OPTIMAL CONTROL OF THERMODYNAMIC PORT-HAMILTONIAN SYSTEMS

BERNHARD MASCHKE 1 , FRIEDRICH PHILIPP 2 , MANUEL SCHALLER 2 , KARL WORTHMANN 2 AND TIMM FAULWASSER 3

ABSTRACT. We consider the problem of minimizing the entropy, energy, or exergy production for state transitions of irreversible port-Hamiltonian systems subject to control constraints. Via a dissipativity-based analysis we show that optimal solutions exhibit the manifold turnpike phenomenon with respect to the manifold of thermodynamic equilibria. We illustrate our analytical findings via numerical results for a heat exchanger.

Keywords. port-Hamiltonian systems, irreversible thermodynamic systems, optimal control, manifold turnpike

1. Introduction

The Hamiltonian formulation of controlled thermodynamic systems is a very active research area with various considered settings ranging from port-Hamiltonian (pH) systems defined on contact manifolds [4, 10, 9, 23, 26], symplectic manifolds [32, 17] to dissipative Hamiltonian (or gradient-Hamiltonian) systems such as GENERIC [18, 13, 14].

With respect to control of thermodynamic pH systems, there are several papers considering passivity-based feedback stabilization using thermodynamic potentials, e.g., the internal energy, eventually augmented with the mechanical or electromagnetic energy or the exergy [29, 31], the availability function [14, 13, 11], or the entropy creation function associated with the irreversible phenomena [22]- The works mentioned above consider classical approaches for pH systems such as passivity-based damping assignment (IDA-PBC), energy function or entropy creation shaping and they do not investigate optimal control.

However, outside the realm of pH systems, there is a series of papers considering dynamic control based on thermodynamic potentials such as the availability function [1, 2, 27, 33], and also the entropy creation [12, 11]. Moreover, there is some effort regarding entropy optimization at steady state for distributed parameter systems [15].

In this work, we consider optimal control of irreversible pH systems [25, 24] accounting both for the energy conservation and the entropy creation. Thereby, we extend our previous works on minimzing the energy supply in the linear pH setting [30, 19, 8] to

¹Univ Lyon, Université Claude Bernard Lyon 1, CNRS, LAGEPP UMR 5007, France (e-mail: bernhard.maschke@univ-lyon1.fr).

²Technische Universität Ilmemau, Institute for Mathematics, Germany (e-mail {friedrich.philipp,manuel.schaller,karl.worthmann}@tu-ilmenau.de)..

³TU Dortmund University, Institute of Energy Systems, Energy Efficiency and Energy Economics, Germany (e-mail: timm.faulwasser@ieee.org).

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the class of nonlinear irreversible pH systems, that is, we aim for a state transition with minimal energy, entropy, or exergy supply, respectively linear combinations thereof. We prove that, under suitable assumptions, a state transition that is optimal with respect to these metrics is always performed in a neighborhood of the set of thermodynamical equilibria for the majority of the time. We embed this intuitive property into the framework of manifold turnpike properties of optimal control problems.

Notation. We denote the gradient of a scalar-valued function $F: \mathbb{R}^n \to \mathbb{R}$ by $\frac{\partial F}{\partial x}$ or just F_x and define the *Poisson bracket* $\{S, H\}_J$ of two functions $S, H: \mathbb{R}^n \to \mathbb{R}$ with respect to a matrix $J \in \mathbb{R}^{n \times n}$ by $\{S, H\}_J(x) = S_x(x)^\top J H_x(x)$.

2. IRREVERSIBLE PORT-HAMILTONIAN SYSTEMS

We commence our analysis by introducing the considered class of systems. The state space is given by \mathbb{R}^n , $n \in \mathbb{N}$, and, as usual in pH Systems, the input and output spaces coincide and are given by \mathbb{R}^m , $m \in \mathbb{N}$.

The definition of an irreversible pH system (IPHS) was introduced by [24], and we slightly adapt it to our setting.

Definition 1. An irreversible port-Hamiltonian system is defined by the state equation (IPHS) $\dot{x}(t) = \gamma(x(t), H_x(x(t)))\{S, H\}_J(x(t))JH_x(x(t)) + g(x, H_x(x))u(t).$

with a skew-symmetric structure matrix $J \in \mathbb{R}^{n \times n}$, a strictly positive continuous function $\gamma : \mathbb{R}^{2n} \to \mathbb{R}$,

- (i) a continuously differentiable non-negative Hamiltonian function $H: \mathbb{R}^n \to \mathbb{R}_0^+$, and
- (ii) an entropy function $S: \mathbb{R}^n \to \mathbb{R}$.

The system is completed with two output variables, the energy-conjugated output y_H and the entropy-conjugated output y_S defined by

(1)
$$y_H := g(x, H_x)^\top H_x \quad \text{and} \quad y_S := g(x, H_x)^\top S_x.$$

Direct calculations show that every trajectory x satisfying the dynamics (IPHS) obeys the energy and entropy balance

(2)
$$\frac{\frac{\mathrm{d}}{\mathrm{d}t}H(x(t)) = y_H(t)^{\top}u(t), \\ \frac{\mathrm{d}}{\mathrm{d}t}S(x(t)) = \gamma(x(t), H_x(x(t)))\{S, H\}_J^2(x(t)) + y_S(t)^{\top}u(t).$$

Here, $y_H(t)^{\top}u(t)$ represents the energy flow, i.e., the power supplied to/extracted from the system, whereas $y_S(t)^{\top}u(t)$ is to be interpreted as the entropy flow injected into/drawn from the system. For closed systems, i.e., $u \equiv 0$, it can be directly inferred from the equations in (2) and the positivity of γ that energy is preserved and entropy is non-decreasing. Hence, the two fundamental laws of thermodynamics hold. In particular, the entropy balance captures the irreversible nature of (IPHS).

2.1. **Example: Heat exchanger.** In this subsection, we introduce the heat exchanger as depicted in Figure 1 in order to motivate the problem formulation and to illustrate our results. The example is slightly adapted from [21].

The thermodynamic properties of each compartment, under the assumption that the walls are non deformable and impermeable, are given by the relation between temperature and entropy

$$T_i(S_i) = T_{\text{ref}} \cdot e^{(S_i - S_{\text{ref}})/c_i}, \quad i = 1, 2,$$

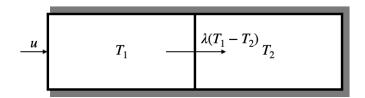


FIGURE 1. Model of a heat exchanger with two compartments

where $S_{\text{ref}} \in \mathbb{R}$ is a reference entropy corresponding to the reference temperature T_{ref} and c_i , i = 1, 2, are heat capacities, cf. [3, Section 2.2]. The energy in each compartment, denoted by $H_i(S_i)$, i = 1, 2, can be obtained by integrating Gibbs' equation $dH_i = T_i dS_i$ as a primitive of the function $T_i(S_i)$, i = 1, 2.

The state vector of the IPHS is composed of the entropies of the compartments $x = (S_1, S_2)^{\top}$ and the total energy (entropy) is given by the sum of the energies (entropies, resp.) in the compartments, i.e.,

$$H(x) = H_1(S_1) + H_2(S_2), \quad S(x) = S_1 + S_2 = (1, 1)^{\top} x.$$

Consider first the situation where the two compartments are isolated and the dynamics only arise from the heat flow through the wall separating the two compartments. Due to Fourier's law, the heat flow is given by

$$\dot{Q} = \lambda (T_1 - T_2),$$

where $\lambda > 0$ is a heat conduction coefficient. By continuity of the heat flux, we have

$$\dot{Q} = -\frac{\mathrm{d}}{\mathrm{d}t}H_1(S_1(t)) = \frac{\mathrm{d}}{\mathrm{d}t}H_2(S_2(t))$$

and hence

$$\lambda(T_1 - T_2) = -T_1 \frac{\mathrm{d}}{\mathrm{d}t} S_1(t) = T_2 \frac{\mathrm{d}}{\mathrm{d}t} S_2(t),$$

which yields the entropy balance equations for each compartment, written as follows

$$\frac{\mathrm{d}}{\mathrm{d}t} \begin{pmatrix} S_1(t) \\ S_2(t) \end{pmatrix} = \lambda \begin{pmatrix} \frac{1}{T_2(t)} - \frac{1}{T_1(t)} \end{pmatrix} \underbrace{\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}}_{-1, I} \begin{pmatrix} T_1(t) \\ T_2(t) \end{pmatrix},$$

hereby matching the definition of the drift term of (IPHS) with

$$\gamma(x, \frac{\partial H}{\partial x}) = \frac{\lambda}{T_1 T_2}, \qquad \{S, H\}_J = \begin{pmatrix} 1 & 1 \end{pmatrix} J \begin{pmatrix} T_1 \\ T_2 \end{pmatrix} = T_1 - T_2.$$

Entropy flow control. The canonical choice of an input would be to consider the entropy flowing into or out of compartment one. In this case, we have

(4)
$$\frac{\mathrm{d}}{\mathrm{d}t} \begin{pmatrix} S_1 \\ S_2 \end{pmatrix} = \gamma(x, H_x) \{ S, H \}_J(x) J H_x + \begin{pmatrix} 1 \\ 0 \end{pmatrix} u.$$

Control by a thermostat. The realizable choice is to induce a heat flow through the external wall connecting compartment two to a thermostat at a controlled temperature T_e . If, e.g., compartment one is not isolated, the heat flow between this compartment and the environment can be described via

$$\dot{Q}_e = \lambda_e (T_e - T_2),$$

with $\lambda_e > 0$ being a heat conduction coefficient. Thus, the energy balance in the first compartment reads

$$T_1 \frac{\mathrm{d}}{\mathrm{d}t} S_1(t) = -\lambda (T_1(t) - T_2(t)) + \lambda_e (T_e(t) - T_1(t))$$

and we obtain the dynamics

(5)
$$\frac{\mathrm{d}}{\mathrm{d}t} \begin{pmatrix} S_1 \\ S_2 \end{pmatrix} = \gamma(x, H_x) \{ S, H \}_J(x) J H_x + \lambda_e \begin{pmatrix} \frac{T_e - T_1}{T_1} \\ 0 \end{pmatrix}.$$

Note that the input map does not correspond to Definition 1, as it is affine in the control: $W(x, H_x) + g(x, H_x)u$ as in [24]. In the sequel, we shall consider the control problem using as input the entropy flow into compartment one (4) which is related to the thermostat temperature control in (5) by the state dependent control transformation $u \to \frac{u-T_1}{T_c}$.

2.2. Optimal Control Problem for IPHS. Considering an optimization horizon $t_f \ge 0$, an initial value $x^0 \in \mathbb{R}^n$, and a terminal region $\Psi \subset \mathbb{R}^n$, we obtain the prototypical Optimal Control Problem (OCP)

(phOCP)
$$\min_{u \in L^{\infty}(0,t_f;\mathbb{U})} \int_0^{t_f} [\alpha_1 y_H(t) - \alpha_2 T_0 y_S(t)]^{\top} u(t) dt$$
s.t. (IPHS), $x(0) = x^0$, $x(t_f) \in \Psi$.

Here, y_H and y_S are given by (1). The set of admissible control values $\mathbb{U} \subset \mathbb{R}^m$ is supposed to contain the origin and to be compact and convex. Then, the feasible set, i.e., the set of all admissible control functions, is given by

$$\mathcal{U}_{t_f} := \{ u \in L^{\infty}(0, t_f, \mathbb{R}^m) \mid u(t) \in \mathbb{U}, x(t_f; x^0, u) \in \Psi \}.$$

In the cost functional, $T_0 > 0$ is a fixed scalar reference temperature and the coefficients $\alpha_1, \alpha_2 \in [0, 1]$ with $\alpha_1 + \alpha_2 = 1$ yield a convex combination of the energy flow and the entropy flow. The three most important cases are the following:

- minimal energy supply, i.e., $\alpha_1 = 1$, $\alpha_2 = 0$,
- minimal entropy extraction, i.e., $\alpha_1 = 0$, $\alpha_2 = 1$,
- minimal exergy supply, i.e., $\alpha_1 = \alpha_2 = \frac{1}{2}$.

Setting $\ell_{\alpha_1,\alpha_2}(x,u) = [\alpha_1 y_H - \alpha_2 T_0 y_s]^{\top} u$ and using the balance equations (2), we obtain the identity

(6)
$$\int_{0}^{t_f} \ell_{\alpha_1,\alpha_2}(x,u) dt = \alpha_1 \left[H(x(t_f)) - H(x(0)) \right] + \alpha_2 T_0 \left(S(x(0)) - S(x(t_f)) + \int_{0}^{t_f} \gamma(x, \frac{\partial H}{\partial x}) \{S, H\}_J^2 dt \right).$$

The following proposition directly follows from [16, Theorem IV.2].

Proposition 2 (Existence of solutions). Let $\Psi = \{0\}$, $x^0 \in \mathbb{R}^n$ and assume that $\mathcal{U}_{t_f} \neq \emptyset$, i.e., there is a feasible control. If state responses to admissible controls are bounded, i.e., for any t_f there is $\alpha \geq 0$ such that

$$||x(t;x^0,u)|| \le \alpha \quad \forall u \in \mathcal{U}_T, \ 0 \le t \le t_f,$$

then there exists an optimal control.

The assumption of a bounded state response is satisfied if, e.g., one has exponential stability of the uncontrolled dynamics and uniform boundedness of the input map g, see [28, Theorem 2.3].

3. Turnpikes towards the manifold of thermodynamic equilibria

To prove the main result of this paper, we will impose the following assumptions on the energy and entropy function.

Assumption 3. Let the following hold.

- (a) $H \in C^2(\mathbb{R}^n, \mathbb{R})$.
- (b) $H_x: \mathbb{R}^n \to \mathbb{R}^n$ is a diffeomorphism,
- (c) the entropy function is linear in the state, i.e., $S(x) = l^{\top}x$ with some $l \in \mathbb{R}^n$.

We briefly discuss the above assumptions. In thermodynamic pH-systems energy H(x) is mostly non-quadratic and, whereas (b) is satisfied for many thermodynamic pH systems, the norm on the inverse of H_x is usually not uniformly bounded on \mathbb{R}^n , cf. the heat exchanger in Section 2.1. The linearity of the entropy function in the state is satisfied by convention for all common models of IPHS, as the total entropy S or the entropies in the subdomains S_i , i = 1, 2 as in the heat exchanger are also considered as a state itself. For various examples we refer to [21, 24].

We define the set of thermodynamic equilibria by

$$\mathcal{T} := \left\{ x \in \mathbb{R}^n : \gamma(x, H_x(x)) \{ S, H \}_J^2(x) = 0 \right\} = \left\{ x \in \mathbb{R}^n : \{ S, H \}_J(x) = 0 \right\},$$

where $\{S, H\}_J(x)$ has the physical interpretation of the driving force of the irreversible phenomenon [24]. In view of linearity of the entropy function (Assumption 3(c)), we compute

$$\{S, H\}_J(x) = S_x(x)^{\top} J H_x(x) = l^{\top} J H_x(x) = -H_x(x)^{\top} J l$$

and hence $\{S, H\}_J(x) = 0$ whenever $H_x(x) \in (Jl)^{\perp}$, i.e.,

$$\mathcal{T} = \frac{\partial H}{\partial x}^{-1} \left((Jl)^{\perp} \right).$$

Further, by differentiating the above expression and due to pointwise invertibility of H_{xx} (Assumption 3(b)), the set \mathcal{T} is a manifold. This manifold is n-dimensional if Jl = 0 and n - 1-dimensional otherwise.

We now recall the manifold turnpike property as introduced by [5] in the context of trim manifolds for Lagrangian and Hamiltonian mechanical systems. For thermodynamic IPHS, the manifold of interest is given by the thermodynamic equilibria.

Definition 4 (Integral state manifold turnpike property). Let $\ell \in C^1(\mathbb{R}^{n+m})$, $\varphi \in C^1(\mathbb{R}^n)$, $\Psi \subset \mathbb{R}^n$ be closed and $f \in C^1(\mathbb{R}^{n+m})$. We say that a general OCP of the form

(7)
$$\min_{u \in L^{1}(0,T;\mathbb{U})} \varphi(x(T)) + \int_{0}^{t_{f}} \ell(x(t), u(t)) dt$$
s.t. $\dot{x} = f(x, u), \quad x(0) = x^{0}, \quad x(t_{f}) \in \Psi$

has the integral state turnpike property on a set $S_{\rm tp} \subset \mathbb{R}^n$ with respect to a manifold $\mathcal{T} \subset \mathbb{R}^n$, if for all compact $K \subset S_{\rm tp}$ there is a constant C_K such that for all $x^0 \in K$ and $t_f > 0$, each optimal pair (x^*, u^*) satisfies

(8)
$$\int_0^{t_f} \operatorname{dist}^2\left(x^{\star}(t), \mathcal{T}\right) dt \le C_K.$$

The previous definition can be interpreted as follows. As the upper bound in (8) is bounded uniformly in t_f , for large time horizons t_f , the positive integrand $\operatorname{dist}^2(x^*(t), \mathcal{T})$ has to be small for the majority of the time. More precisely, for $x^0 \in K \subset S_{\operatorname{tp}}$ and $\varepsilon > 0$ we have

$$\mu(\lbrace t \in [0,T] : \operatorname{dist}(x^{\star}(t),\mathcal{T}) > \varepsilon \rbrace) \leq \frac{1}{\varepsilon^2} \int_0^T \operatorname{dist}^2(x^{\star}(t),\mathcal{T}) dt \leq \frac{C_K}{\varepsilon^2},$$

where μ denotes the standard Lebesgue measure. This behavior of optimal trajectories is called *measure turnpike*, cf. e.g. [7, Definition 2].

Lemma 5. For any compact subset $K \subset \mathbb{R}^n$, there are positive constants c, C > 0 such that

$$c \operatorname{dist}(x, \mathcal{T})^2 \le \gamma(x, H_x(x)) \{S, H\}_J^2(x) \le C \operatorname{dist}(x, \mathcal{T})^2$$

for all $x \in K$.

Proof. The proof is given in the appendix.

As it is typical for thermodynamic systems, neither the Hessian H_{xx} of the Hamiltonian nor its inverse $H_{xx}(\cdot)^{-1}$ are uniformly bounded. For this reason the norm-like equivalence of Lemma 5 could only be proved on compact sets. To apply the above result to optimal trajectories and to render the involved constants uniform in the horizon, we henceforth assume that optimal trajectories are uniformly bounded in the horizon. As we will see later in our heat exchanger example, this property is verified. We comment on future research w.r.t. this assumption in Section 5.

Assumption 6. For any compact set of initial values X^0 , there is a compact set $K \subset \mathbb{R}^n$ such that for all horizons t_f , the corresponding optimal state of (phOCP) with initial datum $x^0 \in X^0$ and horizon t_f is contained in K, i.e.,

$$\forall (x^0, t_f) \in X^0 \times (0, \infty) :$$

 $\forall u^* optimal for (phOCP) : x(t; x^0, u^*) \in K \ \forall t \in [0, t_f]$

To prove the turnpike property we utilize the following notation for initial states that can first be steered to the manifold \mathcal{T} and then to the terminal set Ψ .

$$\mathcal{C}(\mathcal{T}, \Psi) := \{ x^0 \in \mathbb{R}^n \mid \exists t_1 \ge 0, u_1 \in L^{\infty}(0, t_1; \mathbb{U}) \text{ s.t. } x(t_1, u_1, x^0) \in \mathcal{T}, \\ \exists t_2 \ge 0, u_2 \in L^{\infty}(0, t_2; \mathbb{U}) \text{ s.t. } x(t_2, u_2, x(t_1, u_1, x^0)) \in \Psi \}$$

In the following, we denote by $x(\cdot, x^0, u)$ the trajectory emanating from an initial value $x^0 \in \mathbb{R}^n$ when applying a control $u \in L^{\infty}(0, T; \mathbb{R}^m)$. We first provide a result w.r.t. steady states in preparation of our turnpike theorem.

Lemma 7. Every thermodynamic equilibrium is a controlled steady state when choosing $u \equiv 0$, that is, for all $\bar{x} \in \mathcal{T}$

$$x(t; \bar{x}, 0) = \bar{x} \qquad \forall t \ge 0.$$

Proof. The proof immediately follows from the fact that the right-hand side of the dynamics (IPHS) vanishes when plugging in $(\bar{x}, 0)$.

We now state and prove the main result of this paper.

Theorem 8. Let Assumption 6 hold. Then (phOCP) has the integral manifold turnpike on $S_{tp} = \mathcal{C}(\mathcal{T}, \Psi)$ with respect to the manifold of thermodynamic equilibria \mathcal{T} .

Proof. Let (x^*, u^*) be an optimal state-control pair of (phOCP). Then, by optimality, any control $u \in L^{\infty}(0, t_f, \mathbb{U})$ with corresponding state trajectory $x = x(\cdot, u, x^0)$ satisfies

$$\int_0^{t_f} \ell_{\alpha_1,\alpha_2}(x^*(t), u^*(t)) dt \le \int_0^{t_f} \ell_{\alpha_1,\alpha_2}(x(t), u(t)) dt.$$

Abbreviating $R(x) := \gamma(x, H_x(x))\{S, H\}_J^2(x)$, invoking (6) on both sides of the above inequality and cancelling the terms depending on x^0 we obtain

$$\alpha_1 H(x^*(t_f)) + \alpha_2 T_0 \left(-S(x^*(t_f)) + \int_0^{t_f} R(x^*(t)) dt \right)$$

$$\leq \alpha_1 H(x(t_f)) + \alpha_2 T_0 \left(-S(x(t_f)) + \int_0^{t_f} R(x(t)) dt \right).$$

We now will construct a suitable control such that the right-hand side is bounded uniformly in t_f . To this end, by $x^0 \in \mathcal{C}(\mathcal{T}, \Psi)$, we get the existence of $t_1, t_2 > 0$ and corresponding controls u_1, u_2 that steer the initial state into the manifold and to the terminal region, respectively. W.l.o.g., we can assume that $t_f \geq t_1 + t_2$, as the turnpike inequality (8) is of purely asymptotic nature in the horizon and choose

$$u(t) := \begin{cases} u_1(t) & t \in [0, t_1] \\ 0 & t \in (t_1, t_f - t_2) \\ u_2(t - (t_f - t_2)) & t \in [t_f - t_2, t_f]. \end{cases}$$

Thus, using Lemma 7, we have $x(t, x^0, u) = \bar{x} \in \mathcal{T}$ for all $t \in (t_1, t_f - t_2)$. Hence, abbreviating $x(t) = x(t, x^0, u)$, we have

$$\int_0^{t_f} R(x(t)) dt = \int_0^{t_1} R(x(t)) dt + \int_{t_f - t_2}^{t_2} R(x(t)) dt \le c_1(t_1, t_2, u_1, u_2, x^0, \bar{x}).$$

Using non-negativity of the Hamiltonian from below we get

$$\int_0^{t_f} R(x^*(t)) dt \le \frac{1}{\alpha_2 T_0} \left(\alpha_1 H(x(t_f)) + c_1 \right) + ||l|| \left(||x^*(t_f)|| + ||x(t_f)|| \right)$$

Further, by uniform boundedness of the trajectories in the horizon t_f , cf. Assumption 6, we conclude

$$\int_0^{t_f} \gamma(x^*(t), H_x(x^*(t))) \{S, H\}_J^2(x^*(t)) dt = \int_0^{t_f} R(x^*(t)) dt \le c_2$$

with a constant $c_2 > 0$ independent of t_f . Denoting by c the constant appearing in the lower bound of the estimate in Lemma 5, we obtain

$$\int_0^{t_f} \operatorname{dist}\left(x^*(t), \mathcal{T}\right) \, \mathrm{d}t \le \frac{c_2}{c},$$

which is the turnpike property.

Remark 9 (Relation to optimal steady states). The steady-state problem corresponding to (phOCP) reads

$$\min_{(x,u)\in\mathbb{R}^n\times\mathbb{U}} (\alpha_1 y_H + \alpha_2 T_0 y_S)^\top u$$
s.t. $0 = \gamma \left(x, \frac{\partial H}{\partial x}\right) \left\{S, H\right\}_J J \frac{\partial H}{\partial x}(x) + g\left(x, \frac{\partial H}{\partial x}\right) u.$

It can be immediately seen that the choice u=0 leads to zero cost. Further, as the energy balance (6) also holds for steady states this problem is equivalent to

$$\begin{split} \min_{(x,u)\in\mathbb{R}^n\times\mathbb{U}} \alpha_2 T_0 \gamma \left(x,\frac{\partial H}{\partial x}\right) \left\{S,H\right\}_J^2 \\ \text{s.t. } 0 &= \gamma \left(x,\frac{\partial H}{\partial x}\right) \left\{S,H\right\}_J J \frac{\partial H}{\partial x}(x) + g\left(x,\frac{\partial H}{\partial x}\right) u. \end{split}$$

Any optimal control u has to have a cost of at most zero, which means by nonnegativity of the cost functional that $\alpha_2 T_0 \gamma\left(x, \frac{\partial H}{\partial x}\right) \left\{S, H\right\}_J^2 = 0$, i.e, the optimal state is contained in \mathcal{T} . Hence, in order to be feasible, the corresponding optimal control has to satisfy $g(x, \frac{\partial H}{\partial x})u = 0$. Thus, the set of optimal steady states is given by

$$\{(x, u) \in \mathcal{T} \times \mathbb{U} \mid g(x, H_x(x))u = 0\}.$$

4. Set-point transition for a heat exchanger

In this part, we present a numerical case study for the heat exchanger from Subsection 2.1 with entropy flow control (4) to illustrate the manifold turnpike result of Theorem 8. We note that, here, the manifold of thermodynamic equilibria is actually a subspace as $\{S, H\}_J(x) = T_1(S_1) - T_2(S_2)$ and thus

$$\mathcal{T} = \{(S_1, S_2) : T_1(S_1) = T_2(S_2)\} = \{(S_1, S_2) : S_1 = S_2\}$$

where the last equality follows from the injectivity of the exponential function that defines the temperature-entropy relation.

In this part, we set $T_{\text{ref}} = c_1 = c_2 = 1$ and $S_{\text{ref}} = 0$ and obtain the temperature-entropy relation $T_i = e^{S_i}$, i = 1, 2.

We consider the control constraint set $\mathbb{U} = [-10, 10]$ and aim to perform a state

transition within two thermodynamical equilibria: $T_1^0 = T_2^0 = 1$ and $T_1^{t_f} = T_2^{t_f} = 20$. In terms of the optimal control problem (phOCP), this corresponds to the initial value in entropy variables $x^0 = \begin{pmatrix} 0 & 0 \end{pmatrix}^\top$ and the terminal set $\Psi = \left\{ \begin{pmatrix} \ln 20 & \ln 20 \end{pmatrix}^\top \right\}$, by means of the relation $T_i = e^{S_i}$, i = 1, 2.

It is clear that the state transition is only possible through providing heat — or, equivalently, entropy — to the first compartment, cf. Figure 1.

In Figure 2, we observe the distance of optimal state trajectories to the set of thermodynamic equilibria. We can not steer the system from initial to terminal state on this set, as by the form of the input vector in (4), no control action that is non-zero leaves \mathcal{T} invariant. However, for increasing time horizons, the state trajectories remain closer and closer to the manifold, as the necessary control action, that is, the entropy flow, can be chosen smaller and smaller. Furthermore, we observe a turnpike behavior of the control towards zero as this is the only control that leaves the set of thermodynamic equilibria invariant, cf. Remark 9. The states, i.e., the individual entropies in the compartments depicted in the upper plot of Figure 2 indicate a velocity turnpike, cf. [6, 20], that is, their velocity is constant for the majority of the time interval. This can be explained as the Poisson bracket is mostly constant and small — the state has a turnpike towards the manifold — and the control is mostly constant and small — the zero control is the only control that leaves this manifold invariant — and thus the dynamics (IPHS) imply that $\dot{x}_1 = \dot{S}_1 \approx \text{const.}$ and $\dot{x}_2 = \dot{S}_2 \approx \text{const.}$.

We depict the corresponding quantitites extensive variable $H_x(S_1, S_2) = (T_1, T_2)$ in Figure 3. Here, we observe—due to the algebraic relation $T = \exp(S)$ —an exponential behaviour in the upper plot of Figure 3. In the lower plot, we can observe that, the

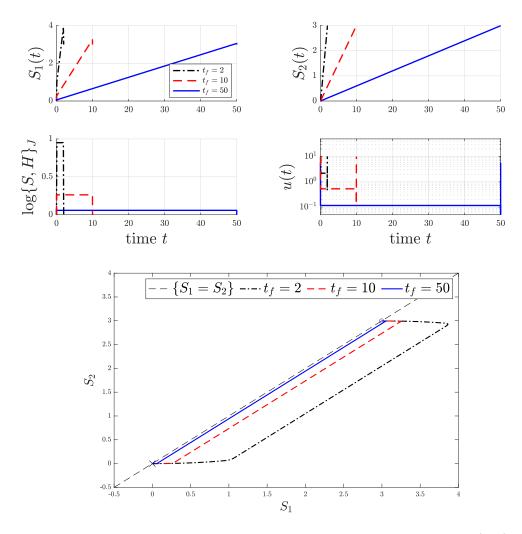


FIGURE 2. Depiction of the optimal intensive variable S over time (top) and in phase space (bottom).

temperature is moving further and further away from the subspace. The reason is that, by means of the turnpike property, we have an optimal rate of travel in the state variable, that is, e.g. for the first compartment, const. = $\dot{S}_1 = \frac{T_1 - T_2}{T_1}$. For increasing temperatures T_1 , the latter fraction can only be constant if also $T_1 - T_2$ increases.

5. Discussion and conclusion

This paper considered optimal state transitions for irreversible port-Hamiltonian systems with minimal supply of energy, entropy, or exergy. We proved a manifold turnpike property w.r.t. the set of thermodynamical equilibria. Moreover, we numerically illustrated our findings drawing upon the example of a heat exchanger.

Future research will consider the relaxation of Assumption 6 used for proving the turnpike theorem. To this end, we aim to show sufficient conditions via a refined argument using optimality, dissipativity, and properties of the input vector field. Put differently,

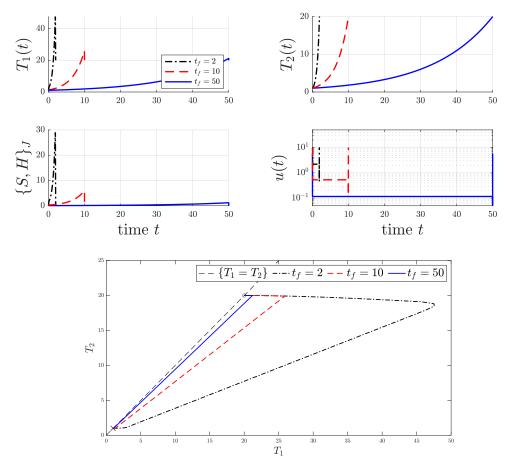


FIGURE 3. Depiction of the optimal extensive variable $T = H_x$ over time (top) and in phase space (bottom).

we will investigate the lack of forward invariance of the manifold of thermodynamic equilibria which is related to $g(x, H_x) \notin T_x \mathcal{T}$ where $T_x \mathcal{T}$ is the tangent space of the manifold \mathcal{T} at x.

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Appendix – Proof of Lemma 5

We will first prove that

(9)
$$c\|x_1 - x_2\| \le \left\| \frac{\partial H}{\partial x}(x_1) - \frac{\partial H}{\partial x}(x_2) \right\| \le C\|x_1 - x_2\|$$

holds for all $x_1, x_2 \in K$. To show the second inequality, we compute

$$||H_x(x_1) - H_x(x_2)|| \le \left(\sup_{\xi \in \text{conv}(K)} ||H_{xx}(\xi)||\right) \cdot ||x_1 - x_2||$$

= $C||x_1 - x_2||$,

where $\operatorname{conv}(K)$ denotes the convex hull of K. For the first inequality of (9) we note that the inverse $[H_{xx}(x)]^{-1}$ is continuous and thus in particular bounded on the compact set $H_x^{-1}(\operatorname{conv}(H_x(K)))$. Hence, for $z_1, z_2 \in H_x(K)$ we have

$$\begin{aligned} & \|H_{x}^{-1}(z_{1}) - H_{x}^{-1}(z_{2})\| \\ & \leq \left(\sup_{\xi \in \text{conv}(\frac{\partial H}{\partial x}(K))} \|(H_{x}^{-1})'(\xi)\|\right) \|z_{1} - z_{2}\| \\ & = \left(\sup_{\xi \in \text{conv}(H_{x}(K))} \|[H_{xx}(H_{x}^{-1}(\xi))]^{-1}\|\right) \|z_{1} - z_{2}\| \\ & = c^{-1} \|z_{1} - z_{2}\|, \end{aligned}$$

which is equivalent to $||H_x(x_1) - H_x(x_2)|| \ge c||x_1 - x_2||$. This proves (9). Now, for $x, v \in \mathbb{R}^n$ we have $|v^\top x| = ||v|| \operatorname{dist}(x, v^\perp)$ and therefore

$$\begin{aligned} \left| \{ S(x), H(x) \}_J \right| &= |H_x(x)^\top J l| = ||J l| \operatorname{dist} \left(H_x(x), (J l)^\perp \right) \\ &= ||J l| \inf_{z \in (J l)^\perp} ||H_x(x) - z|| \\ &= ||J l| \inf_{z \in (J l)^\perp} \left| |H_x(x) - H_x(H_x^{-1}(z))| \right|. \end{aligned}$$

Hence, by (9),

$$\left| \{ S(x), H(x) \}_J \right| \le C \inf_{z \in (Jl)^{\perp}} \|x - H_x(x)^{-1}(z)\|$$
$$= C \inf_{w \in \mathcal{T}} \|x - w\| = C \operatorname{dist}(x, \mathcal{T})$$

and

$$\left| \{ S(x), H(x) \}_J \right| \ge c \inf_{z \in (JI)^{\perp}} \| x - H_x(x)^{-1}(z) \|$$

= $c \inf_{w \in \mathcal{T}} \| x - w \| = c \operatorname{dist}(x, \mathcal{T}).$

The claim now follows from the fact that γ is continuous and positive and K is compact.