \\ t & \in & [qt_0 \quad qt_f] \\ y(t_0) & = & y_0 \\ z(t_0) & = & z_0 \end{array} \right. \tag{3}$$

A direct shooting approach is one of a common used method to simulate the systems described by the nonlinear DAE constraints on the assumed interval of the independent variable (3). The mentioned approach is based on a multiple shooting, where a range of the independent variable $t \in [t_0 \quad t_f]$ is divided on an assumed number N subintervals

$$t^i \in [qt_0^i \quad qt_f^i], \qquad i = 1, \ldots, N \tag{4}$$

where

$$qt_0 = qt_0^1 < qt_f^1 = qt_0^2 < \cdots < qt_f^{N-1} = qt_0^N < qt_f^N. \tag{5}$$

Then, the DAE constraints (3) can be considered on each subinterval independently such, that

$$\Big(DAE^i(q)\Big) \left\{ \begin{array}{rcl} \dot{y}^i(t^i) & = & f^i(y^i(t^i), z^i(t^i), u^i(t^i), p, t^i) \\ 0 & = & g^i(y^i(t^i), z^i(t^i), u^i(t^i), p, t^i) \\ t^i & \in & [qt_0^i \quad qt_f^i] \\ y(t_0^i) & = & y_0^i \\ z(t_0^i) & = & z_0^i \end{array} \right. \tag{6}$$

for $i = 1, \ldots, N$. The variables $y^i(t), z^i(t), u^i(t)$ and p have a similar interpretation like in eq. (1). Moreover, the multiple shooting approach enable us a parametrization of both the state variables $y^i(t^i)$ and $z^i(t^i)$, as well as the input function $u^i(t^i)$, for $i = 1, \ldots, N$.

Assumption 2. On the given subinterval of the independent variable $t^i \in [t_0^i \quad t_f^i]$, the trajectory of the differential state variable $y^i(t^i)$ can be parametrized and represented by a new state variable $\widetilde{y}^i(t^i)$ modeled by a system of linear differential equation of the form

$$\dot{\widetilde{y}}^i(t^i) = D^i \widetilde{y}^i(t^i), \tag{7}$$

for $i = 1, \ldots, N$, where D^i is a $n_{y^i} \times n_{y^i}$ diagonal matrix.

Assumption 3. On the given subinterval of the independent variable $t^i \in [t_0^i \quad t_f^i]$, the trajectory of the algebraic state variable $z^i(t^i)$ can be parametrized and represented by a new state variable $\widetilde{z}^i(t^i)$ modeled by a system of linear algebraic equation of the form

$$0 = \widetilde{z}^i(t^i) - (A_{z^i} t^i + b_{z^i}), \tag{8}$$

for $i = 1, \ldots, N$, where A_{z^i} is a $n_{z^i} \times n_{z^i}$ diagonal matrix and b_{z^i} is a vector with n_{z^i} elements.

Assumption 4. On the given subinterval of the independent variable $t^i \in [t_0^i \quad t_f^i]$, the trajectory of the input function $u^i(t^i)$ can be parametrized and represented by a new input function $\widetilde{u}^i(t^i)$ modeled by a piecewise constant function of the form

$$0 = \widetilde{u}^i(t^i) - (b_{u^i}), \tag{9}$$

for $i = 1, \ldots, N$, where b_{u^i} is a vector with n_{u^i} elements.

Unfortunately, in general, the values of the initial conditions for state variables in shooting points are unknown

$$\mathbf{x_{y_0 z_0}} = \begin{bmatrix} y_0^1 & z_0^1 \\ \vdots & \vdots \\ y_0^N & z_0^N \end{bmatrix}. \tag{10}$$

Therefore, the unknown initial conditions $\mathbf{x_{y_0 z_0}}$ can be treated as an important part of decision variables in a nonlinear optimization task. Moreover, the parametrization variables, which define the trajectories of the state variables and the input function, can be used to built a matrix of decision variables

$$\mathbf{X} = \begin{bmatrix} y_0^1 & z_0^1 & d(A_{z^1}) & b_{z^1} & b_{u^1} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ y_0^N & z_0^N & d(A_{z^N}) & b_{z^N} & b_{u^N} \end{bmatrix}, \tag{11}$$

where an operator $d(B)$ denotes the diagonal elements of the matrix B.

To solve the new system of continuous differential-algebraic constraints, it is enough to assign arbitrary values to the decision variables matrix (11)

$$\Big(\widetilde{DAE^i}(q)\Big) \quad \left\{ \begin{array}{rcl} \dot{\widetilde{y}}^i(t^i) & = & D^i \widetilde{y}^i(t^i) \\ 0 & = & \widetilde{z}^i(t^i) - (A_{z^i} t^i + b_{z^i}) \\ 0 & = & \widetilde{u}^i(t^i) - (b_{u^i}) \\ t^i & \in & [qt_0^i \quad qt_f^i] \\ \widetilde{y}^i(t_0^i) & = & y_0^i \\ \widetilde{z}^i(t_0^i) & = & A_{z^i} t_0^i + b_{z^i} \\ \widetilde{u}^i(t_0^i) & = & b_{u^i} \end{array} \right. \tag{12}$$

for $i = 1, \ldots, N$.

To determine the matrix of decision variables (11), the additional pointwise algebraic constraints were imposed. They were used to force a continuity of the obtained state trajectories $\widetilde{y}(t)$ and $\widetilde{z}(t)$, ensure consistent initial conditions, as well as provide such models of original DAE constraints, that the dynamics of the obtained solutions will meet the primary constraints (1).

This approach results with a system of pointwise equality constraints consisted with concatenated vectors of specified restriction types

$$G(\mathbf{X}) = \begin{bmatrix} G_{cont}(\mathbf{X}) \\ G_{cons}(\mathbf{X}) \\ G_{dyn}(\mathbf{X}) \end{bmatrix} = 0, \tag{13}$$

where

$$G_{cont}(\mathbf{X}) = \begin{bmatrix} \widetilde{y}^1(t_f^1) - y_0^2 \\ \vdots \\ \widetilde{y}^{N-1}(t_f^{N-1}) - y_0^N \end{bmatrix}, \tag{14}$$

is a vector of the continuity constraints,

$$G_{cons}(\mathbf{X}) = \begin{bmatrix} g^1(y_0^1, \widetilde{z}^1(t_0^1), \widetilde{u}^1(t_0^1), p, t_0^1) \\ \vdots \\ g^N(y_0^N, \widetilde{z}^N(t_0^N), \widetilde{u}^N(t_0^N), p, t_0^N) \end{bmatrix}, \tag{15}$$

is a vector of the consistency constraints, as well as

$$G_{dyn}(\mathbf{X}) = $$

$$= \begin{bmatrix} D^1 y_0^1 - f^1(y_0^1, \widetilde{z}^1(t_0^1), \widetilde{u}^1(t_0^1), p, t_0^1) \\ \vdots \\ D^N y_0^N - f^N(y_0^N, \widetilde{z}^N(t_0^N), \widetilde{u}^N(t_0^N), p, t_0^N) \end{bmatrix}, \tag{16}$$

is a vector of the dynamical constraints.

Corollary 5. The $\widetilde{DAE}^i(q)$ model (12) is a special case of a linear differential-algebraic system with time-dependent coefficients

$$\begin{bmatrix} \dot{\widetilde{y}}(t) \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} D & 0 & 0 \\ 0 & I & 0 \\ 0 & 0 & I \end{bmatrix} \begin{bmatrix} \widetilde{y}(t) \\ \widetilde{z}(t) \\ \widetilde{u}(t) \end{bmatrix} - \begin{bmatrix} 0 \\ A_z t + b_z \\ b_u \end{bmatrix}. \tag{17}$$

The proposed methodology can be used to transform the system of highly nonlinear differential-algebraic constraints (1) into the system of linear differential-algebraic constraints (12) with pointwise algebraic constraints related with the continuity, consistency and dynamical constraints (13). The new system of constraints can be considered in the context of nonlinear optimization task

$$\min_{\mathbf{X}} F(\mathbf{X}), \tag{18}$$

where F is a scalar-valued objective function. The additional assumptions related to the F function need to be reflected in a chosen numerical optimization procedure used further in an inner loop of the shortened time horizon optimization algorithm.

III. The new algorithm

The steps of the new optimization approach were presented as the Shortened Time Horizon Optimization (STHO) Algorithm. The designed Algorithm requires some input information, which should be supplied in the Preliminary steps. The defined sequence $\{q_k\}_{k=0}^n$ determines a progress of the shortened time approach (step P 1 in the STHO Algorithm). In the other words, the interval of the independent variable in the kth outer loop iteration is $[q_k t_0 \quad q_k t_f]$. Moreover, the first value $q_0 = 0$ is defined and no more used. Then, the assumed number of shooting subintervals N is constant during the performed computations (P 2). To start the algorithm, the considered DAE constraints (1) are necessary to be inserted (P 3). Moreover, the values of n_y, n_z and n_u with a range of the independent variable $t \in [t_0 \quad t_f]$ are used to obtain the parametrized model of the differential-algebraic constraints. To start the outer loop, the matrix of the initial solution (11) needs to be defined (P 4).

The STHO Algorithm

Preliminaries

P 1 Define a sequence of $n+1$ elements $\{q_k\}_{k=0}^n$, where $q_0 = 0$ and $q_n = 1$.

P 2 Define a number of shooting subintervals $N \in \mathbb{N}^+$.

P 3 Define a system of DAE constraints (1) with values n_y, n_z, n_u and a range of the independent variable $t \in [t_0 \quad t_f]$.

P 4 Choose the initial solution matrix $\mathbf{X_0}$ (11).

The outer loop

FOR $k = 1, 2, \ldots, n$

O 1 Choose a value q_k.

O 2 Define subintervals $t^i \in [q_k t_0^i \quad q_k t_f^i]$, where $i = 1, \ldots, N$.

O 3 Define the new constraints models $\widetilde{DAE}^i(q_k)$.

O 4 Define the vector of algebraic constraints $G(\mathbf{X})$.

The inner loop

Find $\mathbf{X}^\star$ by solving the optimization task

$\min_{\mathbf{X}} F(\mathbf{X})$
subject to
$\widetilde{DAE}^i(q_k), \quad i = 1, \ldots N,$
$G(\mathbf{X}) = 0$

O 5 The obtained solution $\mathbf{X}^\star$ is the new initial solution for the next iteration of the outer loop $\mathbf{X}_0 = \mathbf{X}^\star$

END-FOR.

The optimization method is consisted of two main parts, which will be referred to as an outer- and inner loop. In the inner loop, a numerical optimization procedure solves a parametrized task subject to the differential-algebraic constraints (12), as well as additional equality restrictions (13) resulting from the multiple shooting method. The shortened time approach is a base for the outer loop of the new algorithm. It can take a form of a „for" iterations, where a q parameter is incremented according to the assumed way. The solution obtained as a result at a current iteration of the outer loop, is a starting point for the inner loop in the next outer iteration.

The outer loop is mainly concentrated around a nonlinear optimization task constructing for a given value q_k (O 1). In the steps (O 2) and (O 3), the appropriate subintervals t^i with the new models $\widetilde{DAE}^i$ are defined. Then, the DAE constraints and models $\widetilde{DAE}^i$ (P 3) will be used to calculate the system of pointwise algebraic constraints $G(\mathbf{X})$ (O 4). The constraints $G(\mathbf{X})$ represent similarity between the designed model (12) and the original DAE constraints (1).

The current task is solved in the inner loop by a chosen numerical optimization procedure. The solver can cooperate with a numerical integrator of the differential-algebraic constraints, although the new system of constraints (12) can be solved analytically in many cases. A selection of efficient numerical algorithms for constrained optimization is presented in [10].

IV. COMPUTATIONAL EXPERIMENTS

The algorithm designed in this study was implemented in Matlab environment and applied for solving optimization task of searching for optimal operation of a fed-batch reactor. The considered model is consisted on the differential and algebraic state variables

$$y(t) = [y_1(t) \quad y_2(t) \quad y_3(t) \quad y_4(t) \quad y_5(t)]^T \tag{19}$$

$$z(t) = [z_1(t) \quad z_2(t) \quad z_3(t)]^T, \tag{20}$$

as well as the objective function

$$\max_{u(t)} \quad y_1(t_f)y_5(t_f) \tag{21}$$

The differential-algebraic constraints with initial conditions for the differential state trajectories

$$y(t_0) = [0.0 \quad 0.0 \quad 1.0 \quad 5.0 \quad 1.0]^T \tag{22}$$

are based on the work of Luus and Rosen [8]. The initial conditions for the algebraic state variables $z(t_0)$ can be calculated based on the initial conditions of $y(t_0)$ (22). Moreover, the input function $u(t)$ is constrained by a pair of inequalities

$$0.0 \leq u(t) \leq 10.0 \tag{23}$$

The final value of the state variable y_4 is bounded by

$$y_4(t_f) \leq 14.35 \tag{24}$$

The process duration range was assumed and equal $t \in [0 \quad 25]$. The presented objective function (21) subject to the continuous differential-algebraic constraints, as well as the pointwise constraint (24), was parametrized by a direct shooting method with $N = 25$ subintervals. The parametrization resulted with new decision variables and continuity constraints.

The optimization task with the appropriate parametrization and introduced constraints was solved in three different ways

- case 1: minimization of the objective function extended by a penalty function,
- case 2: optimization with interior-point algorithm implemented in *fmincon* Matlab function,
- case 3: solution by the STHO algorithm presented in this work.

A. The task parametrization

According to the classical multiple shooting rules, the initial conditions of the differential state trajectories are treated as new decision variables. Then, the input function $u(t)$ was parametrized as a piecewise constant trajectory. Therefore, the vector of decision variables $\mathbf{X}$ was consisted of 146 elements. Moreover, to ensure the continuity of the obtained solution, additional 121 equality constraints were take into account. In this set of the decision variables and constraint functions, one decision variable together with one continuity constraint was introduced to represent the inequality (24). This is a basic multiple shooting parametrization used in numerical experiments in the case 1 and case 2.

In the case 3, the parametrization appropriate for the designed STHO algorithm was applied. At the beginning, the initial conditions of the differential state trajectories $\widetilde{y}(t)$, as well as the input function $\widetilde{u}(t)$ are parametrized in the same way like in the cases 1 and 2. Then, the additional variables were introduced to obtain parametrized systems $\widetilde{DAE^i}$: $n_y \times N = 5 \times 25 = 125$ variables for matrices D^i and $n_z \times 2 \times N = 3 \times 2 \times 25 = 150$ variables to parametrize the algebraic state trajectory $\widetilde{z}(t)$.

Moreover, 121 equality continuity constraints $G_{cont}(\mathbf{X})$, $3 \times 25 = 75$ equality consistency constraints $G_{cons}(\mathbf{X})$, as well as $5 \times 25 = 125$ equality dynamical constraints $G_{dyn}(\mathbf{X})$ were introduced. Finally, the optimization task with 421 decision variables, as well as the equality and box constraints was considered.

B. Numerical results

The simulations were started with a similar approach, to the one presented in the article [8]. In the case 1, the objective function was in a form of minimized penalty function

$$\min_{\mathbf{X}} \mathcal{J}_1 = -y_1^{25}(t_f)y_5^{25}(t_f) + \rho\|G_{cont}(\mathbf{X})\|_2^2, \tag{25}$$

where $\|\cdot\|_2$ denotes a l_2 norm and ρ is a penalty parameter. In performed calculation $\rho = 10^4$. The value of the obtained objective function was equal to $\mathcal{J}_1(\mathbf{X}^\star) = -112.71$.

In the case 2, the considered task was taken a form

$$\min_{\mathbf{X}} \mathcal{J}_2 = -y_1^{25}(t_f)y_5^{25}(t_f) \tag{26}$$

subject to

$$G_{cont}(\mathbf{X}) = 0. \tag{27}$$

The solution vector $\mathbf{X}^\star$ was obtained by the interior-point algorithm implemented in the Matlab's *fmincon* function. The obtained value of the minimized objective function was equal to $\mathcal{J}_2(\mathbf{X}^\star) = -112.6231$.

The computational calculations performed in the case 3 were more time-consuming and indicated on some benefits, as well as disadvantages of the STHO algorithm. First of all, the algorithm was working in the outer loop implemented as

for q_k from 0.1 to 1.0 with a step 0.1

The main problem, meet at the beginning of the computations at the first iteration of the outer loop, was to indicate the initial solution near to a such local minimizer, which can fulfill all the constraints $G(\mathbf{X}) = 0$ based on the $\widetilde{DAE^i}(q_k)$ solution. For the $\mathbf{X}_0$ near the local minimizer, the solution was obtained and extended in the next iterations of the outer loop. The figs. 1-2 show the state trajectories $\widetilde{y}_1(t)$ and $\widetilde{y}_2(t)$ obtained for the initial solution near to the local minimizer and calculated for different values of q_k.

The main drawback of the presented solution is related to the construction of $\widetilde{DAE^i}(q_k)$. The models of the linear differential-algebraic constraints systems with variable coefficients result with solutions of a form $Ae^{\lambda t}$ for the differential state variables. Therefore, small modification in the vector of decision variables resulted in significant changes in the solution trajectories. Therefore, the new model of the differential-algebraic constraints $\widetilde{DAE}^i(q_k)$ can show comparable computational difficulties, like an original one (1).

The obtained solution trajectories seems to be piecewise linear, especially, if larger number of subintervals is considered. Therefore, the value $\lambda \approx 0$. This is particular true, if the solution is calculated for higher values of the independent variable.

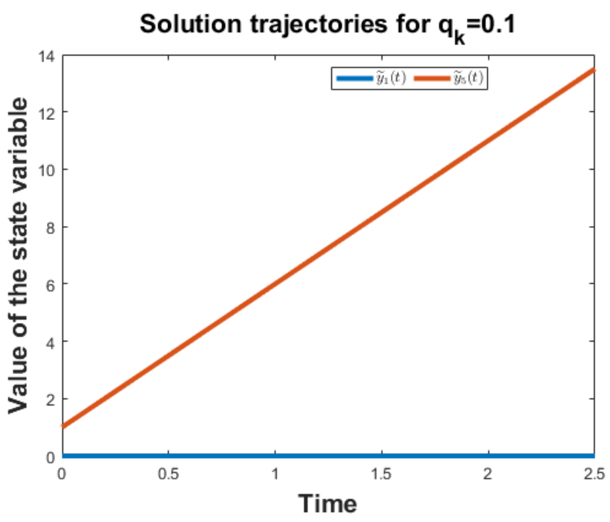

Fig. 1. The trajectories of the state variables $\widetilde{y}_1(t)$ and $\widetilde{y}_5(t)$ obtained for $q_k = 0.1$.

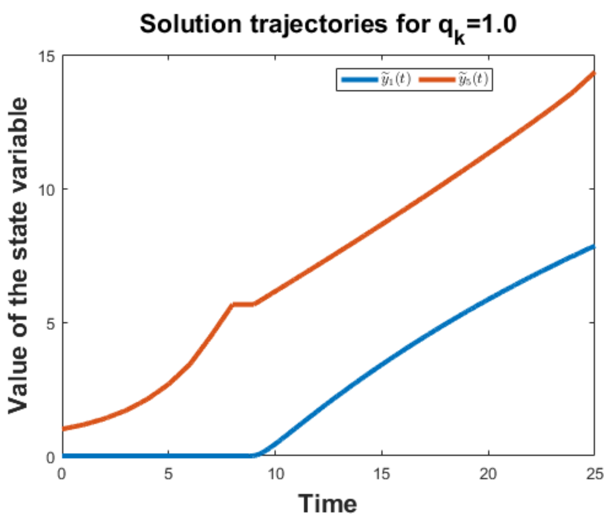

Fig. 2. The trajectories of the state variables $\widetilde{y}_1(t)$ and $\widetilde{y}_5(t)$ obtained for $q_k = 1.0$.

V. Conclusion

In the presented work the STHO Algorithm for optimization with the differential-algebraic constraints was presented. The designed shortened time horizon approach was based on the multiple shooting method, as well as implemented in two main parts - outer in inner iterations. The outer iteration generates the assumed number of subintervals and new constraints models with appropriate vector of pointwise algebraic constraints. In the inner loop, the defined nonlinear optimization tasks with modeled $\widetilde{DAE}^i(q_k)$ constraints and additional equality constraints is solved by a chosen numerical optimization procedure. The final solution of the inner loop is further treated as an initial solution for the next iteration in the outer loop.

The designed algorithm was used to solve the optimization task, where an optimal operation of the fed-batch reactor should be found. The performed computations indicated benefits and drawbacks of the designed procedure. The solution trajectories can be found and simply extended on the wider subintervals, if the appropriate initial solution is known *a priori*.

Acknowledgment

The author would like to thank the anonymous reviewers for thoroughly reading the manuscript and providing valuable comments.

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