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Hamilton–Jacobi–Bellman equations and dynamic programming for power-maximizing relaxation of radiation

Stanislaw Sieniutycz *

Faculty of Chemical and Process Engineering, Warsaw University of Technology, 1 Waryńskiego Street, Warsaw 00-645, Poland

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Abstract

We treat simulation and power optimization of nonlinear, steady and dynamical generators of mechanical energy, in particular radiation engines. In dynamical cases, associated with downgrading of resources in time, real work is a cumulative effect obtained from a nonlinear fluid, set of engines, and an infinite bath. Dynamical state equations describe resources upgrading or downgrading in terms of temperature, work output and process controls. Recent formulae for converter's efficiency and generated power serve to derive Hamilton–Jacobi equations for the trajectory optimization. The relaxation curve of typical nonlinear system is non-exponential. Power extremization algorithms in the form of Hamilton–Jacobi–Bellman equations (HJB equations) lead to work limits and generalized availabilities. Optimal performance functions depend on end states and the problem Hamiltonian, h. As an example of limiting work from radiation, a generalized exergy flux of radiation fluid is estimated in terms of finite rates quantified by Hamiltonian h.

In many systems governing HJB equations cannot be solved analytically. Then the use of discrete counterparts of these equations and numerical methods is recommended. Algorithms of discrete dynamic programming (DP) are particularly effective as they lead directly to work limits and generalized availabilities. Convergence of these algorithms to solutions of HJB equations is discussed. A Lagrange multiplier λ helps to solve numerical algorithms of dynamic programming by eliminating the duration constraint. In analytical discrete schemes, the Legendre transformation is a significant tool leading to the original work function.

1. Introduction

An important class of research on energy limits involves nonlinear systems driven by fluids that are restricted in their amount or flow, i.e. play role of resources. A resource is a valuable substance used in a limited amount in a practical process. Value of the resource can be quantified thermodynamically by specifying its exergy, a maximum work that can be delivered when the resource relaxes to the equilibrium. Reversible relaxation of the resource is associated with the classical exergy. When some dissipative phenomena are allowed generalized exergies are found. They include the resource availability and a minimum work lost during its production. In the classical exergy only the first property is essential.

To calculate an exergy, knowledge of a work integral is required. For thermal problems its integrand is the product of thermal efficiency and the differential of exchanged energy. Various dissipation models lead to diverse thermal efficiencies that deviate from the Carnot efficiency. In fact, generalized exergies quantify somehow these deviations.

Formally, an exergy follows from the principal function of a variational problem for extremum work under suitable boundary conditions. Other components are optimal trajectory and optimal control. In thermal systems the trajectory is characterized by temperature of the resource, $T(t)$, whereas a suitable control is Carnot temperature $T'(t)$ defined in our previous work [1,2]. Whenever $T'(t)$ differs from $T(t)$ the resource relaxes to the environment with a

* Fax: +48 22 251440.
E-mail address: sieniutycz@ichip.pw.edu.pl

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Nomenclature

A^{∞}	generalized exergy density of resource (J m^{-3})
A^{class}	density of classical exergy (J m^{-3})
a	temperature power exponent in kinetic equation (–)
a_{v}	total area of energy exchange per unit volume (m^{-1})
c_{v}	specific heat of unit volume (J m^{-3} K^{-1})
c	specific heats (J g^{-1} K^{-1}, J m^{-3} K^{-1}, J mol^{-1} K^{-1})
D^n,$\widetilde{D}^n$	generalized profit and gauge profit at stage n
DP	dynamic programming
f	rate vector with components $f_1,\ldots,f_k,\ldots,f_s$
f_0, f_i	profit rate and process rates
G	gauge function
$\dot{G}$	resource flux (g s^{-1}, mol s^{-1})
g_1, g	partial and overall conductance (J s^{-1} K$^{-\text{a}}$)
H	Hamiltonian function
h	Hamiltonian density in entropy units (J m^{-3} K^{-1})
l_0	Lagrangian, intensity of generalized cost
p	power output (J s^{-1})
R	minimum performance function (J, or J mol^{-1})
S, S_σ	entropy and entropy produced (J K^{-1})
T	variable temperature of resource fluid (K)
T_1, T_2	bulk temperatures of reservoirs 1 and 2 (K)
$T_{1'}$, $T_{2'}$	temperatures of circulating fluid (Fig. 3) (K)
T^n	temperature after stage n (K)
T^{e}	constant temperature of environment (K)
T'	Carnot temperature control (K)
$\dot{T} = u$	rate of control of T in non-dimensional time (K)
t	physical time (s)
u	control vector
u and v	temperature rate controls, dT/dτ and dT/dt, respectively (K, K s^{-1})
V	maximum performance function (J, or J mol^{-1})
v	velocity (ms^{-1})
W and $\dot{W}$	work and power (J, J s^{-1})
w	work per unit flux of resource (J/mol)
x	state vector
$\tilde{x}$	enlarged state vector including time
z_k	adjoint variable for kth coordinate

Greek symbols

α'	overall heat transfer coefficient (J m^{-2} s^{-1} K^{-1})
β	coefficient, frequency constant (s^{-1})
λ	Lagrange multiplier, time adjoint
$\eta = p/q_1$	first-law efficiency (–)
Φ	factor of internal irreversibility (–)
θ	time interval (s, –)
ξ	intensity index (–)
τ	non-dimensional time or number of heat transfer units (x/H_{TU}) (–)

Subscripts

k	kth state variable
m	molar flow
1,2	first and second fluid
*	modified cost or profit

Superscripts

e	environment
i	initial state
f	final state
′	modified quantity

finite rate and the system's efficiency deviates from that of Carnot. Only in the case when $T'(t) = T(t)$ the efficiency is Carnot, but this corresponds with an infinitely slow relaxation rate of the resource to the thermodynamic equilibrium with the environmental fluid.

The structure of this paper is as follows. Section 2 discusses various aspects of steady and dynamical optimization of power yield. Quantitative analysis of processes with resource's downgrading (in the first reservoir) and issues regarding generalization of the classical exergy for finite rates are presented in Section 3. Sections 4–6 display various Hamilton–Jacobi–Bellman (HJB) and Hamilton–Jacobi equations for extremum power production (consumption). Extensions, highlighting systems with complex kinetics (e.g. radiation) and internal dissipation are treated in Section 7. Analytical formulae for generalized exergies of some nonlinear systems are discussed in Section 8. Next, in view of severe difficulties in getting analytical solutions for systems with nonlinear kinetics discretized (difference) equations and numerical approaches are considered. Section 9 displays difference equations obtained from discretization of the continuous model of power production from the black radiation and presents the dynamic programming equation (DP equation) of the problem. Section 10 discusses convergence conditions of discrete DP schemes to solutions of continuous HJB equations. Section 11 elucidates the solving method by discrete approximations and introduces a Lagrange multiplier as a time adjoint. Section 12 shows the significance of the Legendre transform in recovering original work functions. Section 13 describes numerical procedures using dynamic programming, whereas Section 14 discusses dimensionality reduction in numerical DP algorithms. Section 15 presents most essential conclusions.

The size limitation of the present paper does not allow for inclusion of all suitable derivations to make this paper self-contained, thus the reader may need to turn to some previous works [1,2,4,5].

2. Finite resources and power optimization in steady processes

In a process of energy production two resting reservoirs do interact through an energy generator (engine). The power flow is steady only when two reservoirs are infinite. When one, say, upper, reservoir is finite, its thermal potential must decrease in time, and a dynamical process takes place. From the optimization viewpoint the dynamical process is every one in which sequential changes of state do occur, either in the chronological time or in (spatial) holdup time. Dynamical processes evolving in chronological time take place in non-stationary systems, those evolving in spatial time, in steady-state systems.

The majority of research on energy limits published to date deals with (steady) systems with infinite reservoirs. To this case refer steady-state analyses of the Chambadal–Novikov–Curzon–Ahlborn engine (CNCA engine [6]), where the energy exchange is described by Newtonian law of cooling, or the Stefan–Boltzmann engine, a radiation system with the energy exchange governed by the Stefan–Boltzmann law [7]. As the result of their stationarity (caused by the infiniteness of both reservoirs), controls maximizing power are represented by a fixed point in the state space. In fact, in the CNCA engine, the maximum power point may be related to the optimum value of a free (unconstrained) control variable which can be efficiency η or Carnot temperature T'. In terms of the reservoirs temperatures T_1 and T_2 and the internal irreversibility factor Φ one finds optimal $T'_{\mathrm{opt}} = (T_1 \Phi T_2)^{1/2}$ [4]. For the Stefan–Boltzmann engine the optimal point cannot be determined analytically, yet, this temperature can easily be found graphically from the power diagram $W = f(T\prime)$, Fig. 1.

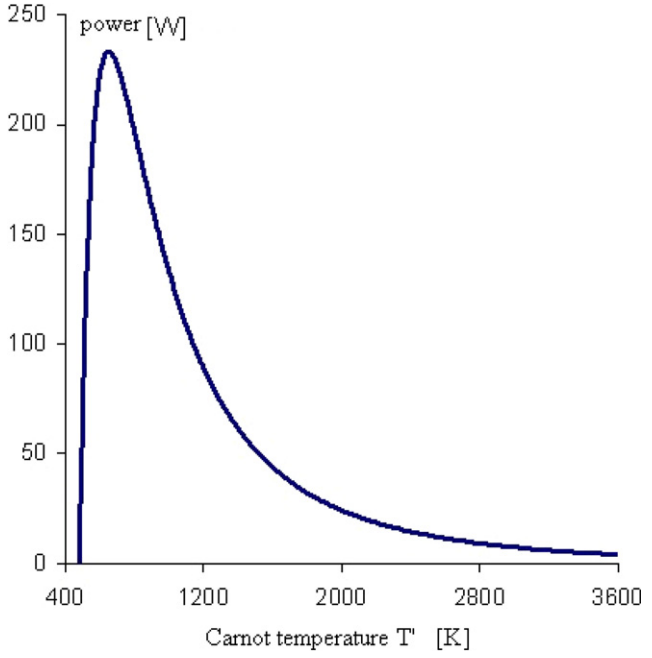

Fig. 1. Maximum of power in a steady radiation system.

Moreover, method of Lagrange multipliers can successfully be applied [8]. As the elimination of these multipliers from a set of resulting equations is quite easy, the problem is broken down to the numerical solving of a nonlinear equation for the optimal control T'.

Finally, the so-called pseudo-Newtonian model [4,5,8], which uses the state or temperature dependent heat exchange coefficient $\alpha(T^3)$, omits many analytical difficulties associated with the use of Stefan–Boltzmann equation in both steady and unsteady situations [4,5].

3. Dynamic optimization and generalized exergies

The prediction of dynamical energy yield requires the evaluation of an extremal curve rather than an extremum point. This is associated with application of variational methods (to handle functional extrema) in place of static optimization methods (to handle extrema of functions). For example, the use of the pseudo-Newtonian model of radiation [5], gives rise to an exponential curve describing the radiation relaxation to the equilibrium. As the consequence of the nonlinear properties of the relaxation dynamics non-exponential are also other curves describing the radiation relaxation, e.g. those following from exact models using the Stefan–Boltzmann equation (symmetric and hybrid, [4,5]).

Analytical difficulties associated with dynamical optimization of relaxing radiation are severe. Optimal (i.e. power-maximizing) relaxation curve $T(t)$ is associated with the optimal control curve $T'(t)$; they both are components of the dynamic optimization solution to a continuous process in which power is produced (consumed) in a sequence of infinitesimal engines, Figs. 2 and 3. Two different works are essential, the first associated with the resource down-

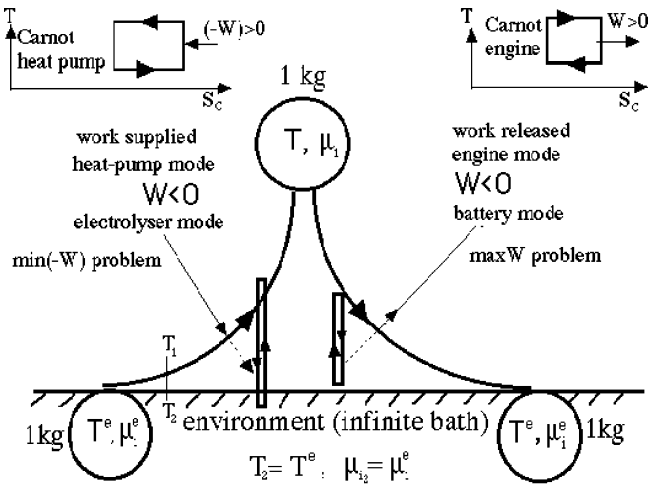

Fig. 2. Work consumed in heat-pump modes is larger than work generated in engine modes. In a problem of maximum work delivery a resource tends to the equilibrium with the thermal reservoir (state downgrading via relaxation from T to T^e, "engine mode"). In a problem of minimum work supply a resource departs from the equilibrium with the thermal reservoir (state upgrading from T^e to T, "heat-pump mode").

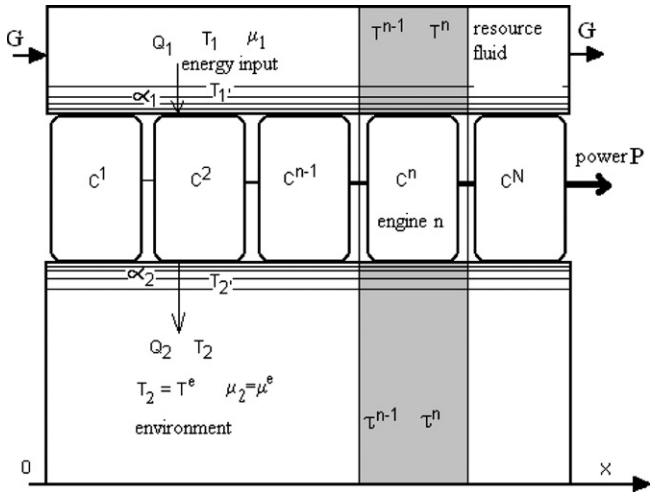

Fig. 3. Cascade scheme of flowing resource downgrading in a power production process. The scheme is a tool for evaluation of a generalized exergy of radiation fluid.

grading during its relaxation to the equilibrium and the second – with the reverse process of resource upgrading, Fig. 2. During the approach to the equilibrium *engine mode* of the system takes place in which work is released, during the departure – *heat-pump mode* occurs in which work is supplied. Work W delivered in the engine mode is positive by assumption (“engine convention”). A sequence of infinitesimal engines (CNCA or Stefan–Boltzmann type) serves to determine a rate-dependent exergy extending the classical exergy for irreversible, finite-rate processes. As an infinitesimal rectangle in Fig. 2 for the heat-pump mode is larger than that for the engine mode, the magnitude of work consumed in energy pumping modes is larger than that in energy generation modes. This effect is, in fact, the manifestation of the second law of thermodynamics.

Before maximization of a work integral, process efficiency η has to be obtained as a function of state T and a control variable, i.e. energy flux q or rate $\mathrm{d}T/\mathrm{d}\tau$, to assure the functional property (path dependence) of the work integral. The integration must be preceded by maximization of power or work at flow w to assure an optimal path. The optimal work is sought in the form of a potential function that depends on the end states and duration. This function is a finite-rate exergy when the final state of engine mode is that of equilibrium with the environment. Another exergy function is obtained for heat-pump mode, when the initial state is close to that of equilibrium with the environment and the resource is upgraded.

In the corresponding discrete problem, Fig. 3, formulated for numerical purposes via discretization, one searches for optimal temperature sequences $\{T^n\}$ and $\{T'^n\}$. Each step is a work-producing (consuming) stage with the energy exchange between two fluids and the thermal machine through finite “conductances”. Each conductance is the product of an effective transfer coefficient and the area. For the radiation (Stefan–Boltzmann) engine it follows from the Stefan–Boltzmann law that the effective transfer coefficient α_1 of the “driving” (radiation) fluid is necessarily temperature dependent, $\alpha_1 = \propto T_1^3$. The second or low-T fluid represents the usual environment, as in the exergy theory. This fluid possesses its own boundary layer as a dissipative component, and the corresponding exchange coefficient is α_2. In the physical space, the flow direction of the resource fluid is along the horizontal coordinate x, corresponding with engines located continuously along x between both fluids.

Diverse optimization methods lead to optimal sequences $\{T^n\}$ and $\{T'^n\}$. They include: direct search, dynamic programming, discrete maximum principle, and combinations of these methods. Minimum power supplied to the system is described by function sequences $R^n(T^n, t^n)$, whereas maximum power produced by functions $V^n(T^n, t^n) = -R^n(T^n, t^n)$. As the systems considered are autonomous, the elimination of duration variable t^n is possible, which improves the accuracy of calculations. The elimination is accomplished by the introduction of a Lagrange multiplier and use of modified power cost functions, Sections 11 and 14.

In the numerical optimization of power (Sections 9–14), one may assume either constant time integrals $\theta = \Delta t$ or admit that these intervals vary with the stage number n. In the second case time intervals θ^n are chosen optimally, so as to optimize the total power form all stages. A freedom in the choice of θ^n is associated with the constancy of a Lagrange multiplier λ. This Lagrange multiplier is the adjoint variable of total time, $t^n = \Sigma\theta^k$.

Importantly, energy limits of dynamical processes are inherently connected with the exergy functions, the classical exergy and its rate-dependent extensions. To obtain the classical exergy from power equations it suffices to assume that the thermal efficiency of the system is the Carnot efficiency. This assumption eliminates the entropy production and the thermodynamic Hamiltonian and leads to work functions dependent only on classical thermodynamic variables (independent of process duration or process rates). For appropriate boundary conditions that assure vanishing of the work potential at the equilibrium, the optimal performance functions become identical with classical exergies.

On the other hand, extended performance functions lead to generalized exergies. The latter depend not only on classical thermodynamic variables but also on their rates. These generalized exergies refer to state changes in a finite time, and can be contrasted with the classical exergies of quasi-static processes. The benefit obtained from generalized exergies is that they define stronger energy limits than those predicted by classical exergies.

Kinetic approach to exergies (classical or generalized) based on work functionals leads to several original results, in particular it explains some unknown properties of exergy of black-body radiation or solar radiation, and proves that the efficiency of a reversible solar flux is equal to the Carnot efficiency [5]. One can also show that the well-known Petela’s equation for the radiation exergy is restricted to the

exergy of enclosed radiation. Yet, this equation ceases to be valid for the exergy transferred with the flux of electromagnetic radiation. Summing up, the kinetic approach helps to solve several basic problems in the literature of classical exergy, and offers a correct generalization of exergy for processes with finite rates.

4. Power functionals and some aspects of analytical HJB theory

Total power obtained from an infinite sequence of infinitesimal engines is determined as the Lagrange functional of the following structure

$$\dot{W}[\mathbf{T}^{\mathrm{i}},\mathbf{T}^{\mathrm{f}}]=\int_{t^{\mathrm{i}}}^{t^{\mathrm{f}}} f_0(T,T')\mathrm{d}t=-\int_{t^{\mathrm{i}}}^{t^{\mathrm{f}}}\dot{G}c(T)\eta(T,T')\dot{T}\,\mathrm{d}t, \tag{1}$$

where f_0 is power generation intensity, $\dot{G}$-resource flux, $c(T)$-specific heat, $\eta(T,T')$-efficiency in terms of state T and control T', $\mathbf{T}$ – enlarged state vector comprising state and time, t – time variable (residence time or holdup time) for the resource contacting with heat transfer surface. Sometimes one uses a non-dimensional time τ, identical with the so-called number of the heat transfer units. Note that, for constant mass flow $\dot{G}$ of a resource, one can extremize power per unit mass flux, the quantity of work dimension. In this case Eq. (1) describes a problem of extremum work. Integrand f_0 is power generation function common for both modes, yet the numerical results it generates for each mode differ by sign. By the "engine convention" f_0 is positive for engine mode and negative for heat-pump mode. Yet f_0 can always be replaced by power consumption function $l_0=-f_0$. Formally, l_0 plays the role of a Lagrangian which is positive in energy consumption modes.

When the resource flux is constant the following work functional can be obtained from Eq. (1) for the *thermal* exergy flux per unit flux of resource

$$w_{\max_{\mathrm{d}T/\mathrm{d}t}}=-\int_{T^{\mathrm{i}}=T}^{T^{\mathrm{f}}=T^{\mathrm{e}}} c(T)\left(1-\frac{T^{\mathrm{e}}}{T'(T,\mathrm{d}t/\mathrm{d}T)}\right)\mathrm{d}T. \tag{2}$$

Note that the independent variable in this equation is different than that in Eq. (1).

The function f_0 in Eq. (1) contains thermal efficiency function, η, described by a practical counterpart of the Carnot formula. When $T>T^{\mathrm{e}}$, efficiency η decreases in the engine mode above η_{c} and increases in the heat-pump mode below η_{c}. At the limit of vanishing rates, $\mathrm{d}T/\mathrm{d}t=0$ and $T'\to T$. Then work of each mode simplifies to the common integral of the classical exergy. For the specific *thermal* exergy

$$w_{\max\limits_{\mathrm{d}T/\mathrm{d}t\to 0}}=-\int_{T^{\mathrm{i}}=T}^{T^{\mathrm{f}}=T^{\mathrm{e}}} c(T)\left(1-\frac{T^{\mathrm{e}}}{T}\right)\mathrm{d}T=h-h^{\mathrm{e}}-T^{\mathrm{e}}(s-s^{\mathrm{e}}). \tag{3}$$

Therefore, with appropriate boundary conditions, Eq. (1) leads to a generalization of thermal exergy for finite time processes. An equivalent form of the work functional has two additive components: the classical (potential or path-independent) part and a non-potential part which depends on the history of the process.

Nonlinearities can have both thermodynamic and kinetic origins; the former refer, for example, to state dependent heat capacity, $c(T)$, the latter to nonlinear energy exchange. Problems with linear kinetics (Newtonian heat transfer) are important subclass of family of problems considered. For example, in problems with linear kinetics, power release per unit mass flow of the fluid (fluid's specific work at flow), w, is described by an equation

$$w[\mathbf{T}^{\mathrm{i}},\mathbf{T}^{\mathrm{f}}]=\dot{W}/\dot{G}=-\int_{T^{\mathrm{i}}}^{T^{\mathrm{f}}} c(T)\left(1-\frac{T^{\mathrm{e}}}{T}\right)\mathrm{d}T - T^{\mathrm{e}}\int_{t^{\mathrm{i}}}^{t^{\mathrm{f}}} c(T)\frac{(T'-T)^2}{T'T}\,\mathrm{d}\tau, \tag{4}$$

where

$$\tau\equiv\frac{x}{H_{\mathrm{TU}}}=\frac{\alpha' a_{\mathrm{v}}F}{\dot{G}c}x=\frac{\alpha' a_{\mathrm{v}}Fv}{\dot{G}c}t \tag{5}$$

is *non-dimensional* time of the process. Eq. (5) assumes that a resource fluid flows with velocity v through cross-section F and contacts with the heat transfer exchange surface per unit volume a_v [1]. Quantity τ is identical with the so-called *number of the heat transfer units*.

Solutions to work extremum problems can be obtained by the variational calculus or maximum principle [8–11]. Yet these methods do not provide a direct information about the optimal work function. This is assured by solving the Hamilton–Jacobi–Bellman equation or a recurrence equation of dynamic programming for 'principal functions' V or R (also called extremum work functions). We shall prove soon that for the example described by Eq. (4)

$$\frac{\partial V}{\partial\tau}+\min_{T'}\left\{\left(\frac{\partial V}{\partial T}+c\left(1-\frac{T^{\mathrm{e}}}{T'}\right)\right)(T'-T)\right\}=0. \tag{6}$$

The extremum work function $V=\max W$ depends on final state of T and total duration, τ. After evaluation of optimal control and its substitution to Eq. (6) one obtains a nonlinear equation

$$\frac{\partial V}{\partial\tau}-c\left\{\sqrt{T^{\mathrm{e}}}-\sqrt{T(1+c^{-1}\partial V/\partial T)}\right\}^2=0 \tag{7}$$

which is the Hamilton–Jacobi equation of the problem. Its solution can be found by the integration of work intensity along an optimal path, for limits T^{i} and T^{f}, as shown in Section 6.

While the final part of this paper offers discrete algorithms whose solutions converge to solutions of HJB equations, these continuous equations have their own analytical theory. This theory is outlined here. Often HJB equations are derived by continuous version of dynamic programming, e.g. Refs. [9–11]. Here a simple and brief approach

exploiting Caratheodory's idea of potentiality of optimal performance function [12] is presented. We also show the role of a Hamiltonian function

$$H = f_0(\mathbf{x},\mathbf{u},t) + \sum_{i=1}^{s}(\partial R/\partial x_i) f_i(\mathbf{x},\mathbf{u},t) \tag{8}$$

in HJB equations. This function contains state vector $\mathbf{x}$, control vector $\mathbf{u}$, rates f_0 and f_i and partial derivatives $z_i = \partial R/\partial x_i$. The latter define the so-called adjoint vector $\mathbf{z}$. The scalar f_0 is the growth rate of a generalized profit (intensity of work yield in our case). Hamiltonian H is an energy-like quantity, constant of an optimal path of an autonomous system. In terms of H and $\mathbf{z} = \partial R/\partial \mathbf{x}$ a general HJB equation is

$$\frac{\partial R}{\partial t} + \max_{\mathbf{u}(t)} H\left(\frac{\partial R}{\partial \mathbf{x}}, \mathbf{x}, \mathbf{u}, t\right) = 0. \tag{9}$$

Let us derive the above equation for the engine mode of an energy process. A control problem of maximum delivery of cumulative power is governed by the characteristic function

$$V(T^{\mathrm{i}}, t^{\mathrm{i}}, T^{\mathrm{f}}, t^{\mathrm{f}}) \equiv \max_{T'(t)} \dot{W}[\mathbf{T}^{\mathrm{i}}, \mathbf{T}^{\mathrm{f}}] = \max_{T'(t)} \left(\int_{t^{\mathrm{i}}}^{t^{\mathrm{f}}} f_0(T, T')\mathrm{d}t \right). \tag{10}$$

As it follows from the above definition of V

$$\max_{T'(t)} \left(\int_{t^{\mathrm{i}}}^{t^{\mathrm{f}}} f_0(T, T')\mathrm{d}t - V(T^{\mathrm{i}}, t^{\mathrm{i}}, T^{\mathrm{f}}, t^{\mathrm{f}}) \right) = 0. \tag{11}$$

Here $f_0 = -l_0$, is the profit generation rate, or, in our case, intensity of power production. Differentiation of Eq. (11) with respect to the upper limit of the integral, t^{f}, yields

$$\max_{T'(t)} \left(f_0^{\mathrm{f}}(T, T') - \frac{\mathrm{d}V(T^{\mathrm{i}}, t^{\mathrm{i}}, T^{\mathrm{f}}, t^{\mathrm{f}})}{\mathrm{d}t^{\mathrm{f}}} \right) = \max_{T'(t)} \left(f_0^{\mathrm{f}}(T, T') - \frac{\partial V}{\partial t^{\mathrm{f}}} - \frac{\partial V}{\partial T^{\mathrm{f}}} f^{\mathrm{f}}(T, T') \right) = 0. \tag{12}$$

All rates (f_0 and f) and partial derivatives of V are evaluated at the final state (the so-called 'forward equation'). In the second expression, total time derivative is expanded in terms of rates. Observe that partial derivative of characteristic function V with respect to time can be taken off this equation and the superfluous index f can be omitted (variable final states). Then, after replacing V by $-R$, a HJB equation is obtained, consistent with Eq. (9)

$$\frac{\partial R}{\partial t} + \max_{T'(t)} \left(\frac{\partial R}{\partial T} f(T, T') - l_0(T, T') \right) = 0. \tag{13}$$

For resources relaxing with *linear kinetics* (Newtonian heat exchange) Eq. (12) yields Eq. (6).

Despite of derivation simplicity, severe difficulties in solving HJB equations call for numerical methods. These methods apply suitable discrete models, for definite rates f_0 (or l_0) and $\mathbf{f}$. Convergence of the DP models to continuous ones is discussed in Section 11, see also [3]. With discrete models the theory can be restated and live with its own life in the realm of difference equations, sums, recurrence relations, two-stage criteria, etc., often achieving a form strongly dissimilar while still equivalent to the original HJB theory [3].

5. HJB equations for complex power generation systems

Detailed derivations of nonlinear models describing sequences of infinitesimal engines are known from previous publications [1,2,4,5]. These models provide both power intensity functions f_0 (or Lagrangians $l_0 = -f_0$) and dynamical constraints, i.e. suitable differential equations. Both f_0 and differential constraints are used in the corresponding HJB equations.

Here we shall display various Hamilton–Jacobi–Bellman equations for power systems described by nonlinear kinetics.

Arbitrary nonlinear kinetics

For an arbitrary work generation function f_0 and nonlinear kinetics $\mathrm{d}T/\mathrm{d}t = f(T, T')$ a HJB equation in terms of work generation function V, final state and final time is

$$-\frac{\partial V}{\partial t} + \max_{T'(t)} \left(f_0(T, T') - \frac{\partial V}{\partial T} f(T, T') \right) = 0. \tag{14}$$

Radiation engine approximated by the pseudo-Newtonian model

A suitable example is a radiation engine whose power integral is expressed as

$$\dot{W} = -\int_{t^{\mathrm{i}}}^{t^{\mathrm{f}}} \dot{G}_m c_m \left(1 - \Phi' \frac{T^{\mathrm{e}}}{T'}\right) \upsilon(T', T)\mathrm{d}t \tag{15}$$

with $\upsilon = \alpha(T^3)(T' - T)$. An alternative form uses Carnot temperature T' explicit in υ [5]. Then

$$\dot{W} = -\int_{T}^{T_0} \dot{G}_m \left(c_{hm}(T) - c_{vm}(T) \frac{T^{\mathrm{e}}}{T} \right) \upsilon \mathrm{d}t - \int_{T}^{T_0} T^{\mathrm{e}} \dot{G}_m \left(c_{vm}(T) \left(\frac{\chi \upsilon^2}{T(T + \chi\upsilon)} + (1 - \Phi)\frac{\upsilon}{T + \chi\upsilon} \right) \right) \mathrm{d}t. \tag{16}$$

This defines f_0 in terms of υ, with the entropy production singled out in the second term. Optimal power function of this problem, $V = \max W$, can be referred to each of these integrals.

Stefan–Boltzmann engine

For *the symmetric model* of radiation conversion (both reservoirs composed of radiation) a power integral has the form

$$\dot{W} = \int_{t^{\mathrm{i}}}^{t^{\mathrm{f}}} \dot{G}_c(T) \left(1 - \frac{\Phi T^{\mathrm{e}}}{T'}\right) \beta \frac{T^a - T'^a}{(\Phi'(T'/T^{\mathrm{e}})^{a-1} + 1) T^{a-1}} \mathrm{d}t. \tag{17}$$

The exponent $a = 4$ for radiation and $a = 1$ for a linear resource. With the state equation [5]

$$\frac{\mathrm{d}T}{\mathrm{d}t}=-\beta\frac{T^a-T'^a}{(\Phi'(T'/T^{\mathrm{e}})^{a-1}+1)T^{a-1}} \tag{18}$$

applied in general Eq. (14) we obtain a HJB equation

$$-\frac{\partial V}{\partial t}+\max_{T'(t)}\left\{\left(\dot{G}_c(T)\left(1-\Phi\frac{T^{\mathrm{e}}}{T'}\right)+\frac{\partial V}{\partial T}\right)\beta\frac{T^a-T'^a}{(\Phi'(T'/T_2)^{a-1}+1)T^{a-1}}\right\}=0. \tag{19}$$

In an optimal case, dynamical equation (18) is the characteristic equation for Eq. (19).

For *the hybrid model* of radiation conversion (lower reservoir Newtonian, [5]) the power integral is

$$\dot{W}=-\int_{\tau^{\mathrm{i}}}^{t^{\mathrm{f}}}G_c(T)\left(1-\frac{\Phi T^{\mathrm{e}}}{(T^a+\beta^{-1}T^{a-1}u)^{1/a}+\Phi\beta^{-1}T^{a-1}ug_1/g_2}\right)u\,\mathrm{d}t \tag{20}$$

and the corresponding Hamilton–Jacobi–Bellman equation is

$$-\frac{\partial V}{\partial t^{\mathrm{f}}}+\max_{T'(t)}\left\{-\left(\dot{G}_c(T)\left(1-\frac{\Phi T^{\mathrm{e}}}{(T^a+\beta^{-1}T^{a-1}u)^{1/a}+\Phi\beta^{-1}T^{a-1}ug_1/g_2}\right)+\frac{\partial V}{\partial T^{\mathrm{f}}}\right)u\right\}=0. \tag{21}$$

6. Analytical solutions in systems with linear kinetics

In all HJB equations extremized expressions are Pontryagin's-type hamiltonians, referred to non-extremal processes rather than extremum hamiltonians resembling energy of classical mechanics. However, in the HJB formalism, as opposed to the canonical Pontryagin's formalism, hamiltonians are defined in the enlarged state space (T,τ) [or (T,t)] rather than in the phase space (T,z,τ). In fact,τ is an extra state variable in the space (T,τ).

For example, Pontryagin's Hamiltonian of linear system (Newtonian energy flow) is

$$\begin{aligned}H&=\left[z-c\left(1-\frac{T^{\mathrm{e}}}{T'}\right)\right](T'-T)\\&=\left[z-c\left(1-\frac{T^{\mathrm{e}}}{T+u}\right)\right]u.\end{aligned} \tag{22}$$

From Eqs. (12) and (22) $z=\partial R/\partial T$, i.e. the temperature adjoint is the gradient of R, or the negative gradient of V. An optimal driving temperature T' is chosen to maximize hamiltonian (22) or HJB expression (12) with respect to T' at each point of the process path. This maximization leads to two equations. The first expresses the optimal control T' through T and z or $\partial R/\partial T$

$$\frac{\partial R}{\partial T}-\frac{\partial l_0(T,T')}{\partial T'}=\frac{\partial R}{\partial T}-c\left(1-\frac{T^{\mathrm{e}}T}{T'^2}\right)=0, \tag{23}$$

whereas the second is the HJB expression without maximizing operation

$$\frac{\partial R}{\partial t}+\frac{\partial R}{\partial T}(T'-T)-c\left(1-\frac{T_2}{T'}\right)(T'-T)=0. \tag{24}$$

To obtain optimal control function $T'(z,T)$ one should solve the second equality in Eq. (23) in terms of T', The result is Carnot control T' in terms of T and $z=\partial R/\partial T$,

$$T'=\left(\frac{T^{\mathrm{e}}T}{1-c^{-1}\partial R/\partial T}\right)^{1/2}. \tag{25}$$

This is next substituted into Eq. (24); the result is the (nonlinear) Hamilton–Jacobi equation

$$\frac{\partial R}{\partial\tau}+cT\left(\sqrt{1-c^{-1}\partial R/\partial T}-\sqrt{T^{\mathrm{e}}/T}\right)^2=0 \tag{26}$$

which contains the extremum Hamiltonian of the extremal process.

$$H\left(T,\frac{\partial R}{\partial T}\right)=cT\left(\sqrt{1-c^{-1}\partial R/\partial T}-\sqrt{T^{\mathrm{e}}/T}\right)^2. \tag{27}$$

Eq. (26) differs from HJB equations as it refers to an extremal path only and H is the extremum Hamiltonian.

Expressing extremum Hamiltonian (27) in terms of state variable T and Carnot control T' yields an energy-like function satisfying the following relations

$$E(T,u)=\frac{\partial l_0}{\partial u}u-l_0=f_0-\frac{\partial f_0}{\partial u}=cT^{\mathrm{e}}\frac{(T'-T)^2}{T'^2}. \tag{28}$$

E is the Legendre transform of the work lagrangian $l_0=-f_0$ with respect to the rate $u=\mathrm{d}T/\mathrm{d}t$.

Assuming a numerical value of the Hamiltonian H, say h,

$$cT\left(\sqrt{1-c^{-1}z}-\sqrt{T^{\mathrm{e}}/T}\right)^2=h, \tag{29}$$

one can exploit the constancy of autonomous Hamiltonians to eliminate adjoint variable z. Combining Eq. (29) with optimal condition (28), or an equivalent equation using energy flow control $u=T'-T$ yields optimal rate $u=\dot{T}$ in terms of temperature T and the constant $H=h$

$$\dot{T}=\left\{\pm\sqrt{h/cT^{\mathrm{e}}}\left(1-\pm\sqrt{h/cT^{\mathrm{e}}}\right)^{-1}\right\}T\equiv\xi(h,T^{\mathrm{e}})T, \tag{30}$$

where

$$\xi(h,T^{\mathrm{e}})\equiv\pm\sqrt{h/cT^{\mathrm{e}}}\left(1-\pm\sqrt{h/cT^{\mathrm{e}}}\right)^{-1} \tag{31}$$

is an intensity index. Positive ξ refer to heating of resources in the heat-pump modes, and the negative – to cooling in engine modes. Eq. (30) describes the optimal trajectory in terms of state variable T and constant h. The corresponding optimal (Carnot) control is

$$T'=(\xi(h,T^{\mathrm{e}})+1)T. \tag{32}$$

Now one can find the *Hamiltonian representation of extremal work*. Substituting Carnot control (32) into work functional (4) and integrating along an optimal path yields an extremal work function

$$V(T^{\mathrm{i}},T^{\mathrm{f}},h)=c(T^{\mathrm{i}}-T^{\mathrm{f}})-cT^{\mathrm{e}}\ln\frac{T^{\mathrm{i}}}{T^{\mathrm{f}}}+cT^{\mathrm{e}}\frac{\xi(h)}{1+\xi(h)}\ln\frac{T^{\mathrm{i}}}{T^{\mathrm{f}}}$$
$$=c(T^{\mathrm{i}}-T^{\mathrm{f}})-cT^{\mathrm{e}}\ln\frac{T^{\mathrm{i}}}{T^{\mathrm{f}}}-cT^{\mathrm{e}}\sqrt{\frac{h}{cT^{\mathrm{e}}}}\ln\frac{T^{\mathrm{i}}}{T^{\mathrm{f}}}. \tag{33}$$

This expression is valid for every process mode. Integration of Eq. (30) subject to boundary conditions $T(\tau^{\mathrm{i}})=T^{\mathrm{i}}$ and $T(\tau^{\mathrm{f}})=T^{\mathrm{f}}$ allows to express Eq. (33) in terms of the process duration

$$V(T^{\mathrm{i}},T^{\mathrm{f}},\tau^{\mathrm{i}},\tau^{\mathrm{f}})=c(T^{\mathrm{i}}-T^{\mathrm{f}})-cT^{\mathrm{e}}\ln\frac{T^{\mathrm{i}}}{T^{\mathrm{f}}}$$
$$-\frac{cT^{\mathrm{e}}[\ln(T^{\mathrm{i}}/T^{\mathrm{f}})]^2}{\tau^{\mathrm{f}}-\tau^{\mathrm{i}}-\ln(T^{\mathrm{i}}/T^{\mathrm{f}})}. \tag{34}$$

Note that the reversible part of this function is the change of the classical exergy between the states i and f.

7. Extensions for systems with nonlinear kinetics and internal dissipation

In systems governed by nonlinear kinetics intensity index ξ is no longer state independent constant. For a class of "pseudo-Newtonian" systems [5] with and internal irreversibility Φ

$$\dot{T}=\xi(h,T,T^{\mathrm{e}},\Phi)T. \tag{35}$$

The presence of resource temperature T in function ξ proves that the relaxation curve is not exponential. An example is the pseudo-Newtonian model of a radiation engine described by the functional [5]

$$\dot{W}=-\dot{V}\int_{T}^{T^{\mathrm{e}}}\left(c_h(T)-c_{\mathrm{v}}(T)\Phi\frac{T^{\mathrm{e}}}{T+\chi\mathrm{d}T/\mathrm{d}t}\right)\mathrm{d}T, \tag{36}$$

where $c_h(T)\equiv c_{\mathrm{v}}(T)+P_T=(16/3)a_0T^3$, $P_T\equiv \mathrm{d}P/\mathrm{d}T=(4/3)a_0T^3$, and $\chi=\rho c_{\mathrm{v}}(a'a_{\mathrm{v}})^{-1}$. Note that ratio $\mathrm{d}t/\chi$ is the differential of non-dimensional number of transfer units, $\mathrm{d}\tau$. An alternative form of this integral is Eq. (16) that has singled out the term with the entropy production.

The application of variational calculus to nonlinear radiation fluids with the variable heat capacity $c_{\mathrm{v}}(T)=4aT^3$, yields pseudo-exponential extremal (35). To single out the environment temperature from $\xi(h,T,T^{\mathrm{e}},\Phi)$, entropy production Hamiltonian $\mathsf{h}_\sigma=h/T^{\mathrm{e}}$ is introduced in place of h. The optimal relaxation curve has then the form

$$\dot{T}=\left(\pm\sqrt{\frac{\mathsf{h}_\sigma}{\Phi c_{\mathrm{v}}(T)}}\left(1-\pm\sqrt{\frac{\mathsf{h}_\sigma}{\Phi c_{\mathrm{v}}(T)}}\right)^{-1}\right)T\equiv\xi(\mathsf{h}_\sigma,\Phi,T)T. \tag{37}$$

Again, the slope of the logarithmic rate $\xi=\mathrm{d}\ln T/\mathrm{d}\tau$ is a state dependent quantity. Operative Carnot control assuring extremum power along an optimal path is $T'=(1+\xi(\mathsf{h}_\sigma,\Phi,T))T$. The slope $\xi(\mathsf{h}_\sigma,\Phi,T)$ is a rate indicator, positive for the resource's heating and negative for cooling. ξ is constant in Newtonian energy exchange for resources with a constant c_{v}. Both ξ and h_σ vanish for quasi-static processes.

For the black radiation fluid $c_{\mathrm{v}}(T)=4a_0T^3$, where a_0 is an universal constant, the optimal trajectory solving Eqs. (37) is

$$\pm(4/3)a_0^{1/2}\Phi^{1/2}\mathsf{h}_\sigma^{-1/2}(T^{3/2}-T^{\mathrm{i}3/2})-\ln(T/T^{\mathrm{i}})=\tau-\tau^{\mathrm{i}}. \tag{38}$$

The integration limits pertain to the initial state (i) and a current state of the radiation fluid, i.e. temperatures T^{i} and T and "times" τ^{i} and τ. Optimal curve (38) is illustrated in Fig. 2 of Ref. [5]. It refers to the case when the radiation relaxation is subject to an operative constraint imposed on T (resulting in non-vanishing partial derivative of V versus T).

Eqs. (37) and (38) are determined by the second (i.e. dissipative) term of Eq. (16). The corresponding extremum work function per unit volume of flowing radiation is

$$V\equiv h_{\mathrm{v}}^{\mathrm{i}}-h_{\mathrm{v}}^{\mathrm{f}}-T^{\mathrm{e}}(s_{\mathrm{v}}^{\mathrm{i}}-s_{\mathrm{v}}^{\mathrm{f}})-(4/3)a_0^{1/2}h_\sigma^{1/2}\Phi^{1/2}T^{\mathrm{e}}(T^{\mathrm{i}3/2}-T^{\mathrm{f}3/2})$$
$$+(4/3)a_0T^{\mathrm{e}}(1-\Phi)(T^{\mathrm{i}3}-T^{\mathrm{f}3}) \tag{39}$$

Explicit analytical form of Eq. (39) is not achievable in models using Stefan–Boltzmann equation without pseudo-Newtonian approximation, for which numerical approaches must be applied. Also, the related exergy function, Eq. (40) below, has an explicit analytical form.

When a constraint on the final temperature of radiation is relaxed, corresponding with local maximum of power at each time instant, the qualitative picture of the relaxation curve may change. Relaxation of local power in this case is illustrated in thesis [13]. This case applies only to engine modes; it is singular from the viewpoint of optimal control theory and refers to vanishing Pontryagin's variables (temperature adjoints) along whole or a finite part of the optimal path. Its physical origin is associated with local maxima of power, and shows a special relation between local and global optima.

8. Analytical formula for generalized exergies in some nonlinear systems

Radiation as a pseudo-Newtonian resource. By using pertinent boundary conditions, a formula for the finite-rate exergy of radiation is obtained from Eq. (39). The particular extremal work which describes an exergy (generalized or classical) should contain the environment temperature as one of the boundary states. The finite-rate exergy is the maximal work $W_{\max}=V(T^{\mathrm{i}},t^{\mathrm{i}},T^{\mathrm{f}},t^{\mathrm{f}})$ with $T^{\mathrm{i}}=T$ and $T^{\mathrm{f}}=T^{\mathrm{e}}$ for the engine mode, and the negative minimal work $(-W)_{\min}=-V=R(T^{\mathrm{i}},t^{\mathrm{i}},T^{\mathrm{f}},t^{\mathrm{f}})$ with $T^{\mathrm{i}}=T^{\mathrm{e}}$ and $T^{\mathrm{f}}=T$ for the heat-pump mode. Eqs. (37)–(39) of pseudo-Newtonian model yield a finite-rate exergy

$$A_{\rm v}(T,T^{\rm e},{\rm h}_\sigma)=A_{\rm v}^{\rm class}(T,T^{\rm e},0)\pm(4/3)a_0^{1/2}{\rm h}_\sigma^{1/2}\Phi^{1/2}T^{\rm e}(T^{3/2}-T^{{\rm e}^{3/2}})+(4/3)a_0T^{\rm e}(1-\Phi)(T^3-T^{{\rm e}^3}). \quad (40)$$

Upper sign refers to the heat-pump mode, lower one – to the engine mode. The classical availability of *radiation at flow* appears in the above equation in Jeter's [14] form

$$A_{\rm v}^{\rm class}(T,T^{\rm e},0)=h_{\rm v}-h_{\rm v}^{\rm e}-T^{\rm e}(s_{\rm v}-s_{\rm v}^{\rm e})=h_{\rm v}(1-T^{\rm e}/T)=(4/3)a_0T^4(1-T^{\rm e}/T). \quad (41)$$

This result proves that the well-known Petela's equation [15,16] should be restricted to the 'enclosed radiation', i.e. it is inapplicable to the exergy flux. As two modes are described, common symbol T in Eqs. (40) and (41) refers to the initial temperature of engine mode or the final temperature of heat-pump mode of the process.

Compressible Newtonian resource without viscous friction. In this case integration can be performed analytically, and leads to the generalized exergy of unit volume in the form

$$A_{\rm v}(T,T^{\rm e},{\rm h}_\sigma)=A_{\rm v}(T,T^{\rm e},0)+c_{p_{\rm v}}T^{\rm e}\left(\frac{\xi}{1+\xi}\right)\ln(T/T^{\rm e})r=c_{p_{\rm v}}T^{\rm e}(T/T^{\rm e}-1)-\ln(T/T^{\rm e})+\ln(P/P^{\rm e})^{\frac{k-1}{k}}+c_{p_{\rm v}}T^{\rm e}\left(\left(\pm\sqrt{\frac{\rm h}{\Phi c_{p_{\rm v}}}}\right)+(1-\Phi)\left(1-\pm\sqrt{\frac{\rm h}{\Phi c_{p_{\rm v}}}}\right)\right)\ln\frac{T}{T^{\rm e}}. \quad (42)$$

Compressibility effect is described by the pressure (P) term. The last line term is non-classical. For vanishing intensities h or ξ the classical thermal exergy is recovered.

Incompressible Newtonian resource without friction and internal dissipation. A simple formula for thermal exergy of an endoreversible system follows in terms of the Hamiltonian

$$A_{\rm v}(T,T^{\rm e},h)=c(T-T^{\rm e})-cT^{\rm e}\ln\frac{T}{T^{\rm e}}\pm cT^{\rm e}\frac{\xi}{1+\xi}\ln\frac{T^{\rm i}}{T^{\rm f}}=c(T-T^{\rm e})-cT^{\rm e}\ln\frac{T}{T^{\rm e}}\pm cT^{\rm e}\sqrt{\frac{h}{cT^{\rm e}}}\ln\frac{T}{T^{\rm e}}=A_{\rm v}(T,T^{\rm e},0)\pm T^{\rm e}s_\sigma \quad (43)$$

or in terms of the non-dimensional duration $\tau=\tau^{\rm f}-\tau^{\rm i}$.

$$A(T,T^{\rm e},\tau^{\rm f}-\tau^{\rm i})=c(T-T^{\rm e})-cT^{\rm e}\ln\frac{T}{T^{\rm e}}\pm\frac{cT^{\rm e}[\ln(T/T^{\rm e})]^2}{\tau^{\rm f}-\tau^{\rm i}\pm\ln(T^{\rm i}/T^{\rm f})}=A(T,T^{\rm e},\infty)\pm T^{\rm e}s_\sigma. \quad (44)$$

$A(T,T^{\rm e},\infty)$ is the classical exergy, and $s_\sigma=\min S_\sigma$ is the related minimum entropy production. The upper sign refers to the heat-pump mode and the lower sign to the engine mode. The final thermodynamic result in the last lines of Eqs. (42)–(44) is in agreement with the second law in the Gouy-Stodola form [17].

By taking into account the entropy production, limits for mechanical energy yield or consumption provided by generalized exergies are stronger than those defined by the classical exergy. This help an engineer in better evaluation of energy limits in practical processes.

However, when models of radiation as a pseudo-Newtonian resource are insufficient and models applying Stefan–Boltzmann equation in an exact way are necessary, HJB and Hamilton–Jacobi equations cannot be solved analytically. Numerical solutions are then necessary, where convergence of discrete optimization algorithms to continuous solutions is important. These issues are discussed in the forthcoming part of this paper, see also [3].

9. A discrete DP model for a nonlinear problem of maximum power from radiation

We begin with the presentation of discrete dynamical methods solving *HJB* equations, either analytically, via discrete approximations, or numerically, with the help of a computer.

As an example, let us recall the problem of minimum work consumed in the radiation system subject to constraints on dynamics and duration [4,5]. For a *symmetric model* of power yield (both reservoirs filled up with radiation) the total power is described by Eq. (17)

$$\dot W=\int_{t^{\rm i}}^{t^{\rm f}}\dot G_c(T)\left(1-\frac{\Phi T^{\rm e}}{T'}\right)\beta\frac{T^a-T'^a}{(\Phi'(T'/T^{\rm e})^{a-1}+1)T^{a-1}}{\rm d}t, \quad (17)$$

where the power exponent $a=4$ for radiation and $a=1$ for a linear resource. The integrand of Eq. (17) represents intensity of generalized profit, f_0. Integral (17) has to be maximized in the engine mode of the process subject to the dynamical constraint (18)

$$\frac{{\rm d}T}{{\rm d}t}=-\beta\frac{T^a-T'^a}{(\Phi'(T'/T^{\rm e})^{a-1}+1)T^{a-1}}. \quad (18)$$

As shown in Section 5, a HJB equation

$$-\frac{\partial V}{\partial t}+\max_{T'(t)}\left\{\left(\dot G_c(T)(1-\Phi\frac{T^{\rm e}}{T'})+\frac{\partial V}{\partial T}\right)\beta\frac{T^a-T'^a}{(\Phi'(T'/T^{\rm e})^{a-1}+1)T^{a-1}}\right\}=0, \quad (19)$$

needs to be solved to determine the extremum conditions for the optimization problem involving Eqs. (17) and (18). Here $V=\max\dot W$. As it is impossible to solve Eq. (19) analytically, except for the case when $a=1$, we describe here a way of numerical solving based on Bellman's method of dynamic programming (DP).

Considering computer needs we introduce a related discrete scheme

$$\dot W^N=\sum_{k=1}^{N}\dot G_c(T^k)\cdot\left(1-\frac{\Phi T^{\rm e}}{T'^k}\right)\beta\frac{T^{k^a}-T'^{k^a}}{(\Phi'(T'^k/T^{\rm e})^{a-1}+1)T^{k^{a-1}}}\theta^k, \quad (45)$$

$$T^k - T^{k-1} = \theta^k \beta \frac{T'^{k^a} - T^{k^a}}{(\Phi'(T'^k/T^e)^{a-1} + 1)T^{k^{a-1}}}, \tag{46}$$

$$\tau^k - \tau^{k-1} = \theta^k. \tag{47}$$

We search for maximum of the sum (45) subject to discrete constraints (46) and (47).

To solve the set of Eqs. (45)–(47) one can use the method of dynamic programming [10,11]. The method is based on Bellman's recurrence equation

$$R^n(\mathbf{x}^n, t^n) = \min_{\mathbf{u}^n, \theta^n} \{ l_0^n(\mathbf{x}^n, t^n, \mathbf{u}^n, \theta^n)\theta^n + R^{n-1}(\mathbf{x}^n - \mathbf{f}^n(\mathbf{x}^n, t^n, \mathbf{u}^n, \theta^n)\theta^n, t^n - \theta^n) \}. \tag{48}$$

Difference models linear in θ^n (those with θ-independent rates f_k) are primary candidates to efficient solving of continuous equations of power systems characterized by their own Hamilton–Jacobi–Bellman equations and Hamilton–Jacobi equations.

We can now return to the difficult radiation problem described by Eqs. (45)–(47). Applying Eq. (48) to this problem, the following recurrence equation is obtained

$$R^n(T^n, t^n) = \min_{\mathbf{u}^n, \theta^n} \left\{ \dot{G}_c(T^n) \cdot \left(1 - \frac{\Phi T^e}{T'^n}\right) \beta \frac{T^{n^a} - T'^{n^a}}{(\Phi'(T'^n/T^e)^{a-1} + 1)T^{n^{a-1}}} \theta^n + R^{n-1}\left(T^n - \theta^n \beta \frac{T'^{n^a} - T^{n^a}}{(\Phi'(T'^n/T^e)^{a-1} + 1)T^{n^{a-1}}}, t^n - \theta^n \right) \right\}. \tag{49}$$

While the analytical solving of Eq. (19) is a tremendous task, it is quite easy to solve recurrence Eq. (49) numerically. Low dimensionality of state vector for Eq. (49) assures a decent accuracy of DP solution. Moreover, an original accuracy can be significantly improved after performing the so-called dimensionality reduction associated with the elimination of time t^n as the state variable. In the transformed problem, without coordinate t^n, accuracy of *DP* solutions is high. Sections 13 and 14 discuss related computational issues.

Our task now is to define conditions when numerical schemes of dynamic programming [e.g. those for the set (45)–(47)] converge to solutions of Hamilton–Jacobi–Bellman equation [e.g Eq. (19)]. The next section analyses this problem for arbitrary objective and constraints.

10. Convergence of discrete DP algorithms to solutions of HJB equations

Conditions determining when discrete optimization schemes converge to solutions of Hamilton–Jacobi–Bellman equations (HJB equations) are quite involved. Moreover, systematic studies of the problem in the literature are seldom [18–20]. To outline these conditions we consider a family of optimization models obtained by discretization of original continuous ones. In this case one has to determine necessary optimality conditions of a general discrete process governed by a work criterion W^N in the sum form

$$W^N = \sum_{n=1}^{N} f_0(\mathbf{x}^n, t^n, \mathbf{u}^n, \theta^n)\theta^n, \tag{50}$$

subject to constraints resulting from difference equations

$$x_i^n - x_i^{n-1} = f_i(\mathbf{x}^n, t^n, \mathbf{u}^n, \theta^n)\theta^n. \tag{51}$$

The scalar f_0 is the rate of the profit generation. Superscripts refer to stages and subscripts to coordinates. The integer n ($n = 1, \ldots, N$) is a discrete time also called stage number, the entity that should be distinguished from continuous time t. The latter is usually the physical time (t is the chronological time in unsteady-state operations and holdup or residence time in steady cascade operations). Both n and t are monotonously increasing. The s-dimensional vector $\mathbf{x} = (x_1, \ldots, x_s)$ is the state vector, and the r-dimensional vector $\mathbf{u} = (u_1, \ldots, u_r)$ is the control vector, where $\mathbf{x}^n \in E^s$, $\mathbf{u}^n \in E^r$ and rate functions f_0^n and f_i^n are continuously differentiable always in $\mathbf{x}$ and θ, but not always in $\mathbf{u}$. While θ^n is a control-type quantity, it is excluded from the coordinates of vector $\mathbf{u}$, i.e. it is treated separately in the optimization model. The rate change of state coordinate x_i in time t is ith component of s-dimensional vector of rates, $\mathbf{f}$. The change of time t through the stage n defined as $\theta^n = t^n - t^{n-1}$ is called the time interval.

The $s+1$-dimensional vector $\tilde{\mathbf{x}} = (\mathbf{x}, t)$ is also used which is the enlarged state vector describing the space-time. Usually one assumes that a control sequence $\{\mathbf{u}^n\}$ and the corresponding trajectory $\{\mathbf{x}^n, t^n\}$ are admissible, i.e. that they satisfy the control constraint $u^n \in U^n$ and the state-space constraint $\tilde{x}^n \in \tilde{X}^n$.

For work production problems criterion (50) is maximized, for work consumption a minimum of the negative of (50) is sought. In optimization problems with constrained duration $t^N - t^0$ (the so-called fixed-horizon problem) discrete model must explicitly include an equation defining time interval θ^n, either as the increment of a monotonously increasing state coordinate satisfying an equation $x_{s+1}^n - x_{s+1}^{n-1} = \theta^n$ or as the increment of usual time

$$t^n - t^{n-1} = \theta^n. \tag{52}$$

The monotonic increase of the time-like coordinate, implying non-negative θ at each stage n, is crucial for many properties of model (50)–(52). Various discretization schemes for constraining differential equations, such as, e.g. Eq. (18), lead to discrete models either linear or nonlinear in θ^n. Throughout the whole paper models with free (unconstrained) intervals θ^n are considered as only those that are able to achieve their own continuous limits.

Two classes of discrete models, linear and nonlinear in free θ^n, are distinguished when considering convergence of their optimality conditions to continuous Hamilton–Jacobi–Bellman (HJB) equations. In the first class HJB equations follow straightforwardly from optimality conditions. In the second class, a condition of weak nonlinearity of the discrete rates with respect to θ^n (discussed below) is sufficient.

In each case stage optimality criteria of Caratheodory–Boltyanskii–Sieniutycz type transferred to discrete systems (*CBS* criteria, [12,21,22]) are valid. For a general function of optimal profit

$$V^n \equiv \max \sum_k^n f_0^k(\mathbf{x}^k, t^k, \mathbf{u}^k, \theta^k)\theta^k \tag{53}$$

a general optimality criterion at stage n that uses the θ-dependent rates has the form

$$0 = \max_{\mathbf{u}^n, \theta^n, \mathbf{x}^n, t^n} \{f_0^n(\mathbf{x}^n, t^n, \mathbf{u}^n, \theta^n)\theta^n - V^n(\mathbf{x}^n, t^n) - V^{n-1}(\mathbf{x}^n - \mathbf{f}^n(\mathbf{x}^n, t^n, \mathbf{u}^n, \theta^n)\theta^n, t^n - \theta^n)\}. \tag{54}$$

(We may also use functions of costs type, local costs $l_0 = -f_0$. and integral optimal costs $R = -V$.)

For a special mode of discretization with θ-free rates $\mathbf{f}$ criterion (54) refers to the "standard" or "canonical" model associated with all involved equations linear in θ^n. It may then be shown that these models [11,18] are characterized by a constant Hamiltonian that satisfies a discrete HJB equation whose convergence to the continuous limit is a relatively easy problem. Yet for θ-dependent rates the situation is more complicated and a condition of a weak dependence of rates on the time interval is required (see below).

Criterion (54) can be applied to derive a set of usable (Hamiltonian-based) optimality conditions including those with respect to $\mathbf{x}^n$ and time t^n. With Eq. (54) one can then pass to an algorithm of discrete maximum principle and related canonical equations. This issue is not discussed in this paper, where a dynamic programming equation [following from Eq. (54) for fixed states and times] is most essential as it provides a direct information about the extremum performance function.

Below we present a set of optimality conditions for the general process with θ-dependent rates. The process is described by Eqs. (50)–(54) with θ-dependent rates. From these conditions those for systems linear in θ^n will easily follow for θ-independent rates and Hamiltonian.

Optimizing in Eq. (54) time intervals θ^n and controls $\mathbf{u}^n$ in the interior of the admissible control set leads respectively to two extremum conditions:

$$-\partial V^{n-1}/\partial t^{n-1} + f_0^n(\mathbf{x}^n, t^n, \theta^n, \mathbf{u}^n) - (\partial V^{n-1}/\partial \mathbf{x}^{n-1}) \cdot \mathbf{f}^n(\mathbf{x}^n, t^n, \mathbf{u}^n, \theta^n) + \theta^n \partial\{f_0^n(\mathbf{x}^n, t^n, \theta^n, \mathbf{u}^n) - (\partial V^{n-1}/\partial \mathbf{x}^{n-1}) \cdot \mathbf{f}^n(\mathbf{x}^n, t^n, \mathbf{u}^n, \theta^n)\}/\partial\theta^n = 0 \tag{55}$$

and

$$\partial\{f_0^n(\mathbf{x}^n, t^n, \theta^n, \mathbf{u}^n) - (\partial V^{n-1}/\partial \mathbf{x}^{n-1}) \cdot \mathbf{f}^n(\mathbf{x}^n, t^n, \mathbf{u}^n, \theta^n)\}/\partial \mathbf{u}^n = 0. \tag{56}$$

For convex functions and constraining set $u^n \in U^n$, stationarity condition (56) allows to find optimal control $\mathbf{u}^n$ from the maximum condition for a Hamiltonian expression

$$\mathbf{u}^n = \arg\max_{\mathbf{u}^n} \{-\partial V^{n-1}/\partial t^{n-1} + f_0^n(\mathbf{x}^n, t^n, \theta^n, \mathbf{u}^n) - (\partial V^{n-1}/\partial \mathbf{x}^{n-1}) \cdot \mathbf{f}^n(\mathbf{x}^n, t^n, \theta^n, \mathbf{u}^n)\}. \tag{57}$$

Eq. (57) describes a maximum principle with respect to $\mathbf{u}^n$ for a 'Hamiltonian', i.e. expression in braces of this equation. The so-called enlarged Hamiltonian expression is used that includes the partial derivative of V with respect to time t.

Discrete HJB equations. Eq. (55) proves that the discrete Hamilton–Jacobi–Bellman structure is not attained when the discrete model is nonlinear in time intervals θ^n. In fact, it follows from Eqs. (55) and (56) that a discrete HJB equation for the optimum profit function

$$-\partial V^{n-1}/\partial t^{n-1} + \max_{\mathbf{u}^n} \{f_0^n(\mathbf{x}^n, t^n, \mathbf{u}^n) - (\partial V^{n-1}/\partial \mathbf{x}^{n-1}) \cdot \mathbf{f}^n(\mathbf{x}^n, t^n, \mathbf{u}^n)\} = 0, \tag{58}$$

or, an equivalent equation, in terms of the cost functions $R = -V$ and $l_0 = -f_0$,

$$\partial R^{n-1}/\partial t^{n-1} + \max_{\mathbf{u}^n} \{-l_0^n(\mathbf{x}^n, t^n, \mathbf{u}^n) + (\partial R^{n-1}/\partial \mathbf{x}^{n-1}) \cdot \mathbf{f}^n(\mathbf{x}^n, t^n, \mathbf{u}^n)\} = 0, \tag{59}$$

cannot be obtained for models nonlinear in θ^n. This is why variable θ^n is absent in rates of Eqs. (58) and (59), i.e. only models linear in θ^n are admitted therein.

Discrete Hamilton–Jacobi equations. When optimal controls θ^n and $\mathbf{u}^n$ are evaluated in terms of $\partial V^{n-1}/\partial \mathbf{x}^{n-1}, \mathbf{x}^n$ and t^n from Eqs. (55) and (56) and next substituted into (55), the result constitutes a discrete counterpart of the Hamilton–Jacobi equation.

For models linear with respect to θ^n one obtains in terms of $R = -V$

$$\partial R^{n-1}/\partial t^{n-1} + H^{n-1}(x_1^n, \ldots, x_s^n, t^n, \partial R^{n-1}/\partial x_1^{n-1} \cdots \partial R^{n-1}/\partial x_s^{n-1}) = 0, \tag{60}$$

whereas for those nonlinear in θ^n Hamiltonian H^{n-1} is replaced by partial derivative $h_\theta \equiv \partial(\theta^n H^{n-1})/\partial\theta^n$

$$\partial R^{n-1}/\partial t^{n-1} + h_\theta^{n-1}(x_1^n, \ldots, x_s^n, t^n, \partial R^{n-1}/\partial x_1^{n-1} \cdots \partial R^{n-1}/\partial x_s^{n-1}) = 0. \tag{61}$$

In fact, the replacement of H^{n-1} by the derivative $h_\theta \equiv \partial(\theta^n H^{n-1})/\partial\theta^n$ in the second case leads to the structure that is explained in the enlarged space-time in terms of (vanishing) partial derivative of the enlarged Hamiltonian function with respect to free control, θ^n [19]. Note that both equations are nonlinear in terms of derivatives $\partial R^{n-1}/\partial \mathbf{x}^{n-1}$.

The above results lead to convergence conditions of discrete computational schemes to continuous Hamilton–Jacobi equations of physical processes. To this end a notion of the weak dependence of the discrete Hamiltonian on θ is important. Note that the Hamiltonian is a weighted measure quantifying dependence of the discrete rate vector on time interval θ.

Definition. The θ-differentiable Hamiltonian function H^{n-1} is said to be weakly dependent on θ^n in a vicinity of $0+$ if for any positive number ε a positive number η exists

such that for a sufficiently small positive $\theta^n \leqslant \eta$ the absolute value of the product $I\theta^n\partial(H^{n-1})/\partial\theta^n I \leqslant \varepsilon$, for $n = 1, 2, \ldots, N$. This means that in a vicinity of 0+ the reciprocal of derivative $\partial(H^{n-1})/\partial\theta^n$ tends to zero slower than θ^n itself or that $\lim(\theta^n\partial(H^{n-1})/\partial\theta^n) = 0$ for $\theta^n \to 0+$ regardless the form of rate functions f_k.

In fact, many popular discretization schemes lead to discrete rates and Hamiltonians weakly dependent on θ^n for positive θ in a vicinity of the point $\theta = 0$. For Hamiltonians weakly dependent on θ^n the following corollary holds.

Corollary. *Assume fixed end states* $(\mathbf{x}^0, \mathbf{x}^N)$, *end times* (t^0, t^N) *and an arbitrarily large number M. For a sufficiently large total number of stages* $N > M$ *each free interval* θ^n *is sufficiently close to zero, i.e.* $\lim\theta^n = 0+$ *for* $N \to \infty$ *by the monotonicity property of time coordinate t. Then for unconstrained intervals* θ^n *and each Hamiltonian function* $H^{n-1}(x_1^n, \ldots x_s^n, t^n, -\partial V^{n-1}/\partial x_1^{n-1} \ldots - \partial V^{n-1}/\partial x_s^{n-1}, \theta^n)$ *weakly dependent on* θ^n *in a vicinity of* 0+ *classical Hamilton–Jacobi equation holds in the limit of* $N \to \infty$.

Proof. For Hamiltonians H^{n-1} weakly dependent on θ^n in a vicinity of 0+ and a sufficiently large N the derivative $\partial(\theta^n H^{n-1})/\partial\theta^n$ is sufficiently close to H^{n-1} for each $n = 1, \ldots N$. In the limiting case of $N \to \infty$ the sequence of free θ^n satisfies the conditions: $\lim\theta^n = 0+$ and $\lim\partial(\theta^n H^{n-1})/\partial\theta^n = \lim H^{n-1} = H(\mathbf{x}, t, \partial R/\partial\mathbf{x})$. Eq. (61) then goes over into the Hamilton–Jacobi equation of a continuous process

$$\partial R/\partial t + H(x_1, \ldots, x_s, t, \partial R/\partial x_1 \cdots \partial R/\partial x_s) = 0. \tag{62}$$

The above corollary assures that the limiting Hamilton–Jacobi equation of a continuous system is obtained in unique form (62), regardless the discretization mode and the form of underlying discrete equation, Eq. (60) or (61). Discrete Hamiltonians weakly dependent on θ^n in a vicinity of 0+ are common in thermodynamic systems described in spaces of arbitrary state variables rather than extensive thermodynamic coordinates. □

11. Discrete approximations and time adjoint as a Lagrange multiplier

In this section we consider another discrete example whose solution converges to that for a continuous problem of power generation. Yet, for brevity of formulas, we restrict ourselves to systems in which nonlinearities are absent in process kinetics although they are still present in the power expression. We obtain the solution of a HJB equation by the discrete approximations produced by the method of dynamic programming and simultaneous state dimensionality reduction (elimination of time coordinate) by using a Lagrange multiplier.

First we shall outline generation of costs in terms of the Lagrangian multiplier λ for the duration constraint. As the time adjoint, λ is constant in autonomous systems.

Consider a minimum of consumed work with constraints imposed on discrete dynamics and process duration

$$R^n(T^n, \tau^n) = \sum_{k=1}^{n} c\left(1 - \Phi'\frac{T^e}{T'^k}\right)(T^k - T^{k-1})$$
$$= \sum_{k=1}^{n} c\left(1 - \Phi'\frac{T^e}{T'^k}\right)(T'^k - T^k)\theta^k, \tag{63}$$

$$T^k - T^{k-1} = \theta^k(T'^k - T^k), \tag{64}$$

$$\tau^k - \tau^{k-1} = \theta^k. \tag{65}$$

Observe that the above difference equations model a continuous problem of minimum work subject to the linear kinetic constraint $\dot{T} = T' - T$ [2].

Exploiting constancy of λ we eliminate state variable τ by introducing a (primed) criterion of modified work

$$R'^n(T^n, \lambda) = \min \sum_{k=1}^{n} \left\{ c\left(1 - \Phi'\frac{T^e}{T'^k}\right)(T^k - T^{k-1}) + \lambda\theta^n \right\}, \tag{66}$$

or, in view of state Eq. (64)

$$R'^n(T^n, \lambda) = \min \sum_{k=1}^{n} \left\{ c\left(1 - \Phi'\frac{T^e}{T'^k}\right) + \frac{\lambda}{T'^k - T^k} \right\}(T^k - T^{k-1}). \tag{67}$$

In this problem, idea of parametric representations for the principal performance function, Lagrange multiplier and process duration had proven its usefulness. While these representations are unnecessary for linear optimization problems, they are quite effective to describe solutions of nonlinear problems, where optimal work, Lagrange multiplier and optimal duration are obtained in terms of an optimal control variable as a parameter.

To begin with we determine optimality conditions from Eq. (67). We consider two initial process stages, 1 and 2. The procedure leading to parametric representations is defined below.

Work equation (or a profit equation) modified by the presence of the Lagrange multiplier λ, yet without a minimization sign

$$R'^1(T^1, T'^1, \lambda) = \left\{ c\left(1 - \Phi'\frac{T_2}{T'^1}\right) + \frac{\lambda}{T'^1 - T^1} \right\}(T^1 - T^0) \tag{68}$$

becomes a component of a parametric representation of $R'^1(T^1, \lambda)$ provided that the following procedure is implemented:

1. λ is determined from the extremum condition of work function R'^1 with respect to a control variable, here with respect to Carnot control T'^1

$$\lambda = c\Phi' T^e \frac{(T'^1 - T^1)^2}{(T'^1)^2}. \tag{69}$$

2. Extremum λ is substituted into the work function R'^1, and the result of this substitution

$$R'^1(T^1,T'^1)=\left\{c\left(1-\Phi'\frac{T^e}{T'^1}\right)+c\Phi\prime T^e\frac{T'^1-T^1}{(T'^1)^2}\right\}(T^1-T^0) \tag{70}$$

is taken together with the expression for stationary λ.

In view of the above, parametric representation of work function $R'^1(T^1,\lambda)$ in terms of Carnot control as a parameter is given by the set of Eqs. (69) and (70). After simplification of work equation the final form of the representation is

$$R'^1(T^1,T'^1)=c\left(1-\Phi' T^e\frac{T^1}{(T'^1)^2}\right)(T^1-T^0)$$

$$\lambda=c\Phi' T^e\left(1-\frac{T^1}{T'^1}\right)^2. \tag{71}$$

In this example it is possible to eliminate the parameter T'^1 which leads to explicit function of work consumption for $n=1$

$$R'^1(T^1,T^0,\lambda)=c(T^1-T^0)-c\Phi' T^e\left(1-\pm\sqrt{\frac{\lambda}{c\Phi' T^e}}\right)^2\left(\frac{T^1-T^0}{T^1}\right). \tag{72}$$

Corresponding optimal control satisfies an equation

$$T'^1=T^1\left(1-\pm\sqrt{\frac{\lambda}{c\Phi' T^e}}\right)^{-1} \tag{73}$$

obtained after solving of Eq. (69) with respect to T'^1.

Yet, the elimination of the parameter is not always possible, and then parameter dependent-functions constitute the only representation of the solution. It is just this case when parametric representations are inevitable and helpful.

Let us proceed further. Optimal work supply to two-stage system $R'^2(T^2,\lambda)$ is described by an equation

$$R'^2(T^2,\lambda)=\min_{T^1}\left\{c(T^2-T^1)-c\Phi' T^e\left(1-\pm\sqrt{\frac{\lambda}{c\Phi' T^e}}\right)^2\left(\frac{T^2-T^1}{T^2}\right)+c(T^1-T^0)-c\Phi' T^e\left(1-\pm\sqrt{\frac{\lambda}{c\Phi' T^e}}\right)^2\left(\frac{T^1-T^0}{T^1}\right)\right\},$$

whence, after making simplifications

$$R'^2(T^2,\lambda)=\min_{T^1}\left\{c(T^2-T^0)-c\Phi' T^e\left(1-\pm\sqrt{\frac{\lambda}{c\Phi' T^e}}\right)^2\times\left(\frac{T^2-T^1}{T^2}+\frac{T^1-T^0}{T^1}\right)\right\}. \tag{74}$$

Optimal interstage temperature between stages 1 and 2, T^1, satisfies the stationarity condition for expression in the large bracket of the above equation

$$\frac{\partial}{\partial T^1}\left(\frac{T^2-T^1}{T^2}+\frac{T^1-T^0}{T^1}\right)=\frac{T^0}{(T^1)^2}-\frac{1}{T^2}=0. \tag{75}$$

Therefore optimal interstage temperature T^1 is the geometric mean of boundary temperatures of both considered stages

$$T^1=(T^0T^2)^{1/2}. \tag{76}$$

The minimum value of optimized expression (75) is

$$\min_{T^1}\left(\frac{T^2-T^1}{T^2}+\frac{T^1-T^0}{T^1}\right)=\frac{T^2-\sqrt{T^0T^2}}{T^2}+\frac{\sqrt{T^0T^2}-T^0}{\sqrt{T^0T^2}}=2(1-\sqrt{T^0/T^2}). \tag{77}$$

This leads to the optimum work function for $n=2$

$$R'^2(T^2,\lambda)=c(T^2-T^0)-2c\Phi' T^e\left(1-\pm\sqrt{\frac{\lambda}{c\Phi' T^e}}\right)^2\left(1-\left(\frac{T^0}{T^2}\right)^{1/2}\right). \tag{78}$$

For $n=3$ we apply an expression for local work

$$K'^3(T^3,T^2,\lambda)=c(T^3-T^2)-c\Phi' T^e\left(1-\pm\sqrt{\frac{\lambda}{c\Phi' T^e}}\right)^2\left(\frac{T^3-T^2}{T^3}\right), \tag{79}$$

which has the same structure as the one-stage function of Eq. (72), but the indices are shifted ahead by the unity. In the recurrence equation for $n=3$, explicit work function $R'^3(T^3,\lambda)$ is the result of optimization described by the following expression

$$R'^3(T^3,\lambda)=\min_{T^2}\left\{c(T^3-T^2)-c\Phi' T^e\left(1-\pm\sqrt{\frac{\lambda}{c\Phi' T^e}}\right)^2\times\left(\frac{T^3-T^2}{T^3}\right)+c(T^2-T^0)-2c\Phi' T^e\times\left(1-\pm\sqrt{\frac{\lambda}{c\Phi' T^e}}\right)^2\left(1-\left(\frac{T^0}{T^2}\right)^{1/2}\right)\right\}.$$

After simplifying we obtain

$$R'^3(T^3,\lambda)=\min_{T^2}\left\{c(T^3-T^0)-c\Phi' T^e\left(1-\pm\sqrt{\frac{\lambda}{c\Phi' T^e}}\right)^2\times\left[\left(\frac{T^3-T^2}{T^3}\right)+2\left(1-\left(\frac{T^0}{T^2}\right)^{1/2}\right)\right]\right\}. \tag{80}$$

Consequently, optimal interstage temperature T^2 satisfies the stationarity condition

$$\frac{\partial}{\partial T^2}\left(\frac{T^3-T^2}{T^3}+2\left(1-\left(\frac{T^0}{T^2}\right)^{1/2}\right)\right)=0. \tag{81}$$

Performing the differentiation with respect to T^2 one obtains in terms of T^0 and T^3

$$T^2 = (T^0)^{1/3}(\mathrm{T}^3)^{2/3} \tag{82}$$

and

$$T^1 = (T^0T^2)^{1/2} = (T^0)^{1/2}[(T^0)^{1/3}(T^3)^{2/3}]^{1/2} = (T^0)^{2/3}(T^3)^{1/3}. \tag{83}$$

Let us eliminate T^0 and determine T^2 in terms of T^1 i T^3. We obtain

$$T^2 = (T^0)^{1/3}(T^3)^{2/3} = (T^1)^{1/2}(T^3)^{-1/6}(T^3)^{2/3} = (T^1)^{1/2}(T^3)^{1/2}. \tag{84}$$

Therefore, as one could expect, also optimal interstage temperature T^2 is the geometric mean of boundary temperatures of two considered stages

$$T^2 = (T^1T^3)^{1/2}. \tag{85}$$

Substitution of temperature $T^2 = (T^0)^{1/3}(T^3)^{2/3}$ into work function (80) yields

$$R'^3(T^3,\lambda) = c(T^3 - T^0) - c\Phi' T^e\left(1 - \pm\sqrt{\frac{\lambda}{c\Phi' T^e}}\right)^2 \times \left[\left(1 - \left(\frac{T^0}{T^3}\right)^{1/3}\right) + 2\left(1 - \left(\frac{T^0}{T^3}\right)^{1/3}\right)\right],$$

which can be simplified to the form

$$R'^3(T^3,\lambda) = c(T^3 - T^0) - 3c\Phi' T^e\left(1 - \pm\sqrt{\frac{\lambda}{c\Phi' T^e}}\right)^2\left(1 - \left(\frac{T^0}{T^3}\right)^{1/3}\right). \tag{86}$$

Comparing this expression with corresponding ones for $n = 1$ and $n = 2$, Eqs. (72) and (78), leads to optimal work function for an arbitrary n

$$R'^n(T^n,\lambda) = c(T^n - T^0) - nc\Phi' T^e\left(1 - \pm\sqrt{\frac{\lambda}{c\Phi' T^e}}\right)^2\left(1 - \left(\frac{T^0}{T^n}\right)^{1/n}\right). \tag{87}$$

The corresponding optimal duration is the partial derivative of optimal work function with respect to Lagrangian multiplier λ

$$\tau^n = \frac{\partial R'^n(T^n,\lambda)}{\partial\lambda} = n\left(1 - \pm\sqrt{\frac{\lambda}{c\Phi' T^e}}\right)\left(\pm\sqrt{\frac{\lambda}{c\Phi' T^e}}\right)^{-1}\left(1 - \left(\frac{T^0}{T^n}\right)^{1/n}\right). \tag{88}$$

Qualitative properties of the duration functions $\tau^n = \Sigma\theta^n$ are illustrated in Fig. 4. Eq. (89) refers to linear kinetics,

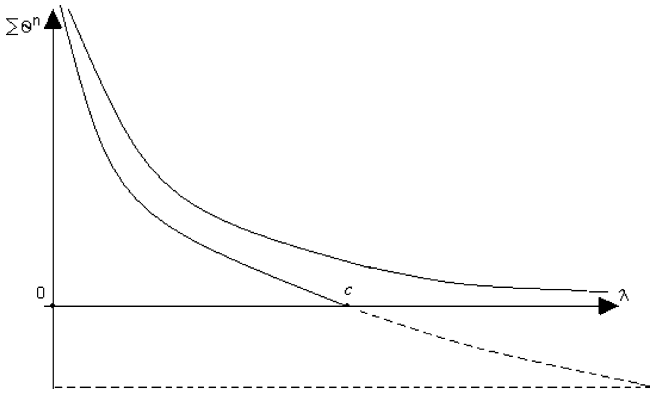

Fig. 4. Two typical functions describing optimal duration $\tau = \Sigma\Theta^n$ in terms of Lagrange multiplier λ in a cascade of power generation units.

in which case the curve intersects the axis of λ for $\lambda = c$. In nonlinear systems with a variable c the intersection point may move to large values of λ, Fig. 4. In any process, linear or not, λ is monotonically decreasing function of duration.

Knowledge of partial derivative of optimal work function with respect to Lagrangian multiplier λ is essential when one wish to return to original work function $R^n(T^n,\tau^n)$ (without Lagrange multiplier term). In this operation the Legendere transformation plays an essential role (Section 12). Yet, before its implementing consider some properties of intensity parameter ξ.

Applying the geometric sequence property for optimal path in the considered example

$$\frac{T^0}{T^n} = \frac{T^0}{T^1}\frac{T^1}{T^2}\cdots\frac{T^{n-1}}{T^n} = \left(\frac{T^{n-1}}{T^n}\right)^n, \tag{89}$$

we obtain

$$\frac{T^{n-1}}{T^n} = \left(\frac{T^0}{T^n}\right)^{1/n}. \tag{90}$$

With these results we can easily prove the equality of a mean rate and a local rate. These rates are described, respectively by the first and the last equality of the following equation

$$\xi \equiv \frac{n}{\tau^n}\left(1 - \left(\frac{T^0}{T^n}\right)^{1/n}\right) = \frac{n}{\tau^n}\left(1 - \frac{T^{n-1}}{T^n}\right) = \frac{T^n - T^{n-1'}}{T^n\theta^n}. \tag{91}$$

Taking into account the limiting value of the expression

$$\lim_{n\to\infty} n\left(1 - (T^0/T^n)^{1/n}\right) = \ln(T^n/T^0),$$

we note that the continuous limit of the mean ξ is the change of the temperature logarithm per unit of time.

Local and mean intensities ξ are in general different quantities. Yet, in processes with linear kinetics, considered in the present example, there is no need to distinguish between them and the same symbol for both is used in equations.

Writing the duration formula, Eq. (88), in the form

$$\xi^{-1} \equiv \frac{\tau^n}{n}\left(1-\left(\frac{T^0}{T^n}\right)^{1/n}\right)^{-1} = \pm\left(\sqrt{\frac{\lambda}{c\Phi' T^e}}\right)^{-1} - 1, \qquad (88')$$

we find an useful equality determining the Lagrange multiplier in terms of the process intensity (mean or instantaneous)

$$\lambda = c\Phi' T^e\left(\frac{\xi}{\xi+1}\right)^2. \qquad (92)$$

Two values of ξ for a given λ correspond with heating and cooling of the resource fluid in heat-pump and engine modes (upgrading and downgrading of the resource). Both λ and ξ vanish in reversible quastitstic processes.

As the following equality is valid

$$1 - \pm\sqrt{\frac{\lambda}{c\Phi' T^e}} = \frac{1}{\xi+1} \qquad (93)$$

optimal work function in terms of ξ assumes the form

$$R'^n(T^n,\xi) = c(T^n - T^0) - \frac{c\Phi' T^e}{(1+\xi)^2} n\left(1-\left(\frac{T^0}{T^n}\right)^{1/n}\right). \qquad (94)$$

We find that the limiting value of function $R'^n(T^n,\xi)$ in a quasi-static ($\xi = 0$) and reversible process ($\Phi = 1$) represents the change of classical thermal exergy.

$$R'^n(T^n,0) = c(T^n - T^0) - cT^e \ln(T^n/T^0). \qquad (95)$$

Therefore optimal work function (94) is a finite-rate exergy of the considered discrete process. In the following section other functions of this kind are obtained.

12. Legendre transform and original work function

The minimum of consumed work (63) is described by original principal function $R^n(T^n,\tau^n)$. This function is the Legendre transform of $R'^n(T^n,\lambda)$ with respect to λ

$$R^n(T^n,\tau^n) = R'^n(T^n,\lambda) - \lambda\tau^n = R'^n(T^n,\lambda) - \lambda\frac{\partial R'^n(T^n,\lambda)}{\partial\lambda}. \qquad (96)$$

For our example we obtain

$$R^n(T^n,\lambda) = c(T^n - T^0) - nc\Phi' T^e\left(1-\pm\sqrt{\frac{\lambda}{c\Phi' T^e}}\right)^2\left(1-\left(\frac{T^0}{T^n}\right)^{1/n}\right) - \lambda n\left(1-\pm\sqrt{\frac{\lambda}{c\Phi' T^e}}\right)\left(\pm\sqrt{\frac{\lambda}{c\Phi' T^e}}\right)^{-1}\left(1-\left(\frac{T^0}{T^n}\right)^{1/n}\right). \qquad (97)$$

which should be transformed to space of variables T^n and τ^n. In transformations we use intensity ξ as an intermediate variable to increase their lucidity. Applying Eq. (92) we obtain

$$\tau^n = \frac{\partial R'^n(T^n,\lambda)}{\partial\lambda} = \frac{n}{\xi}\left(1-\left(\frac{T^0}{T^n}\right)^{1/n}\right) \qquad (98)$$

and

$$R^n(T^n,\xi) = c(T^n - T^0) - c\Phi' T^e\left(\frac{1}{1+\xi}\right)^2 n\left(1-\left(\frac{T^0}{T^n}\right)^{1/n}\right) - \frac{\lambda(\xi)}{\xi} n\left(1-\left(\frac{T^0}{T^n}\right)^{1/n}\right), \qquad (99)$$

where function describing λ in terms of ξ is given by Eq. (92). Using Eq. (93) in (99) we find

$$R^n(T^n,\xi) = c(T^n - T^0) - \frac{c\Phi' T^e}{1+\xi} n\left(1-\left(\frac{T^0}{T^n}\right)^{1/n}\right). \qquad (100)$$

This is also a finite-rate exergy, yet it differs from function $R'^n(T^n,\xi)$ of Eq. (94) by the structure of ξ term. To single out from this equation a ξ-independent term we write $(1+\xi)^{-1}$ as $1 - \xi/(1+\xi)$ and, then,

$$R^n(T^n,\xi) = c(T^n - T^0) - c\Phi' T^e n\left(1-\left(\frac{T^0}{T^n}\right)^{1/n}\right) + \frac{\xi}{1+\xi} c\Phi' T^e n\left(1-\left(\frac{T^0}{T^n}\right)^{1/n}\right). \qquad (101)$$

Eq. (91) can next be used to express the last (rate-dependent) term of Eq. (101) in terms of process duration. We obtain

$$\frac{\xi}{1+\xi} \equiv \frac{n\left(1-\left(\frac{T^0}{T^n}\right)^{1/n}\right)}{\tau^n + n\left(1-\left(\frac{T^0}{T^n}\right)^{1/n}\right)} \qquad (102)$$

and

$$R^n(T^n,\tau^n) = c(T^n - T^0) - c\Phi' T^e n\left(1-\left(\frac{T^0}{T^n}\right)^{1/n}\right) + c\Phi' T^e\left\{n\left(1-\left(\frac{T^0}{T^n}\right)^{1/n}\right)\right\}^2\left(\tau^n + n\left(1-\left(\frac{T^0}{T^n}\right)^{1/n}\right)\right)^{-1}. \qquad (103)$$

First two components of this work function are of static origin. The function describes a minimum work supplied to a resource to upgrade it from T^0 to T^n in a finite (non-dimensional) time τ^n. Like in the case of primed function R' a limiting value of $R^n(T^n,\tau^n)$ in a quasi-static process ($\Phi' = 1, \tau^n \to \infty$) describes a change of classical thermal exergy, Eq. (95).

13. Numerical approaches applying dynamic programming

Numerical aspects of DP algorithms are only briefly mentioned here as there is a literature available that

discusses these issues. Problems of grid expansion and "curse of dimensionality"are usually main difficulties [20,22,23].

Optimal performance functions are direct outcome of numerical methods which apply the dynamic programming. Optimal control problems of both continuous and discrete processes with a single independent variable (time or length) can be treated in the framework of a common discrete formalism. As the computer needs require a discrete set of equations, prior discretizing of ordinary differential equations is required.

Now we describe the numerical generation of optimal function $V^n = \max W$. Assume that at the stage n (duration $\Delta t^n = \theta^n$) a profit function $D^n = D^n(\mathbf{x}^n, t^n, \mathbf{u}^n, \theta^n, n)$ is given. In a maximum work problem $D^n = f_0^n \theta^n$, where D^n is the work produced at stage n. The total work (profit) at the n-stage subprocess equals $\Sigma D^n = \Sigma f_0^m \theta^m$. Along with discrete state equations and local constraints, various data of D^n – analytic, graphic or tabular – are sufficient to develop computational principles for cascade processes with arbitrary number of stages. It is, however, important that D^n is properly expressed at the stage n as a function of state $\mathbf{x}^n$, time t^n, and controls $(\mathbf{u}^n, \theta^n)$. Data of optimal work functions $V^1, \ldots, V^n, \ldots, V^N$ should be generated over subprocesses composed respectively of the stage 1, stages 1 and 2,... stages 1,2,...,n,... and, finally, stages $1, 2, \ldots, N$.

For a given set of difference constraints (51) each profit function, e.g. optimal work potential V^n, is found from Bellman's equation of dynamic programming. A typical form of this equation in terms of enlarged state vector $\tilde{\mathbf{x}}^n \equiv (\mathbf{x}^n, t^n)$ and one-stage profit D^n is

$$V^n(\tilde{\mathbf{x}}^n) = \max_{\mathbf{u}^n, \theta^n} \{D^n(\tilde{\mathbf{x}}^n, \mathbf{u}^n, \theta^n) + V^{n-1}(\tilde{\mathbf{x}}^n - \tilde{\mathbf{f}}^n(\tilde{\mathbf{x}}^n, \mathbf{u}^n, \theta^n)\theta^n)\}. \tag{104}$$

Since one has to generate computational data within a definite domain of the variables $\tilde{\mathbf{x}}$, one can conveniently omit stage superscript n at the (enlarged) state vector of Eq. (104)

$$V^n(\tilde{\mathbf{x}}) = \max_{\mathbf{u}^n, \theta^n} \{D^n(\tilde{\mathbf{x}}, \mathbf{u}^n, \theta^n) + V^{n-1}(\tilde{\mathbf{x}} - \tilde{\mathbf{f}}^n(\tilde{\mathbf{x}}, \mathbf{u}^n, \theta^n)\theta^n)\}. \tag{105}$$

The solution to Eq. (104) or (105) is obtained iteratively in form of tables for $n = 1, 2, \ldots, N$, which describe sequence of functions $V^n(\tilde{\mathbf{x}})$, $\mathbf{u}^n(\tilde{\mathbf{x}})$ and $\theta^n(\tilde{\mathbf{x}})$. The iterative procedure starts with $V^0 = 0$. Potential $V^n(\tilde{\mathbf{x}})$ is in general time dependent even if the process is autonomous.

Organization of calculations requires a suitable computational grid. In the nodes of this grid data of optimal functions and optimal controls are computed and stored. A total number of stages, N, is assumed. Numerical DP algorithm generates potential function $V^n(\tilde{\mathbf{x}})$ from function $V^{n-1}(\tilde{\mathbf{x}})$ of $n-1$ stage subprocess and state transformations, Eqs. (51) and (52). In agreement with Bellman's optimality principle, consistent with Eq. (104), a computer maximizes the sum of optimal cost of all previous $n-1$ stages (optimal function V^n) and non-optimal profit $\widetilde{D}^n$ at the stage n. To determine $V^n(\tilde{\mathbf{x}})$ exactly for a definite n, the computer would have to numerically determine values of this function for every value of $\tilde{\mathbf{x}}$, an impossible task. Therefore, these values are determined on a discrete subset of $\tilde{\mathbf{x}}$, and the data are used in the way that makes possible evaluation of $V^n(\tilde{\mathbf{x}})$ everywhere. If $\langle \tilde{\mathbf{x}}_{\mathrm{I}}, \tilde{\mathbf{x}}_{\mathrm{II}} \rangle$ is the interval of interest, one can take $\tilde{\mathbf{x}}_{\mathrm{I}} = \mathbf{A}\delta$ and $\tilde{\mathbf{x}}_{\mathrm{II}} = \mathbf{B}\delta$, where δ is a small accepted value. The vectors $\mathbf{A}$ and $\mathbf{B}$ are respectively computed as $\tilde{\mathbf{x}}_{\mathrm{I}}/\delta$ and $\tilde{\mathbf{x}}_{\mathrm{II}}/\delta$. The quantity δ cannot be too large, because the results accuracy is then poor. It cannot be too small either, as the computation time becomes very long. The discrete subset of $\tilde{\mathbf{x}}$, for which the values $V^n(\tilde{\mathbf{x}})$ are computed for various n, has the form

$$\tilde{\mathbf{x}} = \mathbf{A}\delta, (\mathbf{A}+1)\delta, \ldots, (\mathbf{B}-1)\delta, \mathbf{B}\delta. \tag{106}$$

This refers to the linear grid of values $\tilde{\mathbf{x}} = \mathbf{a}\delta$, where $\mathbf{a} = \mathbf{A}, \mathbf{A}+\mathbf{1}, \ldots, \mathbf{B}$. Other values of $V^n(\tilde{\mathbf{x}})$, e.g. those in an interval $\langle \mathbf{a}\delta, (\mathbf{a}+1)\delta \rangle$, are defined by accepting $V^n(\mathbf{a}\delta)$ or $V^n[(\mathbf{a}+\mathbf{1})\delta]$ depending on location of $\mathbf{x}\delta$ with respect to $(\mathbf{a}+\mathbf{1}/\mathbf{2})\delta$, or by using interpolation, e.g.

$$V^n(\tilde{\mathbf{x}}) = V^n(\mathbf{A}\delta) + \frac{V^n((\mathbf{A}+1)\delta) + V^n(\mathbf{A}\delta)}{\delta}(\tilde{\mathbf{x}} - \mathbf{a}), \quad \mathbf{a}\delta \leqslant (\mathbf{a}+1)\delta. \tag{107}$$

The discrete subset of admissible controls is defined in a similar way. For example, when constrains imposed on are described by inequality $\mathbf{u}_* \leqslant \mathbf{u}^n \leqslant \mathbf{u}^*$, variable may assume only the discrete values

$$\mathbf{u}^* = \mathbf{E}\gamma + (\mathbf{E}+1)\gamma, \ldots, (\mathbf{F}-1)\gamma, \mathbf{F}\gamma = \mathbf{u}^* \tag{108}$$

for an appropriately small value γ. This refers to the linear grid of controls $\mathbf{u} = \mathbf{b}\delta$, where $\mathbf{b} = \mathbf{E}, \mathbf{E}+\mathbf{1}, \ldots, \mathbf{F}-\mathbf{1}, \mathbf{F}$.

With Eq. (105) optimal controls are determined from the formula

$$\{\mathbf{u}^n(\tilde{\mathbf{x}}), \theta^n(\tilde{\mathbf{x}})\} = \arg\max_{\mathbf{u}^n \theta^n}, \{\tilde{D}^n(\tilde{\mathbf{x}}, \mathbf{u}^n, \theta^n) + V^{n-1}(\tilde{\mathbf{x}} - \tilde{\mathbf{f}}^n(\tilde{\mathbf{x}}, \mathbf{u}^n, \theta^n)\theta^n)\} \tag{109}$$

along with the sequence of the optimal functions V^n. The first optimal function, $V^1(\tilde{\mathbf{x}})$, and the corresponding optimal controls for $n = 1$ follow from the application of the initial condition $V^0(\tilde{\mathbf{x}}) = 0$ in Eqs. (105) and (109); this yields

$$V^1(\tilde{\mathbf{x}}) = \max_{\mathbf{u}^1, \theta^1} \{\widetilde{D}^1(\tilde{\mathbf{x}}, \mathbf{u}^1, \theta^1)\} \tag{110}$$

and

$$\{\mathbf{u}^1(\tilde{\mathbf{x}}), \theta^1(\tilde{\mathbf{x}})\} = \arg\max_{\mathbf{u}^n \theta^n}, \{\widetilde{D}^1(\tilde{\mathbf{x}}, \mathbf{u}^1, \theta^1)\}. \tag{111}$$

To find these functions, the computer chooses the first point $\tilde{\mathbf{x}} = \mathbf{A}\delta = (A_1\delta, A_2\delta)$ and compares $\widetilde{D}^1(\mathbf{A}\delta, E_1\gamma, E_2\gamma)$ with $\widetilde{D}^1(\mathbf{A}\delta, (E_1+1)\gamma, E_2\gamma)$. The larger of these values is stored and compared with $\widetilde{D}^1(\mathbf{A}\delta, (E_1+2)\gamma, E_2\gamma)$, etc. This process is continued until the whole discrete set of controls $(\mathbf{u}^1, \theta^1)$ is exhausted. The largest of the so-obtained values

is always a maximum of $\widetilde{D}^1$ with respect to $(\mathbf{u}^1, \theta^1)$ for a fixed discrete point $\tilde{\mathbf{x}}$. The coordinates of $\mathbf{u}^1$ and θ^1 which maximize $\widetilde{D}^1$ are stored. Analogous operations are next performed for $\tilde{\mathbf{x}} = ((A_1+1)\delta, A_2\delta), ((A_1+2)\delta, A_2\delta)$, and so on. Again, this leads to maximum of $\widetilde{D}^1$ and optimal values of $\mathbf{u}^1$ and θ^1. The generation of data takes place for various points $\tilde{\mathbf{x}}$ (different nodes of the grid).

The computer output are the DP tables with optimal data: $V^1(\tilde{\mathbf{x}})$, $\theta^1(\tilde{\mathbf{x}})$ and $\mathbf{u}^1(\tilde{\mathbf{x}})$.

For $n = 2$ (two-stage process), and for larger n, the procedure is analogous but uses Eqs. (104) and (109) in their complete form. Data of V^{n-1} are found in tables describing previous computations, for cascade with $n-1$ stages. When using these data a difficulty can appear which is called 'the danger of grid expansion'. It follows from the fact that the values $V^{n-1}(\tilde{\mathbf{x}})$ were computed within the range $\tilde{\mathbf{x}}_{\mathrm{I}} \leqslant \tilde{\mathbf{x}} \leqslant \tilde{\mathbf{x}}_{\mathrm{II}}$, but the computation of $V^n(\tilde{\mathbf{x}})$ from Eq. (104) requires the knowledge of $V^{n-1}(\tilde{\mathbf{x}}^{\mathrm{T}})$ for the transformed state $\tilde{\mathbf{x}}^{\mathrm{T}} \equiv \tilde{\mathbf{x}} - \tilde{\mathbf{f}}^n(\tilde{\mathbf{x}}, \mathbf{u}^n, \theta^n)\theta^n$. This means that for some forms of rate functions $\tilde{\mathbf{f}}$ the computation of $V^n(\tilde{\mathbf{x}})$ requires the knowledge of values $V^{n-1}(\tilde{\mathbf{x}})$ for $\tilde{\mathbf{x}}$ located outside of the range $\tilde{\mathbf{x}}_{\mathrm{I}} \leqslant \tilde{\mathbf{x}} \leqslant \tilde{\mathbf{x}}_{\mathrm{II}}$. Therefore, to evaluate $V^n(\tilde{\mathbf{x}})$ within the range satisfying $\tilde{\mathbf{x}}_{\mathrm{I}} \leqslant \tilde{\mathbf{x}} \leqslant \tilde{\mathbf{x}}_{\mathrm{II}}$ it may be necessary to determine $V^{n-1}(\tilde{\mathbf{x}})$ within a boundary which is larger than that described by the inequality $\tilde{\mathbf{x}}_{\mathrm{I}} \leqslant \tilde{\mathbf{x}} \leqslant \tilde{\mathbf{x}}_{\mathrm{II}}$.

The procedure leads to the optimal values of V^n, θ^n and $\mathbf{u}^n$ stored at each node of the grid of $\tilde{\mathbf{x}}$, for each n. These values constitute discrete representations of optimal functions $V^n(\tilde{\mathbf{x}}), \theta^{\mathrm{n}}(\tilde{\mathbf{x}})$ and $\mathbf{u}^n(\tilde{\mathbf{x}})$. Additionally, values of coordinates of the transformed state, $\tilde{\mathbf{x}}^{\mathrm{T}} \equiv \tilde{\mathbf{x}} - \tilde{\mathbf{f}}^n(\tilde{\mathbf{x}}, \mathbf{u}^n, \theta^n)\theta^n$, can be stored. Data of $\tilde{\mathbf{x}}^{\mathrm{T}}$ describe optimal inlet states to the stage n in terms of outlet states from this stage, $\tilde{\mathbf{x}}$.

Backward reading of the solution. Dynamic programming tables, which describe all computed data, can be used to find the solution of a particular (N-stage) problem in which final values of $\tilde{\mathbf{x}}^N \equiv \tilde{\mathbf{x}}^{\mathrm{f}}$and N are prescribed. This is a backward procedure in which we first identify in DP tables the final point $\tilde{\mathbf{x}}^{\mathrm{f}}$ for $n = N$, and, next, in these tables, we read off data of optimal controls $\theta^N(\tilde{\mathbf{x}}^{\mathrm{f}})$ and $\mathbf{u}^N(\tilde{\mathbf{x}}^{\mathrm{f}})$. In the tables we also find transformed outlet states $\tilde{\mathbf{x}}^{\mathrm{T}N} \equiv \tilde{\mathbf{x}} - \tilde{\mathbf{f}}^N(\tilde{\mathbf{x}}, \mathbf{u}^N, \theta^N)\theta^N$, which are inlet states to the stage N.

Now we pass to the $N-1$ stage subprocess. It has its own outlet state $\tilde{\mathbf{x}}^{N-1}$ which was already found as $\tilde{\mathbf{x}}^{\mathrm{T}N}$. By interpolating in the tables for $n = N-1$ we find all suitable data for the state $\tilde{\mathbf{x}} = \tilde{\mathbf{x}}^{N-1}$. We thus find optimal profit $V^{N-1}(\tilde{\mathbf{x}}^{N-1})$, optimal controls $\theta^{N-1}(\tilde{\mathbf{x}}^{N-1})$, $\mathbf{u}^{N-1}(\tilde{\mathbf{x}}^{N-1})$, and inlet states to the stage $N-1$, $\tilde{\mathbf{x}}^{N-2} = \tilde{\mathbf{x}}^{\mathrm{T}N-1}$. Continuing the procedure by the computer, we obtain an optimal solution as a sequence of optimal controls $\mathbf{u}^{\mathrm{N}}, \mathbf{u}^{N-1}, \ldots, u^1$ and $\theta^N, \theta^{N-1}, \ldots, \theta^1$, and an optimal discrete trajectory, $\tilde{\mathbf{x}}^N, \tilde{\mathbf{x}}^{N-1}, \ldots, \tilde{\mathbf{x}}^1, \tilde{\mathbf{x}}^0$. Sequence of optimal costs for all related subprocesses $V^N, V^{N-1}, \ldots, V^1$ also follows. A virtue of the DP method is that it always leads to absolute maximum.

However, in problems with large number of state coordinates a very serious difficulty arises connected with the use of the dynamic programming. This is the so-called 'curse of dimensionality', referred to the large dimensionality of state vector, $\tilde{\mathbf{x}}$. Indeed, for $s = \dim = 1$, a single column of discrete set of $\tilde{\mathbf{x}}$ is sufficient, for $s = 2$ the computational grid must constitute, say, a rectangle. For $s = 3$, however, the grid must be cubic, for $s = 4$ the data must be obtained (and stored) as a set of cubes, etc. Clearly, the number of computational points, and hence the computer memory requirements increase tremendously with state dimensionality s. Problems with $s = 1$ and $s = 2$ are quite easy to solve numerically, problems with higher $s = 3$ are troublesome or serious, and problems with $s \geqslant 5$ are practically intractable if good accuracy is required. Therefore the numerical dynamic programming can effectively be applied only for problems characterized by the small dimensionality of the state vector $\tilde{\mathbf{x}}$; problems of large dimensionality, such as those encountered in the static optimization, are excluded. Fortunately, many dynamical problems of energy yield are of low dimensionality. In the case of high s, other methods, e.g. those applying maximum principles must be applied. They are based on canonical equations, adjoints and a Hamiltonian of these variables, and are described in a number of sources (e.g. [21–25]).

14. Dimensionality reduction in dynamic programming algorithms

Sometimes the dimensionality reduction is possible in DP problems. For the energy problems considered dimensionality reduction is possible in autonomous systems due to the constancy of the time adjoint λ along an optimal path. This is described below.

For V^n regarded as energy production profit, net economic-like profit, or the difference between V^n and the "time penalty cost" $\lambda(t^n - t^0)$, is defined. λ is Lagrange multiplier associated with time t. When a discrete process is autonomous and time interval θ^n is not explicitly present in rates f_k, λ is identical with a constant Hamiltonian $H^{n-1} = H$. Under a weaker assumption of an autonomous process and intervals θ^n explicit in rates f_k, the constancy property refers only to λ. The quantity λ describes the decrease of the original profit when the process duration is increased by one unit.

Applying λ we deal with modified optimal functions, net profits $V^n_* \equiv V^n - \lambda(t^n - t^0)$ or net costs $R^n_* \equiv R^n + \lambda(t^n - t^0)$, both criteria being equivalent because the second is obtained by the multiplication of the first by the minus unity. Local profits and costs are defined in a similar way. For single-stage profit $\widetilde{D}^n$, which appears in Eq. (104), a net profit is $\widetilde{D}^n_* \equiv \widetilde{D}^n - \lambda\theta^n$, where $\theta^n \equiv \Delta t^n$. Similarly total cost at stage $n$is $\widetilde{K}^n_* \equiv \widetilde{K}^n + \lambda\theta^n$, where $\widetilde{K}^n \equiv -\widetilde{D}^n$.

Given net profit $\widetilde{D}^N_*$, optimal process is governed by a sequence of asterisk functions: $V^1_*, \ldots, V^n_*, \ldots, V^{N-1}_*$ and

V^N_*. The sequence of these optimal functions obeys an equation

$$V^n_*(\mathbf{x}^n,\lambda)=\max_{\mathbf{u}^n,\theta^n}\{\widetilde{D}^n_*(\mathbf{x}^n,\mathbf{u}^n,\theta^n,\lambda)+V^{n-1}_*(\mathbf{x}^n-\mathbf{f}^n(\mathbf{x}^n,\mathbf{u}^n,\theta^n)\theta^n,\lambda)\}. \quad (112)$$

This differs from Eq. (104) by the presence of vector $\mathbf{x}$ rather than $\tilde{\mathbf{x}}\equiv(\mathbf{x},t)$. Because of the constancy of λ along an optimal path, state dimensionality of the problem described by Eq. (112) is decreased by 1 in comparison with that for Eq. (104).

The continuous limit of Eq. (112) is a HJB equation

$$\max_u\left\{\tilde{f}_{0*}(\mathbf{x},\mathbf{u},\lambda)-\frac{\partial V_*(\mathbf{x},\lambda)}{\partial\mathbf{x}}f(\mathbf{x},\mathbf{u},\lambda)\right\}=0. \quad (113)$$

It is similar to the Hamilton–Jacobi equation of classical mechanics but contains the maximum sign before a Hamiltonian expression. Eq. (113) refers to an optimal duration $T=(t^{\mathrm{f}}-t^{\mathrm{i}})$ equal to $\partial V_*(\mathbf{x},\lambda)/\partial\lambda$.

Optimal functions of work production, V^n and V^n_*, preserve a number of basic qualitative properties of economic production profits and total economic profits. The same remark refers to functions of work consumption, $R^n=-V^n$ and $R^n_*=-V^n_*$. For multistage control processes, optimal data generated by DP have the form of sequence functions $V^n(\mathbf{x},t)$ or their duals $V^n_*(\mathbf{x},\lambda)$, where $\mathbf{x}$ is process state, t is a time variable and n is the number of stages. Optimal profit functions $V^n(\mathbf{x},t)$ and $V^n_*(\mathbf{x},\lambda)$, or cost functions $R^n(\mathbf{x},t)$ and $R^n_*(\mathbf{x},\lambda)$, are linked by the Legendre transformation [26–28], see the analytical example in Section 12. The limiting case of a continuous process is characterized by functions $V(\mathbf{x},t)$ and $V^n_*(\mathbf{x},\lambda)$, which are mathematical equivalents of Hamilton's principal action and abbreviated action in classical mechanics or related phase functions in optics [26]. The relation between the optimal cost functions generated by dynamic programming and Pontryagin's maximum principle is now well understood [27,28]. The optimal paths of a control problem are equivalent to mechanical paths in mechanics or light rays in optics. The use of dynamic programming in constructing finite-time potentials for discrete and continuous control separation processes has been summarized [18]. Computational examples showing wave-path duality are available for a separation process in which a volatile component is evaporated from a porous, fluidizing solid [18,29].

15. Concluding remarks

In this research we considered energy limits in dynamical energy systems driven by nonlinear fluids that are restricted in their amount or flow, and, as such, play role of resources. We discussed main aspects of analytical HJB theory for continuous systems and various examples of HJB equations in nonlinear power generation systems. Applications of HJB theory, subject to appropriate boundary conditions (the process or its inversion end at the equilibrium with the environment), lead to various finite-rate generalizations of the standard availability (exergy). Processes associated with generalized availabilities are characterized by presence of imperfect phenomena as, e.g., heat conduction or non-ideal compression and expansion. In modes departing from the equilibrium the generalized exergy is larger than in their inversions approaching the equilibrium. Bounds for mechanical energy yield or consumption, provided by generalized exergies, are stronger than those defined by the classical exergy (enhanced bounds).

Analytical solutions are obtained for systems with linear kinetics, and their extensions are discussed for those with nonlinear kinetics and internal dissipation. For radiation fluids analytical difficulties appear, associated with the use of Stefan–Boltzmann equation in its exact form. These difficulties are avoided in the pseudo-Newtonian models [with state dependent exchange coefficients $\alpha(T^3)$] and by use of numerical DP algorithms. Specific results show complex, non-exponential form of the radiation relaxation during the power production process.

We have also considered numerical approaches to power generation problems, which apply the dynamic programming method. Convergence of computational DP algorithms to solutions of corresponding HJB equations was shown. Lagrangian multipliers associated with duration constraint were used to reduce dimensionality of some power production problems. Legendre transform has been applied to recover original work functions.

Other important application of the considered approach involves separation systems, chemical energy systems, and, especially, fuel cells. Fig. 5 depicts work limits for real and reversible heat pumps, separators and energy generators. Systems with work consumption are described by function $R(T,\tau)$, systems with work production – by function $V(T,\tau)$. lbws is a line of lower bound for work supply, ubwp – a line of upper bound for work production. "Endoreversible limits" correspond with curves for $\Phi=1$; weaker reversible limits are represented by the straight line

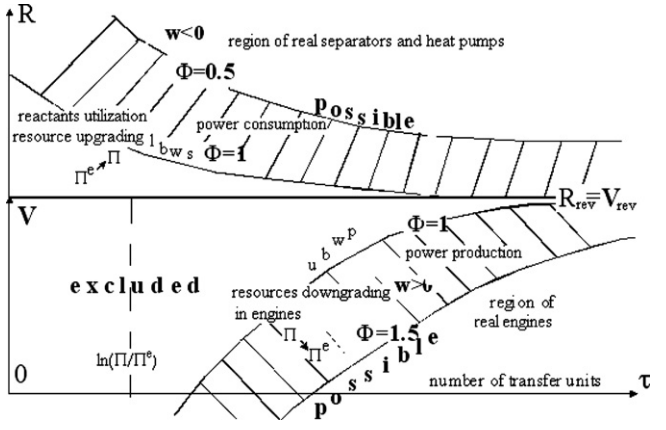

Fig. 5. Influence of internal irreversibilities Φ on limiting finite-rate work generated in engines and consumed in heat pumps ($T_0=T^{\mathrm{e}}$). Example for continuous heat-pump system with $\Phi=0.5$ and engine system with $\Phi=1.5$.

$R_{rev} = V_{rev}$. Dashed lines mark regions of possible improvements when imperfect thermal machines are replaced by those with better performance coefficients, terminating at endoreversible limits with Carnot energy generators.

For a fixed change of system state reversible upper bound V_{rev} achieved in production modes equals to reversible lower bound R_{rev} achieved in consumption modes. For irreversible bounds the equality does not hold, and a lower bound of R is larger than upper bound of V. Note a similarity of this plot to charts characterizing generalized exergies [4]. This similarity is a suitable starting point to investigate energy generation in electrochemical systems.

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