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A General Quasi-Canonical Structure for Hamiltonian Optimization of Sequential Energy Systems*

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Abstract

The mathematical basis of the general theory is Bellman's dynamic programming (DP) and associated maximum principles. Our original contribution develops a generalized theory for multistage discrete processes in which time intervals can reside in the model nonlinearly and can be constrained. The new theory removes the requirement of the free intervals θ^n, yet preserves the most powerful features of the continuous theory of Pontryagin in the discrete context. Applications deal with dynamic optimization of diverse energy and chemical systems in which a minimum of entropy generation is the criterion of performance; from this basic criterion reasonable partial criteria are derived. It is possible to handle optimality conditions for complex systems with state dependent coefficients, and thus to generalize analytical solutions obtained in linear cases to nonlinear situations. Correspondence is shown with basic theoretical mechanics and classical Hamilton-Jacobi theory when the number of stages approaches an infinity.

Key words: optimization, constrained energy systems, discrete control, Hamiltonian theories

1. Introduction

In this paper two Hamiltonian theories are analyzed which are ideally suited for optimization of single-stage and multistage energy systems such as: thermal machines, solar collectors, multi-gap (or tandem) solar cells, heating and drying unit operations, solid handling systems and chemical reactors. The optimization criteria the theories may handle can be arbitrary; in particular they can be constructed on the basis of exergy or economic balance. The first theory is a relatively little known discrete theory with a constant Hamiltonian (Sieniutycz, 1991), and the second one is the new theory which is a quasi-Hamiltonian generalization of the former. The new theory, which is presented in the last section of the paper, synthesizes the two known optimization theories: the traditional (Katz's-Fan's) multistage theory (Fan and Wang, 1964), where the Hamiltonian is not that of Pontryagin (Pontryagin, 1982), and the first theory based on the Pontryagin's like Hamiltonian whose model admits only free residence time intervals, θ^n (Sieniutycz, 1991). The new theory removes the requirement of the free intervals θ^n, yet it transfers the most powerful features of the well-known continuous theory of Pontryagin to the realm of discrete processes.

To formulate the new theory, a class of multistage optimal processes linear with respect to a constrained residence time interval (or a state variable interval) is derived from an arbitrary set of difference constraints. Next, with the help of dynamic programming method (Bellman, 1957; Aris, 1964; Findeisen et. al., 1980), the necessary conditions of optimality are determined in a form which contains a discrete Hamilton-Jacobi

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equation, the optimal control condition and discrete canonical equations. It is then shown that in discrete non-autonomous systems with unconstrained time intervals, θ^n, an enlarged, Pontryagin-like Hamiltonian $\tilde{H}^n$ emerges, which vanishes along the optimal discrete path. In processes with constrained θ^n, the constancy of $\tilde{H}^n$, could still be attained by inclusion of the Lagrange multiplier of the time constraint, λ; yet in terms of $\tilde{H}^n$ the canonical equations are modified by presence of λ-dependent terms. From a physical standpoint, the constancy condition $\tilde{H}^n = 0$ for free optimal θ^n is a sort of tenergy conservation condition as applied to optimal discrete systems.

Applications can be illustrated with the optimization of multistage heat-pump-assisted heating operations and with drying operations which may use solar energy. Applications with thermal machines involve an extension of the classical problem of minimal work to multistage operations with finite heat transfer area. Benefits resulting from power and versatility of both theories when they are applied to optimization of diverse energy systems are explicit. A more detailed account of applications can be found in the forthcoming book (Berry et. al., 2000) and a monograph (Sieniutycz, 2000).

2. Continuous Optimization Problem

To derive necessary optimality conditions, dynamic programming (DP) is applied to both continuous and discrete processes. A discrete approach to sequential systems allows one to pass from DP results to a nontraditional discrete maximum principle which is another powerful computational tool.

Here is an outline of our methodology. We search for a maximum of a Bolza functional S, with a gauging function G, subject to differential constraints for the state vector **x**

$$\frac{d x_i}{dt} = f(\mathbf{x}, t, \mathbf{u}) \tag{1}$$

The control $\mathbf{u} = (u_1, u_2, ...u_r)$ is constrained i.e., $\mathbf{u} \in \mathbf{U}$ where **U** is the admissible set in the control space. We define an optimal performance function $V(\mathbf{x}^i, t^i, \mathbf{x}^f, t^f)$ as max S, i..e

$$\begin{aligned} V(\mathbf{x}^i, t^i, \mathbf{x}^f, t^f) &\equiv \max S \\ &= \max\{\int_{t^i}^{t^f} f_0(\mathbf{x}, t, \mathbf{u}) dt \\ &+ G(\mathbf{x}^f, t^f) - G(\mathbf{x}^i, t^i)\} \end{aligned} \tag{2}$$

Bellman`s optimality then yields the so-called HJB equation (Hamilton-Jacobi-Bellman equation; (Sieniutycz, 1991; Findeisen et. al., 1980)

$$\frac{\partial V}{\partial t} + \min_u\{\frac{\partial V}{\partial \mathbf{x}} . \mathbf{f}(\mathbf{x}, t, \mathbf{u}) - \tilde{f}_0(\mathbf{x}, t, \mathbf{u})\} = 0 \tag{3}$$

where a gauged profit intensity

$$\begin{aligned} \tilde{f}_0(\mathbf{x}, t, \mathbf{u}) &\equiv f_0(\mathbf{x}, t, \mathbf{u}) \\ &+ \frac{\partial G}{\partial t} + \sum_{i=1}^{s} \frac{\partial G}{\partial x_i} f_i(\mathbf{x}, t, \mathbf{u}) \end{aligned} \tag{4}$$

appears in a HJB equation for V. To solve the variational problem of max S we can solve the HJB equation in terms of **u** to obtain u(**p**, t, **x**). When we substitute this function into Eq. (3) the Hamilton-Jacobi equation for V follows

$$-\frac{\partial V}{\partial t} + H(\mathbf{x}, t, -\frac{\partial V}{\partial x_i}) = 0 \tag{5}$$

This form refers to variations of final states and times.

3. Optimization of Discrete Processes

Our first main purpose is to develop a discrete analogy with Eqs. (1) - (5) which would allow description of real multistage processes with small number of finite stages, whereas our second purpose is to exploit this analogy to construct discrete computational algorithms that would numerically solve continuous problems at the limit of very large number of stages, N. Thus we consider the discrete Bolza functional S^N

$$\begin{aligned} S^N &= \sum_{n=1}^{N} f_0(\mathbf{x}^n, t^n, \mathbf{u}^n)\theta^n \\ &+ G(\mathbf{x}^N, t^N) - G(\mathbf{x}^0, t^0) \end{aligned} \tag{6}$$

The maximum for S^N of Eq. (6) is subject to constraints resulting from difference equations

$$x_i^n - x_i^{n-1} = f_i(\mathbf{x}^n, t^n, \mathbf{u}^n)\theta^n. \tag{7}$$

The discrete optimization problem can be stated as that of maximizing S for n = N when the initial point $(\mathbf{x}^0, t^0)$ is fixed. In optimization it is essential to recognize the role of the necessary optimality condition for free intervals of time, θ^n, which yields a vanishing "enlarged Hamiltonian" and the role of generalization of Bellman's recurrence equation to the so-called stage criterion. The latter enables one to include variations of end states and times, thus yielding simultaneously the discrete characteristics and the conditions for an optimal control.

A definition of the optimal performance function V states this function in the form

$$V^n(\mathbf{x}^n, t^n) = \max\{\sum_{k=1}^{n}[f_0^k + (\theta^k)^{-1}(G(\tilde{\mathbf{x}}^k) - G(\tilde{x}^k - f^k\theta^k))]\theta^n\} \equiv \max\{\sum_{k=1}^{n}\tilde{f}_0^k\theta^k\}. \quad (8)$$

where $\tilde{f}_0^k$ is the gauged profit intensity, a discrete analog of that in Eq. (4). The stage criterion

$$0 = \max_{\mathbf{u}^n,\theta^n,\mathbf{x}^n,t^n}\{f_0^n(\mathbf{x}^n, t^n, \mathbf{u}^n)\theta^n - (P^n(\mathbf{x}^n, t^n) - P^{n-1}((\mathbf{x}^n - \mathbf{f}^n(\mathbf{x}^n, t^n, \mathbf{u}^n)\theta^n, t^n - \theta^n))\} \quad (9)$$

where $P^n = G^0 - G(x^n, t^n) + V^n$, is applied to determine the set of necessary optimality conditions including those with respect to $\mathbf{x}^n$ and time t^n. This realizes passage to the algorithm of discrete maximum principle and related canonical equations. Equation (9) yields all relevant information: it leads to HJB equations, definition of H, state adjoints and canonical set. Bellman's equation follows in a 'forward' from the criterion (9) for the fixed final state and time. Thus, starting with $V^0 = 0$ the sequence $V^1,...V^n...V^N$ can be obtained by a recurrence procedure searching for extremum controls $\mathbf{u}^n$ and θ^n at the constant coordinates ($\mathbf{x}^n$, t^n). This leads to the condition:

$$-\partial P^{n-1}/\partial t^{n-1} + \max_{\mathbf{u}^n}\{f_0^n(\mathbf{x}^n, t^n, \mathbf{u}^n) - (\partial P^{n-1}/\partial \mathbf{x}^{n-1}).\mathbf{f}^n(\mathbf{x}^n, t^n, \mathbf{u}^n)\} = 0 \quad (10)$$

which is a discrete HJB equation (Sieniutycz, 1991; Berry et. al., 2000). It represents a maximum principle with respect to $\mathbf{u}^n$ for the 'Hamiltonian', the expression in braces of the above equation. Equation (10) states that the necessary condition for the maximum of S^N with respect to the control sequence $\{\mathbf{u}^n\}$ is that for the Hamiltonian. When the optimal control $\mathbf{u}^n$ is evaluated from Eq. (10) and substituted into it, the result becomes the discrete Hamilton-Jacobi equation

$$H^{n-1}\left(x_1^n,...x_s^n, t^n, -\partial P^{n-1}/\partial x_1^{n-1}... - \partial P^{n-1}/\partial x_s^{n-1}\right) - \partial P^{n-1}/\partial t^{n-1} = 0 \quad (11)$$

which is nonlinear in terms of the derivatives $\partial P^{n-1}/\partial x^{n-1}$. It is written for the *extremum* H^{n-1}. In the limiting case of an infinitesimal sequence of θ^n, this equation goes over into the Hamilton-Jacobi equation of a continuous process.

Let us now fix controls $\mathbf{u}^n$ and θ^n in Eq. (9) and differentiate its expression in braces to determine the stationarity conditions with respect to the final state and time. We obtain an optimal difference set canonical with respect to two sorts of equations, one defining the changes of state and one the related changes of the adjoint variables. Using the phase-space Hamiltonian of energy type

$$H^{n-1}(\mathbf{x}^n, z^{n-1}, t^n, \mathbf{u}^n) \equiv f_0^n(\mathbf{x}^n, t^n, \mathbf{u}^n) + \sum_{i=1}^{s} z_i^n f_i^n(\mathbf{x}^n, t^n, \mathbf{u}^n) \quad (12)$$

the algorithm of the discrete maximum principle follows in the form

$$\frac{x_i^n - x_i^{n-1}}{\theta^n} = \frac{\partial H^{n-1}}{\partial z_i^{n-1}} \quad (13)$$

$$\frac{z_i^n - z_i^{n-1}}{\theta^n} = -\frac{\partial H^{n-1}}{\partial x_i^n} \quad (14)$$

$$\frac{H^n - H^{n-1}}{\theta^n} = -\frac{\partial H^{n-1}}{\partial t^n} \quad (15)$$

$$z_t^{n-1} + \max_{\mathbf{u}^n} H^{n-1}(\mathbf{x}^n, z^{n-1}, t^n, \mathbf{u}^n) = 0 \quad (16)$$

(n=1,...N; i=1,...s and l =1,...r.). For more details, see ref. (Sieniutycz, 1991; Berry et. al., 2000; Sieniutycz, 2000). Quite importantly, Eq. (15) does not follow (as in the continuous version) from the canonical equations for x_i and z_i, but it represents an independent extremum condition associated with the optimal choice of θ^n. In autonomous systems, $H^n = H^{n-1}$, i.e., the Hamiltonian is constant along an optimal discrete path.

4. Some Computational Aspects

Two most effective computational approaches are non-traditional. The primary idea is to solve some underlying equations such as the stage criterion equation (9) or its maximum principle equations (12) - (16), rather than related HJB equation (10) or Hamilton-Jacobi equation (11). This is because the solving methods for the preferred equations are those most efficient. The control theory approach used here differs from the traditional approach in which Hamilton-Jacobi equations are solved. Both continuous and discrete control processes are treated in the framework of the common discrete formalism. In the continuous case prior discretizing of the process differential equations is required. Eq. (9) is solved numerically in the form

$$0 = \max_{\mathbf{u}^n, \theta^n} \{\tilde{D}^n(\tilde{\mathbf{x}}^n, \mathbf{u}^n, \theta^n) + V^{n-1}(\tilde{\mathbf{x}}^n - \tilde{\mathbf{f}}^n(\tilde{\mathbf{x}}^n, \mathbf{u}^n)\theta^n) - V^n(\tilde{\mathbf{x}}^n)\} \quad (17)$$

where the symbol $\tilde{\mathbf{x}}^n$ denotes the enlarged vector ($\mathbf{x}^n$, t^n) and the tilde over D^n refers to the gauged cost including the effect of the state function G. The gauged profit $\tilde{D}^n = \tilde{f}_0^n \theta^n$ is a discrete counterpart of the continuous profit (4).

Now we outline the second basic numerical method. It applies the discrete maximum principle with the energy-type Hamiltonian. The necessary extremum conditions are discrete canonical equations. For numerical applications they are written in a form of algebraic equations which should be solved with a computer. Typical optimization problems lead to two-point boundary conditions. Due to the strong analogy with the Pontryagin's algorithm, procedures which deal with two-point boundary values and control improvement are identical with those applied in the standard continuous algorithm. Methods of trajectory improvement in the state space, and gradient methods in the control space are effective. Quite generally, an approach transforms the discrete maximum principle into a final set

$$F_1(\mathbf{x}^n, \mathbf{x}^{n-1}, \mathbf{z}^n, t^n) = 0 \quad (18a)$$

and

$$F_2(\mathbf{x}^n, \mathbf{z}^{n-1}, \mathbf{z}^n, t^n) = 0 \quad (18b)$$

From this set the state and adjoints before n-th stage, $\mathbf{x}^{n-1}$ and $\mathbf{z}^{n-1}$, and all other quantities are determined, thus the computer may pass to the stage n-1. This is a backward procedure, necessary in the case of complex dependence of the rate functions on the state $\mathbf{x}^n$. See ref. (Sieniutycz, 2000) for more information.

5. Examples of Applications

We now present a review of applications of the theory in multiphase systems. We begin with a process in which work is produced by multistage thermal machines operating between a fluid and a bath, a sequence of 'endoreversible' engines. In an analytical multistage problem one maximizes the work criterion

$$S^n = \sum_{n=1}^{N} f_0^n(T^n, u^n)\theta^n \equiv \sum_{n=1}^{N} c\left(\frac{T^e}{T^n + \chi^n u^n} - 1\right)u^n\theta^n \quad (19)$$

The task is to achieve an extension which could take into account the variability of thermal and transfer coefficients (such as the specific heat capacity c or the overall heat transfer coefficient α' contained in χ) and to include mass transfer. This is important because only numerical solutions are possible for complex profits $\tilde{D}^n$ or $\tilde{f}_0^n$. Therefore, instead of maximizing extensions of Eq. (19) analytically, a computer generates tables of optimal controls and optimal costs through direct extremizing procedure contained in the recurrence equation

$$R_*^n(T^n, X^n) = \min_{u^n, \theta^n, v^n} \{[-f_0^n(T^n, X^n, u^n, v^n) + h]\theta^n + R_*^n(T^n - u^n\theta^n, X^n - v^n\theta^n) \quad (20)$$

where h = H serves as the Lagrange multiplier of time constraint. The X-free truncation of this equation serves to generate numerical solutions for pure heat transfer when both transfer coefficients vary along the process path and an analytical solution cannot be obtained. The classical thermodynamic work is recovered in the reversible limit ($\tau^f \Rightarrow \infty$). The reversible work represents an exact evaluation of the maximum work for infinite size systems only, or for systems with excellent transfer conditions. Clearly, reversible thermostatic limits are too low to be realistic, and the finite-time limits are more useful in practical evaluations.

We now consider another group, the separation processes of drying and adsorption. They do not generate mechanical energy although they may yield valuable products. They often run in cascades of ideally mixed fluidized beds. They are example of processes described by highly nonlinear state equations (sigmoidal equilibrium curves which don't approach straight lines even in limiting cases). Their performance index is an exergy cost which may be written as

$$S^n \equiv -\sum_{n=1}^{N} [eb_g^n(T_g^n, X_g^n) + h]\theta^n \quad (21)$$

where b_g is the specific exergy of a drying gas, and e is the economic value of the exergy unit. The h part of (21) represents the investment costs. To optimize this process, Belman's equation such as Eq. (20) can be solved. However, in this case we use the discrete maximum principle, Eqs. (12)-(16), and the numerical solution is obtained for optimal controls, optimal trajectories and optimal costs. The solutions apply to drying of sugar, porous sorbents and T-sensitive biological materials. These are dried relatively quickly, but otherwise their final T cannot be too high. The results show that the design of expensive apparatus should be associated with intense optimal processes, to assure short process duration.

Now we shall deal with relaxation processes in which state variables are linked by conservation laws for the energy, mass and momentum. This requires an approach which applies Lagrange multipliers to handle dependent rates. The system contains two phases δ and γ which relax to the mutual equilibrium, due to the internal heat and mass transfer between subsystems. In view of state-dependent dissipation, instead of solving a HJB equation we solve a recurrence equation for the minimum of entropy production

$$S_\sigma^n(\mathbf{x}^n) = \min_{v^n,\theta^n,\mu'^n} \{ l_0^n(x^n, \mathbf{v}^n, \mu'^n)\theta^n + S_\sigma^{n-1}(\mathbf{x}^n - v^n\theta^n)\}. \tag{22}$$

where l_0^n is the thermodynamic Lagrangian, the sum of the rate-dependent and state-dependent dissipation functions plus a term with the Lagrange multiplier $\boldsymbol{\mu}'$ as an extra control that handles the conservation law constraint. The superiority of Eq. (22) over a traditional variational formulation follows from arbitrary dependence of resistance functions on the state **x**. The production of the entropy obtained should be subtracted from a fixed final entropy S^f to get the actual entropy of the system.

Now we pass to a problem of least resistivity for heat rays in inhomogeneous systems. When the thermal gradient is prescribed, the flow of thermal energy can be described in terms of 'heat rays', or paths of energy flow in direction of the gradient of T^{-1}. Their deviation from straight lines results from variable thermal conductivity. The heat rays trace paths satisfying the principle of minimum of entropy production which assures the minimum resistivity of the path. The shape of heat rays is an optimal control problem for minimum of the resistance integral

$$(-S) = \int_{t1}^{t2} A_0\rho(x)(1+u^2)dx \tag{23}$$

subject to the control u = dy/dx. A_0 is the constant area of projection of the heat flux tube crossectional area on the surface of constant resistivity. The principal function $R(x^i, y^i, x^f, y^f)$, defined as the minimum of the integral (23), satisfies a HJB equation in which the maximum condition yields an optimal control in the form of the tangent law of bending for a thermal ray, ρ(x)dy/dx = constant. The solution to this HJB can always be broken down to quadratures. However, if the resistivity ρ(x) is too complex, the integrals cannot be evaluated analytically. Hence the role of the discrete approach which solves numerically the recurrence equation

$$R^n(y^n, x^n) = \min_{\mathbf{u}^n,\theta^n} \{A_0^{-1}\rho(x^n)(1+u^2)\theta^n + R^n(y^n - u^n\theta^n, x^n - \theta^n)\}, \tag{24}$$

where $\theta^n = x^n - x^{n-1}$. This does not have an analytical solution for an arbitrary $\rho(x^n)$, thus the sequence R^n is generated numerically. For $N \to \infty$ the numerical solution to Eq. (24) automatically accomplishes the numerical integration.

Our last example deals with chemical waves rotating in porous membranes where propagation of concentration fronts as (bio)chemical waves satisfies the principle of minimum time. The DP approach leads to a HJB equation and its characteristic set for chemical waves. Usually 'geodesic' constraints due to an obstacle influence the state changes and the entering (leaving) conditions of a ray as a tangentiality condition for rays that begin to slide over the boundary of an obstacle. When a function describing the velocity of wave propagation c is known, a HJB equation can be formulated. For a constrained problem of minimum time in 3D systems, a HJB equation is

$$\max_{u,v,\mu'} \left\{ \frac{\partial\gamma}{\partial x}\frac{c(\mathbf{x},u,v)}{\sqrt{1+u^2+v^2}} + \frac{\partial\gamma}{\partial y}\frac{c(\mathbf{x},u,v)u}{\sqrt{1+u^2+v^2}} + \frac{\partial\gamma}{\partial z}\frac{c(\mathbf{x},u,v)v}{\sqrt{1+u^2+v^2}} - (1+\mu'\phi(\mathbf{x})) \right\} = 0 \tag{25}$$

where u = dy/dx, v=dz/dx, and γ is the unknown function which describes the shortest transition time. The constraint $\phi(\mathbf{x})=0$ was built in, operative when the ray slides over the surface of an obstacle; the related Lagrange multiplier is μ. The multipliers of ∂γ/∂x, ∂γ/∂y and ∂γ/∂z in Eq. (25) represent the rates dx/dt, dy/dt and dz/dt that satisfy identically the constraint $(dx/dt)^2 + (dy/dt)^2 + (dz/dt)^2 = c^2(\mathbf{x},u,v)$. The numerical solution can be found by a DP equation for the minimum time $\gamma^n = \Sigma\theta^n$

$$\gamma^n(y,z,x) = \min_{u^n,v^n,\theta^n,\mu'^n} \Big\{(1+\mu'^n\phi(\mathbf{x}))\theta^n + \gamma^{n-1}\Big(y^n - \frac{c(\mathbf{x},u^n,v^n)u^n\theta^n}{\sqrt{1+(u^n)^2+(v^n)^2}}, z^n - \frac{c(\mathbf{x},u^n,v^n)v^n\theta^n}{\sqrt{1+(u^n)^2+(v^n)^2}},$$

$$x^n - \frac{c(\mathbf{x}, u^n, v^n)\theta^n}{\sqrt{1+(u^n)^2+(v^n)^2}}\big)\big\} = 0 \qquad (26)$$

Equation (26) makes possible numerical generation of the function γ(x, y, z) for the case of constrained wave motions in confined regions and in complex media. Experiments confirming the theory are available. Our examples show that highly nonlinear systems can be treated.

6. Outline of Generalized Theory for Arbitrary Discrete Processes

Here we briefly show how the theory can be generalized so that it can handle constrained intervals of time and arbitrary state transformations in which there is originally no control which appears linearly in the optimization model. When optimizing general discrete processes we deal most commonly with state transformations consistent with the backward algorithm of dynamic programming. In this case the original constraints are in the form of s+2 transformations

$$x_k^n = T_k^n(\mathbf{x}^{n-1}, \mathbf{u}^n) \qquad (27)$$

where k= 0, 1,...s, s+1, the 0-th state variable is the profit coordinate and s+1-th state variable is accepted as a time-like coordinate. As long as the coordinate x_{s+1} is the usual time t, the state vector **x** used here includes the space-time vector $\tilde{\mathbf{x}}$. Assuming that changes of the profit coordinate x_0 on the right hand sides of transformations (1) can only be additive, i.e. that T_0^n has the structure $x_0^{n-1} + g_0(\tilde{\mathbf{x}}^{n-1}, \mathbf{u}^n)$ and the remaining T_k^n does not contain x_0^{n-1}, we can deal as before with the optimal functions $V^n = \max S^n$ and $P^n = V^n + G^0 - G^n$. In these functions our present vector $\mathbf{x}^n$ marks solely coordinates of the space-time, without the profit coordinate x_0. Equation (27) represents, in fact, a common description in which each state output x_k^n is expressed in terms of all state inputs x^{n-1} and all controls $\mathbf{u}^n$. To be able to use these expressions in the forward DP algorithm we first invert them to gain transformations $l_k^n(\mathbf{x}^n, \mathbf{u}^n)$ in which each state input x_k^{n-1} is expressed in terms of all state outputs $\mathbf{x}^n$ and controls $\mathbf{u}^n$. With inverted transformations at our disposal we consider constraints in the form of s+2 transformations

$$x_k^{n-1} = l_k^n(\mathbf{x}^n, \mathbf{u}^n) \qquad (28)$$

By introducing the s+2 functions $g_k(\mathbf{x}^n, \mathbf{u}^n)$ defined as follows

$$g_k(\mathbf{x}^n, \mathbf{u}^n) \equiv x_k^n - l_k^n(\mathbf{x}^n, \mathbf{u}^n) \qquad (29)$$

the inverted transformations (28) take the form of difference equations

$$x_k^n - x_k^{n-1} = g_k(\mathbf{x}^n, \mathbf{u}^n) \qquad (30)$$

where k= 0, 1...s+1.

Now we introduce the interval of the time-like variable either as $\theta^n \equiv t^n - t^{n-1}$ (whenever $x_{s+1} \equiv t$) or as the quantity defined by an equation

$$x_{s+1}^n - x_{s+1}^{n-1} = \theta^n \qquad (31)$$

Note that the function $g_{s+1} \equiv g_t$ in Eq. (30) constraints intervals of time; they must satisfy Eq. (30) for k = s+1. We also define functions of relative rates

$$f_k(\mathbf{x}^n, \mathbf{u}^n) \equiv \frac{g_k(\mathbf{x}^n, \mathbf{u}^n)}{g_{s+1}(\mathbf{x}^n, \mathbf{u}^n)} \qquad (32)$$

Clearly, $f_{s+1} \equiv 1$. Applying these definitions in Eq. (30), we recover the basic difference model (7) as the substructure of the following s+ 2 equations of state

$$x_k^n - x_k^{n-1} = g_k(\mathbf{x}^n, \mathbf{u}^n)\theta^n, \qquad (33)$$

(k= 0, 1...s+1 and $f_{s+1} \equiv 1$), However, in this model the controls ($\mathbf{u}^n$, θ^n) should not only satisfy the standard constraint $\mathbf{u}^n \in \mathbf{U}$ but also one extra constraint

$$\theta^n - g_{s+1}(\mathbf{x}^n, \mathbf{u}^n) = 0 \qquad (34)$$

which limits the time intervals. Later we consider a generalization of Eq. (34) in which the inequality constraint $\theta^n - g_{s+1} \le 0$ replaces the original equation (34).

In the present notation, the discrete Bolza criterion S^N, Eq. (6), has the form

$$S^N = \sum_{n=1}^{N} f_0(\mathbf{x}^n, t^n, \mathbf{u}^n)\theta^n + G(\mathbf{x}^N, t^N) - G(\mathbf{x}^0, t^0). \qquad (35)$$

This quantity should attain a maximum subject the above set of constraints. As the profit generation intensity is independent of the coordinate x_0, the latter does not appear in Eqs. (32), (34) and (35).

The presence of the constraint (34) changes the form of the effective profit intensity which has to be applied in the stage criterion when deriving a canonical set from this criterion. A modified profit function $\widetilde{f}^n_{0\lambda}$ which adjoints constraint (34) to the original function $\widetilde{f}^n_0$ by a Lagrange multiplier λ be used in the stage criterion of the DP type. In the present case the stage criterion has the form

$$0 = \max_{\mathbf{u}^n, \theta^n, \mathbf{x}^n} \{f^n_0(\mathbf{x}^n, \mathbf{u}^n)\theta^n + \lambda^n(\theta^n - g_{s+1}(\mathbf{x}^n, \mathbf{u}^n)$$
$$- P^n(\mathbf{x}^n) - P^{n-1}((\mathbf{x}^n - \mathbf{f}^n(\mathbf{x}^n, \mathbf{u}^n)\theta^n))\} \quad (36)$$

Dealing with this criterion we define state adjoints in the manner consistent with the Hamiltonian (12)

$$z^{n-1}_k \equiv \frac{\partial P^{n-1}(\mathbf{x}^{n-1})}{\partial x^{n-1}_k} \quad (37)$$

(k = 1...s, s+1). Here, however, we shall use the *enlarged* Hamiltonian (including the time adjoint)

$$\widetilde{H}^{n-1}(\mathbf{x}^n, z^{n-1}, \mathbf{u}^n)$$
$$\equiv f^n_0(\mathbf{x}^n, \mathbf{u}^n) + \sum_{k=1}^{s+1} z^{n-1}_k f^n_k(\mathbf{x}^n, \mathbf{u}^n). \quad (38)$$

From Eq. (36), the necessary condition for maximum of S^N with respect to intervals θ^n is

$$[\widetilde{H}^{n-1}(\mathbf{x}^n, z^{n-1}, \mathbf{u}^n)]\delta\theta^n \le 0 \quad (39)$$

and that with respect to controls $\mathbf{u}^n$ is

$$\theta^n \left(\frac{\partial \widetilde{H}^{n-1}}{\partial \mathbf{u}^n} - \lambda^n \frac{\partial \ln g^n_{s+1}}{\partial \mathbf{u}^n}\right).\delta\mathbf{u}^n \le 0 \quad (40)$$

Equation (39) implies that for stationary and positive intervals θ^n, Eq. (31), and active constraint (34) the enlarged Hamiltonian is not constant as in the free-θ theory but satisfies the condition

$$\widetilde{H}^{n-1}(\mathbf{x}^n, z^{n-1}, \mathbf{u}^n) + \lambda^n = 0 \quad (41)$$

Equation (40) shows that interior optimal controls $\mathbf{u}^n$ satisfy the condition

$$\frac{\partial \widetilde{H}^{n-1}}{\partial \mathbf{u}^n} - \lambda^n \frac{\partial \ln g^n_{s+1}}{\partial \mathbf{u}^n} = 0 \quad (42)$$

which becomes the local maximum condition for $\widetilde{H}^{n-1}$ (and sometimes H^{n-1}) only in case of unconstrained θ^n. Equation (41) shows that the negative value of the Lagrange multiplier for the active local constraint (34) equals the value of the enlarged Hamiltonian function.

Now we perform variation of state and time coordinates in the stage criterion (36). Splitting the effect of space and time and using condition (41) we get a 'quasicanonical' set of optimality conditions

$$\frac{x^n_k - x^{n-1}_k}{\theta^n} = \frac{\partial \widetilde{H}^{n-1}}{\partial z^{n-1}_k} \quad (43)$$

$$\frac{x^n_{s+1} - x^{n-1}_{s+1}}{\theta^n} = \frac{\partial \widetilde{H}^{n-1}}{\partial z^{n-1}_{s+1}} = f^n_{s+1} \equiv 1, \quad (44)$$

$$\frac{z^n_k - z^{n-1}_k}{\theta^n} = -\frac{\partial H^{n-1}}{\partial x^n_k} - \widetilde{H}^{n-1}\frac{\partial \ln g^n_{s+1}}{\partial x^n_k} \quad (45)$$

$$\frac{z^n_{s+1} - z^{n-1}_{s+1}}{\theta^n} = -\frac{\partial H^{n-1}}{\partial t^n} - \widetilde{H}^{n-1}\frac{\partial \ln g^n_{s+1}}{\partial t^n} \quad (46)$$

and

$$\left(\frac{\partial \widetilde{H}^{n-1}}{\partial \mathbf{u}^n} + \widetilde{H}^{n-1}\frac{\partial \ln g^n_{s+1}}{\partial \mathbf{u}^n}\right).\delta\mathbf{u}^n \le 0, \quad (47)$$

where k = 1...s. The above set is purposely written in the form suitable to comprise both the present theory of constrained θ^n and that of free θ^n described at the beginning. For the former the identification $\theta^n = g_{s+1}$ should be made on the left hand sides of Eqs. (43)-(47). For the latter, constraint (34) is absent or the corresponding inequality $\theta^n - g_{s+1} \le 0$ is inactive, in which cases $\lambda^n = 0$ and θ^n is free; then the basic algorithm, derived at the beginning, is recovered. In this case the enlarged Hamiltonian $\widetilde{H}^{n-1}$ vanishes and the set (43)-(47) becomes canonical. With the general model (43)-(47) we can treat optimization of arbitrary discrete processes. Examples of applications for systems in which θ^n are free (the case when $\widetilde{H}^{n-1}=0$) are known (Sieniutycz, 1991; Berry et. al., 2000; Sieniutycz, 2000). Examples of application for systems with locally-constrained θ^n will be reported.

6. Conclusions

We have synthesized powerful mathematical approaches to dynamic optimization of nonlinear active and inactive sequential energy systems. Applications which deal with diverse energy and chemical systems lead to optimal performance functions, optimal trajectories and optimal controls that are found in terms of end states, process duration and number of stages, N. The canonical and quasicanonical structure of equations describing optimal processes is shown.

The new, most general, theory synthesizes the two known optimization theories: the traditional multistage theory, where the Hamiltonian is not that of Pontryagin, and the first theory based on the Pontryagin's like Hamiltonian whose model admits only unconstrained residence time intervals, θ^n. The new theory removes the requirement of the free intervals θ^n, yet it preserves the most powerful features of the continuous theory of Pontryagin in the discrete context. Our approach makes it possible to determine optimality conditions for complex systems with state dependent coefficients, and thus to generalize analytical solutions obtained in linear cases to nonlinear situations. Optimal performance functions that describe extremal values of optimization criteria are found in terms of end states, process duration and number of stages, N. Alternatively, Legendre transforms of original functions with respect to the time t are generated; then the optimal functions are found in terms of end states, a Hamiltonian and N. With the help of our theory, general limits for energy consumption (production) are found for finite durations; they bound the consumption of the classical work potential (exergy) in a given finite time.

As pointed out earlier, one of main goals of this work is a discrete analogy with the continuous theory which would allow description of real multistage processes with small number of finite stages. As pointed out by the referee of this paper, in relation to that goal, it is known that even the simplest of the discrete (fixed N) problems are rife with local optima, thus the mere stating of necessary optimality conditions, such as the Hamiltonian-based canonical and quasicanonical sets may be insufficient. In this regard it is worth stressing that, as opposed to the Hamiltonian-based algorithms, the stage criterion (36) constitutes quite generally also the locally-sufficient optimality condition. This is, in fact, the criterion, that is capable of yielding a computational scheme for a computable suboptimal solution whose deviation from optimality is small and can be estimated in terms of N. A related issue is that, in the case of free θ^n, the difficulties associated with local optima are reduced due to vanishing second order terms in Taylor expansions of optimal performance functions. For this issue, see Refs. (Findeisen et. al., 1980) and (Berry et. al., 2000) which also discuss the convergence conditions for discrete solutions to achieve the continuous limit.

Optimal-performance-based choice of time intervals, which involves global or integral criteria, may be compared with the group of special-purpose integration methods for OD equations called collectively the structure-preserving integrators (also called mechanical or geometric integrators). In these methods local discretizing structure may be established without explicit recourse to an optimization criterion although it has to preserve *exactly* a number of important properties known for OD equations. Examples are symplectic integrators for Hamiltonian OD equations, volume-preserving integrators for divergence-free OD equations, time-reversing symmetries preserving integrators, and integrators preserving the structure of gradient and Lyapunov systems (McLachlan et. al., 1999; McLachlan and Quispel, 1998).

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Nomenclature

A	available energy (exergy)
A, a	cumulative and local heat exchange area, respectively
a_v	specific area of heat exchange (per unit volume)
b_g	specific exergy of controlling gas
c	specific heat at the constant pressure
D^n	profit at stage n
$\tilde{D}^n$	gauged profit at stage n
e	economic value of the exergy
F	cross-sectional area of the system
f_0	profit intensity
f_0^n	profit at stage n
$\tilde{f}_0^n$	gauged profit intensity
$\mathbf{f} = (f_1 ... f_s)$	vector of process rates
$\mathbf{f}^n$	rate vector at stage n
$G(\mathbf{x}, t)$	gauging function depending on state **x** and time t
g	conductance
$H(\mathbf{x}, \mathbf{u}, \mathbf{z}, t)$	standard Hamiltonian function of a continuous process
$H^{n-1}(\mathbf{x}^n, \mathbf{u}^n, \mathbf{z}^{n-1}, t^n)$	Hamiltonian function of a discrete process at stage n
$\tilde{H}^{n-1}(\mathbf{x}^n, t^n, \mathbf{u}^n, \mathbf{z}^{n-1}, z_t^{n-1}, t^n)$	enlarged Hamiltonian at stage n
h	numerical Hamiltonian, Lagrange multiplier of time constraint
$l_0^n = - f_0^n$	process Lagrangian at stage n
l	distance variable in an exchanger
N	total number of stages
n	current stage number
$P = G^i - G + V$	effective optimal profit function with gauging term
P^n	optimal gauged profit at n-th stage
R	universal gas constant

R	total resistance of a thermal path
$R^n(\mathbf{x}, t)$	optimal cost function at stage n
$R_*^n(\mathbf{x}^n, h)$	modified optimal cost
S	thermodynamic entropy
S^N	performance index, optimization criterion for N-stage process
s	number of coordinates
S_σ	integral entropy production
$\mathbf{T}^n(\mathbf{x}^n, \mathbf{u}^n)$	state transformation function
T	temperature of key phase
T^e	temperature of reservoir
T^n	temperature of flux from stage n
T_g^n	temperature of gas phase at stage n
t	holdup time
U	admissible control set
$\mathbf{u} = (u_1, u_2, ..u_r)$	control vector
$\tilde{\mathbf{u}}^n$	enlarged control vector at stage n
u^n, v^n	rates of change as controls
$V \equiv \max S$	optimal performance function of profit type
$V^n(\mathbf{x}, t)$	optimal profit function at n-th stage of the process
X	concentration, gas humidity
X_g^n	absolute humidity of gas at stage n
$\mathbf{x} = (x_1, x_2, ...x_i...x_s)$	state vector of a general process
x, y, z	Cartesian coordinates
$\tilde{\mathbf{x}}$	enlarged state vector with the last coordinate $x_{s+1} \equiv t$
x_0	performance coordinate
$\mathbf{z}^n$	adjoint vector of a general process
$z_i^{n-1} = -\partial P^{n-1}/\partial x_i^{n-1}$	adjoint variable for coordinate x_i^n

Greek symbols

∇	nabla operator
θ^n	free interval of an independent variable or time interval at stage n
Λ	generalized Lagrangian
$\boldsymbol{\mu}' \equiv$	vector of Lagrange multipliers
ρ	thermal resistance
σ	entropy production of unit volume
Υ	passage time for a chemical wawe
τ	nondimensional time
$\phi_a(\mathbf{x}, t)$	constraining function

Subscripts

i	i-th state variable;
σ	dissipative quantity
0	zero-th variable, profit, reference state
*	transformed or modified quantity

Superscripts

e	environment
f	final state
i,	initial state;
k or n	number of k^{-th} or n^{-th} stage
$\tilde{q}$	enlarged quantity q

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