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OPTIMAL DISCRETE PROCESSES, NONLINEAR IN TIME INTERVALS: THEORY AND SELECTED APPLICATIONS

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Abstract

In the present paper we investigate the Hamiltonian-based optimization algorithms for inherently discrete processes, i.e. those in which state changes at the process stage are finite and may be large. Their mathematical models (difference equations) refer either for processes which are discrete by nature or are obtained from continuous (differential) models by suitable discretization. We show that, when discrete time intervals are linear in the discrete model, the optimal discrete process is described by a Hamiltonian of Pontryagin's type which is constant along the discrete path. However, for models with nonlinear time intervals, the constancy of the optimal discrete Hamiltonian is lost and, instead, an extra difference equation constitutes a model component describing the change of the Hamiltonian. Selected applications of the obtained algorithms in evaporation and drying operations are presented, which involve models with linear and nonlinear time intervals.

Key words

Optimization, Hamiltonian, maximum principle, optimization algorithm.

1 Introduction

One of the key reasons for the development of process modeling is the necessity to optimize the processes already in the design. The development of mathematical models of processes and the increase of their complexity requires a development of the method and algorithms for optimization, because optimization algorithms applied to simple models cannot be used in case of more complex models. In the case of multistage or continuous processes, one of the most effective optimization methods are algorithms of Maximum Principle.

The first continuous version of optimization algorithm of Maximum Principle was formulated by Pontryagin and co-workers in 1956. Next, Gamkrelidze, Boltyanski and Rozonoer [Pontryagin *et al.*, 1962], and, independently, Fan [Fan, 1966], have given some modifications, generalizations and proofs of the continuous algorithm. The first discrete algorithm of the Maximum Principle type was presented in 1960 by Katz [Fan and Wang, 1964] and Fan [Boltyanski, 1973]. However, the algorithms of Katz's and Fan's have a completely different structure than Pontryagin's continuous algorithm. In 1972, by using the method of dynamic programming Sieniutycz [Sieniutycz, 1974] revealed a constant Hamiltonian algorithm for discrete processes described by an optimization model linear with respect to one arbitrary decision, which is essentially a finite time interval, replacing an infinitesimal, differential interval in Pontryagin's algorithm. This paper shows that a new discrete algorithm can be derived resembling the continuous version of Pontriagin's principle. Similarly like in Pontriagin's algorithm, in Sieniutycz's algorithm the Hamiltonian maintains a constant value along an optimal trajectory. In further studies Kafarow, Polak, Zangwill and Szwast obtained a weak version of the discrete algorithm with constant Hamiltonian (Weak Maximum Principle) by using the method of Lagrange's multipliers [Szwast, 1994], [Szwast, 1979]. Next, studies carried out by Szwast conducted to derive an enhanced version of this algorithm (Strong Maximum Principle) [Szwast, 1988]).

The classical version of the discrete algorithm with constant Hamiltonian is limited by a requirement of linearity of the optimization model with the respect of one distinguished decision variable – "finite interval of time". This requirement is satisfied by many models describing many processes of chemical engineering, but not by all. Obviously Katz' and Fan's algorithms can be used, but the discrete algorithm with a constant Hamiltonian has some advantages in comparison with

Katz' and Fan's algorithms. One of these advantages is the fact that a physical meaning can be attributed to Hamiltonian and adjoint variables in the algorithm with constant Hamiltonian whereas this is impossible for Katz' and Fan's algorithm. The advantage is especially apparent if solving of an optimization problem demands an iterative method (some values of adjoint variables and Hamiltonian must be assumed). Hence the idea arises to generalize the classical version of the discrete algorithm with constant Hamiltonian, so that it could be used to optimize linear and nonlinear problems.

The generalized version of the discrete algorithm with a constant Hamiltonian is presented in this paper.

2 Classical Version of the Discrete Algorithm with Constant Hamiltonian

The scheme of considered multistage processes is presented in Figure 1, where $\mathbf{x}^n$, $\mathbf{u}^n$ and $\mathbf{z}^n$ are vectors of state variables, decision variables and adjoint variables respectively; θ^n is "the time interval", a decision variable with respect of which the process model is linear by assumption, and t^n is an additive time-like state variable referred to "the time". While t^n may represent the reagents residence time or the process chronological time it may also be a measure of these quantities. The variables θ^n and t^n satisfy the following relation:

$$\theta^n = t^n - t^{n-1} \tag{1}$$

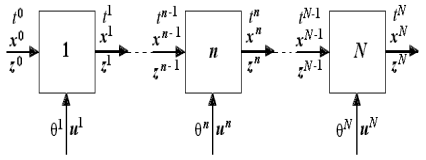

Figure 1. Scheme of considered multistage processes

Discrete algorithm with constant Hamiltonian can be used to resolve an optimization problem for which the optimization model is linear with the respect of θ^n. Linearity of the optimization model requires both state equations (transformations) and performance index to be linear with the respect of this variable.

The considered performance index takes a following Lagrange's form (other forms of performance index can be found in literature, e. g. [Fan, 1966], [Fan and Wang, 1964], [Boltyanski, 1973]):

$$I = \sum_{n=1}^{N} f_0\left(\mathbf{x}^n, \mathbf{u}^n, t^n\right)\theta^n \tag{2}$$

The state equations (called also state transformations) are derived from equations of mathematical model of process. For each state variable, a state equation describes a change of this variable value through the *n*-th stage of cascade. General form of the state transformations takes a following form, which is right for all cascade stage ($n = 1..N$) and for all state variables ($i = 1..s$; where s is a number of state variables):

$$x_i^n - x_i^{n-1} = f_i^n\left(\mathbf{x}^n, \mathbf{u}^n, t^n\right)\theta^n \tag{3}$$

The function f_i appearing in the equation (3) can be a function of time, t^n, but in any case, it can't be a function of time-interval, θ^n.

The Hamiltonian (Hamilton's function) is defined in following form:

$$H^{n-1}\left(\mathbf{x}^n, \mathbf{u}^n, \mathbf{z}^n, t^n\right) = f_0^n\left(\mathbf{x}^n, \mathbf{u}^n, t^n\right) + \\ + \sum_{i=1}^{s} z_i^{n-1} f_i^n\left(\mathbf{x}^n, \mathbf{u}^n, t^n\right) \tag{4}$$

where z_i^{n-1} are a component of adjoint vector, $\mathbf{z}^{n-1}$ for $n = 1..N$ and $i = 1..s$.

Necessary conditions for optimality of performance index (2) are described by canonical set of equations (5) and (6), equation (7), which describes a weak condition of optimality with respect to decisions variables, $\mathbf{u}^n$, and equation (8) describing changes of the Hamiltonian along an optimal trajectory. Equation (8) is, in fact, a condition of optimality for decision θ^n. These equations are valid for all stages of the cascade, $n = 1..N$, for all state and adjoint variables, $i = 1..s$, and for all decisions being a component of the vector un, $j = 1..r$, where r is the number of decision variables excluding θ^n.

$$\frac{\partial H^{n-1}\left(\mathbf{x}^n, \mathbf{u}^n, \mathbf{z}^n, t^n\right)}{\partial z_i^{n-1}} = \frac{x_i^n - x_i^{n-1}}{\theta^n} = \\ = f_i^n\left(\mathbf{x}^n, \mathbf{u}^n, t^n\right) = \tag{5}$$

$$-\frac{\partial H^{n-1}\left(\mathbf{x}^n, \mathbf{u}^n, \mathbf{z}^n, t^n\right)}{\partial x_i^n} = \frac{z_i^n - z_i^{n-1}}{\theta^n} \tag{6}$$

$$\frac{\partial H^{n-1}\left(\mathbf{x}^n, \mathbf{u}^n, \mathbf{z}^n, t^n\right)}{\partial u_j^n} = 0 \tag{7}$$

$$\frac{H^n - H^{n-1}}{\theta^n} = \frac{\partial H^{n-1}\left(\mathbf{x}^n, \mathbf{u}^n, \mathbf{z}^n, t^n\right)}{\partial t^n} \tag{8}$$

The Hamiltonian (4) is valid both for the autonomous processes and for non autonomous processes. For the autonomous processes Hamiltonian (2) in not explicit function of time t^n, whereas for non autonomous ones time t^n is an explicit argument of the Hamiltonian. In agreement with equation (8) the Hamiltonian is constant along an optimal trajectory of an autonomous process.

Although the equations presented above are sufficient to solve all problems defined by performance index (2) and state equations (1) and (3), an enlarged Hamiltonian is often introduced. The enlarged Hamiltonian is always constant and, moreover, it always equal to 0. The enlarged Hamiltonian takes a following form

$$\begin{aligned}&\tilde{H}^{n-1}\left(\mathbf{x}^n,\mathbf{u}^n,\mathbf{z}^n,t^n,z_t^{n-1}\right)=\\&=H^{n-1}\left(\mathbf{x}^n,\mathbf{u}^n,\mathbf{z}^n,t^n\right)+z_t^{n-1}\end{aligned}\tag{9}$$

where z_t^{n-1} is a adjoint variable connected with the time, t^n.

The optimality condition presented by equations (5)–(7) can be redefined using the enlarged Hamiltonian. In redefined equations the traditional Hamiltonian (of energy type) is substituted by the enlarged Hamiltonian:

$$\begin{aligned}&\frac{\partial\tilde{H}^{n-1}\left(\mathbf{x}^n,\mathbf{u}^n,\mathbf{z}^n,t^n,z_t^{n-1}\right)}{\partial z_i^{n-1}}=\\&=\frac{x_i^n-x_i^{n-1}}{\theta^n}=f_i^n\left(\mathbf{x}^n,\mathbf{u}^n,t^n\right)\end{aligned}\tag{10}$$

$$-\frac{\partial\tilde{H}^{n-1}\left(\mathbf{x}^n,\mathbf{u}^n,\mathbf{z}^n,t^n,z_t^{n-1}\right)}{\partial x_i^n}=\frac{z_i^n-z_i^{n-1}}{\theta^n}\tag{11}$$

$$\frac{\partial\tilde{H}^{n-1}\left(\mathbf{x}^n,\mathbf{u}^n,\mathbf{z}^n,t^n,z_t^{n-1}\right)}{\partial u_j^n}=0\tag{12}$$

Equation (8), describing changes of the traditional Hamiltonian along an optimal trajectory, is replaced by the following equation

$$\frac{z_t^n-z_t^{n-1}}{\theta^n}=-\frac{\partial\tilde{H}^{n-1}\left(\mathbf{x}^n,\mathbf{u}^n,\mathbf{z}^n,t^n,z_t^{n-1}\right)}{\partial x_i^n}\tag{13}$$

which describing changes of adjoint variable, z_t^{n-1}.

Because the adjoint variable z_t^{n-1} is an additional variable, which doesn't appear in equations (5) – (8), the set of equations (10) – (13) must be completed by a new equation. The additional equation results form fact that the enlarged Hamiltonian is always equal to zero, so the additional equation takes the following form:

$$\begin{aligned}&\tilde{H}^{n-1}\left(\mathbf{x}^n,\mathbf{u}^n,\mathbf{z}^n,t^n,z_t^{n-1}\right)=f_0^n\left(\mathbf{x}^n,\mathbf{u}^n,t^n\right)+\\&+\sum_{i=1}^{s}z_i^{n-1}f_i^n\left(\mathbf{x}^n,\mathbf{u}^n,t^n\right)+z_t^{n-1}=0\end{aligned}\tag{14}$$

2.1 Boundary Conditions

To solve the discrete optimization problem considered above, some boundary conditions for state and adjoint variables are needed. In the simplest (but most often used) form of boundary conditions some initial and final values of state variables are determined. For typical problems all the initial values of state variables are usually known, whereas some final values can be known and some ones can be undetermined. Analogically, the initial value of time, t^n, is usually accepted as equal to zero ($t^0=0$), whereas the final value can be fixed or free.

The form of the boundary conditions for adjoint variables comes from the form of performance index and conditions for state variables. Therefore, for the performance index described by the Lagrange form, equation (2), the following holds: if the value of the state variable is undetermined then right adjoint variable is equal zero, whereas if the value of the state variable is fixed then the value of related adjoint variable is free. Similarly if the time, t^n, is free, then the Hamiltonian H^n is equal to zero, whereas if the time, t^n, is fixed then the Hamiltonian is undetermined. In the case when the enlarged Hamiltonian is used, conditions presented above take the following form: if the time is free the variable adjoint with the time, z_t^{n-1}, equals zero, whereas if the time is fixed the adjoint variable is undetermined.

Above conditions can be summarized in the following form:

$$\begin{aligned}x_i^n-\text{fixed}&\Rightarrow z_i^n-\text{undetermined}\\t^n-\text{fixed}&\Rightarrow H^n\text{ or }z_t^n-\text{undtermined}\\x_i^n-\text{undetermined}&\Rightarrow z_i^n=0\\t^n-\text{undetermined}&\Rightarrow H^n=0\text{ or }z_t^n=0\end{aligned}\tag{15}$$

One should underline that the boundary conditions discussed above are valid for the performance index given by equation (2) (Lagrange's form). The boundary conditions for other forms of the performance index and for more complicated conditions for initial and final state variables can be found in the literature [Fan, 1966; Fan and Wang, 1964; Boltyanski, 1973].

3 Generalized Version of the Discrete Algorithm with Constant Hamiltonian

The classical version of the discrete algorithm with constant Hamiltonian is limited by the requirement of the linearity of the process optimization model, including all state equations and performance index, with the

respect to a distinguished decision variable. This requirement is satisfied by many models of engineering processes, but not by all. Obviously, Katz' and Fan's algorithms can be used, but the discrete algorithm with constant Hamiltonian has some advantages in comparison with Katz' and Fan's algorithm. One of these advantages is the fact that a physical meaning can be attributed to Hamiltonian and adjoint variables in the algorithm with the constant Hamiltonian whereas similar interpretations are quite limited for Katz' and Fan's algorithms. This advantage is especially apparent for an optimization problem wherein a solving procedure demands to use an iterative method in which some values of adjoint variables and Hamiltonian must be assumed. Therefore, the natural idea emerges to generalize the classical version of the discrete algorithm with constant Hamiltonian, so as it could be used for nonlinear optimization problem. By the nonlinear problem we mean here the one in which one cannot find any control variable with respect to which all equations of optimization model are linear. In brief, this means that variables θ^n may appear nonlinearly in the process model.

We recall that the equations presented above are linear with respect to decision θ^n. This is too restrictive for some models of heat and chemical cascades, and for computational difference models obtained by the discretization of continuous (differential) equations. Therefore a generalized version of the discrete Hamiltonian algorithm is derived below by using the method of Lagrange's multipliers. As mentioned above, the generalized version does not require all equations of the optimization model (for the performance index and state transformations) to be linear with respect of a selected decision variable. A derivation of the generalized version is presented below.

In the derivation presented below we concentrate on some differences between classical and generalized version of the discrete algorithm with constant Hamiltonian, whereas some considerations about features common for both versions are omitted. This omission mainly concerns boundary conditions, which are the same for both versions, so the equations of the boundary conditions for the state variables and the (derivation of) boundary conditions for the adjoint variables are not taken into consideration. The broadened information concerning the problem of the derivation of boundary conditions can be found in the literature [Fan, 1966], [Fan and Wang, 1964], [Boltyanski, 1973].

The considered performance index for the generalized version of discrete algorithm with constant Hamiltonian takes a following general form:

$$I = \sum_{n=1}^{N} f_0^n \left(\mathbf{x}^n, \mathbf{u}^n, t^n, \theta^n\right) \theta^n \tag{16}$$

While the performance index (16) is quite similar to the performance index described by equation (2), one should note that the profit rate function f_0^n can explicitly contain the variable θ^n. This shows a significant difference between both performance indices (equations (2) and (16)) because the profit rate in the classical version of the algorithm cannot be a function of θ^n.

State equations for $n = 1, ..N$ and $i = 1, ..s$ take a general form

$$x_i^n - x_i^{n-1} = f_i^n \left(\mathbf{x}^n, \mathbf{u}^n, t^n, \theta^n\right) \theta^n \tag{17}$$

Analogously to the performance index, also rates in state equations f_i^n contain explicitly the decision variable θ^n, in contrary to the functions f_i^n of classical version, which cannot contain the control θ^n as an explicit argument. The state equation (1) for the state variable t^n remains valid for both versions of the algorithm.

For the optimization problem defined by equations (16) and (17), the Lagrange function takes the following form:

$$\begin{gathered} L\left(x_1^1..x_s^N, u_1^1..u_r^N, t^1..t^N, \theta^1..\theta^N, \lambda_1^0..\lambda_s^N, \lambda_t^0..\lambda_t^N\right) = \\ = \sum_{n=1}^{N} f_0^n \theta^n + \sum_{n=1}^{N}\sum_{i=1}^{s} \lambda_i^{n-1}\left(f_i^n \theta^n - x_i^n + x_i^{n-1}\right) + \\ + \sum_{n=1}^{N} \lambda_t^{n-1}\left(\theta^n - t^n + t^{n-1}\right) + \sum_{i=1}^{l} \lambda_i^N \left(c_i - x_i^N\right) + \\ + \lambda_t^N \left(t_k - t^N\right) \end{gathered} \tag{18}$$

where λ_i^{n-1} and λ_t^{n-1} are Lagrange multipliers, c_i are the fixed final values of state variables, whereas l is a number of fixed final values of state variables, and t_k is a fixed final value of time. As mentioned above, all initial values of state variables are usually fixed, therefore they are not arguments of the Lagrange function.

Substituting the enlarged Hamiltonian defined in the following form

$$\begin{gathered} \tilde{H}\left(\mathbf{x}^n, \mathbf{u}^n, t^n, \theta^n, \boldsymbol{\lambda}^n, \lambda_t^n\right) = \\ = f_0^n + \sum_{i=1}^{s} \lambda_i^{n-1} f_i^n + \lambda_t^n \end{gathered} \tag{19}$$

into equation (18) we obtain the following new form of the Lagrange function:

$$\begin{gathered} L\left(.....\right) = \sum_{n=1}^{N} \tilde{H}\left(\mathbf{x}^n, \mathbf{u}^n, t^n, \theta^n, \boldsymbol{\lambda}^n, \lambda_t^n\right) \theta^n + \\ + \sum_{n=1}^{N}\sum_{i=1}^{s} \lambda_i^{n-1}\left(-x_i^n + x_i^{n-1}\right) + \\ + \sum_{n=1}^{N} \lambda_t^{n-1}\left(-t^n + t^{n-1}\right) + \sum_{i=1}^{l} \lambda_i^N \left(c_i - x_i^N\right) + \\ + \lambda_t^N \left(t_k - t^N\right) \end{gathered} \tag{20}$$

The necessary condition for an extremum of the performance index (16) requires that the partial derivatives of Lagrange function (20) with respect to all state variables, all decisions and all Lagrange multipliers must be equal to zero.

The derivatives of equation (20) for all components of vector $\boldsymbol{\lambda}^{n-1}$ and for λ_t^{n-1} ($n = 1...N$) take the following forms

$$\frac{\partial L\left(...\right)}{\partial \lambda_i^{n-1}} = \frac{\partial \tilde{H}^{n-1}}{\partial \lambda_i^{n-1}}\theta^n - x_i^n + x_i^{n-1} = 0 \qquad (21)$$

$$\frac{\partial L\left(...\right)}{\partial \lambda_t^{n-1}} = \frac{\partial \tilde{H}^{n-1}}{\partial \lambda_t^{n-1}}\theta^n - t^n + t^{n-1} = 0 \qquad (22)$$

where the symbol $L\left(...\right)$ signifies a short notation of the Lagrange function with its all arguments. From the derivatives of L with respect to the multipliers with the superscript N, λ_i^N and λ_t^N, conditions for final values of state variables are obtained:

$$\begin{aligned} c_i - x_i^N &= 0 \\ t_k - t^N &= 0 \end{aligned} \qquad (23)$$

Next, after deriving all suitable derivatives of L with respect to all components of state vector $\mathbf{x}^n$ ($n = 1...N$) and time t^n we obtain the following equations:

$$\frac{\partial L\left(...\right)}{\partial x_i^n} = \frac{\partial \tilde{H}^{n-1}}{\partial x_i^n}\theta^n + \lambda_i^n - \lambda_i^{n-1} = 0 \qquad (24)$$

$$\frac{\partial L\left(...\right)}{\partial t^n} = \frac{\partial \tilde{H}^{n-1}}{\partial t^n}\theta^n + \lambda_t^n - \lambda_t^{n-1} = 0 \qquad (25)$$

The weak optimality condition for the decision variables - the components of vector $\mathbf{u}^n$ takes a following form

$$\frac{\partial L\left(...\right)}{\partial u_j^n} = \frac{\partial \tilde{H}^{n-1}}{\partial u_j^n}\theta^n = 0 \qquad (26)$$

whereas the optimality condition for the decision variable θ^n is found as:

$$\frac{\partial L\left(...\right)}{\partial \theta^n} = \frac{\partial \tilde{H}^{n-1}}{\partial \theta^n}\theta^n + \tilde{H}^{n-1} = 0 \qquad (27)$$

In algorithms of Maximum Principle the Lagrange's multipliers are substituted by the adjoint variables. For the optimization problem defined above by equations (1) – (3) the adjoint variables are equal to the Lagrange's multipliers. Replacing the Lagrange multipliers by the adjoint variables, the generalized Hamiltonian, equation (19), can be rewritten to the form:

$$\tilde{H}^{n-1} = f_0^n + \sum_{i=1}^{s} z_i^{n-1} f_i^n + z_t^{n-1} = 0 \qquad (28)$$

With adjoint variables taken in place of Lagrange multipliers, equations (21), (22) and (24) (27) can be rewritten to the following form:

$$\frac{\partial \tilde{H}^{n-1}}{\partial z_i^{n-1}} = \frac{x_i^n - x_i^{n-1}}{\theta^n} \qquad (29)$$

$$-\frac{\partial \tilde{H}^{n-1}}{\partial x_i^n} = \frac{z_i^n - z_i^{n-1}}{\theta^n} \qquad (30)$$

$$-\frac{\partial \tilde{H}^{n-1}}{\partial t^n} = \frac{z_t^n - z_t^{n-1}}{\theta^n} \qquad (31)$$

$$\frac{\partial \tilde{H}^{n-1}}{\partial u_j^n} = 0 \qquad (32)$$

$$\frac{\partial \tilde{H}^{n-1}}{\partial \theta^n} + \frac{\tilde{H}^{n-1}}{\theta^n} = 0 \qquad (33)$$

Equations (29)–(30) are quite similar to those describing the classical version of the discrete algorithm with a constant Hamiltonian. The only difference, equation (33), is caused by the generalized property of enlarged Hamiltonian, which is an explicit function of time intervals θ^n. As we already know, in the classical version of the algorithm, control variables θ^n cannot be an explicit argument of the Hamiltonian.

Equation (33) is not present in the traditional structure of the constant Hamiltonian algorithm. Yet, this equation appears in the generalized algorithm (28)-(33) in place of equation (14) which is limited to the traditional version (and which states that the optimal enlarged Hamiltonian is always equal to zero). One should easily note that if the Hamiltonian is not an explicit function of control variable θ^n then equation (33) reduces to equation (14). So, we may conclude that the discrete constant-Hamiltonian algorithm is a particular, discrete counterpart of the continuous algorithm of Maximum Principle.

Boundary conditions for adjoint variables connected with all state variables and time are the same for both versions of the discrete algorithm.

4 Course of Calculations

In the typical problems initial values of all state variables are usually known, while final ones are known only for some state variables whereas the others are undetermined. Such a case is described below but the calculation procedure is the same if the some initial values are undetermined. Only conditions for the termination of calculation are different.

Final values of adjoint variables result from boundary conditions. Thus the values of adjoint variables are undetermined if the values of corresponding state variables are known, and the adjoint variables are equal zero if the corresponding state variables are free. Therefore in the first step of calculation procedure unknown values of state and adjoint variables must be assumed.

The optimization calculation can be accomplished by the following procedure:

1. Unknown final values of state and adjoint variable are assumed.

2. For the last stage of cascade ($n = N$) the set of equations (29) (33) is solved; All values of state and adjoint variables before the last stage, x^{N-1} and z^{N-1}, are obtained along with values of decision variables, $\mathbf{u}^N$ and θ^N, moreover the values of t^{N-1} and are found.

3. Next, n is decreased by taking successively values $N-1$, $N-2$, ... 2, 1, and the set of equations (29) (33) is solved again for all values of n; all values of state and adjoint variables before the stage n, $\mathbf{x}^{n-1}$ and $\mathbf{z}^{n-1}$ as well the values of decision variables at this stage, $\mathbf{u}^n$ and θ^n are obtained. For each stage the values of t^{n-1} and z_t^{n-1} are obtained.

4. After solving the set of equations for $n = 1$ the values of state and adjoint variables before of cascade, $\mathbf{x}^0$, $\mathbf{z}^0$, t^0 and z_t^0 are calculated. The procedure is terminated if the calculated values of state and adjoint variables are equal to the fixed values of these variables; if not, new values of final unknown variables must be assumed in the first step.

Termination of above optimization procedure follows if the fixed values of state and adjoint are achieved by calculated values of these variables. In the case when all initial values of state variables are fixed all values of adjoint variables are free, so only fixed and calculated values of state variables are compared. In the case when some initial values of state variables are know and some are undetermined, calculated values of state variables are compared with the fixed ones, whereas calculated adjoint variables connected with state variables, which are undetermined, must be equal to zero.

5 Example of Application

Applications of optimal control can be discussed for a number of unit processes including transport phenomena, separation systems, and energy systems. The potential application of the optimization algorithm presented above and some examples for all these systems was reported on Sieniutycz [Sieniutycz, 2006]. Whereas the below example concerns the problem of maximizing profit in a cascade of chemical reactors with ideal mixing.

5.1 Profit Maximization for Chemical Reaction

The performance index accepted in our consideration describes a profit obtained from sale of reaction product and reduced by cost of reactors. The obtained profit is proportional to final concentration of product, whereas the cost of reactor is proportional to the reactor volume involution m, so the performance index takes a form

$$I = \sum_{n=1}^{N} c_R \left(x^n - x^{n-1}\right) - \frac{b_R}{\tau_u} \left(V_R^n\right)^m \tag{34}$$

where c_R is a price of reaction product, b_R and m are a coefficients in the reactor cost equation and τ_u is an utilization time. The first-order reversible catalytic reaction proceeding in cascade of ideally mixed reactors is considered in this paper. The increase of reaction product on the stage n is given by following form

$$x^n - x^{n-1} = \left[k_1 a\left(t^n\right)\left(1 - x^n\right) - k_2 a\left(t^n\right) x^n\right] \theta^n \tag{35}$$

where x is a product concentration; k_1 and k_2 are the reaction-rate constants; θ^n is a holdup time on the stage n; $a(t^n)$ is a catalyst activity factor and it is a function of a state variable called a time, t^n. The catalyst activity decreases during the reaction and it is described by following expression:

$$a = a_0 e^{-kt} \tag{36}$$

The equation (34) describing a performance index can't be directly used in optimization algorithm, so above equation must be transformed to the following form

$$I = \sum_{n=1}^{N} \left[\begin{array}{c} k_1 a\left(t^n\right)\left(1 - x^n\right) + \\ -k_2 a\left(t^n\right) x^n - \beta \left(\theta^n\right)^m \end{array}\right] \theta^n \tag{37}$$

where coefficient β is defined by expression:

$$\beta = \frac{b_R q}{\tau_u c_R} \tag{38}$$

In accordance with optimization algorithm presented above the Hamiltonian for stage n takes a following form

$$\begin{aligned} \tilde{H} = \left(1 + z^{n-1}\right) \left[k_1 a\left(t^n\right)\left(1 - x^n\right) - k_2 a\left(t^n\right) x^n\right] + \\ -\beta \left(\theta^n\right)^{m-1} + z_t^{n-1} \end{aligned} \tag{39}$$

The conditions for optimality of decision variables, temperature and holdup time, are described by following equations, respectively:

$$\frac{\partial \tilde{H}^{n-1}}{\partial T^n} = \\ = \left(1+z^{n-1}\right)\begin{bmatrix} k_1 a\left(t^n\right)\left(1-x^n\right)\frac{E_1}{R(T^n)^2}+ \\ -k_2 a\left(t^n\right)x^n\frac{E_2}{R(T^n)^2}\end{bmatrix} = 0 \tag{40}$$

$$\tilde{H}^{n-1}+\theta^n\frac{\partial \tilde{H}^{n-1}}{\partial \theta^n} = \\ \left(1+z^{n-1}\right)\left[k_1 a\left(t^n\right)\left(1-x^n\right)-k_2 a\left(t^n\right)x^n\right]+ \\ -\beta\left(\theta^n\right)^{m-1}-\beta\left(m-1\right)\left(\theta^n\right)^{m-1}+z_t^{n-1}=0 \tag{41}$$

The equation (40) allow us to determine the optimal temperature, which depends only on the current degree of conversion x^n at each stage.

$$T^n = \frac{E_2-E_1}{R\ln\left(\frac{k_{20}E_2}{k_{10}E_1}\frac{x^n}{1-x^n}\right)} \tag{42}$$

The adjoint equations describing changes of adjoint variables on the stage n take a following forms:

$$\frac{\partial \tilde{H}^{n-1}}{\partial x^n} = -\frac{z^n-z^{n-1}}{\theta^n} = \\ = \left(1+z^{n-1}\right)\left[-k_1 a-k_2 a\right]=0 \tag{43}$$

$$\frac{\partial \tilde{H}^{n-1}}{\partial t^n} = -\frac{z_t^n-z_t^{n-1}}{\theta^n} = \\ = -\left(1+z^{n-1}\right)\left[-k_1\left(1-x^n\right)-k_2 x^n\right]a_0 k e^{-kt^n}=0 \tag{44}$$

Because final values of reaction product concentration, x^N, and the time, t^N, are free the final values of right adjoint variables are equal zero (z^N and z_t^N). At the beginning of calculations the final values of state variables x^N and t^N have to be assumed, next the set of equations (34-44) from the last stage to the first stage must be resolved and finally one ought to compare calculated initial values of state variables (x^0 and t^0) with required ones. If calculated values are right the calculation are finished, if not the new final values of state variables must be assumed.

6 Summary

The paper presents two versions of the Hamiltonian optimization algorithm for discrete systems: the traditional version and a generalized version. Traditional version of the discrete Hamiltonian algorithm, relatively unknown in the literature, requires the optimization model (performance index and state transformations) to be linear with the respect of one, distinguished control variable, usually the time interval. This requirement is a considerable restriction for using this algorithm. Still, there is a clear advantage of the algorithm, namely, the well defined meaning of adjoint variables, which are the same as in continuous systems (Pontryagin's adjoints, identical with the Lagrange multipliers of the state equations). This possibility doesn't occur in other discrete algorithm (Katz' and Fan's algorithm). It was thus reasonable to develop a new optimization algorithm which, while still preserving Pontryagin's definition of state adjoints, could be used to optimize discrete models nonlinear in time intervals. In this paper, we have used the method of Lagrange's multipliers to derive such a generalized version of discrete algorithm with constant Hamiltonian for the Lagrange form of performance index. This new version of the discrete algorithm can be used to solve both linear and nonlinear optimization problems.

The use of the generalized version is exemplified by optimizing a chemical reaction problem in Section 5. In this problem the state transformations are linear with respect to the holdup time, but the performance index is linear for the exponent $m = 1$ and nonlinear for the exponent $m \neq 1$. Therefore classical version of discrete algorithm with constant Hamiltonian could not be used, but the generalized one could be applied for both non and linear problems. Other examples of optimization solutions are obtained for difficult (heterogeneous) models of fluidization, with bubling and other imperfections [Poswiata, 2003)], [Poswiata, 2004].

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