PHYSCON 2009, Catania, Italy, September, 1–September, 4 2009

DYNAMIC PROGRAMMING APPROACHES TO THE HAMILTON-JACOBI-BELLMAN THEORY OF ENERGY SYSTEMS

Piotr Kuran
Faculty of Chemical Engineering
Warsaw University of Technology
Warsaw, Poland
Kuran@ichip.pw.edu.pl

Stanisław Sieniutycz
Faculty of Chemical Engineering
Warsaw University of Technology
Warsaw, Poland
Sieniutycz@ichip.pw.edu.pl

Abstract.
Dynamical problems of maximum power produced in thermal systems and associated problems of minimum entropy production are governed by Hamilton–Jacobi–Bellman (HJB) equations which describe corresponding optimal functions and associated controls. Systems with nonlinear kinetics (e.g. radiation engines) are particularly difficult (the optimal relaxation curve is non-exponential), thus, discrete counterparts of original HJB equations and numerical approaches are applied. We investigate convergence of discrete algorithms to solutions of HJB equations, discrete approximations of controls, and role of Lagrange multiplier λ associated with the duration constraint. In analytical discrete schemes, the Legendre transformation is a significant tool leading to the original work function. We also describe numerical algorithms of dynamic programming and consider dimensionality reduction in these algorithms.

Nomenclature

a temperature power exponent in kinetic equation [-]
c specific heat [$Jg^{-1}K^{-1}$, $Jm^{-3}K^{-1}$, $Jmol^{-1}K^{-1}$]
$\dot{G}$ resource flux [gs^{-1}, $mols^{-1}$]
f rate vector with components f_1, ..f_k.. f_s
f_0 intensity of generalized profit
H Hamiltonian function
R minimum performance function [J, or $Jmol^{-1}$]
S entropy [JK^{-1}]
T variable temperature of resource fluid [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 time [s]
u control vector
u temperature rate control, $dT/d\tau$ [K]
V maximum performance function [J, or $Jmol^{-1}$]
W and $\dot{W}$ work and power [J, Js^{-1}]
x state vector
$\tilde{x}$ enlarged state vector including time

Greek symbols

β coefficient, frequence constant [s^{-1}]
λ Lagrange multiplier, time adjoint
η first-law efficiency [-]
θ time interval [s,-]
Φ factor of internal irreversibility [-]
ξ intensity factor [-]
τ nondimensional time or number of heat transfer units (x/H_{TU}) [-]

Superscripts

e environment
i initial state
n- stage number
f initial state
‘ modified quantity

1. Introduction

In this paper we consider analytical and computational aspects of energy limits in dynamical systems propelled by nonlinear fluids that are restricted in their amount or flow, and, as such, play role of resources. In practical processes of engineering and technology a resource is a useful, valuable substance of a limited amount or flow. Value of the resource can be quantified thermodynamically by specifying its exergy, a maximum work that can be delivered when the resource is downgraded to the equilibrium with the environment. Reversible relaxation of the resource is associated with the classical exergy, when some dissipative phenomena are allowed generalized exergies are obtained. Generalized exergies incorporate both limited availability of the resource and a minimum work lost during its production. In the classical exergy only the first property is taken into account [1].

To calculate any exergy function knowledge of a work integral is required [2, 3]. For thermal systems this integral involves the product of thermal efficiency and the differential of exchanged energy. Various process models lead to diverse formulas for thermal efficiencies, which show how efficiency of a practical system deviates from the Carnot efficiency. In thermal systems the trajectory is characterized by the temperature of the resource fluid $T(t)$, whereas the control variable may be efficiency η or Carnot temperature $T'(t)$. The latter quantity, defined in our previous work [3], is particulary suitable in describing of driving forces in energy systems. Whenever $T'(t)$ differs from $T(t)$ the resource relaxes to the environment with a finite rate associated with the efficiency deviation from the Carnot efficiency. Only 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.

In this research we apply the theory for Hamilton-Jacobi-Bellman (HJB) and Hamilton-Jacobi equations to nonlinear thermal systems with power generation. In order to obtain generalized exergies (or corresponding functions describing limits on entropy production) one has to solve appropriate HJB equations. The problem is, however, that most of optimal solutions cannot be obtained in the form of explicit analytical formulae (especially systems with nonlinear kinetics e.g. radiation systems). To overcome the difficulty, discrete counterparts of continuous equations are solved in numerical approaches to HJB equations. Especially a few forms of discrete dynamic programming algorithms are efficient to solve continuous HJB equations.

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

In our earlier papers [4]-[5] we considered mathematical modeling for continuous, active (work producing) systems working with finite rates. Systems producing mechanical energy from radiation were especially considered as suitable example of nonlinear energy systems. As a representative problem of minimum work consumed in a system subject to constraints imposed on dynamics and duration we consider a dynamical system producing power from radiation. It is characterized by a highly nonlinear kinetics [4, 5]. For a *symmetric model* of power yield from radiation (both reservoirs consist of radiation) a power integral is [5]

$$\dot{W} = \int_{t^i}^{t^f} \dot{G}_c(T)\left(1-\frac{\Phi T^e}{T'}\right)\beta\frac{T^a - T'^a}{\left(\Phi'\left(\frac{T'}{T^e}\right)^{a-1}+1\right)T^{a-1}}dt \quad (1)$$

In the physical space, power exponent a = 4 for radiation and a = 1 for a linear resource. Integral (1) has to be maximized in the engine mode of the process subject to the dynamical constraint ('state equation'). A standard way to determine the extremum conditions for the dynamic optimization problem requires solving the HJB equation

$$-\frac{\partial V}{\partial t} + \max_{T'(t)}\left\{\left(\dot{G}_c(T)\left(1-\Phi\frac{T^e}{T'}\right)+\frac{\partial V}{\partial T}\right)\beta\frac{T^a - T'^a}{\left(\Phi'\left(\frac{T'}{T^e}\right)^{a-1}+1\right)T^{a-1}}\right\} = 0 \quad (2)$$

where $V = \max\dot{W}$. As it is extremely difficult to solve Eq. (2) analytically except for the case when a = 1 we focus here on numerical solving based on Bellman's method of dynamic programming (DP). A nice summary of this method is given in Aris's book [6].

Considering computer needs we introduce a related discrete scheme

$$\dot{W}^N = \sum_{k=1}^{N} \dot{G}_c(T^k)\left(1-\frac{\Phi T^e}{T'^k}\right)\beta\frac{T^{k^a} - T'^{k^a}}{(\Phi'(T'^k/T^e)^{a-1}+1)T^{k^{a-1}}}\theta^k \quad (3)$$

$$T^k - T^{k-1} = \theta^k\beta\frac{T'^{k^a} - T^{k^a}}{(\Phi'(T'^k/T^e)^{a-1}+1)T^{k^{a-1}}} \quad (4)$$

$$\tau^k - \tau^{k-1} = \theta^k \quad (5)$$

We search for maximum of the sum (3) subject to discrete constraints (4) and (5).

3. 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 [6-8]. 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

$$W^N = \sum_{n=1}^{N} f_0(\mathbf{x}^n, t^n, \mathbf{u}^n, \theta^n)\theta^n . \tag{6}$$

subject to constraints resulting from difference equations

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

The scalar f_0 is the rate of the profit generation. Superscripts refer to stages and subscripts to coordinates. The integer n (n = 1…N) is usually called discrete time, 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 $\mathbf{x} = (x_1, ..x_s)$ is the state vector, and the r-dimensional vector $\mathbf{u} = (u_1…u_r)$ 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 $\mathbf{u}$. The rate change of state coordinate x_i in time t is i-th component of s-dimensional vector of rates, **f.** The change of time t through the stage n defined as $\theta^n = t^n - t^{n-1}$ is called the time interval.

Various discretization schemes for constraining differential equations lead to discrete models either linear or nonlinear in θ^n. 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 model.

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

$$t^n - t^{n-1} = \theta^n . \tag{8}$$

The monotonic increase of the time-like coordinate, implying nonnegative θ at each stage n, is crucial for many properties of this model. Two classes of discrete models, linear and nonlinear in free θ^n, should be 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 must be satisfied. Discretizations which produce process rates weakly dependent on θ^n are sufficient to assure the convergence of the dynamic programming solutions to the solutions of continuous HJB and Hamilton-Jacobi equations.

4. Dynamic programming equation for maximum power from radiation

Equations modeling limiting continuous processes (including, of course, equations of power systems considered) can be solved numerically by a discrete algorithm associated with stage criterion. Especially, one can use the dynamic programming (DP) algorithm. The latter is associated with Bellman's recurrence equation

$$\begin{aligned} R^n(\mathbf{x}^n, t^n) = \min_{\mathbf{u}^n, \theta^n} \{ & l_0^n(\mathbf{x}^n, t^n, \mathbf{u}^n, \theta^n)\theta^n + \\ & + R^{n-1}((\mathbf{x}^n - \mathbf{f}^n(\mathbf{x}^n, t^n, \mathbf{u}^n, \theta^n)\theta^n, t^n - \theta^n)\} \end{aligned} \tag{9}$$

Difference models linear in θ^n (those with θ-independent rates f_k) are primary candidates to efficient solving 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. Applying equation (9) to this problem, the following recurrence equation is obtained

$$\begin{aligned} R^n(T^n, t^n) = \min_{\mathbf{u}^n, \theta^n} \left\{ \dot{G}_c(T^n) \left(1 - \frac{\Phi T^e}{T'^n}\right) \beta \frac{T^{na} - T'^{na}}{\left(\Phi' \left(\frac{T'^n}{T^e}\right)^{a-1} + 1\right) T^{na-1}} \theta^n \right\} + \\ + R^{n-1} \left(T^n - \theta^n \beta \frac{T'^{na} - T^{na}}{\left(\Phi' \left(\frac{T'^n}{T^e}\right)^{a-1} + 1\right) T^{na-1}}, t^n - \theta^n \right) \end{aligned} \tag{10}$$

It is quite easy to solve recurrence equation (10) numerically. Low dimensionality of state vector for Eq. (10) 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.

5. Discrete approximations and time adjoint as a Lagrange multiplier

We consider solutions of *HJB* equations by discrete approximations (produced by the method of dynamic programming) in association with state dimensionality reduction (elimination of time coordinate) by using a Lagrange multiplier.

First we outline the generation of costs in terms of the Lagrangian multiplier λ associated with the duration constraint. As the time adjoint, λ is constant in autonomous systems. Exploiting constancy of λ we eliminate state variable τ by introducing a (primed) criterion of modified work

$$R'^n\left(T^n,\lambda\right)=\min\sum_{k=1}^{n}\left\{c\left(1-\Phi'\frac{T^e}{T'^k}\right)\left(T^k-T^{k-1}\right)+\lambda\theta^n\right\} \quad (11)$$

or, in view of state equation

$$R'^n(T^n,\lambda)=\min\sum_{k=1}^{n}\left\{c\left(1-\Phi'\frac{T^e}{T'^k}\right)+\frac{\lambda}{T'^k-T^k}\right\}\left(T^k-T^{k-1}\right) \quad (12)$$

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 equation (12). We consider two initial stages, 1 and 2. A procedure leading to parametric representations is defined below.

Equation of work modified by the presence of the Lagrange multiplier λ, yet without a minimization sign becomes a component of a parametric representation of $R'^1(T^1,\lambda)$:

$$R^{'1}\left(T^1,T'^1,\lambda\right)=\left\{c\left(1-\Phi'\frac{T_2}{T'^1}\right)+\frac{\lambda}{T'^1-T^1}\right\}\left(T^1-T^0\right) \quad (13)$$

In this example we can present function of work consumption for n=1 and corresponding optimal control, and going further we can show optimal work supply to two-stage system $R^{'2}(T^2,\lambda)$ and optimal interstage temperature T^1 which is the geometric mean of boundary temperatures of both considered stages $T^1=\left(T^0T^2\right)^{1/2}$. Further considerations leads to optimal work function for an arbitrary n

$$R^{'n}(T^n,\lambda)=c(T^n-T^0)-$$
$$nc\Phi'T^e\left(1-\pm\sqrt{\frac{\lambda}{c\Phi'T^e}}\right)^2\left(1-\left(\frac{T^0}{T^n}\right)^{1/n}\right). \quad (14)$$

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

$$\tau^n=\frac{\partial R^{'n}(T^n,\lambda)}{\partial\lambda}=\frac{\left(1-\pm\sqrt{\frac{\lambda}{c\Phi'T^e}}\right)}{\left(\pm\sqrt{\frac{\lambda}{c\Phi'T^e}}\right)}n\left(1-\left(\frac{T^0}{T^n}\right)^{1/n}\right). \quad (15)$$

Properties of duration function is illustrated in Fig. 1. In any process, linear or not, λ is monotonically decreasing function of duration.

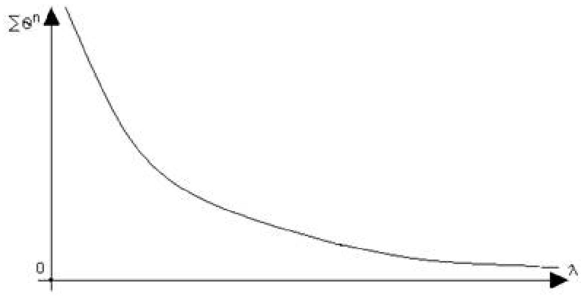

Figure 1 Dependence of Lagrange multiplier λ.on optimal duration $\tau=\Sigma\Theta^n$ in a cascade of power generation systems.

6. Mean and local intensities in discrete processes

Further transformations are easier if the following intensity criterion is introduced

$$\xi\equiv\frac{n}{\tau^n}\left(1-\left(T^0/T^n\right)^{1/n}\right) \quad (16)$$

The ξ defined by equation (16) is a discrete counterpart of a *mean* relaxation rate of the temperature logarithm for the *n*-stage process. For an arbitrary stage *n* we can also introduce a local intensity of a discrete process

$$\xi^n \equiv \frac{T^n - T^{n-1}}{T^n \theta^n} \qquad (17)$$

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

$$\lambda = c\Phi' T^e \left(\frac{\xi}{\xi + 1} \right)^2 \qquad (18)$$

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 quasistatic processes. Optimal work function in terms of ξ assumes:

$$R'^n(T^n, \xi) = c(T^n - T^0) - \frac{c\Phi' T^e}{(1+\xi)^2} n \left(1 - \left(\frac{T^0}{T^n} \right)^{1/n} \right) \qquad (19)$$

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

$$R'^n(T^n, 0) = c(T^n - T^0) - cT^e \ln(T^n / T^0) \qquad (20)$$

Therefore optimal work function (19) is a finite-rate exergy of the considered discrete process.

7. Legendre transform and original work function

The minimum of consumed work is described by original principal function $R^n\left(T^n, \tau^n\right)$. This function is the Legendre transform of $R'^n\left(T^n, \lambda\right)$ with respect to λ. In transformations we use intensity ξ as an intermediate variable to increase lucidity of formulas. We obtain

$$\tau^n = \frac{\partial R'^n(T^n, \lambda)}{\partial \lambda} = \frac{n}{\xi} \left(1 - \left(\frac{T^0}{T^n} \right)^{1/n} \right) \qquad (21)$$

$$R^n(T^n, \xi) = c(T^n - T^0) - c\Phi' T^e \left(\frac{1}{1+\xi} \right)^2 n \left(1 - \left(\frac{T^0}{T^n} \right)^{\frac{1}{n}} \right) - \frac{\lambda(\xi)}{\xi} n \left(1 - \left(\frac{T^0}{T^n} \right)^{\frac{1}{n}} \right) \qquad (22)$$

where function describing λ in terms of ξ is given by Eq. (15). A complementary formula expressing λ in terms of duration τ follows from Eq. (15)

$$\lambda = c\Phi' T^e \left(\tau^n / n \left[1 - \left(T^0 / T^n \right)^{1/n} \right] + 1 \right)^{-2} \qquad (23)$$

Monotonic decrease of λ with τ is a general property of both linear and nonlinear processes.

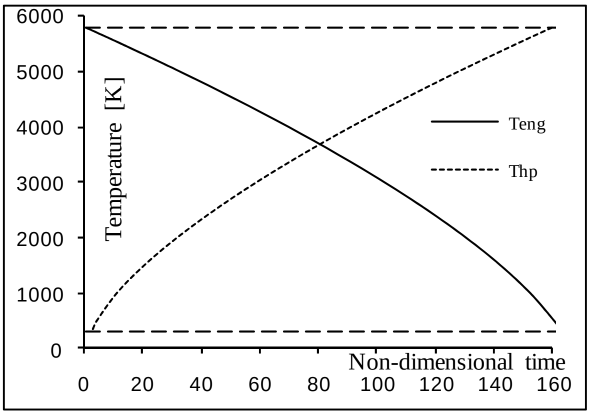

Figure 2. Decreasing temperature of radiation relaxing in engine mode and increasing temperature of radiation utilized in heat pump mode in terms of non-dimensional time τ, for Φ'=1 and the Lagrange multiplier $\lambda = 1*10^{-8}$ [$JK^{-1}m^{-3}$].

We obtain

$$R^n\left(T^n, \tau^n\right) = c\left(T^n - T^0\right) - c\Phi' T^e n \left(1 - \left(\frac{T^0}{T^n} \right)^{\frac{1}{n}} \right) + c\Phi' T^e \left\{ n \left(1 - \left(\frac{T^0}{T^n} \right)^{\frac{1}{n}} \right) \right\}^2 \left(\tau^n + n \left(1 - \left(\frac{T^0}{T^n} \right)^{\frac{1}{n}} \right) \right)^{-1} \qquad (24)$$

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 reversible and quasistatic process ($\Phi' = 1, \tau^n \to \infty$) describes a change of classical thermal exergy (20).

This approach can also be organized in the entropy representation, where principal function $R_\sigma'^n$ is the minimum entropy production modified by Lagrange multiplier term.

10. Concluding Remarks

In this paper we have presented a basic formuation for maximum power in nonlinear dynamical systems with radiation and considered convergence of discrete computational algorithms to solutions of corresponding HJB equations. Lagrangian multipliers associated with duration constraint have been used to reduce dimensionality of power yield problems. Analytical and numerical approaches, applying the dynamic programming method, are described. Legendre transform is applied to recover optimal work as function $R^n(T^n, \tau)$.

Generalized (time dependent) work potentials are found for nonlinear systems. They lead to thermodynamic bounds on power produced (consumed) in a finite time, which are stronger than classical thermodynamic bounds due to extra constraints coming from process kinetics.

Other important application of the considered approach involves chemical energy systems, and, especially, fuel cells.

Acknowledgements

This research was supported in part by The Polish Ministry of Science, grant NN208 019434: Thermodynamics and Optimization of Chemical and Electrochemical Energy Generators with Applications to Fuel Cells.

References

1. T. J. Kotas, *Exergy Method of Thermal Plant Analysis*, Butterworths, Borough Green,1985.
2. S. Sieniutycz, Nonlinear thermokinetics of maximum work in finite time, Int. J. Engng Sci. 36, 557-597 (1988).
3. S. Sieniutycz, Carnot controls to unify traditional and work-assisted operations with heat & mass transfer, *International J. of Applied Thermodynamics,* **6,** 59-67 (2003), see also S. Sieniutycz in *Open Sys. & Information Dynamics,* **10**, 31-49 (2003).
4. S. Sieniutycz and P. Kuran, Nonlinear models for mechanical energy production in imperfect generators driven by thermal or solar energy, *Intern. J. Heat Mass Transfer,* **48**, 719-730 (2005).
5. S. Sieniutycz and P. Kuran, Modeling thermal behavior and work flux in finite-rate systems with radiation, *Intern. J. Heat and Mass Transfer* **49**, 3264-3283 (2006).
6. R. Aris, *Discrete Dynamic Programming*, Blaisdell, New York, pp. 10-39, 1964.
7. S. Sieniutycz, State transformations and Hamiltonian structures for optimal control in discrete systems, *Reports on Mathematical Physics*, **49**, 789-795, (2006).
8. R. E. Bellman, *Adaptive Control Processes: a Guided Tour*, pp. 1-35, Princeton University Press, Princeton, 1961.