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Hamilton–Jacobi–Bellman analysis of irreversible thermal exergy

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Abstract—A dissipative extension of the classical Carnot problem of maximum work extracted from a system of two bodies with different temperatures is analysed. In the classical problem the instantaneous rates do vanish due to a reversibility requirement imposed on the process, in the extended problem some inevitable, rate-related irreversibilities are allowed, in particular those occurring in boundary layers. In our analysis, nonlinear thermodynamic modeling is inherently linked with ideas and methods of the optimal control. In this paper, we consider a somewhat special but important case in which the thermal capacity of the second body is very large and its intensive parameters do not change. This case may also be referred to the active energy exchange between the fluid of a limited thermal capacity and ambient or environmental fluid. Our variational theory treats an infinite sequence of infinitesimal Curzon–Ahlborn–Novikov processes (CAN processes), as the pertinent theoretical model to develop a finite time theory of a body in a bath, when the indirect exchange of the energy occurs through the working fluid of participating engines, refrigerators or heat pumps. These applications refer, in particular, to the extension of the classical thermodynamic problem of maximum work (exergy) delivered from the system of a finite exchange area or of a finite contact time. The dissipative exergy is discussed in terms of the finite process intensity and finite duration. An analytical formalism, strongly analogous to those in analytical mechanics and optimal control theory, is an effective tool in the thermodynamic optimization. In this paper, a novel approach is worked out which is based on the Hamilton–Jacobi–Bellman equation for the dissipative exergy and related work functionals (HJB theory). The HJB formulation is important for finding the work potentials by numerical methods which use the related Bellman's recurrence equation. The latter is practically the sole method of extremum seeking for functionals with constrained rates and states, and for complex boundary conditions. It will certainly be inevitable in the case of the problem generalization to mass transfer and chemical reactions. The optimality of a definite irreversible process is pointed out for a finite duration. The connection is shown between the process duration, optimal dissipation and the optimal intensity measured in terms of a Hamiltonian. An essential decrease of the maximal work received from an engine system and increase of minimal work added to a heat pump system is shown in the high-rate regimes and for short durations of thermodynamic processes. The results prove that criteria known from the classical availability theory should be replaced by stronger limits obtained for finite time processes, which are closer to reality. Hysteretic properties are effective, which cause the difference between the work supplied and delivered, for the inverted end states of the process.

1. INTRODUCTION

Recently, considerable progress has been achieved in understanding the thermodynamics of finite rate and finite time systems, including the theory of Curzon–Ahlborn–Novikov (CAN) engine [1–4]. In particular, the theory of infinite sequence of infinitesimal CAN processes arranged sequentially in order to accomplish the active (work producing) exchange of heat between two fluids (in particular fluid and bath) was worked out [5, 6]. It was shown that the sequence is the basic theoretical tool to define a rate dependent and duration-dependent function of available energy (exergy) which generalizes the classical thermal exergy for finite time processes with dissipation occurring in associated resistances. Some works on the finite-time exergy, published to date, suffer an absence of exact functional formulations, which could comprise, within a single expression, the potential property of the classical reversible component and the path-dependent property of the irreversible component. Moreover, these works do not make a distinction between the finite time exergy of processes approaching and leaving equilibrium. This property was first emphasized only recently [10, 11]. The property is lost in the reversible case of quasistatic processes, when the effect of resistances does vanish, and the extended exergy simplifies to the classical exergy, inherently associated with infinite durations. The classical exergy is known from many sources [12–14].

We shall distinguish two classes of active (work exchanging) nonequilibrium systems. When the system is approaching the equilibrium the work is released and the system plays the role of an engine. This case is called the engine mode of the system. The delivered work W is positive by assumption. Otherwise, when the system is departing from the equilibrium the work must be supplied, and the system plays the role of a heat pump. This is the so-called heat-pump mode of the system. The work W is then

NOMENCLATURE

A	cumulative heat exchange area
a_v	specific area of heat exchange (per unit volume)
$B = E_x^{\infty}$	classical exergy of mass unit
c	specific heat capacity
E_x	generalized (dissipative) exergy of mass unit
F	cross-sectional area of the system
$\mathbf{f}$	rate vector of the general process
f_0	rate of work production, profit rate $(-L)$
G	fluid mass flux
H, h	extremum Hamiltonian function and numerical Hamiltonian, respectively
H_{TU}	heat of transfer unit
I	optimal performance function for the work integral
Q_1, Q_2	cumulative heat fluxes for upper and lower reservoir, respectively
$\mathbf{Q} \equiv Q_1(\gamma)$	function describing the driving heat flux along the conductance coordinate γ
S_σ	dissipated entropy per unit mass flux of driving fluid
s	specific entropy
t	contact time of the driving fluid with the exchange surface
$\mathbf{T} = (T, \tau)$	vector composed of the temperature and the number of heat transfer units
T_1, T_2	temperatures of upper and lower reservoirs (usually $T_2 = T^e$, and $T_1 \equiv T$)
T^e	constant temperature of environment
$T_{1'}, T_{2'}$	upper and lower temperature of the Carnot engine as the part of the CAN engine
$\mathbf{u}$	control vector of the generalized process
$u = \mathrm{d}T/\mathrm{d}\tau$	rate of the temperature change of the first fluid as the process control
V	wave-front function, defined in the text
v	linear velocity of the driving fluid (fluid 1)
$\mathcal{W}$	cumulative power output
$W \equiv \mathcal{W}/G$	total specific work or total power per unit mass flux
$\mathbf{x}$	enlarged vector of state with coordinates W, T and τ
x	transfer area coordinate
z	adjoint variable of the work minimization problem, momentum-type variable $\partial L/\partial \dot{T}$
z_σ	adjoint variable of the entropy generation minimization, momentum-type variable $\partial L_\sigma/\partial \dot{T}$.

Greek symbols

α	overall heat transfer coefficient
$\Omega\Gamma$	gauging function
γ_1, γ_2	coordinates of partial conductances
γ	coordinate of overall cumulative conductance
λ	adjoint variable of work maximization problem, momentum-type variable $\partial f_0/\partial \dot{T}$
$\eta = \mathrm{d}W/\mathrm{d}Q_1$	local efficiency
τ	dimensionless contact time, number of the heat transfer units (x/H_{TU})
ξ	logarithmic intensity
Θ^i, Θ^f	optimal performance functions for the initial and final work coordinates
σ_s	entropy production.

Subscripts

C	Carnot point
s	entropy related quantity
v	per unit volume
σ	dissipative quantity
1,2	first and second fluid, respectively.

Superscripts

e	environment, equilibrium
f	final state
i	initial state
^	external value.

negative, which means that the positive work $(-W)$ must be supplied to the system. To obtain a generalized exergy, optimization problems are considered in this paper, which involve the maximum of the work delivered [max W] and the minimum of the work supplied [min$(-W)$].

The classical thermal exergy (availability) is the nonnegative quantity. It is reversible in the sense that the magnitude of the work delivered during the reversible approaching of the system to equilibrium is equal to the magnitude of the work supplied, after the initial and final states are interchanged. The first case corresponds to the engine mode of the system, the second to the heat-pump mode of the system. The classical exergy is the quantity which defines bounds on work delivered from (or supplied to) very slow, reversible processes. Our research is directed toward the generalization of this classical idea for the finite rate transitions. We show that while the reversibility property is lost for the generalized nonclassical exergy, the thermokinetic bounds formed by the dissipative exergy are stronger and, hence, more useful than classical thermostatic bounds. This substantiates the role of the generalized exergy for the evaluation of the energy limits in practical systems [15].

In this paper, we briefly recapitulate some basic issues associated with the derivation of basic work functionals, and then direct our analysis towards a new aspect, which is the derivation of the Hamilton–Jacobi–Bellman theory (HJB theory) for functionals of dissipative exergy and work. The HJB theory is known as a basic ingredient of variational calculus and optimal control [16–20]. The HJB formulation is important for the purpose of finding the dissipative exergy and/or related work potentials by numerical methods. These methods, along with the associated Pontryagin's maximum principle [21], are the main effective extremum seeking methods for functionals in the case of constrained rates and states, and some complex boundary conditions [22]. They will certainly be inevitable in the case of the problem generalization to include the mass transfer (in separation units) and chemical reactions. However, the Pontryagin's maximum principle algorithm, as itself, does not generate the optimal performance function (principal function), which is, in our case, the generalized work potential or the dissipative exergy, the main result which is sought. Otherwise, when the HJB equation is known, the exergy (or work) function is explicit therein, and a discretization approach can transform the problem into the Bellman's functional equation, which can be solved by standard solving techniques of discrete dynamic programming [23].

2. EXTREMUM WORK FOR INFINITE SEQUENCE OF INFINITESIMAL CAN PROCESSES

However, for the purpose of the dissipative extension of the exergy no analysis of a single CAN unit is sufficient, rather a treatment of a complex system composed of infinite number of infinitesimal CAN units is necessary. This abstract system, which is shown in Fig. 1, is still a work-producing system in which the active heat exchange occurs between the two real fluids of finite thermal conductivities and containing their own boundary layers as dissipative elements. The differential Carnot engines are located continuously between two separated boundary layers of the fluids, so that they work between their interfaces. This quite abstract model of the active energy exchange, associated with the power production, is a finite-rate generalization of the corresponding classical model of the available energy for the reversible energy exchange between two fluids. In both cases (reversible and not), the amount or flow of the second fluid is infinite and, hence, it plays the role of the bath or an infinite reservoir [12].

Let us consider an infinitesimal CAN process at the steady-state [6]. In the steady process the conservation balances refer to the fluxes rather than to amounts. The first fluid (subscript 1) flows in the direction parallel to the x-axis with a finite mass flux G. Between the working fluid of the Carnot engine and each of the two fluids (each of a finite thermal conductivity) the differential conductances $d\gamma_1$ and $d\gamma_2$ are present, as the system dissipative elements.

The conductances link the heat sources with the working fluid of the engine at high and low tempera-

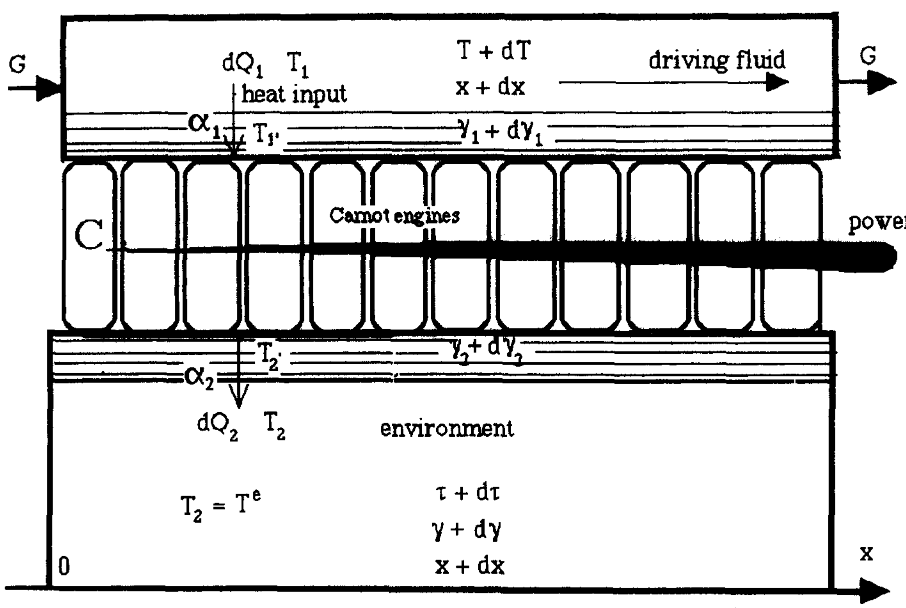

Fig. 1. Model of power production and dissipative exergy of flowing fluid accomplished in infinite sequence of infinitesimal Curzon–Ahlborn–Novikov engines.

tures, and they can be expressed as $d\gamma_1 = \alpha_1 dA_1$ and $d\gamma_2 = \alpha_2 dA_2$, where α_1 and α_2 are the heat transfer coefficients, and dA_1 and dA_2 are the upper and lower exchange surface areas (the components of the total differential area dA). For the differential length dx (the area dA) the fluid delivers the driving heat power dQ_1 to the working medium of the infinitesimal Carnot engine. The temperature of the driving fluid (fluid 1) decreases slightly along its path, since this fluid releases the heat to run the engine. In the range $T_1 > T^e$ the differential dT_1 is negative for the engine and positive for the heat pump. The differential of the driving heat flux, dQ_1, describes the heat power subtracted from the flowing driving fluid when its temperature decreases from T_1 to $T_1 + dT_1$.

We designate $T_{1'}$ and $T_{2'}$ as the upper and lower temperatures of the working agent which circulates in each differential Carnot engine. The high-grade heat dQ_1 reaches the engine part at $T_{1'}$. In the simplest case of the Newtonian heat exchange, which we consider here, this heat is proportional to the temperature difference $T_1 - T_{1'}$. Otherwise, the low-temperature part of the Carnot subsystem releases the pure heat to an environment (or fluid 2) through another conductance, $d\gamma_2$. The flux of the released heat is proportional to the difference $T_{2'} - T_2$. This low-grade heat flows between the low-temperature part of the engine (at $T_{2'}$) and the environmental fluid, and reaches this fluid at the low temperature $T_2 = T^e$. We are dealing with the case when the temperature of the bath fluid is constant and equal to that of an environment (infinite bath of the second fluid, $T_2 = T^e$).

While the first-law efficiency of such infinitesimal unit is still described by the Carnot formula

$$\eta = 1 - \frac{T_{2'}}{T_{1'}} \tag{1}$$

this efficiency is, nonetheless, lower than the efficiency of the unit working between the boundary temperatures T_1 and $T_2 = T^e$, as the former applies to the intermediate temperatures $T_{1'}$ and $T_{2'}$. The intermediate temperatures are unknown, but they can be expressed in terms of the boundary temperatures T_1 and T_2 and the efficiency, η. By solving equation (1), along with the reversible entropy balance of the Carnot differential subsystem,

$$\frac{d\gamma_1(T_1 - T_{1'})}{T_{1'}} = \frac{d\gamma_2(T_{2'} - T_2)}{T_{2'}} \tag{2}$$

one obtains the primed temperatures as certain functions of the variables T_1, $T_2 = T^e$ and η. The associated driving heat flux $dQ_1 = d\gamma_1(T_1 - T_{1'})$ is then found in the form

$$dQ_1 = d\gamma\left[T_1 - \frac{1}{(1-\eta)}T_2\right] \tag{3}$$

from which the efficiency-power characteristic follows as:

$$\eta = 1 - \frac{T_2}{T_1 - dQ_1/d\gamma}. \tag{4}$$

In equations (3) and (4), γ is an appropriately defined overall conductance of the traditional heat transfer theory [6]. The conductance $d\gamma$ may be expressed as the product $\alpha' dA$ which further leads to the expression

$$d\gamma = \alpha' dA = \alpha' a_v F dx = \alpha' a_v F v\, dt. \tag{5}$$

Here α' is the overall heat transfer coefficient referred to the total differential area dA, a_v is the total specific exchange area per unit volume of the driving fluid system and F is the system cross-sectional area, perpendicular to x. The symbol v refers to the linear velocity of the driving fluid and t is the contact time of this fluid with the heat exchange surface.

Now one can introduce the quantity

$$\frac{Gc}{\alpha' a_v F} = H_{TU} \tag{6}$$

which has the length dimension and is known from the heat transfer theory as the so-called 'height of the heat transfer unit' (H_{TU}). In equation (6) it is referred to the driving fluid (fluid 1).

A nondimensional length $x/H_{TU} = vt/H_{TU}$ can next be defined which is known as the 'number of transfer units'. Since it measures the extent of the system and it is proportional to the contact time of the driving fluid with the energy exchange area, it also plays the role of a nondimensional time, and this is why it is designated by τ

$$\tau \equiv \frac{x}{H_{TU}} = \frac{\alpha' a_v F}{Gc} x = \frac{\alpha' a_v F v}{Gc} t. \tag{7}$$

In what follows, the subscript 1, designating the first fluid (driving fluid), will be omitted for simplicity of the equations. From the energy balance of the driving fluid, the heat power variable, Q_1, satisfies $dQ = -Gc\,dT$, where dT is the differential temperature drop of the first (driving) fluid, and c is its specific heat. With the above definitions and the differential heat balance of the driving fluid, the control term $dQ_1/d\gamma$ of eq. (4), may be written in the form

$$dQ/d\gamma \equiv -u = -Gc\,dT/\alpha' dA = -Gc\,dT/\alpha' a_v F dx$$
$$= -Gc\,dT/\alpha' a_v F v\,dt = -dT/d\tau \tag{8}$$

(subscript 1 omitted). The negative of the derivative $dQ/d\gamma$ is the control variable u of the process. In short, the above equation says that $u = \dot{T}$, that is, the control variable u equals the rate of the temperature change with respect to the nondimensional time τ. The control u has the temperature dimension.

With the help of equations (5)–(8), the efficiency formula (4) becomes

$$\eta = 1 - \frac{T^e}{T + \dot{T}}. \tag{9}$$

When $T > T^e$ the derivative $\dot{T}$ is negative for the engine mode. This is because the driving fluid must release the energy to the engine to assure the work production. Similarly, $\dot{T}$ is positive for the heat-pump mode. In the engine case $\eta \leqslant \eta_C$, whereas in the heat-pump mode $\eta \geqslant \eta_C$. When $T < T^e$ the efficiencies (as the first-law efficiencies do) become negative, nonetheless in each case the efficiency of a finite time process deviates adversely from the Carnot efficiency.

For any process mode, the cumulative power delivered per unit fluid flow, $\mathscr{W}/G$, is obtained by integration of the product of η and $dQ/G = -c\,dT$, between an arbitrary initial temperature T^i and an arbitrary final temperature T^f of the fluid. This integration yields the specific work of the flowing fluid in the form of the functional

$$W_{[\mathbf{T}^i,\mathbf{T}^f]} \equiv \mathscr{W}/G = -\int_{T^i}^{T^f} c\left(1-\frac{T^e}{\dot{T}+T}\right)\dot{T}\,d\tau. \quad (10)$$

The notation $[\mathbf{T}^i, \mathbf{T}^f]$ means the passage of the vector $\mathbf{T} \equiv (T, \tau)$ from its initial state, $\mathbf{T}^i$, to its final state, $\mathbf{T}^f$. For the above functional, the work maximization problem can be stated for the engine mode of the process.

$$(W)_{\max} = \max\left\{-\int_{\tau^i}^{\tau^f} L(T,\dot{T})\,d\tau\right\}$$
$$= \max\left\{-\int_{\tau^i}^{\tau^f} c\left(1-\frac{T^e}{\dot{T}+T}\right)\dot{T}\,d\tau\right\} \quad (11)$$

whereas for the heat-pump mode (fluid heating process), one states the minimization problem

$$(-W)_{\min} = \min_{dT/d\tau}\int_{\tau^i}^{\tau^f} L(T,\dot{T})\,d\tau$$
$$= \min_{dT/d\tau}\int_{\tau^i}^{\tau^f} c\left(1-\frac{T^e}{\dot{T}+T}\right)\dot{T}\,d\tau. \quad (12)$$

For each process mode, a dissipative exergy of the finite time process is obtained as the extremal value of the related functional with the appropriate integration limits ($T^i = T$ and $T^f = T^e$ for the engine mode of the process and $T^i = T^e$ and $T^f = T$ for the heat-pump mode of the process).

The above Lagrange functional represents the total power per unit mass flux of the fluid which is the quantity of the specific work dimension, hence its direct relation to the specific exergy of the fluid at flow. In the quasistatic limit of vanishing rates, $dT/d\tau = 0$, the above work functional represents the change of the classical exergy

$$W_{(dT/d\tau\to 0)} = -\int_{T^i}^{T^f} c\left(1-\frac{T^e}{T}\right)dT. \quad (13)$$

This functional leads to the classical exergy in case of appropriate boundary temperatures, $T^i = T$ and $T^f = T^e$. Consequently, equation (10) represents the dissipative exergy change for the finite time processes in which irreducible dissipative phenomena occurring in the boundary layers are essential. For the engine mode of the process, the dissipative exergy itself is obtained as the maximum of the functional (10), with the integration limits $T^i = T$ and $T^f = T^e$, for the heat-pump mode—as the minimum of the negative of this functional, with the integration limits $T^i = T^e$ and $T^f = T$.

The alternative form of the specific work (10), can be written as the functional

$$W_{[\mathbf{T}^i,\mathbf{T}^f]} \equiv \mathscr{W}/G$$
$$= -\int_{T^i}^{T^f} c\left(1-\frac{T^e}{T}\right)dT - T^e\int_{T^i}^{T^f} c\frac{\dot{T}^2}{T(T+\dot{T})}\,d\tau \quad (14)$$

in which the first term is the classical reversible term and the second term is the product of the equilibrium temperature and the entropy production

$$S_{\sigma[\mathbf{T}^i,\mathbf{T}^f]} = \int_{T^i}^{T^f} c\frac{\dot{T}^2}{T(T+\dot{T})}\,d\tau. \quad (15)$$

This has been shown elsewhere [6].

3. SOME PROPERTIES OF EXTREMAL SOLUTIONS

Applying the maximum operation for the basic functional (14) at the fixed end temperatures and time it is seen that the role of the first (potential) term is inessential, and the problem of the maximum released work, max W, is equivalent to the associated problem of the minimum entropy production. Similarly, performing the minimum operation for the negative of this functional (the role of the first term is inessential again) it is seen that the problem of the minimum supplied work, min$(-W)$, is again equivalent with the problem of the minimal entropy production. This confirms the crucial role of the entropy generation minimization in the context of the extremum work problems, for each mode of the process. The consequence of this conclusion is that a problem of the extremal work and an associated fixed-end problem of the minimum entropy generation have the same solutions. Yet, considerations involving the entropy production are unnecessary when the work functionals are given.

For each process mode, the work extremization problems can be broken down to variational calculus for the Lagrangian

$$L = c\left(1-\frac{T^e}{\dot{T}+T}\right)\dot{T}. \quad (16)$$

The Euler–Lagrange equations for the problems of extremal work and the minimum entropy production lead to the same second-order differential equation

$$T\ddot{T}-\dot{T}^2=0 \tag{17}$$

which characterizes the optimal trajectories of all considered processes. It has been proven [6] that the extremal rate, $\dot{T}$, satisfies the Legendre condition for the minimum work supply in the case of the heat-pump mode and for the maximum work delivery in the engine mode, and that each of these two situations is associated with the minimum entropy generation. For a given duration and the prescribed end temperatures T^i and T^f, the extremal function $T(\tau)$, which satisfies equation (17), is described by the equation

$$T(\tau,\tau^f,T^i,T^f)=T^i(T^f/T^i)^{\tau/\tau^f}. \tag{18}$$

One also obtains a momentum-like quantity, a formal analog of the mechanical momentum

$$z\equiv\frac{\partial L}{\partial\dot{T}}=c\left(1-\frac{T^eT}{(\dot{T}+T)^2}\right) \tag{19}$$

and the first integral

$$E\equiv\frac{\partial L}{\partial\dot{T}}\dot{T}-L=c\frac{T^eT^2}{(\dot{T}+T)^2} \tag{20}$$

which is a formal analog of the mechanical energy. An equation for the optimal temperature follows from the condition $E=h$

$$\dot{T}=\frac{\pm T\sqrt{\dfrac{h}{cT^e}}}{1-\pm\sqrt{\dfrac{h}{cT^e}}}\equiv\xi T \tag{21}$$

and the integration of this equation for the fixed-end boundary conditions leads to equation (18). The coefficient ξ is a process intensity constant, which can be determined from the boundary conditions of the fixed-end problem

$$\xi=\frac{\ln T^f/T^i}{\tau^f-\tau^i}. \tag{22}$$

ξ is positive for the fluid heating process and negative for the fluid cooling process. In what follows we shall assume $\tau^i=0$, then the total duration will be represented by the time τ^f.

Equation (21) shows that, for the same h, the heat-pump heating processes run faster than the engine cooling processes (larger ξ and shorter durations in the engine case than in the heat-pump case). On the other hand, as shown by the function $E(\xi)=cT^e\xi^2(1+\xi)^{-2}$ obtained from equation (20), for the two values of ξ of the same magnitude, but of opposite signs and for the same durations, the values $E=h$ are larger for the engine mode than for the heat-pump mode of the process.

4. DYNAMIC PROGRAMMING: CHARACTERISTIC FUNCTIONS

Our problem of generalized exergy falls into the category of certain finite-time potentials, an evergreen problem of contemporary thermodynamics [24]. The power of the dynamic programming method (DP) as applied to problems of this sort lies in its important property: regardless of local constraints on controls or state variables the optimal performance functions satisfy an equation of Hamilton–Jacobi–Bellman (HJB equation) with the same state variables as those for the unconstrained problem. Only numerical values of optimizing control sets and those of the optimal performance functions differ in constrained and unconstrained cases. Although in the case of pure heat transfer problem most components of the solution can be obtained analytically, even then formulations exist in which the analytical solutions are not possible. Such are those with free boundary conditions, non-Newtonian heat transfer and constraints imposed on rate change of state and state itself (rate change of the temperature and T itself in our one-dimensional case). Otherwise, the state function property of dynamic programming potentials should prove to be priceless for more complex problems, such as those with mass transfer and chemical reactions. Therefore, the test of the HJB method in the context of the heat transfer problem and associated exergy is highly desirable. This test should initiate a systematic search towards the properties and implications of HJB equations in thermodynamics. In particular, the test performed in this work shows that our problems may be correctly described by two sorts of the HJB equations, a backward HJB equation and a forward HJB equation. The former is associated with the optimal work or exergy as an optimal integral function (I) defined on the initial states (temperatures), and accordingly refers to the engine mode or processes approaching the equilibrium. On the other hand, the forward HJB deals with the exergy (work) as the function ($-I$) defined on the final states, and accordingly refers to the heat-pump mode or processes leaving the equilibrium (see Section 10).

Amongst the work extremization problems considered, the problem of the maximal work delivery (constrained or not) is governed by the characteristic function

$$I(\tau^f,T^f,\tau^i,T^i)\equiv\max W_{\mathrm{IT^i,T^f I}}$$

$$=\max\left\{-\int_{T^i}^{T^f}c\left(1-\frac{T^e}{T+u}\right)u\,\mathrm{d}\tau\right\}. \tag{23}$$

In equation (23) $u=\dot{T}$ is the rate control variable defined by equation (8). This equation refers to the engine mode or to processes approaching equilibrium. For heat-pump mode and processes departing from equilibrium one can define the optimal function as

$$-I(\tau^{f}, T^{f}, \tau^{i}, T^{i}) \equiv \min(-W_{[T^{i},T^{f}]})$$

$$= \min\left\{\int_{T^{i}}^{T^{f}} c\left(1-\frac{T^{e}}{T+u}\right)u\,d\tau\right\}. \quad (24)$$

Indeed, since for arbitrary quantity W for the same change of the end states and times, the components of the vector $\mathbf{T} = (T, \tau)$, the following holds

$$\max W_{[\mathbf{T}^{i},\mathbf{T}^{f}]} = -\min(-W_{[\mathbf{T}^{i},\mathbf{T}^{f}]}) \quad (25)$$

the common extremal function $I(\tau^{f}, T^{f}, \tau^{i}T^{i})$ describes the two modes, yet each mode refers to a different region in the space $\mathbf{T}$. Clearly, the quantity I describes the extremal value of the work integral $W[\mathbf{T}^{i}, \mathbf{T}^{f}]$, equation (10). It characterizes the extremal value of the work released for the prescribed temperatures T^{i} and T^{f} when the total process duration is $\tau^{f}-\tau^{i}$. (The invariance of the integral value with respect to the variation of one of the end times when the total duration is fixed is consistent with existence of the energy-like integral for the problem.)

Here, this problem is transformed into the equivalent problem in which one seeks a maximum of the final work coordinate $x_0^{f} = W^{f}$ for the system described by the following set of the differential equations

$$\frac{dW}{d\tau} = -c\left(1-\frac{T^{e}}{u+T}\right)u \equiv f_0(T, u) \quad (26)$$

$$\frac{dT}{d\tau} = u \equiv f_1(T, u) \quad (27)$$

$$\frac{d\mathbf{x}_2}{d\tau} = 1 \equiv f_2(T, u). \quad (28)$$

The state of the above system is described by the enlarged state vector $\mathbf{x}$, which is composed of the three state coordinates, $\mathbf{x}_0 = W$, $\mathbf{x}_1 = T$ and $\mathbf{x}_2 = \tau$. The last equation of the set states that the state coordinate $\mathbf{x}_2 = \tau$ has been chosen as the independent variable of the system. The sole control variable u in the system is simply the rate of the temperature change in time τ. Supposedly, more involved models of this problem might exist, with a vector of control variables, $\mathbf{u}$, hence the symbol $\mathbf{u}$ rather than u is used in our general formulas below.

While the knowledge of the characteristic function I is only sufficient for a complete description of the extremal properties of the problem, other functions of this sort are nonetheless very suitable for the problem characterization. One of these functions, Θ^{i}, works in the space of one dimension larger than I and involves the work coordinate $x_0 = W$

$$\max_{\mathbf{u}} W^{f} \equiv \Theta^{i}(W^{i}, \tau^{i}, T^{i}, \tau^{f}, T^{f}) = W^{i} + I(\tau^{i}, T^{i}, \tau^{f}, T^{f}). \quad (29)$$

This structure is the consequence of the fact that the state variable W is not explicitly present in the rates of the state equations (26)–(28). In this paper, we do not consider more general cases.

In the still enlarged space of variables $(W^{i}, t^{i}, T^{i}, W^{f}, t^{f}, T^{f})$ we also introduce the (non-extremal) wave-front function V defined as

$$V \equiv W^{f} - \Theta^{i}(W^{i}, \tau^{i}, T^{i}, \tau^{f}, T^{f})$$

$$= W^{f} - W^{i} - I(\tau^{i}, T^{i}, \tau^{f}, T^{f}). \quad (30)$$

Its two mutually-equal maxima, at the constants W^{i} and W^{f}, are described by the extremal functions $V^{i}(W^{i}, t^{i}, T^{i}, t^{f}, T^{f}) = V^{f}(t^{i}, T^{i}, W^{f}, t^{f}, T^{f}) \equiv 0$, which vanish identically along all optimal paths. They are associated, respectively, with the maximum of the free final coordinate W^{f} in the subspace of variables $(W^{i}, t^{i}, T^{i}, t^{f}, T^{f})$ and the minimum of free initial coordinate W^{i} in the subspace $(t^{i}, T^{i}, W^{f}, t^{f}, T^{f})$.

Regardless of the state variables being constrained or not, the partial derivatives of the extremal performance function Θ^{i} with respect to its 'working state' [the initial enlarged state (W^{i}, τ^{i}, T^{i})] and those of the wave-front function $V = W^{f} - \Theta^{i}(W^{i}, \tau^{i}, T^{i} \ldots)$ do coincide modulo to sign. One can, therefore, use the negative partial derivatives $(-\partial V/\partial T^{i}, -\partial V/\partial \tau^{i}$ and $-\partial V/\partial W^{i})$ instead of $(\partial\Theta^{i}/\partial T^{i}, \partial\Theta^{i}/\partial\tau^{i}$ and $\partial\Theta^{i}/\partial W^{i})$ in any equation of the backward DP algorithm (the standard algorithm in which the initial set of the coordinates W^{i}, T^{i}, τ^{i} forms the state variables).

On the other hand, one can also formulate a dual problem of a minimal initial work coordinate W^{i}, when the final work coordinate W^{f} is fixed. This minimum is described by the extremal performance function

$$\min_{u} W^{i} \equiv \Theta^{f}(W^{f}, t^{f}, T^{f}, t^{i}, T^{i}) = W^{f} - I(t^{f}, T^{f}, t^{i}, T^{i}) \quad (31)$$

which is related to the wave-front function V as follows

$$V = \Theta^{f}(W^{f}, t^{f}, T^{f}, t^{i}, T^{i}) - W^{i}$$

$$= W^{f} - W^{i} - I(\tau^{i}, T^{i}, \tau^{f}, T^{f}) \quad (32)$$

[compare equation (30) for V in terms of Θ^{i}]. Of course, the following equalities hold along an extremal path

$$\max W^{f} - W^{i} - I(\tau^{f}, T^{f}, \tau^{i}, T^{i})$$

$$= W^{f} - \min W^{i} - I(\tau^{f}, T^{f}, \tau^{i}, T^{i}) = 0. \quad (33)$$

They can be written in terms of the wave-front function V as follows

$$\max V = \max\{W^{f} - W^{i} - I(\tau^{f}, T^{f}, \tau^{i}, T^{i})\} = 0. \quad (34)$$

The partial derivatives of the extremal performance function Θ^{f} with respect to its 'coordinates of working state' [the final coordinates (W^{f}, T^{f}, τ^{f}) which are varied in the forward DP equation] and those of $V = \Theta^{f} - W^{i}$ do coincide. One may, therefore, use the partial derivatives ($\partial V/\partial T^f, \partial V/\partial t^f$ and $\partial V/\partial W^f$) instead of ($\partial \Theta^f/\partial T^f, \partial \Theta^f/\partial t^f$ and $\partial \Theta^f/\partial W^f$) in any equation of the forward DP algorithm (the algorithm where the final coordinates W^f, T^f, t^f are the state variables). These properties are exploited below.

We search for a dynamic programming equation by applying the Bellman's optimality principle [16, 17] for a control $\mathbf{u}$, in an admissible set U, which makes the final work coordinate $\mathbf{x}_0(\tau^f) \equiv W^f$ a maximum or the initial work coordinate, $\mathbf{x}_0(\tau^i) = W^i$, a minimum. We use the enlarged state vector $\mathbf{x}$ as the vector including the work coordinate $x_0 = W$ and the coordinates T and τ, and the optimality principle in a relatively seldom form which links the original and dual optimization problem. This form states that the optimal final value of an optimized quantity is a function of the initial state, whereas the optimal initial value of the optimized quantity is a function of the final state. Accordingly, the 'original' problem of the maximal final work coordinate is described by the function $\Theta^i(\mathbf{x}^i) \equiv \Theta^i(W^i, \tau^i, T^i)$, equation (29), the 'dual' problem of minimal initial work coordinate—by the function $\Theta^f(\mathbf{x}^f) \equiv \Theta^f(W^i, \tau^i, T^i)$, equation (31). In the first function, the complete set of the initial coordinates is necessary, in the second the complete set of the final coordinates must be used. Taking this into account, we will occasionally omit, for the brevity of formulas, the remaining variables in these functions which can be regarded as parameters. We apply the original and dual form of the optimality principle, respectively, for the initial and final part of a path, to show that the conclusions obtained from DP equations can be read in terms of the single, common wave-front function $V(\mathbf{x}^i, \mathbf{x}^f)$ which treats the initial and final states in the enlarged space $\mathbf{x}$ on an equal footing. While the accepted independent variable can be to a large extent arbitrary (its monotonicity property in time is the suitable limitation), we will assume the time coordinate τ as the independent variable. We also assume that the rate $\mathrm{d}W/\mathrm{d}\tau \equiv \mathrm{d}x_0/\mathrm{d}\tau$ is known in the form $f_0(\mathbf{x}, \mathbf{u}) = -L(\mathbf{x}, \mathbf{u})$, where L is the integrand in equation (12) with $\dot{T} = u$. By passing to the usual residence time t (in seconds) and taking into account the explicit presence of transfer coefficients in f_0, one could admit the possibility of 'aging' of the system, however, this extension is omitted in this paper. While we derive below the DP equations for $\Theta^i(\mathbf{x}^i)$ or $\Theta^f(\mathbf{x}^f)$ only, the related equation for the integral work function $I(T^i, t^i, T^f, t^f)$ in the narrowed space of the coordinates (T, τ) follows immediately from the condition $V = 0$.

5. DYNAMIC PROGRAMMING: HJB EQUATIONS

The problem can be treated mathematically as follows. Let us write our system of the three state equations [equations (26)–(28)] with the state variables $\mathbf{x}_0 = W$, $x_1 = T$ and $x_2 = \tau$ in a general form

$$\frac{\mathrm{d}\mathbf{x}_\beta}{\mathrm{d}\tau} = \mathbf{f}_\beta(\mathbf{x}, \mathbf{u}) \quad \beta = 0, 1, 2 \tag{35}$$

($f_2 \equiv 1$). Let us assume differentiability of the optimal performance function $\Theta^i(\mathbf{x}^i)$ and consider the control $\mathbf{u}$ in intervals $\langle \tau^i, \tau^i + \Delta t \rangle$ and $\langle \tau^i + \Delta\tau, \tau^f \rangle$, where $\Delta\tau$ is a small quantity. In order to take the variations of the initial state in $\Theta^i(\mathbf{x}^i)$ into account, we assume that the 'long', final segment of trajectory, for τ in the interval $\langle \tau^i + \Delta\tau, \tau^f \rangle$, is optimal, The performance index of this segment equals $\Theta^i(\mathbf{x}^i + \Delta\mathbf{x})$. Therefore, the optimal final work for the whole path in the interval $\langle \tau^i, \tau^f \rangle$ is the maximum of the criterion

$$W^f \equiv \Theta^i(\mathbf{x}^i + \Delta\mathbf{x}) = \Theta^i(W^i + \Delta W, T^i + \Delta T, \tau^i + \Delta\tau). \tag{36}$$

The maximization is with respect to the control vector $\mathbf{u}^i$ at the constant $\mathbf{x}^i$, for the small initial (non-optimal) part of the path. It is performed at the constant $\mathbf{x}^i$ subject to all constraints, i.e. including the differential transformations of state, equations (27) and (28). Restricting to linear terms of expansion of Θ^i, equation (36), in the Taylor series one finds

$$\begin{aligned} W^f &= \Theta^i(\mathbf{x}^i) + \frac{\partial \Theta^i}{\partial \mathbf{x}^i_\beta}\Delta\mathbf{x}_\beta + 0(\varepsilon^2) \\ &= \Theta^i(W^i, T^i, \tau^i) + \frac{\partial \Theta^i}{\partial W^i}\Delta W \\ &\quad + \frac{\partial \Theta^i}{\partial T^i}\Delta T + \frac{\partial \Theta^i}{\partial \tau^i}\Delta\tau + 0(\varepsilon^2). \end{aligned} \tag{37}$$

In equation (37) the symbol $0(\varepsilon^2)$ means the second-order and higher terms. They possess the property $\lim\,[0(\varepsilon^2)/\Delta\tau] \to 0$ when $\Delta\tau \to 0$.

Similarly, one may consider the variation of the final coordinates of the state vector $\mathbf{x} = \mathbf{x}^f$. One then assumes that a 'long' initial segment of a trajectory is optimal. The performance index of this optimal segment equals $\Theta^f(\mathbf{x}^f - \Delta\mathbf{x})$. In this case the control $\mathbf{u} = \mathbf{u}^f$ should be properly adjusted along a 'short' nonoptimal final part of the path. The optimal initial work coordinate W^i, for the whole path in the interval $\langle \tau^i, \tau^f \rangle$, is the minimum of the criterion

$$W^i = \Theta^f(\mathbf{x}^f - \Delta\mathbf{x}) = \Theta^f(W^f - \Delta W, T^f - \Delta T, \tau^f - \Delta\tau). \tag{38}$$

Now the minimization is with respect to the control $\mathbf{u}^f$, at the constant $\mathbf{x}^f$ and subject to all constraints, i.e. including the differential transformations, equations (26)–(28). Restricting to linear terms of expansion of Θ^f, equation (38), in the Taylor series one obtains

$$\begin{aligned} W^i &= \Theta^f(\mathbf{x}^f) - \frac{\partial \Theta^f}{\partial \mathbf{x}^i_\beta}\Delta\mathbf{x}_\beta + 0(\varepsilon^2) \\ &= \Theta^f(W^f, T^f, \tau^f) - \frac{\partial \Theta^f}{\partial W^f}\Delta W \\ &\quad - \frac{\partial \Theta^f}{\partial T^f}\Delta T - \frac{\partial \Theta^f}{\partial \tau^f}\Delta\tau + 0(\varepsilon^2). \end{aligned} \tag{39}$$

In equations (37) and (39) the state changes are connected with controls $\mathbf{u}$ by the state equations (35), hence for small $\Delta\tau$

$$\Delta \mathbf{x}_\beta = \mathbf{f}_\beta(\mathbf{x}, \mathbf{u})\, \Delta\tau + 0(\varepsilon^2). \quad (40)$$

After substituting equation (40) into equations (37) and (39), and performing the appropriate extremizations in accordance with the Bellman's principle of optimality, one obtains for the variations of the initial point

$$\max_{\mathbf{u}^i} W^f = \max_{\mathbf{u}^i} \left\{ \Theta^i(\mathbf{x}^i) + \frac{\partial \Theta^i}{\partial \mathbf{x}^i_\beta} f_\beta(\mathbf{x}, \mathbf{u})\, \Delta\tau + 0(\varepsilon^2) \right\} \quad (41)$$

and for the variations of the final point

$$\min_{\mathbf{u}^f} W^i = \min_{\mathbf{u}^f} \left\{ \Theta^f(\mathbf{x}^f) - \frac{\partial \Theta^f}{\partial \mathbf{x}^f_\beta} f_\beta(\mathbf{x}, \mathbf{u})\, \Delta\tau + 0(\varepsilon^2) \right\}. \quad (42)$$

Equations (41) and (42) can then be simplified on the basis of definition of the optimal performance functions Θ^i and Θ^f, equations (29) and (31), and using the property that these functions are independent of the control $\mathbf{u}$. After the reduction of Θ^i and Θ^f and the division of both sides of equations (41) and (42) by $\Delta\tau$, the passage to the limit $\Delta\tau \to 0$ subject to the condition $\lim\,[0(\varepsilon^2)/\Delta\tau] \to 0$ yields, respectively, the backward and forward Hamilton–Jacobi–Bellman equations (HJB equations) of the optimal control problem.

For the initial point of the extremal path one finds as the backward DP equation

$$\max_{\mathbf{u}^i} \left\{ \frac{\partial \Theta^i}{\partial \mathbf{x}^i_\beta} f_\beta(\mathbf{x}, \mathbf{u}) \right\} = \max_{\mathbf{u}^i} \left\{ \frac{\partial \Theta^i}{\partial W^i} \dot{W}^i(T^i, \mathbf{u}^i) + \frac{\partial \Theta^i}{\partial T^i} \dot{T}^i(T^i, \mathbf{u}^i) + \frac{\partial \Theta^i}{\partial \tau^i} \right\} = \max_{\mathbf{u}^i} \left(\frac{\mathrm{d}\Theta^i}{\mathrm{d}\tau^i} \right)$$
$$= -\min_{\mathbf{u}^i} \left(\frac{\mathrm{d}V}{\mathrm{d}\tau^i} \right) = \max_{\mathbf{u}^i} \left(\frac{\mathrm{d}V}{\mathrm{d}(-\tau^i)} \right) = 0. \quad (43)$$

On the other hand, for the final point of the extremal path one finds the forward DP equation

$$\min_{\mathbf{u}^f} \left\{ -\frac{\partial \Theta^f}{\partial \mathbf{x}^f_\beta} f_\beta(\mathbf{x}, \mathbf{u}) \right\} = -\max_{\mathbf{u}^f} \left\{ \frac{\partial \Theta^f}{\partial W^f} \dot{W}^f(T^f, \mathbf{u}^f) + \frac{\partial \Theta^f}{\partial T^f} \dot{T}^f(T^f, \mathbf{u}^f) + \frac{\partial \Theta^f}{\partial \tau^f} \right\} = \min_{\mathbf{u}^f} \left(-\frac{\mathrm{d}\Theta^f}{\mathrm{d}\tau^f} \right)$$
$$= \min_{\mathbf{u}^f} \left(-\frac{\mathrm{d}V}{\mathrm{d}\tau^f} \right) = -\max_{\mathbf{u}^f} \left(\frac{\mathrm{d}V}{\mathrm{d}\tau^f} \right) = 0. \quad (44)$$

The properties of $V = W^f - \Theta^i = \Theta^f - W^i$ have been used in the second lines of the above equations. The rates $\mathrm{d}\mathbf{x}_i/\mathrm{d}\tau$ should necessarily be considered in terms of the state variables and control(s). One concludes that the optimal motion of the wave always maximizes the speed of the advancing wave front $\mathrm{d}V/\mathrm{d}\tau^f$ or the speed of the retreating wave front $\mathrm{d}V/\mathrm{d}(-\tau^i)$.

The partial derivative of V with respect to the independent variable τ can remain outside of the bracket of this equation as well. Taking this into account as well as using in equations (43) and (44) the relations $\partial V/\partial W^i = -\partial\Theta^i/\partial W^i = -1$, $\partial V/\partial W^f = \partial\Theta^f/\partial W^f = 1$ and $\dot{W} = f_0 = -L$, one finds

$$\frac{\partial V}{\partial \tau^i} + \min_{u^i} \left\{ \frac{\partial V}{\partial T^i} u^i + L^i(T^i, u^i) \right\} = 0 \quad (\max W^f) \quad (45)$$

$$\frac{\partial V}{\partial \tau^f} + \max_{u^f} \left\{ \frac{\partial V}{\partial T^f} u^f - L^f(T^f, u^f) \right\} = 0 \quad (\min W^i). \quad (46)$$

In terms of the integral function of optimal work, $I = W^f - W^i - V$, these equations become, respectively,

$$\frac{\partial I}{\partial \tau^i} + \max_{u^i} \left\{ \frac{\partial I}{\partial T^i} u^i + f^i_0(T^i, u^i) \right\} = 0 \quad (47)$$

$$\frac{\partial I}{\partial \tau^f} + \min_{u^f} \left\{ \frac{\partial I}{\partial T^f} u^f - f^f_0(T^f, u^f) \right\} = 0. \quad (48)$$

In all equations of this sort the extremized expression are some Hamiltonians. In fact, they are Pontryagin's type, nonextremal Hamiltonians. The optimal control u, which solves the optimal work problem, is chosen in order to extremize a Hamiltonian at each point of the extremal path, which means extremizing the wave-front velocity $\mathrm{d}V/\mathrm{d}\tau$ in the considered HJB equation.

6. PASSAGE TO HAMILTON–JACOBI EQUATION

For the process Lagrangians (functions L or $-f_0$) the extremum condition of the Pontryagin's Hamiltonian links the derivatives of L or $-f_0$ with respect to the process rate $u = \dot{T}$ with the adjoint variable $z = \partial V/\partial T = \partial I/\partial T$. For concreteness, we will work with equation (48) in which the index f is omitted. The minimization of this equation with respect to the rate u leads to the two equations of which the first describes the optimal control u expressed through the variables T and $\lambda \equiv \partial I/\partial T$.

$$\frac{\partial I}{\partial T} = \frac{\partial f_0(T, u)}{\partial u} \quad (49)$$

and the second is the original equation (48) without the extremization sign

$$\frac{\partial I}{\partial \tau} + \frac{\partial I}{\partial T} u - f_0(T, u) = 0. \quad (50)$$

With the momentum-type variable $\lambda \equiv \partial I/\partial T$ and equation (49) written in the form

$$\lambda = \frac{\partial f_0(T,u)}{\partial u} \quad (51)$$

one can solve the above equation in terms of u to obtain the function $u(\lambda, T)$. Next one substitutes this function into the last two terms on the left-hand side of equation (50). [This is just the minimal form of equation (48).] One obtains the energy-type Hamiltonian of the extremal process

$$H(T,\tau,\lambda) = \lambda u(\lambda, T) - f_0(\lambda, T). \quad (52)$$

With this Hamiltonian and using $\lambda \equiv \partial I/\partial T$ one obtains from equation (50) the Hamilton–Jacobi equation for the integral I

$$\frac{\partial I}{\partial \tau} + H\left(T, \frac{\partial I}{\partial T}\right) = 0. \quad (53)$$

(In our example both functions f_0 and H do not contain time explicitly.) This equation differs from the HJB equations as it refers to an extremal path only and H is the extremal Hamiltonian. In Section 8 we apply the above formulae to our concrete Lagrangian (16).

A brief heuristic approach to derivation of equation (53) along the lines of reasoning first introduced to variational calculus by Caratheodory is insightful [25–27]. As follows from the definition of the maximum performance function I for the work functional (23)

$$\max_{\{u(\tau)\}} \left\{ \int_{t^i}^{t^f} f_0(T,u)\,d\tau - I(T^i, \tau^i, T^f, \tau^f) \right\} = 0. \quad (54)$$

The differentiation of this equation with respect to τ^f proves that the total time derivative of I satisfies the equation

$$\max_u \left\{ f_0^f(T^f, u^f) - \frac{dI(T^i, \tau^i, T^f, \tau^f)}{d\tau^f} \right\} = 0 \quad (55)$$

which describes the vanishing maximum of the power f_0 gauged by the total derivative of the optimal performance function. Expanding in this equation the total time derivative and changing signs (associated with change of the extremum operation) yields

$$\min_{u^f} \left\{ \frac{\partial I}{\partial \tau^f} + \frac{\partial I}{\partial T^f} u^f - f_0^f(T^f, u^f) \right\} = 0 \quad (56)$$

which is equivalent with equation (48) and leads to the Hamilton–Jacobi equation (53).

7. HAMILTON–JACOBI EQUATIONS FOR EXTREMAL WORK AND EXERGY

Let us apply the above procedure to the basic integral (10) written in the form

$$W_{T^iT^f} = \int_{t^i}^{t^f} \left\{ -c\left(1 - \frac{T^e}{T+u}\right)u \right\} d\tau \quad (57)$$

whose extremal value is the function $I(T^i, \tau^i, T^f, \tau^f)$. The integrand of this integral is the function $f_0(T,u)$. The momentum-like variable (equal to the temperature adjoint) is then

$$\lambda \equiv \frac{\partial f_0}{\partial u} = -c\left(1 - \frac{T^e T}{(T+u)^2}\right). \quad (58)$$

Hence the rate control u in terms of T and its adjoint $\lambda = \partial I/\partial T$.

$$u = \sqrt{\frac{T^e T}{1+\lambda/c}} - T. \quad (59)$$

The energy-like function $E(T,u)$ of the engine mode problem is the rate representation of the extremal Hamiltonian

$$E(T,u) = \frac{\partial f_0}{\partial u} u - f_0 = -cT^e \frac{u^2}{(T+u)^2}. \quad (60)$$

The extremal Hamiltonian itself is E expressed in terms of the adjoint λ

$$H(T,\lambda) = c\left(\sqrt{\frac{T^e T}{1+\lambda/c}} - T\right)\left(\lambda/c + 1 - \frac{T^e}{\sqrt{\frac{T^e T}{1+\lambda/c}}}\right). \quad (61)$$

After rearrangements and simplifications

$$H(T,\lambda) = 2c\sqrt{T^e T(1+\lambda/c)} - cT(1+\lambda/c) - cT^e$$
$$= -c(\sqrt{T^e} - \sqrt{T(1+\lambda/c)})^2. \quad (62)$$

The Hamiltonian in terms of the derivative $\partial I/\partial T$ is then

$$H(T, \partial I/\partial T) = -c(\sqrt{T^e} - \sqrt{T(1+c^{-1}I/T)})^2. \quad (63)$$

While one could obtain a positively-defined H by changing signs at the adjoint variables, we retain the Hamiltonian (63) negative, as the formal property reflecting the dissipation of the mechanical energy.

The Hamilton–Jacobi partial differential equation for the maximum work problem (the engine mode of the system) is

$$\partial I/\partial \tau - c(\sqrt{T^e} - \sqrt{T(1+c^{-1}I/T)})^2 = 0. \quad (64)$$

Note, however, that equation (64) is valid not only for the engine mode, but also for the heat-pump mode, the conclusion which is true even if different definitions are applied in the heat-pump case. Indeed, for the heat-pump mode one has to minimize the time integral over the Lagrangian $L = -f_0(T,u)$, and the procedure leads to the extremal function $-I(T^i, \tau^i, T^f, \tau^f)$. The adjoint variables and the Hamiltonian change their signs ($\lambda = -z$, $H_\lambda = -H_z$, where $z = -\partial I/\partial T$. Consistently, the new Hamilton–Jacobi equation takes the same form as the equation given above. In our earlier work [10], the definitions of

Lagrangians and characteristic functions were different to those of this paper, associated with different signs in Hamiltonians and characteristic functions. We believe that the definitions used here have the virtue of greater coherency than those previous ones, restricted to particular cases.

8. HAMILTON–JACOBI EQUATION FOR MINIMAL ENTROPY PRODUCTION

As shown in a previous paper [11], the variational fixed-end problem of the maximum work W is equivalent to the variational fixed-end problem of the minimum entropy production. Let us, however, compare the Hamilton–Jacobi equations of these two problems. The specific entropy production is described by the functional [11]

$$S_\sigma = \int_0^{\tau^f} L_\sigma \, d\tau \equiv \int_0^{\tau^f} c\frac{u^2}{T(T+u)} d\tau. \tag{65}$$

Assume that the minimum of this functional is described by the optimal function $I_\sigma(T^i, \tau^i, T^f, \tau^f)$. We shall find the Hamilton–Jacobi equation for this function. For an extremal path, the partial derivative $\partial I_\sigma/\partial T$ satisfies the maximum Hamiltonian condition

$$z_\sigma \equiv \frac{\partial I_\sigma}{\partial T} = \frac{\partial L_\sigma}{\partial u}. \tag{66}$$

In our case

$$\frac{\partial L_\sigma}{\partial u} = \frac{c}{T}\left[1 - \frac{T^2}{(u+T)^2}\right] \tag{67}$$

whence

$$\frac{T}{u+T} = \sqrt{1 - Tz_\sigma/c}. \tag{68}$$

From this equation one finds the rate control $u = dT/d\tau$ in terms of the temperature T and its adjoint $z_\sigma = \partial I_\sigma/\partial T$

$$u = T\left(\frac{1}{\sqrt{1 - Tz_\sigma/c}} - 1\right). \tag{69}$$

The energy-like integral of the entropy functional is

$$E_\sigma = \frac{\partial L_\sigma}{\partial u}u - L_\sigma = c\frac{u^2}{(T+u)^2}. \tag{70}$$

Moreover, we find from equations (60) and (70) for the definitions used in this paper

$$E = -T^e E_\sigma. \tag{71}$$

This means that in the energy representation of thermodynamics (primed quantities), the equality $E = -E'_\sigma$ holds, where $E'_\sigma \equiv T^e E_\sigma$. The equality (71) is true for each mode of the system. For the modified definitions, described at the end of Section 8, which are particularly convenient for the heat-pump mode, $E = E'_\sigma$.

The entropy production Hamiltonian H_σ is the representation of E_σ in terms of T and z_σ

$$H_\sigma = c\frac{u^2}{(T+u)^2}$$

$$= c\left(\frac{T}{\sqrt{1 - Tz_\sigma/c}} - T\right)^2 \left(\frac{T}{\sqrt{1 - Tz_\sigma/c}}\right)^{-2} \tag{72}$$

whence

$$H_\sigma = c(1 - \sqrt{1 - Tz_\sigma/c})^2. \tag{73}$$

Clearly, from equations (66), (67) and (70), the case of vanishing z_σ implies $H_\sigma = 0$ identically, which refers to the reversible quasistatic process. The Hamilton–Jacobi partial differential equation for the minimum entropy generation problem (both modes of the system) is

$$\partial I_\sigma/\partial\tau + c(1 - \sqrt{1 - c^{-1} T \partial I_\sigma/\partial T})^2 = 0. \tag{74}$$

This can be compared to equation (64), which describes the extremal work problems based on the work Hamiltonian H, equation (63). In spite of the equality, $E = E'_\sigma$, the partial derivatives of both extremal functions with respect to T, $\partial I/\partial T$ and $\partial I'_\sigma/\partial T$, differ. Since, however, the two functionals (that of the work and that of the entropy generation) yield the same extremal, the connection between them can be determined. The procedure is based on the canonical transformation theory which leads to the conclusion that the lost power $L'_\sigma \equiv T^e L_\sigma$ can be gauged by addition of the total time derivative $d\Omega/d\tau$ of a gauging function $\Omega(T)$. Taking into account the change in the type of the extremum operation, in order to preserve unchanged equation of the extremal curve, the following general equation must link the momentum-type variables

$$\frac{\partial f_0}{\partial u} = \frac{\partial \Omega}{\partial T} - \frac{\partial L'_\sigma}{\partial u}. \tag{75}$$

For the engine mode of our example this reads

$$-c\left[1 - \frac{T^e T}{(\dot{T}+T)^2}\right] = \frac{d\Omega(T)}{dT} - \frac{cT^e}{T}\left[1 - \frac{T^2}{(\dot{T}+T)^2}\right]. \tag{76}$$

This relationship links the Lagrangians of the entropy and work. The equality $E'_\sigma = E$ proves that we deal with a time independent gauging function, hence the ordinary derivative $d\Omega/dT$ in equation (76). The above equation yields

$$\frac{d\Omega(T)}{dT} = -c\left(1 - \frac{T^e}{T}\right) \tag{77}$$

whence after integration between T^i and T^f

$$\Omega(T) = c(T^i - T^f) - cT^e \ln\left(\frac{T^i}{T^f}\right) = -\Delta B(T) \tag{78}$$

which is the change of the classical thermal exergy. Therefore, the change of the classical exergy is just the Hamiltonian-preserving gauging function for the dissipated availability functional based on the integrand $L'_\sigma \equiv T^e L_\sigma$. The equalities (71) and (76) may be viewed as equations linking the two functionals, the entropy functional and the generalized exergy functional, along an extremal. Subtraction of the classical exergy change from the dissipated availability functional is that form of gauging which preserves the same extremal trajectories and dissipative Hamiltonians of the two fixed-end problems considered.

9. PRINCIPAL FUNCTIONS FOR WORK AND EXERGY PROBLEMS

Let us now discuss the solutions of the Hamilton–Jacobi equations for the considered problems. From equation (23), by integration along an extremal path, one finds the function which describes the optimal specific work

$$I(T^i, T^f, \tau^i, \tau^f) = c(T^i - T^f) - \frac{T^e}{1+\xi} c \ln \frac{T^i}{T^f}. \quad (79)$$

This is the expression which generalizes changes of the exergy to processes with a finite rate $dT/d\tau = \xi T$. In a finite rate process this work depends explicitly on the process duration.

From the above equation and after using the end conditions to evaluate the intensity ξ in terms of the boundary temperatures and times

$$\xi = \frac{\ln (T^f/T^i)}{\tau^f - \tau^i} = -\frac{\ln(T^i/T^f)}{\tau^f - \tau^i} \quad \text{(each mode)} \quad (22')$$

the extremal specific work between two arbitrary states follows for every process mode in the form

$$\begin{aligned} &I(T^i, T^f, \tau^i, \tau^f) \\ &= c(T^i - T^f) - cT^e \ln \frac{T^i}{T^f} + c\left(T^e - \frac{T^e}{1+\xi}\right) \ln \frac{T^i}{T^f} \\ &= cT^i - T^f) - cT^e \ln \frac{T^i}{T^f} + cT^e \left(\frac{\xi}{1+\xi}\right) \ln \frac{T^i}{T^f} \\ &= c(T^i - T^f) - c(T^e \ln \frac{T^i}{T^f} - cT^e \frac{\ln(T^i/T^f)^2}{\tau^f - \tau^i - \ln(T^i/T^f)}. \end{aligned} \quad (80)$$

The particular extremal work which describes the (generalized) exergy should contain the environment temperature as one of the boundary states. The exergy, the always-positive quantity at the classical limit, is the maximal work $W_{max} = I(T^i, \tau^i, T^f, \tau^f)$ with $T^i = T$ and $T^f = T^e$ for the engine mode, and the negative minimal work $(-W)_{min} = -I(T^i, \tau^i, T^f, \tau^f)$ with $T^i = T^e$ and $T^f = T$ for the heat-pump mode of the system. For $\xi = 0$ the change of the classical thermal exergy is recovered.

From equation (80) with $T^i = T$ and $T^f = T^e$ one finds the dissipative exergy of the engine mode

$$E_x(T, T^e, \tau^i, \tau^f) = c(T - T^e) - cT^e \ln \frac{T}{T^e} - cT^e \frac{(\ln (T/T^e))^2}{\tau^f - \tau^i - \ln(T/T^e)}. \quad (81)$$

It may be verified that this function satisfies the Hamilton–Jacobi equation (64) with the $I = E_x$. Otherwise, one obtains the exergy of the heat-pump mode for the function $-I(T^i, \tau^i, T^f, \tau^f)$ with $T^i = T^e$ and $T^f = T$

$$E_x(T, T^e, \tau^i, \tau^f) = c(T - T^e) - cT^e \ln \frac{T}{T^e} + cT^e \frac{(\ln (T/T^e))^2}{\tau^f - \tau^i + \ln (T/T^e)}. \quad (82)$$

This function satisfies the Hamilton–Jacobi equation (64) with $I = -E_x$. Taking into account that the last term of the above equation contains the minimal integral of the entropy production

$$S_\sigma(T, T^e, \tau^i, \tau^f) = c \frac{(\ln(T/T^e))^2}{\tau^f - \tau^i \pm \ln(T/T^e)} \quad (83)$$

the general formula for the dissipative exergy is

$$\begin{aligned} E_x(T, T^e, \tau^f) &= c(T - T^e) - cT^e \ln \frac{T}{T^e} \pm cT^e \frac{(\tau^f)^{-1}[\ln(T/T^e)]^2}{1 + \pm (\tau^f)^{-1} \ln(T/T^e)} \\ &= E_x(T, T^e, \infty) \pm T^e S_\sigma \end{aligned} \quad (84)$$

where $E_x(T, T^e, \infty)$ is the classical exergy and we have assumed without any losses in generality that $\tau^i = 0$. In the above equations the upper sign refers to the heat-pump mode and the lower sign to the engine mode. An alternative form of the generalized exergy contains the height of the transfer unit $H_{TU} = \mathscr{L}/\tau$ and the contact length $\mathscr{L}$.

$$E_x(T^f, T^e, \tau) = E_x(T^f, T^e, \infty) \pm cT^e \frac{H_{TU}(\ln(T^f/T^e))^2}{\mathscr{L} \pm H_{TU} \ln(T^f/T^e)}. \quad (85)$$

It follows that the classical exergy yields an exact estimation of the extremal work for small H_{TU}, i.e. for the excellent transfer conditions, or for infinitely long times of the energy exchange. The heat-pump mode exergy $E_x = (-W)_{min}$, which defines the lower bound on the work consumption, can be significantly higher than the minimal work of classical thermodynamics. For state changes occurring in short times, this work may differ from the classical work substantially. This result explains the restrictive applicability of the classical thermodynamic bounds when they are applied to real processes, and it shows that these bounds should be replaced by stronger bounds obtained from non-equilibrium thermodynamics.

10. FINAL REMARKS

The irreversible or hysteretic properties of our generalized exergy as a finite-time work function are important. They are associated with different values of the work function obtained when the process, which leaves the equilibrium, is compared to the inverse process, which approaches the equilibrium. The first process corresponds with the heat-pump mode, associated with the supply of the work to the system, the second with the engine mode, characterized by the delivery of the work from the system.

While in the classical reversible thermodynamics these two modes can be accomplished with exactly the same magnitude of work, in our dissipative theory the works consumed and produced in two modes running between the two fixed states are no longer equal. A significant decrease of the maximal work received from the engine system and an increase of the minimal work added to the heat pump system is shown in the high-rate regimes and for short durations of thermodynamic processes. These results show that limits known from the classical availability theory should be replaced by stronger limits obtained for finite time processes, which are closer to reality.

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APPENDIX

Alternative notation of HJB equation

Frequently the subscript f is omitted in equations which operate with final coordinates meaning that one is allowed to consider arbitrary final states and times, for example

$$\frac{\partial V}{\partial \tau} + \max_{u} \left\{ \frac{\partial V}{\partial T} u - L(T, u) \right\} = 0 \quad (\min W^{i}) \qquad \text{(A1)}$$

which corresponds with the function V written in the form

$$V(W, T, \tau) = W - \Theta^{i} = \Theta - W^{i} = W - W^{i} - I(\tau^{i}, T^{i}, \tau, T). \qquad \text{(A2)}$$