

Simulated annealing with constraints aggregation for control of the multistage processes

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Abstract—In the article the control and optimization of multistage technological processes were discussed. In the presented research, it was assumed, that in the complex technological processes, the multistage differential-algebraic constraints with unknown consistent initial conditions were considered. To rewrite the infinite-dimensional optimal control problem into the finite-dimensional optimization task, the direct shooting method was applied. Simulated annealing algorithm was proposed as the method for solving nonlinear optimization problem with constraints. Stretching function was used to allow us to locate the globally optimal solution. The complex process constraints were treated using constraints aggregation methods. The presented methodology was tested with optimal control problem of the two-reactors system. The numerical simulations were executed in MATLAB environment using Wrocław Center for Networking and Supercomputing.

Index Terms—optimal control, DAE systems, simulated annealing, constraints aggregation, stretching function.

I. INTRODUCTION

NOWADAYS, technological processes have been modeled using more general and complex systems of equations. To model technological processes in such branch of industry, like chemical engineering, biotechnology and aerospace engineering, both dynamics and physical conservation laws have been under consideration [2], [3], [8], [16]. Then, a validated model of the process can be applied to control and optimize the technological systems. In the other words, to ensure an efficient and trouble free technological processes, an optimization problem subject to nonlinear differential-algebraic constraints need to be solved [4], [13].

In the last years, deterministic, as well as stochastic optimization algorithms, are adjusted to solve new advanced technological problems. New methods in modeling, algorithmic procedures and globalization of the obtained solutions can be observed in all areas of optimization [9], [10], [26]. In the presented work we would like to indicate the simulated annealing algorithm, which has been seen as one of the main global optimization procedures. In this work the new aspects of the simulated annealing algorithm were given and discussed.

Direct shooting method enables us to transform the optimal control problem into medium- or large-scale nonlinear optimization problem. Then, using aggregation and disaggregation procedures, the considered model can be represented

by other system, which reflects the most important features of the original process, but is better adjusted for computational optimization methods [14]. Then, the obtained results can be applied to control the original system.

The presentation of new methodology was performed in the following way. In the next section optimal control with differential-algebraic constraints was introduced. Then, in section III, optimization with aggregated constraints was discussed. "Stretching" function technique in optimization procedures was presented in section IV. Then, a new simulated annealing algorithm with constraints was given and tested in sections IV and V. The considerations were concluded in section VI.

II. OPTIMAL CONTROL WITH DIFFERENTIAL-ALGEBRAIC CONSTRAINTS

The optimal control algorithms are highly connected with the available modeling methods. The main objective of the control is always the same - we need to find the control function, which optimizes one of the known forms of the process performance index. But the assumptions, conditions and complexity of the considered processes are increasingly challenging and difficult to solve.

In the last years, new particular types of systems have become popular due to many practical applications. There are the multistage dynamical systems and processes with differential-algebraic equations, which are more general, than the pure dynamical processes.

The most important common features of the systems mentioned above, is the presence of the dynamics in the model. The difference, which has a far-reaching consequences in the calculation methods comes from the non-dynamical part of the model.

In the multistage processes, the state variables have to be continuous across the stages. It means, that in the known points, at the interface between the processes, algebraic continuity constraints are introduced. Therefore, the additional algebraic constraints have a pointwise character.

In processes with differential-algebraic constraints, the algebraic relations are justified by physical laws, which take place in the process and are reflected in the model. In this way, both the differential and algebraic equations have a continuous

character and can be treated as a one differential-algebraic system [6].

The presented work concerns the case, when the process is multistage and each stage was described using its own system of differential-algebraic equations. In this way, new theoretical assumptions have to be made and new computational concepts should be designed and implemented.

The features presented above lead us to the optimal control problems in the known form. At first, the process performance index, which can be treated as the measure of the control quality, has to be defined as follows

$$\min_{u(t)} Q = \int_0^{t_F} \mathcal{L}(y(t), z(t), u(t), p, t) dt + \mathcal{E}(y(t_F), z(t_F), t_F) \quad (1)$$

with single system of differential-algebraic constraints in semi-explicit form

$$\begin{aligned} B(t)\dot{y}(t) &= f(y(t), z(t), u(t), p, t) \\ 0 &= g(y(t), z(t), u(t), p, t), \end{aligned} \quad (2)$$

where $y(t) \in \mathcal{R}^{n_y}$ is a differential state, $z(t) \in \mathcal{R}^{n_z}$ is an algebraic state and $u(t) \in \mathcal{R}^{n_u}$ denotes the unknown control function. The independent variable (e.g. time or length of the chemical reactor) is denoted as $t \in \mathcal{R}$. As $p \in \mathcal{R}^{n_p}$ was denoted the vector of global parameters constant in time. The variables in the process are defined by vector-valued functions:

$$f : \mathcal{R}^{n_y} \times \mathcal{R}^{n_z} \times \mathcal{R}^{n_u} \times \mathcal{R}^{n_p} \times \mathcal{R} \rightarrow \mathcal{R}^{n_y} \quad (3)$$

and

$$g : \mathcal{R}^{n_y} \times \mathcal{R}^{n_z} \times \mathcal{R}^{n_u} \times \mathcal{R}^{n_p} \times \mathcal{R} \rightarrow \mathcal{R}^{n_z}. \quad (4)$$

To ensure, that the system (2) consists of differential-algebraic equations in semi-explicit form, it is assumed, that the matrix $B(t)$ is invertible for all values of t .

As it was mentioned, the quality of the process is measured by the value of $Q \in \mathcal{R}$. It is an important assumption, that quality of the whole complex process can be specified by only one real number.

When the multistage processes are considered, then each stage can be described using its own system of differential-algebraic equations

$$\begin{aligned} B^i(t)\dot{y}^i(t) &= f^i(y^i(t), z^i(t), u^i(t), p, t) \\ 0 &= g^i(y^i(t), z^i(t), u^i(t), p, t), \end{aligned} \quad (5)$$

where NS denotes number of the stages in the considered process.

One of the most important progresses in the optimal control methods has been connected with parametrization of the control problem. Because in this way the optimal control problem can be treated as a nonlinear optimization problem, efficient numerical optimization algorithms can be applied.

The parametrization of the control function has been proposed in the article [24] in 1994. Today, the piecewise continuous control parametrization using constant, linear or quadratic functions has been a commonly used approach.

In this way, instead to search for optimal solution using advanced analytical methods, the efficient algorithm of numerical optimization can be applied to obtain the best solution in the assumed class of piecewise continuous functions [7].

The parametrization of the control function in optimal control problems has been often used together with the multiple shooting technique. The multiple shooting method is appropriate to decompose the complex technological processes as well as to stabilize the solutions of both the unstable and highly nonlinear systems.

The multiple shooting method together with the control function parametrization lead us to the direct shooting approach. In this methodology, at the first step, the independent variable domain is divided into the assumed number of intervals

$$t = \bigcup_{i=1}^{NS-1} [t_{i-1} \quad t_i] \cup [t_{NS-1} \quad t_{NS}], \quad (6)$$

where t_0 is the time instant, when the process starts and t_{NS} is the final time.

Therefore, the control function as well as the differential-algebraic system can be parametrized in each interval. In practical applications, when the control function is parametrized as piecewise constant, then

$$u^i(t) = u_i, \quad i = 1, \dots, NS. \quad (7)$$

The differential-algebraic model of the technological process is parametrized in the sense of the unknown initial conditions. This approach enables us to solve the DAE system using the efficient numerical procedures [17]. The initial conditions of differential-algebraic system can be parametrized in the following way

$$\begin{aligned} y^i(t_{i-1}) &= s_y^i \\ z^i(t_{i-1}) &= s_z^i \end{aligned} \quad (8)$$

for $i = 1, \dots, NS$.

Therefore, the differential-algebraic constraints have been obtained the new form

$$\begin{aligned} B^i(t)\dot{y}^i(t) &= f^i(y^i(t), z^i(t), u^i, p, t^i) \\ 0 &= g^i(y^i(t), z^i(t), u^i, p, t^i), \end{aligned} \quad (9)$$

with $t^i \in [t_{i-1} \quad t_i]$ and $i = 1, \dots, NS$. Because the consistent initial conditions are needed to solve the DAE systems, the algebraic part can be extended by damping factor α

$$0 = g^i(y^i(t), z^i(t), u^i, p, t^i) + \alpha^i(t)g^i(s_y^i, s_z^i, u^i, p, t^i) \quad (10)$$

for $t^i \in [t_{i-1} \quad t_i]$ and $i = 1, \dots, NS$.

The process performance index has been rewritten as follows

$$\min_{s_y^i, s_z^i, u^i} \hat{Q} = \sum_{i=1}^{NS} \int_{t_{i-1}}^{t_i} \mathcal{L}(s_y^i, s_z^i, u^i, p, t) dt + \mathcal{E}(s_y^{NS}, s_z^{NS}, t_F). \quad (11)$$

It is worth to note, that the trajectories of the differential states are continuous. It means, that the additional relations have to be incorporated to the model

$$y^i(t_i) = y^{i+1}(t_i) = s_y^{i+1}, \quad i = 1, \dots, NS - 1, \quad (12)$$

which results as additional pointwise algebraic constraints of the following form

$$y^i(t_i) - s_y^{i+1} = 0, \quad i = 1, \dots, NS - 1. \quad (13)$$

In the most practical situations, the unknown parameters have their physical interpretation. Among them can be distinguished an unknown volume of the chemical reactor, concentration of the substrates or value of the temperature. The interpretation of the decision variables and technological restrictions defines the feasible region and can be rewritten as the inequality constraints in the form of lower and upper bounds.

Direct shooting approach enables us to transform the optimal control problem into the nonlinear programming problem with the vector of decision variables designed as

$$x = [s_y^i \quad s_z^i \quad u_i \quad p]^T, \quad (14)$$

the process performance index in the form of the objective function

$$\min_x \hat{Q}(x) \quad (15)$$

differential-algebraic constraints

$$\begin{aligned} B^i(t) \dot{y}^i(t) &= f^i(y^i(t), z^i(t), u^i, p, t^i) \\ 0 &= g^i(y^i(t), z^i(t), u^i, p, t^i), \end{aligned} \quad (16)$$

consistency constraints

$$0 = g^i(y^i(t), z^i(t), u^i, p, t^i) + \alpha^i(t) g^i(s_y^i, s_z^i, u^i, p, t^i) \quad (17)$$

continuity constraints

$$y^i(t_i) - s_y^{i+1} = 0, \quad (18)$$

and the constraints of upper and lower bounds type

$$x_L \leq x \leq x_U \quad (19)$$

for $t^i \in [t_{i-1} \quad t_i]$ and $i = 1, \dots, NS$.

This causes, that the various numerical optimization algorithms can be treated as an important part of the control algorithms [18]. This transformation is a main effect of the direct shooting method applied in the optimal control problems.

III. OPTIMIZATION WITH AGGREGATED CONSTRAINTS

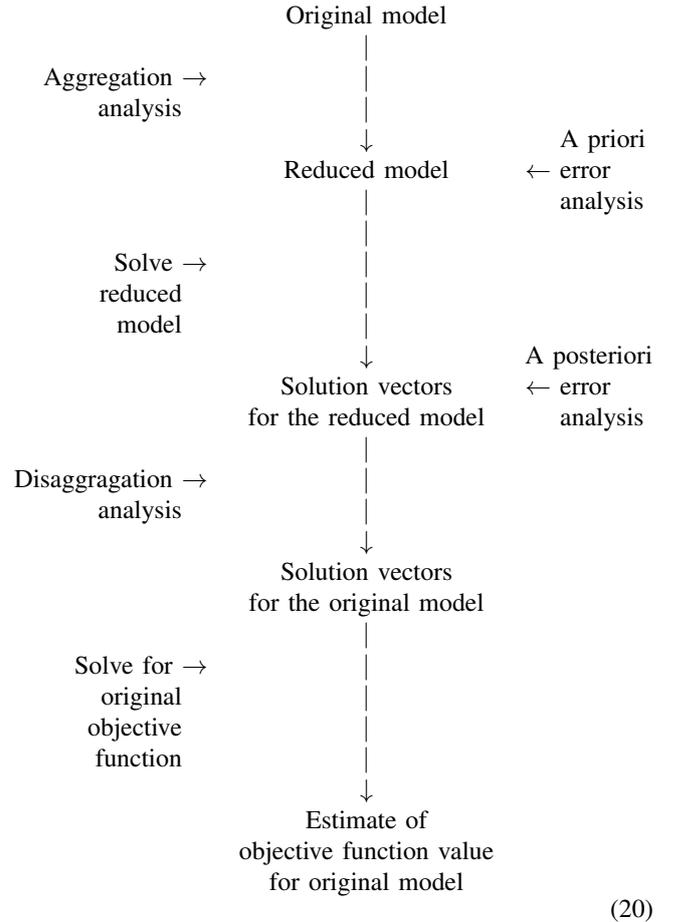
The complexity of the considered models and large number of decision variables makes, that the analytical solutions and some intuitive numerical approaches can be inappropriate in the control of the real-life technological processes.

One of the most important question in modern optimization and control theory is, how to solve the problems with thousands or millions variables and comparable number of equality and inequality constraints. The second important question is, how to compare two unfeasible solutions and to make a decision, which one proposed solution is better than the others.

To analyze the complex process, both the aggregation and disaggregation techniques were used. There is a general methodology, how to obtain useful information about the process by a possibly little model modifications and computations amount [5].

In the previous section, the optimal control problem was reformulated as a middle- or large-scale nonlinear optimization problem. To do this, the direct shooting method was applied. At this point, the consecutive question cannot more wait for the answer - how to treat optimization problems with so many variables and subject to huge number of constraints? The question, which has been just imposed, is considered in this section.

The general way to obtain the useful information about the complex process can be constructed as follows [23]



In a general sense, in model aggregation, large-scale optimization models are reformulated as less complex systems. The obtained in this way models reflect the most important features of the original systems, but should be much more suitable to perform numerical simulations.

In the other words, the aggregation technique is a method to specified parts of the model, which can be described using only one single element. At this step, the new single element should be explicitly defined. Therefore, aggregation analysis consists of two levels:

- process of determining, which data are in some sense similar and can be considered as elements in the same group; this step is known as cluster analysis,
- the method of combining the clustered data to define the reduced model.

In contrast to the aggregation analysis, the disaggregation is a method, which can derive the information about the complex model using results obtained by reduced system analysis. The disaggregation analysis, often known as the reversal aggregation analysis, enables us to estimate the solution of the original system using only results obtained from solving the reduced model.

The last stage, which is connected with aggregation and disaggregation methodology, is an error analysis. The error analysis determines the resulting error, which can be introduced by algorithms with aggregate models and disaggregate solutions. From practical point of view, the error analysis can be useful for selection of appropriate aggregation and disaggregation procedures. In the literature two main types of error are defined

a) a priori error bounds, which are the bounds placed upon the optimal value of an original optimization model after aggregation stage, but before the aggregate model is solved,

b) a posteriori error bounds are the bounds placed upon the optimal value of an original optimization model after the aggregated model has been formed and solved.

In practical applications, the iterative optimization algorithms with successive aggregation-disaggregation schemes are used. Such procedures are known as an Iterative Aggregation-Disaggregation (IAD) technique.

As it was mentioned, the direct shooting method allows us to transform the optimal control problem into a nonlinear optimization problem. Therefore, solution of the original infinite-dimensionally task can be obtained by solving finite-dimensional optimization problem. But the question posed in this section does not refer to the optimal control problems. It concerns the much more fundamental task - how to solve medium- and large-scale optimization problems?

It is expected, that the efficient numerical optimization methods enable us to solve optimal control problems.

Therefore, we would like to propose aggregation methods, which can be useful to define new reduced process performance index, as well as reduced constraints.

At this place, we would like to focus on the constraints function aggregation. It was mentioned, that two main types of the constraints need to be considered in the process - there are continuous and pointwise constraints. In particular, it means, that some group of functions are connected with process description by continuous differential-algebraic constraints. There is the second group of constraints, which denotes the additional constraints at the prescribed time instances in the process.

Let us consider the system of the continuous differential-algebraic equations. This particular system can be solved by implementation of efficient numerical algorithms. After that, the process performance index, as well as fulfillment of the constraint can be determined. There is an important question, which refers to consistent initial conditions, which enables us to solve the differential-algebraic system. Although the initial conditions are defined at the specific point, they strictly refer

to the continuous process constraints and should be perceived with continuous differential-algebraic constraints. In this work, we refer to this type of constraints as *the consistency constraints* and denote as

$$c_{cons}(\{s_y^i, s_z^i, u^i, p, t_{i-1}\}_{i=1}^{NS}) = \begin{bmatrix} g^1(s_y^1, s_z^1, u^1, p, t_0) \\ g^2(s_y^2, s_z^2, u^2, p, t_1) \\ \vdots \\ g^{NS}(s_y^{NS}, s_z^{NS}, u^{NS}, p, t_{NS-1}) \end{bmatrix} = 0. \quad (21)$$

The other group of constraints represents the pointwise constraints, which are connected with the fact, that the multistage system is considered. In the other words it means, that the differential state trajectories are continuous across the process stages. The vector of pointwise algebraic constraints denoted as c_{cont} is defined as follows

$$c_{cont}(\{s_y^{i+1}, s_z^{i+1}, u^i, p, t_i\}_{i=1}^{NS-1}) = \begin{bmatrix} y^1(t_1) - s_y^2 \\ y^2(t_2) - s_y^3 \\ \vdots \\ y^{NS-1}(t_{NS-1}) - s_y^{NS} \end{bmatrix} = 0. \quad (22)$$

In some numerical optimization algorithms, e.g. Sequential Quadratic Programming, it is suggested to treat each constraint function in the same way. Therefore, in each iteration, a large-scale and possibly structured matrix of constraint functions derivatives can be obtained. In general case, when the structure of the process constraints is unknown, the matrix of partial derivatives of the constraints might be time and memory consuming.

If, in general, $c(x)$ denotes

$$c(x) = \begin{bmatrix} c_1(x) \\ c_2(x) \\ \vdots \\ c_{NS}(x) \end{bmatrix} = 0, \quad (23)$$

then the vector of the constraint functions can be replaced using one of the following real-valued aggregated functions

$$\tilde{c}(x) = \|c(x)\|_1, \quad (24)$$

$$\tilde{c}(x) = \|c(x)\|_2 \quad (25)$$

or

$$\tilde{c}(x) = \|c(x)\|_\infty. \quad (26)$$

One cannot determine, which one measure of the constraints infeasibility has the best features. The constraints aggregation function can be chosen depending on the considered process, optimization methods and, first of all, available computing resources.

The other question is, how to treat the process performance index. Parametrization of the control function, as well as differential and algebraic states, enables us to rewrite the

process performance index as the objective function in non-linear optimization problem. In some applications the penalty function approach and many variations of it can be observed. Advanced optimization methods focus on methods without penalty function [12], [22]. For these reasons, in presented methodology, the objective function $\hat{Q}(x)$, which represents control quality index, was remained unchanged.

IV. STRETCHING FUNCTION

In the previous section it has been indicated, how to apply the direct shooting method to transform the optimal control problem into the nonlinear optimization task. In general, the presented methodology enables us to consider the optimization problem over the feasible region

$$\min_x f(x), \quad \forall x \in \mathcal{A}, \quad (27)$$

where $f(x)$ is a real-valued objective function

$$f: \mathcal{A} \rightarrow \mathcal{R} \quad (28)$$

where $\mathcal{A} \subseteq \mathcal{R}^D$ is the D-dimensional compact set.

The important question is, how to treat the nonlinear optimization problem with the large number of equality, as well as inequality constraints.

To solve the optimization problem on the compact set, the "stretching" technique for the objective function can be applied [19].

Let us consider the objective function $f(x)$ defined on the compact set. Let the objective function f get the local minimum in a point x^* . Therefore, the point x^* is a local minimizer of the function f . As a consequence, it means, that in the neighborhood \mathcal{NB} of the point x^* , the inequality

$$f(x^*) \leq f(x) \quad (29)$$

is satisfied for all $x \in \mathcal{NB}$.

In real-life optimization and control problems, it is highly undesirable, that one of the low quality local minima can be treated as the global solution. The "stretching" function method was designed as a remedy for described situation. This method enables us to alleviate the local minimum using the following two-step transformation.

Let x^* be the local minimum of the function f , then in the step 1, the function $f(x)$ elevates and all the local minima, which are above the point $f(x^*)$, disappear

$$\mathcal{G}(x) = f(x) + \frac{\gamma_1}{2} \|x - x^*\| \left(\text{sign}(f(x) - f(x^*)) + 1 \right) \quad (30)$$

In the step 2, the neighborhood of the point x^* is stretched upwards, in this way, that it assigns higher values of those points

$$\begin{aligned} \mathcal{S}(f(x)) &= f^{\mathcal{S}}(x) = \mathcal{H}(x) = \\ &= \mathcal{G}(x) + \frac{\gamma_2 \left(\text{sign}(f(x) - f(x^*)) + 1 \right)}{2 \tanh \left(\mu (\mathcal{G}(x) - \mathcal{G}(x^*)) \right)}. \end{aligned} \quad (31)$$

The parameters γ_1 , γ_2 and μ are the positive constants with arbitrary chosen value. The authors, who proposed the "stretching" function technique as the global optimization method, suggested the values of the mentioned parameters as $\gamma_1 = 10000$, $\gamma_2 = 1$, $\mu = 10^{-10}$. It was suggested, that the choice of the considered parameters seems not to be critical for the success of the optimization, but they can influence the convergence rate. For these reasons, the parameter tuning was suggested [20].

It is an important question, how the "stretching" function technique can be applied for optimization problems, when a feasible region is no more a compact set? The mentioned situation can be met in all cases, when optimization problems with equality constraint are considered [21].

To find the answer for the question posed above, the constraints aggregation methodology is very helpful.

V. SIMULATED ANNEALING WITH CONSTRAINTS

The main ideas connected with simulated annealing algorithm have their origin in thermodynamics. The physical laws, which governs cooling of molten metal in annealing process, have been used to design new optimization methods. After slow cooling in annealing process, the metal tends to reach a state with a low energy. In general, the state with the minimum energy is desired. In analogy to annealing process, the energy represents the possible solution of the optimization problem. Therefore, the state with the minimal energy represents the solution in the optimization algorithm [15], [25].

The simulated annealing algorithm is constructed as follows.

The simulated annealing algorithm

```

Initialization ( $x_0, T_0$ )
Calculation of  $f(x_0)$ 
Until convergence
  Generation of new state  $x_1$ 
  if  $f(x_1) < f(x_0)$ 
     $x_0 = x_1$ 
  else
    if  $\exp\left(\frac{f(x_0) - f(x_1)}{T}\right) > \text{Rand}(0, 1)$ 
      Accept new solution  $x_0 = x_1$ 
    else
      Reject new solution
      Decrease the temperature
end (Until)

```

At this moment we would like to introduce new simulated annealing method for optimal control of the multistage differential-algebraic systems. We start the presentation with some remarks.

Remark 1. *The optimal control problem with index-1 differential-algebraic constraints using the direct shooting approach has been transformed into nonlinear optimization*

problem with equality constraints of the following form

$$\begin{aligned} \min_x \hat{Q}(x) \\ c_{cons}(x) = 0 \\ c_{cont}(x) = 0. \end{aligned} \quad (32)$$

Remark 2. The quality \mathcal{Q} of any proposed solution x can be specified using a triple

$$\mathcal{Q}(x) = \begin{bmatrix} q_1(x) \\ q_2(x) \\ q_3(x) \end{bmatrix} = \begin{bmatrix} \hat{Q}(x) \\ c_{cons}(x) \\ c_{cont}(x) \end{bmatrix}. \quad (33)$$

Remark 3. The "stretching" function technique applied for some proposed solution transforms the vector, which parametrized the quality of the proposed solution

$$\mathcal{S}(\mathcal{Q}(x)) = \mathcal{Q}^S(x) = \begin{bmatrix} q_1^S(x) \\ q_2^S(x) \\ q_3^S(x) \end{bmatrix} = \begin{bmatrix} \hat{Q}^S(x) \\ c_{cons}^S(x) \\ c_{cont}^S(x) \end{bmatrix}. \quad (34)$$

The decisions of the new solution acceptance can be made by quality comparison of the considered solutions

Definition 4. Any two values \mathcal{Q}_a and \mathcal{Q}_b are in the relation \oplus if

$$\begin{aligned} q_1(a) \oplus q_1(b) \\ q_2(a) \oplus q_2(b) \\ q_3(a) \oplus q_3(b) \end{aligned} \quad (35)$$

Theorem 5. Let x_0 and x_1 be any two solutions. The solution x_0 is unconditionally better than solution x_1 if and only if

$$\mathcal{Q}(x_0) < \mathcal{Q}(x_1). \quad (36)$$

Let us transform the triple, which defines the quality of the solution, using the "stretching" function technique.

Theorem 6. Let x_0 and x_1 be any two solutions. If

$$\begin{aligned} q_1^S(x_0) < q_1^S(x_1) \\ q_2^S(x_0) < q_2^S(x_1) \\ q_3^S(x_0) < q_3^S(x_1) \end{aligned} \quad (37)$$

then

$$\mathcal{Q}(x_0) < \mathcal{Q}(x_1). \quad (38)$$

The question is, how to compare two solutions, which are not in the relation presented in Theorem 6.

One of the most important features of simulated annealing algorithm is a possibility of accepting a step, which does not improve the current solution. Therefore, to compare any two solution, which are not in clear relation, a conditional acceptance mode can be applied. In simulated annealing methodology, it is known as *an acceptance with probability*. In the presented work, because of three-dimensional quality solution index $\mathcal{Q}(x)$ under considerations, a new extended method of acceptance with probability was proposed.

Proposition 7. Let x_0 be the current solution and x_1 be any other solution generated by simulated annealing algorithm from the neighborhood of the point x_0 , and T denote the value of the temperature in the current iteration. If the point x_1 cannot be unconditionally accepted as a new solution, then it can be accepted with the probability $p \in \mathcal{N}(0,1)$. The

acceptance probability is dependent on the index quality in the following way

$$\exp\left(-\frac{\hat{Q}^S(x_1) - \hat{Q}(x_0)}{T}\right) > p$$

or

$$\exp\left(-\frac{c_{cons}^S(x_1) - c_{cons}(x_0)}{T}\right) > p$$

or

$$\exp\left(-\frac{c_{cont}^S(x_1) - c_{cont}(x_0)}{T}\right) > p.$$

There are two important remarks connected with the presented acceptance condition

Remark 8. The multiple conditions increase the general acceptance probability of the worse solution.

Remark 9. Application of the "stretching" function technique transforms the bad solution in the worse one. Moreover, "stretching" function technique supports searching for better solutions and alleviate the local minima.

The presented simulated annealing "stretching" function algorithm with new conditional solution acceptance approach was applied to solve the optimal control problem of the multistage reactors system.

VI. NUMERICAL EXAMPLES

The presented methodology was tested on the optimization problem of the three-stage technological process. The presented system consists of two chemical reactors with mixing [24]. The sketch of the process was presented in the Fig. 1.

At the beginning, the first reactor was loaded with the substrate A with the volume 0.1 m^3 and concentration 2000 mol/m^3 . Due to reactions taking place in the system, the products B and C are obtained according to the following scheme



Additionally, the first reactor was equipped with a heating exchanger, which can be used to control the process temperature and in this way - to influence the trajectories of the process variables. The concentrations of the substrate and products were changing in the following way

$$\dot{C}_A = -2k_1(T)C_A^2 \quad (40)$$

$$\dot{C}_B = 2k_1(T)C_A^2 - k_2(T)C_B \quad (41)$$

$$\dot{C}_C = k_2(T)C_B \quad (42)$$

with the kinetics constraints

$$k_1(T) = 0.0444 \exp(-2500/T) \quad (43)$$

and

$$k_2(T) = 6889.0 \exp(-5000/T). \quad (44)$$

Then, in the mixing stage at the time t_1 , the component B of concentration $C_B^0 = 600 \text{ mol/m}^3$ and some volume S was added. Therefore, the volume and concentrations of the substrates were changing, so the following relations were satisfied

$$V_2 C_A(t_2^0) = V_1 C_A(t_1) \quad (45)$$

$$V_2 C_B(t_2^0) = V_1 C_B(t_1) + S C_B^0 \quad (46)$$

$$V_2 C_C(t_2^0) = V_1 C_C(t_1) \quad (47)$$

where V_1 is the volume of substrates loaded at the beginning of the first reactor. Therefore, the volume V_2 in the second reactor was given by

$$V_2 = V_1 + S \quad (48)$$

The volume S is a decision parameter with

$$0 \leq S \leq 0.1(m^3) \quad (49)$$

After the mixing stage, the substrates were loaded into the last reactor, where three reactions were taking a place



In the 2nd reactor, the reactions take place under isothermal conditions. The state variables are changing in the following way

$$\dot{C}_A = 0 \quad (53)$$

$$\dot{C}_B = -0.02C_B - 0.05C_B - 2 \times 4.0 \times 10^{-5}C_B^2 \quad (54)$$

$$\dot{C}_C = 0 \quad (55)$$

$$\dot{C}_D = 0.02C_B \quad (56)$$

$$\dot{C}_E = 0.05C_B \quad (57)$$

$$\dot{C}_F = 4.0 \times 10^{-5}C_B^2 \quad (58)$$

The combined processing time for both reactors is equal to 180 min

$$t_1 + t_2 = 180, \quad (59)$$

$$t_1 > 0, \quad t_2 > 0. \quad (60)$$

The decision variables are the profile of the temperature $T(t)$, the duration time of the reactions in each stage, and the amount S of component B , which is added at the mixing step.

The process is aimed to maximize the amount of the product D at the output of the 2nd reactor

$$\max_{t_1, t_2, S, T(t)} V_2 C_D(t_2) \quad (61)$$

subject to the constraints on the temperature profile

$$298 \leq T(t) \leq 398(K), \quad t \in [0 \quad t_1]. \quad (62)$$

The direct shooting method enables us to transform the multistage optimal control problem as an nonlinear optimization problem with both continuous and pointwise constraints. In classical approaches, the nonlinear optimization problem with constraints can be solved using penalty function approach or NLP algorithms, like Sequential Quadratic Programming or Barrier methods. In this way, the process in first reactor was divided into 10 equidistance intervals. Additionally, the initial conditions for the second reactor should be consistent with the results of the mixing stage. Therefore, the considered NLP

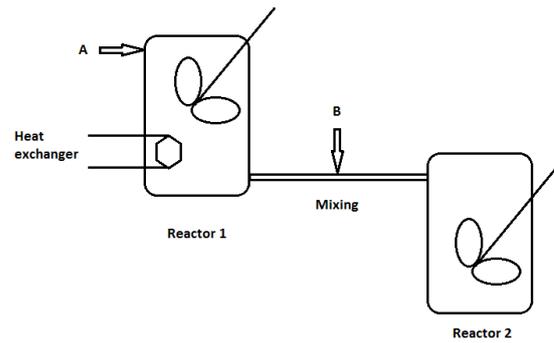


Fig. 1. System of the two-reactors with mixing.

problem consisted of 27 continuity constraints, 3 consistency constraints and 42 decision variables.

The aggregated model was defined using 3 scalar functions

$$\hat{Q}(x) = Q(x) \quad (63)$$

$$c_{cont}(x) = \sum_{i=1}^{27} \|c_{cont,i}(x)\|_1 \quad (64)$$

$$c_{cons}(x) = \sum_{i=1}^3 \|c_{cons,i}(x)\|_1 \quad (65)$$

In the next step, all three function were transformed using "stretching" function technique

$$\mathcal{S}(\hat{Q}(x)) = \hat{Q}^S(x) \quad (66)$$

$$\mathcal{S}(c_{cont}(x)) = c_{cont}^S(x) \quad (67)$$

$$\mathcal{S}(c_{cons}(x)) = c_{cons}^S(x) \quad (68)$$

and optimized using presented simulated annealing algorithm with new acceptance method.

The parameters of the methods were adjusted automatically. Therefore, the simulations were performed with the following parameters

- number iterations in the outer loop $MaxIter = 500$,
- inner iterations in cooling loop $MaxIterCool = 10$,
- diameter of the considered neighborhood $\alpha = 0.4$
- initial temperature $T_0 = 100$,
- temperature update factor $T_{i+1} = \beta T_i$ is $\beta = 0.6$.

The obtained results, which were obtained for the aggregated model, were applied to the original model of the considered process. After 702 model evaluations, the final value of the original process performance index was equal to 22.7233 mol. The obtained state trajectories were presented in the Fig. 2.

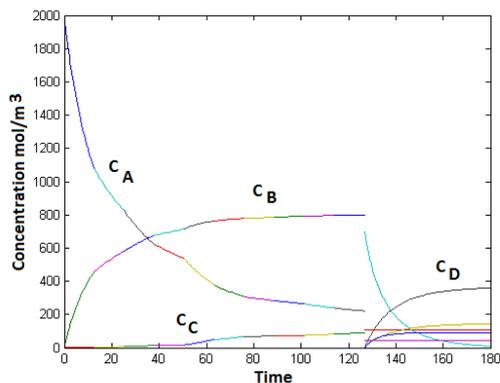


Fig. 2. Trajectories of the state variables.

VII. CONCLUSION

In the article a problem of solving complex multistage technological processes was considered. The new methodology, which was presented, applies aggregation-disaggregation approach. The optimal control problem was transformed into the nonlinear optimization problem using the direct shooting approach. Then, the NLP problem has been defined using only three functions, which reflects the characteristics features of the process. The first one denotes the value of the process performance index. Then, the second one is connected with the continuity of the differential state trajectories, and the last one denotes the consistent initial conditions of the process. The quality of the proposed solution was defined using only values of these three functions. To compare any two proposed solutions, the new decision approach was proposed. The presented methodology was applied to the two-stage reactor system.

The future research will be devoted to error analysis of the aggregation-disaggregation procedures for control and optimization of the multistage technological processes with nonlinear differential-algebraic constraints.

ACKNOWLEDGMENT

Many thanks are due to two anonymous referees, whose constructive suggestions led to improvement of the original article.

The project was supported by the grant Młoda Kadra B40099/I6 at Wrocław University of Technology.

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