Stability Analysis of Thermodynamic Systems: Heat Conduction in Solids ⋆

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Abstract: This paper addresses the fundamental difference between equilibria of thermodynamic systems and equilibria of autonomous state space systems. The notion of stability of thermodynamic equilibria is analyzed in terms of an entropy generating function that classifies as a Lyapunov function to prove asymptotic stability of thermal equilibria. The stability analysis is performed for both finite and infinite dimensional systems. It is shown how the proposed Lyapunov function naturally extends to assess stability of interconnected thermal systems. A number of examples is given to demonstrate the time evolution of the Lyapunov function.

Keywords: Thermal stability, Lyapunov functions, Thermal equilibria.

1. INTRODUCTION

The understanding of thermal behaviour plays an increasingly important role to further enhance performance of high-precision systems. In particular, the compensation of thermally induced deformations of materials are among the most important challenges in lithographic machines, electron microscopes and in technical metrology. Although many methods and tools van den Hurk et al. (2018) have been developed for the modeling, simulation and controller synthesis of multi-physical systems, a rigorous integration of first principle thermal features in multi-physics models is often lacking. First principle methods are among the key tools to explicitly describe energy flows, heat transfers, and energy conversions among different components, different subsystems or different physical domains.

At the abstract level, conservation laws and energy functions are often used to prove stability of equilibria of systems, to analyze their behavior, and for purposes of control and optimization. The role of Lyapunov functions in autonomous systems, together with their generalizations in the direction of open dynamical systems, passive and dissipative dynamical systems, bond-graph theory and port-Hamiltonian systems are fundamental in modern systems theory Khalil (2002); Willems (1972a,b). The essence of these frameworks lies in the observation that the efficiency of many physical processes is limited by their energy storage and the amount of energy that has been supplied by its environment. Indeed, Carnot's principle claims the limited efficiency of heat engines; in Hamiltonian and Lagrangian mechanics, the recoverable energy is always bounded by the Hamiltonian or Lagrangian function; in an ideal reversible thermodynamical process, all heat can be converted into work.

In the last decades, non-equilibrium thermodynamics has been developed as a research field, aimed at describing

physics of thermal processes beyond and away from thermodynamic equilibrium. In particular, it aims at incorporating the time-course of intensive variables such as temperature and pressure and to generalize the concept of entropy to thermal states that are not in equilibrium. Starting with Onsager's reciprocal relations Onsager (1931a,b) in 1931, important contributions on non-equilibrium thermodynamics have been made by Denbigh Denbigh (1951) on steady state principles, De Groot's work on linear irreversible processes De Groot (1952); De Groot and Mazur (1962) and Prigogine's minimum entropy production principle Prigogine (1947) that has been extended to the theory of entropy generation minimization by Bejan Bejan (1996). This theory claims that the maximum efficiency of a thermodynamic system is achieved while the dissipated energy is minimal.

For many applications, quadratic Lyapunov functions have been widely used to provide insight in the qualitative behavior of systems. Although in Delvenne and Sandberg (2017), a quadratic function of temperature is proposed to satisfy Lyapunov stability criteria, these functions do not naturally inherit the energy attributes of thermodynamic systems. In In this paper, we propose an alternative function, directly related to entropy increase, to prove stability properties of thermal systems that are away from their thermodynamic equilibrium.

The main contributions of this work can be summarized as follows: (1) We formally distinguish between the concept of an equilibrium of a dynamical system described by differential equations and a thermal equilibrium of a thermodynamic system. We show that not every equilibrium is a thermodynamic equilibrium. (2) We propose a physically relevant Lyapunov function, which characterizes thermal dissipation by entropy generation. It is shown that this function characterizes the Lyapunov stability of any thermodynamic equilibrium. (3) We show the usage of this function for both distributed and lumped thermodynamic models describing thermal conduction.

The paper is organized as follows. Section 2 introduces a number of fundamental concepts of quasi-static and time-dependent thermodynamics. These include entropy balance (second law of thermodynamics), and the definition of thermal equilibria. In Section 3, we give the derivation of the physical relevant Lyapunov function and the corresponding stability analysis for both infinite-dimensional and finite-dimensional systems. In Section 4, some simulation results are given to validate the equilibrium analysis and the stability analysis based on the proposed Lyapunov function. Conclusions are given in Section 5.

We first give some notational conventions that will be used in the paper. The col operator stacks its arguments in a column vector as in $x = \mathrm{col}(x_1, \cdots, x_n)$. ∇ is the gradient operator with $\nabla u := \mathrm{col}(\frac{\partial u}{\partial x_i} \mid i = 1, \ldots, n)$ for a differentiable function $u : \mathbb{R}^n \to \mathbb{R}$. Its divergence $\nabla \cdot u = \sum_{i=1}^{n} \frac{\partial u}{\partial x_i}$ and its Laplacian $\nabla^2 u = \nabla \cdot (\nabla u) = \sum_{i=1}^{n} \frac{\partial^2 u}{\partial x_i^2}$. The directional derivative $\frac{\partial u}{\partial \bar{n}} = \nabla u \cdot \bar{n}$.

A real-valued continuously differentiable function $V : \mathcal{G} \to \mathbb{R}$ is *positive definite* on a neighborhood $\mathcal{G}$ of x^* if $V(x^*) = 0$ and $V(x) > 0$ for any $x \neq x^*$ in $\mathcal{G}$. If it satisfies $V(x) \geq 0$ for any $x \neq x^*$ in $\mathcal{G}$, then V is said to be *positive semidefinite*. A function $\alpha : [0, a) \to \mathbb{R}_+ = [0, \infty)$ is of class $\mathcal{K}$ if it is continuous, strictly increasing, and $\alpha(0) = 0$.

2. THERMODYNAMICS FUNDAMENTALS

This section briefly reviews a number of classical concepts from thermodynamics and proceeds with quasi-static processes so as to incorporate the time evolution of intensive variables. Furthermore, the concept of entropy, together with the second law of thermodynamics, is presented.

Following the authoritative work of Callen (1998), a (macroscopic homogeneous) thermodynamic system is described by *extensive* and *intensive* variables whose behavior is a subset

$$\mathcal{T} \subset \mathcal{X}^{ext} \times \mathcal{X}^{int} \qquad (1)$$

where the extensive variables

$$x^{\mathrm{ext}} = \mathrm{col}(U, S, V, N_1, \cdots, N_r) \in \mathcal{X}^{\mathrm{ext}}$$

consist of internal energy U, entropy S, volume V and the mole numbers N_i of the r constituent chemical components. The intensive variables

$$x^{\mathrm{int}} = \mathrm{col}(T, P, \mu_i, \cdots, \mu_r) \in \mathcal{X}^{\mathrm{int}}$$

consist of temperature T, pressure P and the electrochemical potentials μ_i of each component. The extensive variables x^{ext} define the thermodynamic equilibria and are related either by an *energetic fundamental relation*

$$U = U(S, V, N_1, \cdots, N_r) \qquad (2)$$

or an *entropic fundamental relation*

$$S = S(U, V, N_1, \cdots, N_r). \qquad (3)$$

Either of these relations define the intensive variables x^{int} through the partial derivatives

$$T := \frac{\partial U}{\partial S}, \quad P := -\frac{\partial U}{\partial V}, \quad \mu_i := \frac{\partial U}{\partial N_i}. \qquad (4)$$

See Callen (1998); Sandler (2017). The first law of thermodynamics claims the preservation of internal energy is expressed by Gibbs' equation. A similar expansion applies to the entropic representation and reads

$$dS = \frac{1}{T}dU + \frac{P}{T}dV - \sum_{i=1}^{r} \frac{\mu_i}{T}dN_i. \qquad (5)$$

Under the assumption that x^{ext} and x^{int} represent a *quasi-static process* consisting of an ordered succession of equilibrium states Callen (1998); Landsberg (1956), we may derive the time evolution of state variables from Gibbs' relation according to

$$\frac{dU}{dt} = T\frac{dS}{dt} - P\frac{dV}{dt} + \sum_{i=1}^{r} \mu_i \frac{dN_i}{dt}. \qquad (6)$$

The time evolution of the balance equation may be viewed as an extension of the first law of thermodynamics to non-equilibrium state, introduced in Demirel and Sandler (2004). A wide range of macroscopic systems has been studied in this context. See, e.g., De Groot and Mazur (2013); Kuiken and Kuiken (1994); Fitts (1962); Denbigh (1951); Prigogine (1947); Keizer (1978).

2.1 Entropy generation

According to the fundamental postulate of thermodynamics De Groot and Mazur (2013), the entropy change of a system can be decomposed according to

$$\frac{dS_{sys}}{dt} = \frac{dS_e}{dt} + \frac{dS_i}{dt}, \qquad (7)$$

where S_e is the entropy production from its surrounding across the external boundary of the system and dS_i denotes the entropy production due to processes in the interior of the system. The change in the entropy of a system is associated with the heat flow and the mass flow but not the work flow $P\frac{dV}{dt}$ Sandler (2017). Irreversibility is the difference between reversible work and actual work and leads to a net increase in entropy. Specifically, we have the following entropy balance equation

$$\frac{dS_{sys}}{dt} = \sum_{i=1}^{N} \dot{m}_i \hat{s}_i + \frac{\dot{Q}}{T} + S_{gen}, \qquad (8)$$

where $\dot{m}_i$ denotes the net rate of the ith mass flow into or out of the system and $\hat{s}_i$ is the entropy per unit mass. $\dot{Q}/T$ represents the rate of entropy flow due to the heat flow across the boundary and S_{gen} characterizes the internal entropy generation within the system (7). The entropy generation rate is

$$S_{gen} = \frac{dS_i}{dt}. \qquad (9)$$

It is important to remark that $S_{gen} = 0$ for reversible processes, while $S_{gen} > 0$ for irreversible processes.

2.2 Thermodynamic equilibria

In this paper we distinguish between thermodynamic equilibria and an equilibria (or fixed points) of autonomous differential equations. In order to avoid confusion in the sequel, $(\cdot)^\star$ denotes the thermodynamic equilibrium and we refer the $(\cdot)^*$ to the equilibrium in the sense of system theory.

A thermodynamic equilibrium is defined by Sandler (2017) as a state $x = \mathrm{col}(x^{\mathrm{ext}}, x^{\mathrm{int}})$ that (1) does not vary

with time; (2) is spatially uniformly distributed, e.g., without temperature or pressure gradients; (3) causes no flow of heat, mass, or work between the system and its surroundings; (4) causes the net rate of all chemical reactions to be zero.

The first requirement demands a state variable at equilibrium $x^\star$ in (6) to be time-independent:

$$x^\star \in \mathcal{X}^{ext} \times \mathcal{X}^{int} \implies \frac{\mathrm{d}x^\star}{\mathrm{d}t} = 0. \qquad (10)$$

The second requirement imposes a *consensus constraint*, addressed by Olfati-Saber and Murray (2004) and Callen (1998), which states that the equilibrium is uniformly established at all compartments of a composite system. This phenomenon is known as the *equipartition of energy*, that was elaborated by Bernstein and Hyland (1993), Lyon (1975),Pearson and Johnson (1987), requires a uniform spatial distribution of state variables in thermodynamic equilibrium:

$$x^\star \in \mathcal{X}^{ext} \times \mathcal{X}^{int} \implies \nabla x^\star = 0. \qquad (11)$$

The third condition states that

$$x^\star \in \mathcal{X}^{ext} \times \mathcal{X}^{int} \implies \nabla x^\star \cdot \bar{n} = 0 \text{ on } \partial\mathcal{G} \qquad (12)$$

where $\partial\mathcal{G}$ denotes the boundary of the geometry of the system and $\bar{n}$ is an outward pointing unit vector at the boundary. The fourth condition establishes the chemical equilibrium Smith (1950) $\sum_{i=1}^{r} \mu_i^\star v_i^\star = 0$ where v_i denote the stoichiometric coefficients.

Definition 1. For a dynamic system $\dot{x} = f(x,t)$ defined on a geometric domain $\mathcal{G}$, let $\nabla x \cdot \bar{n}$ be constant on the boundary $\partial\mathcal{G}$. A point $x^\star$ is in *thermodynamic equilibrium* (in the absence of chemical reactions) if

(1) it is time-invariant: $\frac{dx^\star}{dt} = 0$,
(2) it satisfies the equipartition property $\nabla x^\star = 0$,
(3) it is independent of interaction across the boundary $\nabla x^\star \cdot \bar{n} = 0$ on $\partial\mathcal{G}$.

For (autonomous) dynamical systems described by ordinary differential equations, an *equilibrium point* is a constant solution to the differential equation. This only meets the first requirement in Definition 1. In particular, a dynamical system can still be at equilibrium while the inflow rate is equal to the outflow rate. Hence, a dynamical system can be at equilibrium without being at thermodynamic equilibrium if (2) or (3) are not satisfied. See Fig. 1 for an illustration of the various requirements.
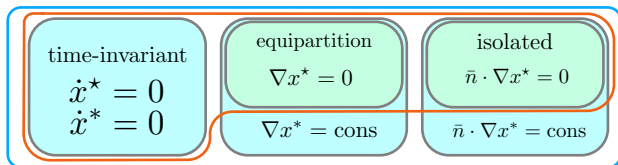

Fig. 1. A set of equilibrium x^* (blue frame) and its subset of thermodynamic equilibrium $x^\star$ (red frame).

3. STABILITY OF THERMODYNAMIC SYSTEMS

In this section, we analyse the stability of thermodynamic equilibria. For an example of thermal conduction in a system described by partial differential equations, we present a Lyapunov function that warrants stability of a

thermodynamic equilibrium. A similar example is given in the second subsection for a system described by ordinary differential equations.

3.1 Equilibria in distributed systems

Consider a model of 1-dimensional thermal conduction in a solid, as depicted in Fig. 2, whose governing equation, boundary conditions and initial condition are given by
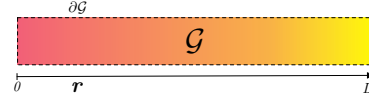

Fig. 2. Heat conduction in a solid with geometry $\mathcal{G}$ and boundary $\partial\mathcal{G}$ (dashed line).

$$\rho C_{\mathrm{p}} \frac{\partial T}{\partial t} + \nabla \cdot J = 0 \quad \text{in } \mathcal{G}, \qquad (13a)$$
$$\nabla T(r,t) \cdot \bar{n} = \gamma \qquad \text{on } \partial\mathcal{G}, \qquad (13b)$$
$$T(r,0) = T_0(r) \qquad \text{at initial time } t = 0. \qquad (13c)$$

Here, $T : \mathcal{G} \times \mathbb{R}_{\geq 0} \to \mathbb{R}_{>0}$ is an analytic function of the 1-dimensional domain $\mathcal{G}$ that represents temperature. The heat flux $J(r) := -\kappa \nabla T(r)$, $r \in \mathcal{G}$ where $\kappa > 0$ represents the heat transfer coefficient. Density and heat capacity of the solid are defined by ρ and C_{p}, respectively. The case where $\gamma = 0$ corresponds to an isolated system. We assume a time-independent non-positive constant γ. For every time instance $t \geq 0$, the temperature $T(\cdot,t)$ is assumed to be a mapping from $\mathcal{G}$ to $\mathbb{R}_{>0}$. The set of all such mappings is denoted by $\mathcal{D}$. With a given initial condition $T_0 \in \mathcal{D}$ and γ defined on $\partial_\mathcal{G}$, we will assume that $T(r,t)$, with $r \in \mathcal{G}$, $t \geq 0$ is uniquely defined by (13).

Let $\mathcal{D}$ be equipped with an inner product

$$\langle T_1, T_2 \rangle := \int_\mathcal{G} T_1(r)T_2(r) \,\mathrm{d}r \qquad (14)$$

where $T_1, T_2 \in \mathcal{D}$. Then $(\mathcal{D}, \langle \cdot, \cdot \rangle)$ becomes an inner product space with induced norm $\|T\| := \sqrt{\langle T, T \rangle}$. The entropy balance equation then reads

$$\dot{S}_{sys} = \boxed{-\int_{\partial\mathcal{G}} \nabla \cdot \frac{J(r)}{T(r)} \,\mathrm{d}r} + \boxed{\int_\mathcal{G} J(r) \cdot \nabla \frac{1}{T(r)} \,\mathrm{d}r}.$$

The first term represents the entropy flux across the boundary. The second term denotes the entropy generation within the system, that we will propose as candidate Lyapunov function. Let $S_{gen} : \mathcal{D} \to \mathbb{R}$ be defined as

$$S_{gen}(T) = \int_\mathcal{G} J(r) \cdot \nabla \frac{1}{T}(r) \,\mathrm{d}r = -\kappa \int_\mathcal{G} \nabla T \cdot \nabla \frac{1}{T(r)} \,\mathrm{d}r$$
$$\stackrel{\text{def}}{=} \kappa \|\nabla(\ln T)\|^2. \qquad (15)$$

Thus, $S_{gen}(T)$ is a positive semidefinite function on $\mathcal{D}$. Equilibrium solutions T^* of (13a) satisfy $\kappa \nabla^2 T^* = 0$ and therefore have constant gradient ∇T^*. This means that $S_{gen}(T^*)$ not necessarily vanishes at equilibria T^*. In particular, S_{gen} is not strict positive definite on a neighborhood of T^*.

Theorem 1. Let $\mathbb{E}$ denotes the set of all thermodynamic equilibrium points of the system (13). Then any $T^\star \in \mathbb{E}$ is Lyapunov stable. Moreover, the function $S_{gen} : \mathcal{D} \to \mathbb{R}$ defined by (15) is a Lyapunov function in the sense that

S_{gen} is positive definite on a neighborhood of T^* in $\mathcal{D}$ and $\dot{S}_{gen}(T) \leq 0$ for all $T \in \mathcal{D}$.

Proof. Let $T^\star \in \mathbb{E}$ and consider S_{gen} defined in (15). Then $S_{gen}(T) \geq 0$ and since $T^\star$ satisfies (11), it follows from (15) that $S_{gen}(T^\star) = 0$. S_{gen} is therefore positive definite on a neighborhood of $T^\star$. Using the chain rule, the time derivative $\dot{S}_{gen}(T)$ of $S_{gen}(T(r,t))$ along solutions of (13) is given by

$$\dot{S}_{gen}(T) = -\kappa \int_{\mathcal{G}} \left[(\frac{\partial}{\partial t}\nabla T)\cdot\nabla\frac{1}{T} + \nabla T\cdot(\frac{\partial}{\partial t}\nabla\frac{1}{T}) \right] \mathrm{d}r$$
$$= -\kappa \int_{\mathcal{G}} \left[\nabla\dot{T}\cdot\nabla\frac{1}{T} + \nabla T\cdot\nabla(\frac{\partial}{\partial t}\frac{1}{T}) \right] \mathrm{d}r. \quad (16)$$

Using integration by parts it follows that

$$\nabla\dot{T}\cdot\nabla\frac{1}{T} = \nabla\cdot(\dot{T}\nabla\frac{1}{T}) - \dot{T}\nabla^2\frac{1}{T}, \quad (17)$$

$$\nabla T\cdot\nabla(\frac{\partial}{\partial t}\frac{1}{T}) = \nabla\cdot(\frac{\partial}{\partial t}\frac{1}{T}\nabla T) - \frac{\partial}{\partial t}\frac{1}{T}\nabla^2 T. \quad (18)$$

Substitute (17),(18) in (16) to infer that

$$\dot{S}_{gen}(T) = -\kappa \int_{\mathcal{G}} \left[\nabla\cdot(\frac{\partial}{\partial t}\frac{1}{T}\nabla T) + \nabla\cdot(\dot{T}\nabla\frac{1}{T}) \right. $$
$$\left. - \dot{T}\nabla^2\frac{1}{T} - (\frac{\partial}{\partial t}\frac{1}{T})\nabla^2 T \right] \mathrm{d}r. \quad (19)$$

After applying the divergence theorem, the first three terms at the right-hand side of (19) can be rewritten as

$$-\kappa \int_{\mathcal{G}} \left[\nabla\cdot(\frac{\partial}{\partial t}\frac{1}{T}\nabla T) + \nabla\cdot(\dot{T}\nabla\frac{1}{T}) - \dot{T}\nabla^2\frac{1}{T} \right] \mathrm{d}r$$
$$= -\kappa \int_{\partial\mathcal{G}} [\frac{\partial}{\partial t}\frac{1}{T}\nabla T + \dot{T}\nabla\frac{1}{T}]\cdot\bar{n}\mathrm{d}\bar{r} + \kappa \int_{\mathcal{G}} \dot{T}\nabla\cdot(\nabla\frac{1}{T})\,\mathrm{d}r$$
$$= \kappa \int_{\partial\mathcal{G}} \frac{2}{|T|^2}\dot{T}\nabla T\cdot\bar{n}\,\mathrm{d}\bar{r} - \kappa \int_{\mathcal{G}} \dot{T}\nabla\cdot(\frac{1}{|T|^2}\nabla T)\,\mathrm{d}r$$
$$= \kappa \int_{\partial\mathcal{G}} \frac{1}{|T|^2}\dot{T}\nabla T\cdot\bar{n}\,\mathrm{d}\bar{r}. \quad (20)$$

which vanish because of the boundary condition (13b). The derivative (19) is therefore equal to

$$\dot{S}_{gen}(T) = \kappa \int_{\mathcal{G}} (\frac{\partial}{\partial t}\frac{1}{T})\nabla^2 T\,\mathrm{d}r = -\kappa \int_{\mathcal{G}} \frac{1}{|T|^2}\dot{T}\nabla^2 T\,\mathrm{d}r.$$

By substituting the model equation (13a) this gives

$$\dot{S}_{gen}(T) = -\frac{\kappa^2}{\rho C_\mathrm{p}}\|\frac{\nabla^2 T}{T}\|^2. \quad (21)$$

It follows that $\dot{S}_{gen}(T) \leq 0$ for all $T \in \mathcal{D}$ and $\dot{S}_{gen}(T^\star) = 0$. Conclude that S_{gen} is a Lyapunov function proving Lyapunov stability of $T^\star \in \mathbb{E}$. $\square$

Theorem 1 proves stability of thermodynamic equilibrium points of (13), not their asymptotic stability. Indeed, the set $\mathbb{E}$ generally does not consist of isolated equilibrium points, which means that $\dot{S}_{gen}$ is not negative definite in an open neighborhood of $T^\star \in \mathbb{E}$. The following result establishes uniform asymptotic stability to the set $\mathbb{E}$. For this, let the distance between $T \in \mathcal{D}$ and the set $\mathbb{E}$ of thermodynamic equilibria of (13) be defined by

$$\mathrm{dist}(T, \mathbb{E}) := \inf_{T^\star \in \mathbb{E}} \|T - T^\star\|^2.$$

Theorem 2. Let $\mathbb{E}$ denote the set of all thermodynamic equilibrium points of the system (13). Then $\mathbb{E}$ is uniformly asymptotically stable in the sense that $\lim_{t\to\infty}\mathrm{dist}(T,\mathbb{E}) = $

0 for any solution T of (13). In particular, there exist functions $\alpha_1, \alpha_2, \alpha_3$ of class $\mathcal{K}$ such that

$$\alpha_1(\mathrm{dist}(T, \mathbb{E})) \leq S_{gen}(T) \leq \alpha_2(\mathrm{dist}(T, \mathbb{E}))$$
$$\dot{S}_{gen}(T) \leq -\alpha_3(\mathrm{dist}(T, \mathbb{E}))$$

for all $T \in \mathcal{D}$.

Proof. This proof follows a similar reasoning as in [114, Theorem 4.1] Khalil (2002). The difference is that the upper and lower bound on S_{gen} are measures of $\mathrm{dist}(T, \mathbb{E})$. We claim that the distance from $T \in \mathcal{D}$ to the set $\mathbb{E}$ of thermodynamic equilibria is $\mathrm{dist}(T, \mathbb{E}) = \|\nabla T\|^2$. For $1 \leq T < \infty$ and $\kappa > 0$ we have

$$S_{gen}(T) = \kappa\|\frac{\nabla T}{T}\|^2 \leq \kappa\bar{\nu}^2\|T\|^2 = \alpha_2(\mathrm{dist}(T, \mathbb{E}))$$

where $0 < \sup_{1\leq T<\infty} T^{-1} = \bar{\nu} \leq 1$. Similarly, for the lower bound, we have

$$S_{gen}(T) = \kappa\|\frac{\nabla T}{T}\|^2 \geq \kappa\underline{\nu}^2\|\nabla T\|^2 = \alpha_1(\mathrm{dist}(T, \mathbb{E}))$$

where $0 < \inf_{1\leq T<\infty} T^{-1} = \underline{\nu} \leq 1$. By construction, $\alpha_1(\mathrm{dist}(T^\star, \mathbb{E})) = \alpha_1(0) = 0$ and $\alpha_2(\mathrm{dist}(T^\star, \mathbb{E})) = \alpha_2(0) = 0$. Next, we claim for all real positive $\rho C_\mathrm{p} \in \mathbb{R}_{>0}$,

$$\dot{S}_{gen} = -\frac{\kappa^2}{\rho C_\mathrm{p}}\|\frac{\nabla^2 T}{T}\| \leq -\frac{\kappa^2}{\rho C_\mathrm{p}}\|\nabla^2 T\underline{\nu}\|^2 \quad (22)$$
$$= -\frac{\nu^2\kappa^2}{\rho C_\mathrm{p}}\|\nabla^2 T\|^2 \leq -\frac{\nu^2\kappa^2\lambda}{\rho C_\mathrm{p}}\|\nabla T\|^2.$$

We prove this claim as follows. Using integration by parts, $\|\nabla T\|^2$ infers

$$\int_{\mathcal{G}} \nabla T \cdot \nabla T\,dr = -\int_{\mathcal{G}} T\cdot\nabla^2 T\,dr + \int_{\mathcal{G}} \nabla\cdot(T\,\nabla T)dr$$
$$\leq -\int_{\mathcal{G}} T\cdot\nabla^2 T\,dr + \gamma\max\{T(0),T(L)\}$$
$$\leq \int_{\mathcal{G}} -T\cdot\nabla^2 T\,dr. \quad (23)$$

Notice that the $\gamma\max\{T(0),T(L)\} \leq 0$ is derived by the divergence theorem and the $\max\{T(0),T(L)\}$ denotes the highest boundary temperature. Using Holder's inequality, (23) can be rewritten as

$$\int_{\mathcal{G}} \nabla T\,\nabla T\,dr \leq \int_{\mathcal{G}} -\nabla^2 T\,T\,dr$$
$$\leq \left(\int_{\mathcal{G}} |-\nabla^2 T|^2 dr\right)^{\frac{1}{2}}\left(\int_{\mathcal{G}} |T|^2 dr\right)^{\frac{1}{2}}.$$

We note that for the given boundary condition (13b), there exist such an eigenvalue

$$\lambda = \min_{T\in\mathcal{D},T\neq 0} \frac{\int_{\mathcal{G}} |\nabla T|^2 dr}{\int_{\mathcal{G}} |T|^2 dr} \geq 0. \quad (24)$$

(See Evans (2010)). Consequently, we have

$$\|\nabla T\|^2 \leq \lambda^{-1}\|\nabla^2 T\|^2. \quad (25)$$

By substituting the (25) into (22), we prove the claim

$$\dot{S}_{gen} \leq -\frac{\nu^2\kappa^2\lambda}{\rho C_\mathrm{p}}\|\nabla T\|^2 = -\alpha_3(\mathrm{dist}(T, \mathbb{E})).$$

Therefore, $\dot{S}_{gen} \leq -\alpha_3(\mathrm{dist}(T, \mathbb{E}))$ for a function α_3 of class $\mathcal{K}$ is proved. $\square$

3.2 Equilibria in lumped composite systems

Consider a spatial partitioning of the geometry $\mathcal{G}$ depicted in Fig. 2, leading to the composite system shown in Fig. 3 with two disjoint geometries $\mathcal{G}_1$ and $\mathcal{G}_2$.
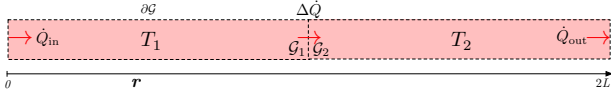

Fig. 3. Composite system of two compartments: $\mathcal{G}_1 \cup \mathcal{G}_2$.

In this formulation, the system dynamics of the two components are described by

$$\rho_1 C_{\mathrm{p}_1} \dot{T}_1(t) = \dot{Q}_{\mathrm{in}} - \Delta\dot{Q} \quad \text{in } \mathcal{G}_1, \tag{26a}$$

$$\rho_2 C_{\mathrm{p}_2} \dot{T}_2(t) = \Delta\dot{Q} - \dot{Q}_{\mathrm{out}} \quad \text{in } \mathcal{G}_2 \tag{26b}$$

with initial conditions $T_1(0) = T_{0,1}, T_2(0) = T_{0,2}$. Here $\Delta\dot{Q}$ denotes the rate of heat flow between $\mathcal{G}_1$ and $\mathcal{G}_2$, represented by Fourier's law $\Delta\dot{Q} = \kappa(T_1 - T_2)$ where $\kappa > 0$. The density and the specific heat capacity of each subsystem are given by ρ_i and C_{p_i}, $i = 1, 2$, respectively. The rate of heat inflow to $\mathcal{G}_1$ is denoted by $\dot{Q}_{\mathrm{in}}$, the rate of heat outflow from $\mathcal{G}_2$ is $\dot{Q}_{\mathrm{out}}$.

From the governing equations, the entropy balance (7) can be derived by dividing (26) by T_1 and T_2. This gives

$$\rho_1 C_{\mathrm{p}_1} \frac{\dot{T}_1}{T_1} = \frac{\dot{Q}_{\mathrm{in}}}{T_1} - \frac{\Delta\dot{Q}}{T_1}, \quad \rho_2 C_{\mathrm{p}_2} \frac{\dot{T}_2}{T_2} = \frac{\Delta\dot{Q}}{T_2} - \frac{\dot{Q}_{\mathrm{out}}}{T_2}. \tag{27}$$

The left-hand sides of the equality in (27) can be rewritten as $\rho_i C_{\mathrm{p}_i} \frac{\dot{T}_i}{T_i} = \rho_i C_{\mathrm{p}_i} \frac{d}{dt}[\ln T_i(t)]$. This logarithmic form, also derived in Haddad et al. (2009), shares the form of Boltzmann's entropy formula. For the composite system, the first law of thermodynamics is obtained by adding the equations (26) which gives

$$\rho_1 C_{\mathrm{p}_1} \dot{T}_1 + \rho_2 C_{\mathrm{p}_2} \dot{T}_2 = \dot{Q}_{\mathrm{in}} - \dot{Q}_{\mathrm{out}}. \tag{28}$$

Similarly, the entropy balance in inferred by adding (27),

$$\frac{\mathrm{d}S_{sys}}{dt} = \frac{\mathrm{d}}{\mathrm{d}t}\left[\ln(\rho_1 C_{\mathrm{p}_1} \dot{T}_1) + \ln(\rho_2 C_{\mathrm{p}_2} \dot{T}_2)\right]$$

$$= \frac{\dot{Q}_{\mathrm{in}}}{T_1} - \frac{\dot{Q}_{\mathrm{out}}}{T_2} + S_{gen}(T_1, T_2) \tag{29}$$

where the entropy production is

$$S_{gen}(T_1, T_2) = \kappa\frac{(T_1 - T_2)^2}{T_1 T_2}. \tag{30}$$

In this derivation, we set $\dot{Q}_{\mathrm{in}} = \dot{Q}_{\mathrm{out}} = 0$ as an input-free system. Notice that $S_{gen}(T_1, T_2) \geq 0$. Taking the time derivative of S_{gen} along solutions (T_1, T_2) of (26) gives

$$\dot{S}_{gen}(T_1, T_2) = -\kappa\frac{(T_1^2 - T_2^2)(T_1\dot{T}_2 - T_2\dot{T}_1)}{T_1^2 T_2^2} \tag{31}$$

Substitute (26) to infer that

$$\dot{S}_{gen} = -\kappa^2\frac{(T_1 - T_2)^2(T_1 + T_2)}{T_1^2 T_2^2}\left(\frac{T_1}{\rho_2 C_{\mathrm{p}_2}} + \frac{T_2}{\rho_1 C_{\mathrm{p}_1}}\right). \tag{32}$$

This proves that S_{gen} is a Lyapunov function for the thermodynamic equilibria of the composite system.

Theorem 3. The set $\mathbb{E} = \{(T_1, T_2) \mid T_1 = T_2\}$ are the thermodynamic equilibrium points of the system (26). Any $(T_1^\star, T_2^\star) \in \mathbb{E}$ is Lyapunov stable. Moreover, the function S_{gen} defined in (30) is a Lyapunov function.

Next, we derive the equivalent of Theorem 2 for the composite system. Let

$$\mathrm{dist}((T_1, T_2), \mathbb{E}) := \inf_{(T_1^\star, T_2^\star)\in\mathbb{E}} \omega_1(T_1 - T_1^\star)^2 + \omega_2(T_2 - T_2^\star)^2.$$

where $\omega_1 > 0$ and $\omega_2 > 0$ are positive weights. The weighting factors ω_i can be made material dependent and, for example, be chosen as $\omega_i = \rho_i C_{\mathrm{p}_i}$.

Theorem 4. Let $\mathbb{E} := \{(T_1^\star, T_2^\star) \mid T_1^\star = T_2^\star\}$ be the set of all thermodynamic equilibria of (26). Then $\mathbb{E}$ is uniformly asymptotically stable in the sense that $\lim_{t\to\infty} \mathrm{dist}(T_i(t), \mathbb{E}) = 0$ for any solution $T_i(t)$ of (26) and any positive weights ω_1, ω_2. In particular, there exist functions $\alpha_1, \alpha_2, \alpha_3$ of class $\mathcal{K}$ such that

$$\alpha_1(\mathrm{dist}((T_1, T_2), \mathcal{E})) \leq S_{gen}(T_1, T_2) \leq \alpha_2(\mathrm{dist}((T_1, T_2), \mathcal{E}))$$

$$\dot{S}_{gen}(T_1, T_2) \leq -\alpha_3(\mathrm{dist}((T_1, T_2), \mathcal{E}))$$

for all $T \in \mathcal{D}$.

Proof: The proof follows the same lines as the proof of Theorem 2. $\qquad\square$

4. NUMERICAL EXAMPLE

In this section we provide a computation of the temperature distribution in the 1D heat conduction example given in Fig. 2. Consider the spatial geometry $\mathcal{G} = [0, L]$ with $L > 0$ the length of a beam. Let its temperature distribution be described by (13a) with Dirichlet/Neumann boundary conditions and initial conditions given by

Dirichlet & IC:
$$\begin{cases} T(0, t) = T_0(t) \\ T(L, t) = T_L(t) \\ T(r, 0) = \beta\sin(\frac{\pi}{L}r) + T_{0L}(r) \end{cases}$$

where $T_{0L}(r) = T_0 + r\frac{T_L - T_0}{L}$.

Neumann & IC:
$$\begin{cases} \frac{\partial T(0,t)}{\partial r} = 0 \\ \frac{\partial T(L,t)}{\partial r} = 0 \\ T(r, 0) = \cos(\frac{\pi r}{L}) + \xi, \quad \xi > 0 \end{cases}$$

The solutions are obtained by separation of variables and read for the Dirichlet conditions

$$T(r, t) = T_{0L}(r) + \beta\sin(\frac{\pi r}{L})\exp(-\frac{\pi^2}{L^2}\frac{\kappa}{\rho C_{\mathrm{p}}}t)$$

with $\beta > 0$, and for the Neumann conditions

$$T(r, t) = \xi + \cos(\frac{\pi r}{L})\exp(-\frac{\pi^2}{L^2}\frac{\kappa}{\rho C_{\mathrm{p}}}t).$$

For $t \to \infty$ the two types of boundary conditions exhibit two different stable thermodynamic equilibria as depicted in Fig. 4 and Fig. 5.

Note that the equilibrium in Fig 4 is not a thermodynamic equilibrium since the equipartition condition does not hold, while the steady state in Fig 5 is a thermodynamic equilibrium. The time evolution of the proposed Lyapunov function, together with the time derivative are both given in the following Fig 6.

5. CONCLUSION

This paper considers thermodynamical systems beyond their quasi-static behavior. We make an important conceptual distinction between thermodynamic equilibria of
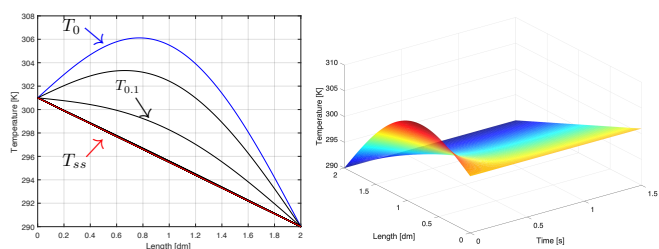
Fig. 4. Spatial temperature profiles with Dirichlet boundary condition. The temperature distribution $T_0, T_{0.1}$ and T_{ss} represent the time at $t = [0, 0.1]$ and the steady state, respectively.
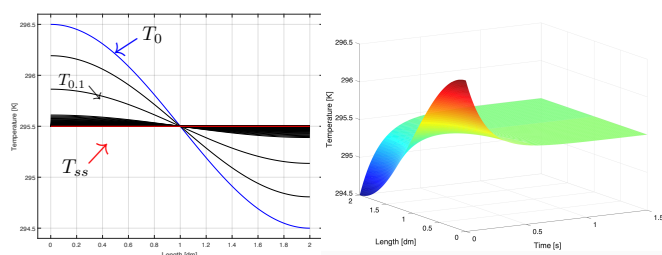

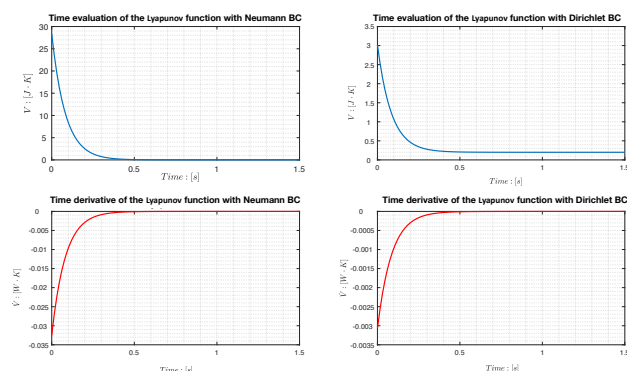Fig. 5. Spatial temperature profiles with Neumann boundary condition.

Fig. 6. Time evolution of the Lyapunov function with two different boundary conditions.

a system and equilibria in the sense of constant (time-positive invariant) solutions of autonomous systems described by differential equations. We proved the stability of thermodynamic equilibria in a distributed thermodynamical model and in a composite lumped thermodynamical model. In both cases, a suitable Lyapunov function has been derived from first principle properties of the entropy balance equation of the system. It is shown that this function represents entropy generation at the state of irreversible thermal processes and decays along solutions of the system towards thermodynamic equilibria. The set of thermodynamic equilibria is proven to be uniform asymptotically stable.

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