# Boundary controlled irreversible port-Hamiltonian systems

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## Abstract

Boundary controlled irreversible port-Hamiltonian systems (BC-IPHS) defined on a 1-dimensional spatial domain are defined by extending the formulation of reversible BC-PHS to irreversible thermodynamic systems controlled at the boundaries of their spatial domain. The structure of BC-IPHS has clear physical interpretation, characterizing the coupling between energy storing and energy dissipating elements. By extending the definition of boundary port variables of BC-PHS to deal with the irreversible energy dissipation, a set of boundary port variables are defined such that BC-IPHS are passive with respect to a given set of conjugated inputs and outputs. As for finite dimensional IPHS, the first and second laws of Thermodynamics are satisfied as a structural property of the system. Several examples are given to illustrate the proposed approach.

*Keywords:* Port-Hamiltonian systems, irreversible thermodynamics, infinite dimensional systems

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## 1. Introduction

The control of processes in Chemical Engineering is a highly difficult problem due to the nonlinearities induced as well by their thermodynamic properties as their flux relations. One very fruitful approach for the synthesis of nonlinear controllers is to use the properties of the dynamical models arising from first principle modeling such as symmetries, invariants and more generally balance equations of particular thermodynamic potential functions such as the entropy. These balance equations may be used as dissipation inequalities in passivity-based control as introduced in (62) and is now a well-developed branch of control (57; 8).In the case of chemical engineering processes, various thermodynamic potentials, such as the entropy or Helmholtz free energy, may be used as storage functions for control design methods based on Lyapunov control functions (11; 10) and passivity (1; 2; 3; 54).

The derivation of these Lyapunov functions and control Lyapunov functions are in most cases, based on the axioms of Equilibrium and Irreversible Thermodynamics and the structure of the dynamical models for these systems. A variety of such "thermodynamic" dynamical models have been suggested which are generalization of gradient control systems (12), Lagrangian control systems (40), Hamiltonian control systems (7; 38),(32, chap. 7) or Port Hamiltonian systems (33; 58; 15; 56) in the sense that they should account both for the conservation of the total energy and for the irreversible entropy production.

A first class of these thermodynamic control systems is defined by pseudo-gradient systems (17; 19), meaning that they are redefined with respect to a pseudo-metric, in a very similar way as suggested for electrical circuits in (6; 55). A second class of systems is defined as metriplectic systems (sum of Hamiltonian and gradient systems) with one or two generating functions (22; 41; 37; 49; 23; 24). A third class of systems is defined as nonlinearly constrained Lagrangian systems (20). A fourth class of systems is defined as implicit Hamiltonian control systems, in the sense that they are defined on a submanifold of some embedding space (the Thermodynamic Phase space or its symplectic extension), by control Hamiltonian systems defined on contact manifolds (36; 16; 18; 45; 44; 47; 35) or their symplectization (60).

In this paper a formalism that threats irreversible thermodynamic system within the framework of PHS, allowing to model thermo-mechanical systems in an unified manner is proposed, namely Boundary Controlled Irreversible Port-Hamiltonian Systems (BC-IPHS). We expect that the proposed formalism will allow to extend control design methods of BC-PHS to BC-IPHS like passivity-based and geometric control approaches, such as methods based on invariance (21), Casimir functions (31; 30) or (non)-linear dynamic boundary control (43; 52). To this end BC-IPHS on 1-dimensional spatial domains are defined by extending the formulation of reversible BC-PHS (59) to irreversible thermodynamic systems controlled at the boundaries of their spatial domain. The structure of BC-IPHS has clear physical interpretation, characterizing the coupling between energy storing and energy dissipating elements. By extending the definition of boundary port variables of BC-PHS (29; 25) to deal with the irreversible dissipation of energy, a set of boundary port variables are defined such that BC-IPHS are passive with respect to a given set of conjugated inputs and outputs. As for finite dimensional IPHS (45; 46), the first and second laws of Thermodynamics are satisfied as a structural property of the system. Several examples are given to illustrate the proposed approach. Note that a first approach in this line was given in (50) for a diffusion process. Interesting is to notice that when no irreversible phenomena is considered the definition of BC-IPHS reduces to the definition of a BC-PHS.

The paper is organized as follows. In Section 2 we recall the definition of BC-PHS corresponding to models of reversible systems and then motivate the paper using the example of a 1-D fluid, in the reversible and irreversible case when its viscosity is taken into account. Section 3 presents the main contribution of the paper, namely the definition of BC-IPHS on a 1D spatial domain. Section 4 gives two important lemmas regarding the passivity of the system, namely the energy conservation and the irreversible entropy production. In Section 5 the IPHS model of a general diffusion-reaction process is presented, and finally in Section 6 some conclusions and comments on future work are given.

## 2. Preliminaries and motivating example

This section presents preliminaries on boundary controlled port-Hamiltonian systems (BC-PHS) on a 1-D spatial domain. The example of a 1-D fluid is used to illustrate the approach and the importance of extending BC-PHS to BC-IPHS when viscous damping is considered.

### 2.1. Boundary Controlled PHS

An infinite dimensional PHS defined on a 1-D spatial domain is characterized by the following PDE

$$\frac{\partial x}{\partial t}(t,z) = P_1 \frac{\partial}{\partial z}\left(\frac{\delta H}{\delta x}(t,z)\right) + (P_0 - G_0)\frac{\delta H}{\delta x}(t,z), \qquad (1)$$

with $z \in (a,b)$, $P_1 \in M_n(\mathbb{R})^1$ a nonsingular symmetric matrix, $P_0 = -P_0^\top \in M_n(\mathbb{R})$, $G_0 \in M_n(\mathbb{R})$ with $G_0 \geq 0$ and $x$ taking values in $\mathbb{R}^n$. The functional $H(x)$ is the Hamiltonian and $\frac{\delta H}{\delta x}$ its variational derivative. The controlled (and homogeneous) boundary conditions of (1) are characterized by a matrix $W_B$ of appropriate size such that

$$v(t) = W_B \begin{bmatrix} \frac{\delta H}{\delta x}(t,b) \\ \frac{\delta H}{\delta x}(t,a) \end{bmatrix}$$

Considering the above boundary conditions as the input of the system, we can define an associate boundary output as

$$y(t) = W_C \begin{bmatrix} \frac{\delta H}{\delta x}(t,b) \\ \frac{\delta H}{\delta x}(t,a) \end{bmatrix}.$$

If $W_B$ and $W_C$ satisfy

$$\begin{aligned} W_B \tilde{\Sigma} W_B^\top &= W_C \tilde{\Sigma} W_C^\top = 0 \\ W_B \tilde{\Sigma} W_C^\top &= W_C \tilde{\Sigma} W_B^\top = I \end{aligned} \qquad (2)$$

with $\tilde{\Sigma} = \begin{bmatrix} P_1^{-1} & 0 \\ 0 & -P_1^{-1} \end{bmatrix}$, then the change of energy of the system becomes

$$\dot{H}(t) = y^\top(t)v(t) - \int_a^b \frac{\delta H}{\delta x}^\top(t,z) G_0 \frac{\delta H}{\delta x}(t,z)dz$$

The reader is referred to (29; 25) for details. We can see from this equation that the dissipation in the system is characterized by the matrix $G_0$. Indeed, since the input and output act and sense at the boundary of the spatial domain, in the absence of internal dissipation ($G_0 = 0$) the system only exchanges energy with the environment through the boundaries. In this case the PHS fullfils

$$\dot{H}(t) = y^\top(t)v(t),$$

and the PHS is called conservative. This formulation has proven to be extremely useful to study the existence and uniqueness of solutions for the linear case, and to perform control synthesis for the general class of PHS (29; 25; 43; 31; 52). One interesting feature of PHS is that they are applicable to hyperbolic systems and can be extended to parabolic systems, however the PHS formulation of parabolic systems leads necessary to an implicit system.

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[1] $M_n(\mathbb{R})$ denote the space of real $n \times n$ matrices

### 2.2. *The isentropic fluid: the reversible case*

Let us first consider the dynamic behavior of an 1-D isentropic fluid in Lagrangian coordinates, also known as *p-system*, and recall its port Hamiltonian formulation (34). The 1-D spatial domain is the interval $[a, b] \ni z$, $a$, $b \in \mathbb{R}$, $a < b$. Using as state variables the specific volume $\phi(t, z)$ and the velocity $\upsilon(t, z)$ of the fluid, the dynamical model of the fluid is given by the system of two conservation laws first of the mass (expressed in terms of the specific volume) and second of the momentum (expressed in terms of the velocity seen as "momentum density")

$$\frac{\partial \phi}{\partial t}(t,z) = \frac{\partial \upsilon}{\partial z}(t,z) \tag{3}$$

$$\frac{\partial \upsilon}{\partial t}(t,z) = -\frac{\partial p}{\partial z}(t,z) \tag{4}$$

where $p(\phi)$ is the pressure of the fluid. The Hamiltonian formulation is obtained by considering the total energy of the system which consists in the sum of the kinetic and the internal energy, denoting the internal energy density by $u(\phi)$

$$H(\upsilon, \phi) = \int_a^b \left(\frac{1}{2}\upsilon^2 + u(\phi)\right) dz$$

The variational derivative of the total energy yields $\frac{\delta H}{\delta \upsilon} = \upsilon$ and $\frac{\delta H}{\delta \phi} = \frac{\partial u}{\partial \phi} = -p$ and the system (3)-(4) may be written as the *Hamiltonian system*

$$\begin{bmatrix} \frac{\partial \phi}{\partial t} \\ \frac{\partial \upsilon}{\partial t} \end{bmatrix} = P_1 \frac{\partial}{\partial z}\left(\begin{bmatrix} \frac{\delta H}{\delta \phi} \\ \frac{\delta H}{\delta \upsilon} \end{bmatrix}\right), \qquad \text{with} \quad P_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \tag{5}$$

and $P_1 \frac{\partial}{\partial z}$ is a *Hamiltonian operator* (39). Considering an open system, when there is mass and energy flow through the boundary (at the points $a$ and $b$), the Hamiltonian system (5) is completed with conjuguated *boundary port variables*

$$\begin{bmatrix} v \\ y \end{bmatrix} = \begin{bmatrix} W_B \\ W_C \end{bmatrix} \begin{bmatrix} \frac{\delta H}{\delta \phi}(b) \\ \frac{\delta H}{\delta v}(b) \\ \frac{\delta H}{\delta \phi}(a) \\ \frac{\delta H}{\delta v}(a) \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} -p(t,b) \\ \upsilon(t,b) \\ -p(t,a) \\ \upsilon(t,a) \end{bmatrix}$$

yielding a BC-PHS (59). These boundary port variables are the velocity and the pressure at the boundary $v(t) = \begin{bmatrix} -p(t,b) \\ p(t,a) \end{bmatrix}$ and $y(t) = \begin{bmatrix} \upsilon(t,b) \\ \upsilon(t,a) \end{bmatrix}$. The choice of inputs and outputs satisfies (2) yielding the energy balance equation $\dot{H}(t) = y^\top(t) v(t)$.

### 2.3. *The non-isentropic fluid: the irreversible case*

Consider that there is dissipation in the system given by viscous damping. The momentum obeys the following balance equation

$$\frac{\partial \upsilon}{\partial t}(t,z) = -\frac{\partial p}{\partial z}(t,z) - \frac{\partial \tau}{\partial z}(t,z) \tag{6}$$

where $\tau$ is the viscous force defined as $\tau = -\hat{\mu}\frac{\partial \upsilon}{\partial z}$, with $\hat{\mu}$ the viscous damping coefficient. The system contains dissipation, i.e., a irreversible phenomenon induced by the viscosity of the fluid. Therefore we account for the thermal domain and consider Gibbs' equation $du = -p d\phi + T ds$ where $s$ denotes the entropy density (which is now varying) and $T$ the temperature. The total energy of the system is still the sum of the kinetic and the internal energy

$$H(\upsilon, \phi, s) = \int_a^b \left(\frac{1}{2}\upsilon^2 + u(\phi, s)\right) dz$$

The mass balance (3) and momentum balance equations (6) are then augmented with the entropy balance equation

$$\frac{\partial s}{\partial t}(t,z) = \frac{\hat{\mu}}{T}\left(\frac{\partial \upsilon}{\partial z}\right)^2 (t,z)$$

and the system of balance equations may be written as the quasi-Hamiltonian system

$$\begin{bmatrix} \frac{\partial \phi}{\partial t} \\ \frac{\partial \upsilon}{\partial t} \\ \frac{\partial s}{\partial t} \end{bmatrix} = \begin{bmatrix} 0 & \frac{\partial(\cdot)}{\partial z} & 0 \\ \frac{\partial(\cdot)}{\partial z} & 0 & \frac{\partial}{\partial z}\left(\frac{\hat{\mu}}{T}\left(\frac{\partial \upsilon}{\partial z}\right)(\cdot)\right) \\ 0 & \frac{\hat{\mu}}{T}\left(\frac{\partial \upsilon}{\partial z}\right)\frac{\partial(\cdot)}{\partial z} & 0 \end{bmatrix} \left(\begin{bmatrix} \frac{\delta H}{\delta \phi} \\ \frac{\delta H}{\delta \upsilon} \\ \frac{\delta H}{\delta s} \end{bmatrix}\right)$$

As the differential matrix operator depends on the co-energy variable $T = \frac{\delta H}{\delta s}$, it is only a quasi-Hamiltonian operator and hence does not fall into the definition of BC-PHS given in Section 2.

In the following section this latter formulation will be used to define BC-IPHS, extending the framework originally proposed in (45; 46) for irreversible thermodynamic systems on finite dimensional spaces to systems defined on infinite dimensional spaces.

## 3. Boundary IPHS

In this section, we introduce the Boundary Controlled Irreversible Port Hamiltonian System (BC-IPHS) defined on a 1D spatial domain $z \in [a, b]$, $a$, $b \in \mathbb{R}$, $a < b$. The state variables of the system are the $n + 1$ *extensive variables*[2]. The following partition of the state vector $\mathbf{x} \in \mathbb{R}^{n+1}$ shall be considered: the first $n$ variables

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[2] A variable is qualified as extensive when it characterizes the thermodynamic state of the system and its total value is given by the sum of its constituting parts.

by $x = [q_1, \dots, q_n]^\top \in \mathbb{R}^n$ and the entropy density by $s \in \mathbb{R}$. The thermodynamic properties of the system are expressed by Gibbs' equation (9), which we give here in its local form with pairs of specific energy-conjugated variables (15, Chapter 3)

$$dh = T ds + p_i \sum_{i=1}^{n} dq_i$$

where $T$ is the temperature, conjugated to the entropy density, and the variables $p_i$ denote the *intensive variables*, which are conjugated to the $q_i$ variables. Gibbs' equation is here understood in a general context in order to account for coupled thermo-electro/magnetic/mechanical systems. Gibbs' equation is equivalent to the existence of an energy functional

$$H(x, s) = \int_a^b h\,(x(z), s(z))\, dz \tag{7}$$

where $h(x, s)$ is the energy density function. The total entropy functional is denoted by

$$S(t) = \int_a^b s(z, t) dz \tag{8}$$

In the sequel we shall furthermore use the following notation. For any two functionals $H_1$ and $H_2$ of the type (7) and for any matrix differential operator $\mathcal{G}$ we define the pseudo-brackets

$$\begin{aligned} \{H_1|\mathcal{G}|H_2\} &= \begin{bmatrix} \frac{\delta H_1}{\delta x} \\ \frac{\delta H_1}{\delta s} \end{bmatrix} \begin{bmatrix} 0 & \mathcal{G} \\ -\mathcal{G}^* & 0 \end{bmatrix} \begin{bmatrix} \frac{\delta H_2}{\delta x} \\ \frac{\delta H_2}{\delta s} \end{bmatrix}, \\ \{H_1|H_2\} &= \frac{\delta H_1}{\delta s}^\top \left( \frac{\partial}{\partial z} \frac{\delta H_2}{\delta s} \right) \end{aligned} \tag{9}$$

where $\mathcal{G}^*$ denotes the formal adjoint operator of $\mathcal{G}$.

We shall first define a system of balance equations in terms of an Irreversible (quasi-)Hamiltonian system.

**Definition 1.** *An infinite dimensional IPHS undergoing $m$ irreversible processes is defined by*

- *a pair of functionals: the total energy (7) and the total entropy (8)*
- *a pair of matrices $P_0 = -P_0^\top \in \mathbb{R}^{n\times n}$ and $P_1 = P_1^\top \in \mathbb{R}^{n\times n}$*
- *a pair of matrices $G_0 \in \mathbb{R}^{n\times m}$, $G_1 \in \mathbb{R}^{n\times m}$ with $m \leq n$ and the strictly positive real-valued functions $\gamma_{k,i}\left(x, z, \frac{\delta H}{\delta x}\right)$ $k = 0,\ 1;\ i \in \{1, \dots m\}$*
- *a pair of real-valued functions $\gamma_s\left(x, z, \frac{\delta H}{\delta x}\right) > 0$ and $g_s(x)$*

*and the PDE*

$$\frac{\partial}{\partial t} \begin{bmatrix} x(t,z) \\ s(t,z) \end{bmatrix} = \begin{bmatrix} P_0 & G_0 \mathbf{R_0} \\ -\mathbf{R}(\mathbf{x})^\top G_0^\top & 0 \end{bmatrix} \begin{bmatrix} \frac{\delta H}{\delta x}(t,z) \\ \frac{\delta H}{\delta s}(t,z) \end{bmatrix} + \begin{bmatrix} P_1 \frac{\partial (.)}{\partial z} & \frac{\partial (G_1 \mathbf{R_1} .)}{\partial z} \\ \mathbf{R_1}^\top G_1^\top \frac{\partial (.)}{\partial z} & g_s \mathbf{r_s} \frac{\partial (.)}{\partial z} + \frac{\partial (g_s \mathbf{r_s} .)}{\partial z} \end{bmatrix} \begin{bmatrix} \frac{\delta H}{\delta x}(t,z) \\ \frac{\delta H}{\delta s}(t,z) \end{bmatrix} \tag{10}$$

*with vector-valued functions $\mathbf{R_l}\left(\mathbf{x}, \frac{\delta H}{\delta \mathbf{x}}\right) \in \mathbb{R}^{m\times 1}$, $l = 0, 1$, defined by*

$$R_{0,i} = \gamma_{0,i}\left(x, z, \frac{\delta H}{\delta x}\right) \{S|G_0(:, i)|H\}$$

$$R_{1,i} = \gamma_{1,i}\left(x, z, \frac{\delta H}{\delta x}\right) \left\{S|G_1(:, i)\frac{\partial}{\partial z}|H\right\}$$

*and*

$$r_s = \gamma_s\left(x, z, \frac{\delta H}{\delta x}\right) \{S|H\}$$

*where the notation $G(:, i)$ indicates the i-th column of the matrix $G$.*

This definition may be commented with respect to physical systems' modeling as follows. The pair of matrices $P_0$ and $P_1$ corresponds to reversible coupling phenomena as it appears in the example of the isentropic fluid with $P_0 = 0$ and $P_1$ given in (5). The pair of matrices $G_0$ and $G_1$ corresponds to the irreversible coupling phenomena. In the example of the non-isentropic fluid, $G_0 = 0$ and $G_1 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$ which indicates that the irreversible phenomenon associated with the viscosity of the fluid, couples the momentum and the entropy balance equations. The functions $\gamma_{k,i}$ and $\gamma_s$ define the constitutive relations of the irreversible phenomena and the functions $\{S|G_0(:, i)|H\}$, $\left\{S|G_1(:, i)\frac{\partial}{\partial z}|H\right\}$ and $\{S|H\}$ correspond to their driving forces. In the example of the non-isentropic fluid, $\left\{S|G_1(:, i)\frac{\partial}{\partial z}|H\right\} = \frac{\partial v}{\partial s}$ is indeed the driving force of the viscosity and $\gamma_{1,1} = \frac{\hat{\mu}}{T}$ with $T = \frac{\delta H}{\delta s}$ is indeed a strictly positive function containing the viscosity parameter and defining the constitutive relation of the viscosity.

**Remark 1.** *Setting the matrices $P_1$ and $G_1$ to zero, reduces the PDE (10) to*

$$\frac{d}{dt} \begin{bmatrix} x(t,z) \\ s(t,z) \end{bmatrix} = \begin{bmatrix} P_0 & G_0 \mathbf{R_0}(\mathbf{x}) \\ -\mathbf{R_0}(\mathbf{x})^\top G_0^\top & 0 \end{bmatrix} \begin{bmatrix} \frac{\delta H}{\delta x}(t,z) \\ \frac{\delta H}{\delta s}(t,z) \end{bmatrix}$$

*which is formally the definition of finite-dimensional IPHS in (45; 46) for the case $m = 1$ or (48; 51) for $m > 1$. In this sense the Definition 1 is an infinite-dimensional extension of the definition of IPHS.*

In the sequel we shall complete the IPHS defined above with port variables enabling to write the interaction of the system with its environment or other physical systems, in a very similar way as for reversible PHS presented in the Section 2.

**Definition 2.** *A Boundary Controlled IPHS (BC-IPHS) is an infinite dimensional IPHS according to Definition 1 augmented with the boundary port variables*

$$v(t) = W_B \begin{bmatrix} e(t,b) \\ e(t,a) \end{bmatrix}, \qquad y(t) = W_C \begin{bmatrix} e(t,b) \\ e(t,a) \end{bmatrix} \tag{11}$$

*as linear functions of the modified effort variable*

$$e(t,z) = \begin{bmatrix} \frac{\delta H}{\delta x}(t,z) \\ \mathbf{R}(\mathbf{x}, \frac{\delta H}{\delta \mathbf{x}})\ \frac{\delta H}{\delta s}(t,z) \end{bmatrix}, \tag{12}$$

*with* $\mathbf{R}(\mathbf{x}, \frac{\delta H}{\delta \mathbf{x}}) = \begin{bmatrix} 1 & \mathbf{R_1}(\mathbf{x}, \frac{\delta \mathbf{H}}{\delta \mathbf{x}}) & \mathbf{r_s}(\mathbf{x}, \frac{\delta \mathbf{H}}{\delta \mathbf{x}}) \end{bmatrix}^\top$ *and*

$$W_B = \left[ \tfrac{1}{\sqrt{2}} \left( \Xi_2 + \Xi_1 P_{ep} \right) M_p \quad \tfrac{1}{\sqrt{2}} \left( \Xi_2 - \Xi_1 P_{ep} \right) M_p \right],$$
$$W_C = \left[ \tfrac{1}{\sqrt{2}} \left( \Xi_1 + \Xi_2 P_{ep} \right) M_p \quad \tfrac{1}{\sqrt{2}} \left( \Xi_1 - \Xi_2 P_{ep} \right) M_p \right],$$

*where* $M_p = (M^\top M)^{-1} M^\top$*,* $P_{ep} = M^\top P_e M$ *and* $M \in \mathbb{R}^{(n+m+2)\times k}$ *is spanning the columns of* $P_e \in \mathbb{R}^{n+m+2}$ *of rank* $k$*, defined by*[3]

$$P_e = \begin{bmatrix} P_1 & 0 & G_1 & 0 \\ 0 & 0 & 0 & g_s \\ G_1^\top & 0 & 0 & 0 \\ 0 & g_s & 0 & 0 \end{bmatrix} \tag{13}$$

*and where* $\Xi_1$ *and* $\Xi_2$ *in* $\mathbb{R}^{k\times k}$ *satisfy* $\Xi_2^\top \Xi_1 + \Xi_1^\top \Xi_2 = 0$ *and* $\Xi_2^\top \Xi_2 + \Xi_1^\top \Xi_1 = I$*.*■

The definition of the boundary port variables (11) and (12) shall not be justified here as for reversible BC-PHS to define a Stokes-Dirac structure, as the nonlinear operator in (10) is not a Hamiltonian operator but rather by the energy balance equation established in the Section 4.

**Remark 2.** *Setting the matrices* $G_0$ *and* $G_1$ *to zero as well as* $g_s$*, the system is reversible and the functions* $R_0$*,* $R_1$ *and* $r_s$ *are all zero. As a result the dynamics of the entropy is trivial and the entropy is constant. Moreover the dynamics of the remaining extensive variables* $x$ *and the port boundary variables reduces to the (conservative) BC-PHS presented in the section 2. Therefore the BC-IPHS may be seen as a generalization of BC-PHS (29) with first-order differential operators.*

**Example 1.** *Recalling the 1D fluid model in Section 2.3, its BC-IPHS formulation is given by* $P_0 = 0, G_0 = 0, g_s = 0$*,* $P_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$ *and* $G_1 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$ *with* $x = \begin{bmatrix} \phi \\ \upsilon \end{bmatrix}$ *and* $R_{11} = \gamma_1 \{S | G_1(:,1) \frac{\partial}{\partial z} | H\}$ *with* $\gamma_1 = \frac{\hat{\mu}}{T} > 0$*. In this case* $n = 2$*,* $m = 1$ *and the boundary port variables may be computed as follows, starting with*

$$P_e = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

*of rank* $k = 2$ *which gives* $M = \begin{bmatrix} \frac{1}{2} & 0 & 0 & \frac{1}{2} & 0 \\ 0 & 1 & 0 & 0 & 0 \end{bmatrix}^\top$*,* $M_P = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 \end{bmatrix}$ *and* $P_{ep} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$*. Choosing the parametrization*

$$\Xi_1 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 0 \\ 1 & 0 \end{bmatrix}, \quad \Xi_2 = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & 1 \\ 0 & -1 \end{bmatrix}$$

*define the following boundary inputs and outputs*

$$v(t) = \begin{bmatrix} -p(t,b) + \frac{\hat{\mu}}{T} \frac{\partial \upsilon}{\partial z}(t,b) \\ p(t,a) - \frac{\hat{\mu}}{T} \frac{\partial \upsilon}{\partial z}(t,a) \end{bmatrix}, \qquad y(t) = \begin{bmatrix} \upsilon(t,b) \\ \upsilon(t,a) \end{bmatrix}.$$

*As for the reversible case, the boundary inputs and outputs correspond, respectively, to the pressure and the velocity evaluated at the boundary points* $a$ *and* $b$*. Note however that this time the pressure is the sum of the static and hydrodynamic pressure. If there is no dissipation in the system,* $\hat{\mu} = 0$ *and the boundary inputs and outputs are exactly the same as for the reversible case.*

**Example 2.** *Consider the heat conduction with heat diffusion over a 1D spatial domain, for instance a rod with cylindrical symmetry. We assume the medium to be undeformable, i.e. its deformations are neglected, and consider only one physical domain, the thermal domain and its dynamics. The conserved quantity is the density of internal energy and the state reduces to a unique variable. Choose the internal energy density* $u = u(s)$ *as thermodynamic potential function (and* $U(s) = \int_a^b u dz$*), in this case Gibbs relation defines the temperature as intensive variable conjugated to the extensive variable, the entropy by* $T = \frac{du}{ds}(s)$*. This leads to write the following entropy balance equation (15)*

$$\frac{\partial s}{\partial t} = -\frac{1}{T} \frac{\partial}{\partial z} \left( -\lambda \frac{\partial T}{\partial z} \right)$$

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[3] 0 has to be understood as the zero matrix of proper dimensions.

*where, according to Fourier's law, $\lambda$ denotes the heat conduction coefficient and $-\lambda\frac{\partial T}{\partial z} = f_Q$ corresponds to the heat flux. Alternatively the heat conduction can be written in terms of the entropy flux $f_S = \frac{1}{T} f_Q = -\frac{\lambda}{T}\frac{\partial T}{\partial z}$,*

$$\frac{\partial s}{\partial t} = \frac{\partial}{\partial z}\left(\frac{\lambda}{T}\frac{\partial T}{\partial z}\right) + \frac{\lambda}{T^2}\left(\frac{\partial T}{\partial z}\right)^2 \tag{14}$$

*from where the entropy production $\sigma_s = \frac{\lambda}{T^2}\left(\frac{\partial T}{\partial z}\right)^2$ is identified. This balance equation is also known as Jaumann's entropy balance (14; 5; 26). Recalling that $\frac{\delta U}{\delta s} = T$, the IPHS formulation of the heat conduction is obtained from (14),*

$$\frac{\partial s}{\partial t} = \frac{\lambda}{T^2}\frac{\partial T}{\partial z}\frac{\partial}{\partial z}\left(\frac{\delta U}{\delta s}\right) + \frac{\partial}{\partial z}\left(\frac{\lambda}{T^2}\frac{\partial T}{\partial z}\left(\frac{\delta U}{\delta s}\right)\right)$$

*which is equivalent to* (10) *where $P_0 = 0$, $P_1 = 0$, $G_0 = 0$, $G_1 = 0$, $g_s = 1$ and $r_s = \gamma_s\{S|U\}$ with $\gamma_s = \frac{\lambda}{T^2}$ and $\{S|U\} = \frac{\partial T}{\partial z}$. In this case $P_e = \frac{1}{2}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$, $n = 1$ and $m = 1$. Choosing $\Xi_1 = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 0 \\ 1 & 0 \end{bmatrix}$, $\Xi_2 = \frac{1}{\sqrt{2}}\begin{bmatrix} 0 & 1 \\ 0 & -1 \end{bmatrix}$ the boundary inputs and outputs of the system are*

$$v(t) = \begin{bmatrix} \left(\frac{\lambda_s}{T}\frac{\partial T}{\partial z}\right)(t,b) \\ -\left(\frac{\lambda_s}{T}\frac{\partial T}{\partial z}\right)(t,a) \end{bmatrix}, \qquad y(t) = \begin{bmatrix} T(t,b) \\ T(t,a) \end{bmatrix},$$

*respectively the entropy flux and the temperature at each boundary.*

## 4. Energy and entropy balance equations

BC-IPHS encode the first and second laws of Thermodynamics, i.e., the conservation of the total energy and the irreversible production of entropy as stated in the following lemmas.

**Lemma 1.** *(First law of Thermodynamics) The total energy balance is*

$$\dot{H} = y(t)^\top v(t)$$

*which leads, when the input is set to zero, to $\dot{H} = 0$ in accordance with the first law of Thermodynamics.*

**Proof.** The variation of the total energy with respect to time is

$$\dot{H} = \int_a^b \frac{\partial h}{\partial t} dz = \int_a^b \left(\frac{\delta H}{\delta x}^\top \frac{\partial x}{\partial t} + \frac{\delta H}{\delta s}^\top \frac{\partial s}{\partial t}\right) dz$$
$$= \int_a^b \left[\frac{\delta H}{\delta x}(t,z)^\top \quad \frac{\delta H}{\delta s}(t,z)\right] \mathcal{J}_e \begin{bmatrix} \frac{\delta H}{\delta x}(t,z) \\ \frac{\delta H}{\delta s}(t,z) \end{bmatrix} dz$$

with

$$\mathcal{J}_e = \begin{bmatrix} P_1 \frac{\partial (.)}{\partial z} & \frac{\partial (G_1 \mathbf{R_1}(\mathbf{x}).)}{\partial z} \\ \mathbf{R_1}(\mathbf{x})^T G_1^T \frac{\partial (.)}{\partial z} & g_s \mathbf{r_s}(\mathbf{x}) \frac{\partial (.)}{\partial z} + \frac{\partial (g_s \mathbf{r_s}(\mathbf{x}).)}{\partial z} \end{bmatrix}$$

where we have used the skew symmetry of the matrix of zero order operators

$$\begin{bmatrix} P_0 & G_0 \mathbf{R_0}(\mathbf{x}) \\ -\mathbf{R_0}(\mathbf{x})^T G_0^T & 0 \end{bmatrix}.$$

Noticing that

$$\int_a^b \frac{\delta H}{\delta x}^\top P_1 \frac{\partial}{\partial z}\left(\frac{\delta H}{\delta x}\right) dz = \frac{1}{2}\left[\frac{\delta H}{\delta x}^\top P_1 \frac{\delta H}{\delta x}\right]_a^b$$

that

$$\int_a^b \left(\frac{\delta H}{\delta s}\mathbf{R_1}(\mathbf{x})^T G_1^T \frac{\partial}{\partial z}\left(\frac{\delta H}{\delta x}\right) + \frac{\delta H}{\delta x}^\top \frac{\partial}{\partial z}\left(G_1 \mathbf{R_1}(\mathbf{x})\frac{\delta H}{\delta s}\right)\right) dz$$
$$= \left[\frac{\delta H}{\delta s}\mathbf{R_1}(\mathbf{x})^\top G_1^\top \frac{\delta H}{\delta x}\right]_a^b$$

and that

$$\int_a^b \left(\frac{\delta H}{\delta s} g_s \mathbf{r_s}(\mathbf{x}) \frac{\partial}{\partial z}\left(\frac{\delta H}{\delta s}\right) + \frac{\delta H}{\delta s}\frac{\partial}{\partial z}\left(g_s \mathbf{r_s}(\mathbf{x})\frac{\delta H}{\delta s}\right)\right) dz$$
$$= \left[\frac{\delta H}{\delta s} g_s \mathbf{r_s}(\mathbf{x})\left(\frac{\delta H}{\delta s}\right)\right]_a^b$$

we have

$$\dot{H} = \left[\begin{bmatrix} \frac{\delta H}{\delta x} \\ \frac{\delta H}{\delta s} \\ \mathbf{R_1}(\mathbf{x}) G_1^T \frac{\delta H}{\delta s} \\ g_s \mathbf{r_s}(\mathbf{x}) \frac{\delta H}{\delta s} \end{bmatrix}^\top P_e \begin{bmatrix} \frac{\delta H}{\delta x} \\ \frac{\delta H}{\delta s} \\ \mathbf{R_1}(\mathbf{x}) G_1 \frac{\delta H}{\delta s} \\ g_s \mathbf{r_s}(\mathbf{x}) \frac{\delta H}{\delta s} \end{bmatrix}\right]_a^b$$

with $P_e$ defined in (13). Using the parametrization proposed in (29; 28) ($P_e$ is potentially not full rank), it is possible to write

$$\begin{bmatrix} u(t) \\ y(t) \end{bmatrix} = \frac{1}{\sqrt{2}}\begin{bmatrix} \Xi_1 & \Xi_2 \\ \Xi_2 & \Xi_1 \end{bmatrix}\begin{bmatrix} P_{1p} M_p & -P_{1p} M_p \\ M_p & M_p \end{bmatrix}\begin{bmatrix} e(t,b) \\ e(t,a) \end{bmatrix}$$

with $\Xi_i$, $M_P$ and $P_{1p}$ defined in Definition 2, from where it is obtained that $\dot{H} = y(t)^\top u(t)$. If the input of the system is zero, i.e., $u = 0$, then $\dot{H} = 0$ in accordance with the first law of Thermodynamics. ■

**Lemma 2.** *(Second law of Thermodynamics) The total entropy balance is given by*

$$\dot{S} = \int_a^b \sigma_t dz - y_S^\top v_s$$

*where $y_s$ and $v_s$ are the entropy conjugated input/output and $\sigma_t$ is the total internal entropy production. This leads, when the input is set to zero, to $\dot{S} = \int_a^b \sigma_t dz \geq 0$ in accordance with the second law of Thermodynamics.*

**Proof.** Let's consider the total entropy balance

$$\begin{aligned}\dot{S} &= \int_a^b \frac{\partial s}{\partial t} dz \\ &= \int_a^b \Bigg(\mathbf{R_0}(\mathbf{x})^\top G_0^\top \frac{\delta H}{\delta x} + \mathbf{R_1}(\mathbf{x})^\top G_1^\top \frac{\partial}{\partial z}\frac{\delta H}{\delta x} + \\ & g_s \mathbf{r_s}(\mathbf{x}) \frac{\partial}{\partial z}\frac{\delta H}{\delta s} + \frac{\partial}{\partial z}\left(g_s \mathbf{r_s}(\mathbf{x}) \frac{\delta H}{\delta x}\right)\Bigg) dz\end{aligned}$$

The first three terms define the internal entropy production related to the operators of order zero and one

$$\begin{aligned}\mathbf{R_0}(\mathbf{x})^\top G_0^\top \frac{\delta H}{\delta x} &= \sum_i^m \left(R_{0,i}(x) G_0(:,i)^\top \frac{\delta H}{\delta x}\right) \\ &= \sum_i^m \gamma_{0,i} \{S|G_0(:,i)|H\}^2 = \sum_i^m \sigma_{0i} \geq 0, \\ \mathbf{R_1}(\mathbf{x})^\top G_1^\top \frac{\partial}{\partial z}\frac{\delta H}{\delta x} &= \sum_i^m \left(R_{1,i}(x) G_1(:,i)^\top \frac{\partial}{\partial z}\frac{\delta H}{\delta x}\right) \\ &= \sum_i^m \gamma_i \left\{S|G_1(:,i)\frac{\partial}{\partial z}|H\right\}^2 = \sum_i^m \sigma_{1i} \geq 0, \\ g_s \mathbf{r_s}(\mathbf{x}) \frac{\partial}{\partial z}\frac{\delta H}{\delta s} &= \gamma_s \{S|H\}^2 = \sigma_s \geq 0,\end{aligned}$$

where $\sigma_{0i}$ and $\sigma_{1i}$ are, respectively, the zero and first order internal entropy productions due to the $i$-th irreversible thermodynamic processes, and $\sigma_s$ is the internal entropy production due to entropy (heat) flux. Since the total internal entropy production is the sum of the internal entropy production of all irreversible processes $\sigma_t = \sum_i^m (\sigma_{0i} + \sigma_{1i} + \sigma_s)$ we have

$$\begin{aligned}\dot{S} &= \int_a^b \sigma_t dz + \int_a^b \frac{\partial}{\partial z}\left(g_s \mathbf{r_s}(\mathbf{x}) \frac{\delta H}{\delta x}\right) dz \\ &= \int_a^b \sigma_t dz + \left(g_s \mathbf{r_s}(\mathbf{x}) \frac{\delta H}{\delta x}(b,t) - g_s \mathbf{r_s}(\mathbf{x}) \frac{\delta H}{\delta x}(a,t)\right) \\ &= \int_a^b \sigma_t dz - (f_s(b,t) - f_s(a,t)).\end{aligned}$$

from where we have the supply rate $y_S^\top v_s = (f_s(b,t) - f_s(a,t))$, representing the entropy flux at the boundaries. Hence, the total entropy variation is equal to the internal entropy production minus what is flowing in/out through the boundaries. If the entropy conjugated input is zero, i.e., $v_s = 0$, then $\dot{S} = \int_a^b \sigma_t dz \geq 0$ in accordance with the second law of Thermodynamics. ■

## 5. Example: the diffusion-reaction process

Diffusion-reaction processes are systems in which the changes in the mole number per unit volume are due to transport of particles, through processes such as diffusion and convection, and due to chemical reactions. This is the case for instance for tubular reactors (4; 27; 53). We shall assume a diffusion reaction-process without convection involving $n$ species and $j$ chemical reactions in which the molar concentrations and the temperature are non-uniform over a 1-D spatial domain. Viscous phenomena shall be neglected and no external forces are supposed to be present. Under these conditions the pressure is uniform over the system if we assume that mechanical equilibrium is rapidly established, as is the case for systems confined to closed reservoirs (14; 5; 26).The diffusion-reaction process is described by the following set of PDEs

$$\begin{aligned}\frac{\partial c_i}{\partial t} &= -\frac{\partial f_{ci}}{\partial z} + \sum_{k=1}^{j} \bar{\nu}_{ki} r_k, \qquad i = 1, \ldots, n \\ \frac{\partial s}{\partial t} &= -\frac{\partial f_s}{\partial z} + \sum_{k=1}^{n} \sigma_{c_k} + \sum_{k=1}^{j} \sigma_{r_k} + \sigma_s.\end{aligned} \tag{15}$$

where $c_i$ is the molar concentration per unit volume of the $i$-th species and $s$ is the entropy density. The chemical potential of the $i$-th species is denoted by $\mu_i$. The molar flux of the $i$-th species is modeled according to Fick's law as $f_{ci} = -L_i \frac{\partial \mu_i}{\partial z}$ where $L_i$ is the positive diffusion coefficient of the $i$-th species (13; 61). According to Fourier's law $f_s = -\frac{\lambda}{T}\frac{\partial T}{\partial z}$ corresponds to the entropy flux, with $\lambda$ the positive heat conduction coefficient. According to the law of mass action $\bar{\nu}_i$ is the signed stoichiometric coefficient of the reactant $i$ in the $k$-th reaction: $\bar{\nu}_{ki} = -\nu_{ki}$ if it appears on the left hand side of the reaction scheme, $\bar{\nu}_{ki} = \nu_{ki}$ in the other case. The reaction rate of the $k$-th reaction is $r_k$, which depends on the temperature and on the molar concentrations. The thermodynamic driving forces are, respectively, $\frac{\partial \mu_i}{\partial z}$ for the diffusion of the $i$-th species, $\frac{\partial T}{\partial z}$ for the heat conduction and the chemical affinity of the $k$-th reaction $\mathcal{A}_k = -\sum_{i=1}^n \bar{\nu}_{ki}\mu_i$ for the $k$-th chemical reaction. The internal entropy production of the process is due to irreversible diffusion, heat conduction and to the chemical reactions. In (15) the internal entropy production terms are respectively, $\sigma_{c_i} = -\frac{1}{T} f_{ci} \frac{\partial \mu_i}{\partial z} = \frac{L_i}{T}\left(\frac{\partial \mu_i}{\partial z}\right)^2$ for the diffusion of the $i$-th species, $\sigma_{r_k} = \frac{1}{T} r_k \mathcal{A}_k = -\frac{r_k}{T}\sum_{i=1}^{n-1} \bar{\nu}_{ki}\mu_i$ for the $k$-th chemical reaction and $\sigma_s = -\frac{1}{T} f_s \frac{\partial T}{\partial z} = \frac{\lambda}{T^2}\left(\frac{\partial T}{\partial z}\right)^2$ for the heat conduction.

### 5.1. The IPHS model

**Proposition 1.** *Consider the diffusion-reaction process with $x = [c_1, \ldots, c_n]^\top \in \mathbb{R}^n$. Then (15) can be written* *as the infinite dimensional IPHS (Definition 1)*

$$\frac{\partial}{\partial t}\begin{bmatrix} x(t,z) \\ s(t,z)\end{bmatrix} = \begin{bmatrix} 0 & G_0\mathbf{R_0}(\mathbf{x}) \\ -\mathbf{R_0}(\mathbf{x})^\top G_0^\top & 0\end{bmatrix}\begin{bmatrix} \frac{\delta H}{\delta x}(t,z) \\ \frac{\delta H}{\delta s}(t,z)\end{bmatrix} +$$
$$\begin{bmatrix} 0 & \frac{\partial(G_1\mathbf{R_1}(\mathbf{x})\cdot)}{\partial z} \\ \mathbf{R_1}(\mathbf{x})^\top G_1^\top \frac{\partial(\cdot)}{\partial z} & g_s\mathbf{r_s}(\mathbf{x})\frac{\partial(\cdot)}{\partial z} + \frac{\partial(g_s\mathbf{r_s}(\mathbf{x})\cdot)}{\partial z}\end{bmatrix}\begin{bmatrix} \frac{\delta H}{\delta x}(t,z) \\ \frac{\delta H}{\delta s}(t,z)\end{bmatrix} \quad (16)$$

*The modulating function of the mass diffusion of the i-th species is*

$$R_{1i} = \gamma_{1i}\{S|G_1(:,1)\tfrac{\partial}{\partial z}|U\} = \frac{1}{T}L_i\frac{\partial\mu_i}{\partial z}$$

*with* $\gamma_{ci} = \frac{1}{T}L_i > 0$, $\{S|G_1(:,i)\frac{\partial}{\partial z}|U\} = \frac{\partial\mu_i}{\partial z}$ *and the matrices of the operators of order one* $G_1 = I_n$. *The modulating function of the heat diffusion is*

$$r_s = \gamma_s\{S|U\} = \frac{1}{T}\left(\frac{\lambda}{T}\right)\frac{\partial T}{\partial z}$$

*with* $\gamma_s = \frac{1}{T}\left(\frac{\lambda}{T}\right) > 0$, $\{S|U\} = \frac{\partial T}{\partial z}$ *and* $g_s = 1$. *The modulating function of the* $j$*-th chemical reaction is*

$$R_{0j} = \gamma_{0j}\{s|G_0(:,j)|U\} = \frac{1}{T}\left(\frac{r_j}{\mathcal{A}_j}\right)\mathcal{A}_j$$

*with* $\gamma_{r_j} = \frac{1}{T}\left(\frac{r_j}{\mathcal{A}_j}\right) > 0$, $\{S|G_{0j}|U\} = \mathcal{A}_j$ *and the matrix of the operator of order zero* $G_0 = I_n$.

*Furthermore, consider the following set of boundary inputs and outputs, respectively,*

$$v = \begin{bmatrix} \mathbf{f}(t,a) \\ \mathbf{f}(t,b)\end{bmatrix}, \qquad y = \begin{bmatrix} -\frac{\delta H}{\delta x}(t,b) \\ -\frac{\delta H}{\delta s}(t,b) \\ \frac{\delta H}{\delta x}(t,a) \\ \frac{\delta H}{\delta s}(t,a)\end{bmatrix}, \qquad (17)$$

*with* $\mathbf{f} = [f_{c1},\dots,f_{cn},f_s]^\top$ *the vector of fluxes, then (16) with (17) is a BC-IPHS (Definition 2).*

**Proof.** The pseudo-brackets related to mass and heat diffusion correspond to the respective thermodynamic driving forces. The non-linear functions $\gamma_{ci}$ and $\gamma_s$ are positive since the mass diffusion coefficients $L_i$, the thermal conductivity coefficient $\lambda$ and the temperature are always positive. For the thermodynamic driving force of the chemical reaction, consider in a first instance only the $j$-th reaction term. The pseudo-bracket for the $j$-th chemical reaction is

$$\{S|G_{0j}|U\} = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ 1\end{bmatrix}^\top \begin{bmatrix} 0 & \dots & 0 & \bar{\nu}_{j1} \\ & & & \vdots \\ 0 & \dots & 0 & \\ 0 & \dots & 0 & \bar{\nu}_{jn} \\ -\bar{\nu}_{j1} & \dots & -\bar{\nu}_{jn} & 0\end{bmatrix}\begin{bmatrix} \mu_1 \\ \vdots \\ \\ \mu_{n-1} \\ T\end{bmatrix} = \mathcal{A}_j.$$

On the other hand from De Donder's fundamental equation (42) it has been shown in (45) that $\gamma_{r_j} = \frac{1}{T}\left(\frac{r_j}{\mathcal{A}_j}\right) > 0$. The same applies for the other reactions. Regarding the boundary inputs and outputs, we have that

$$P_e = \begin{bmatrix} 0 & 0 & I_n & 0 \\ 0 & 0 & 0 & 1 \\ I_n & 0 & 0 & 0 \\ 0 & 1 & 0 & 0\end{bmatrix}$$

since $P_1 = 0, G_1 = I_n$ and $g_s = 1$. This implies $M_p = P_{ep} = M = P_e$, hence choosing the parametrization

$$\Xi_1 = \frac{1}{\sqrt{2}}\begin{bmatrix} 0 & 0 & -I_n & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & I_n & 0 \\ 0 & 0 & 0 & 1\end{bmatrix}, \quad \Xi_2 = \frac{1}{\sqrt{2}}\begin{bmatrix} I_n & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ I_n & 0 & 0 & 0 \\ 0 & 1 & 0 & 0\end{bmatrix}$$

we obtain the boundary inputs/outputs (17). ■

### *5.2. A simple application case*

Consider a simple diffusion-reaction process on $z \in [a,b]$ involving only two species and obeying the following reaction scheme

$$A \xrightarrow{r} B \qquad (18)$$

This simple reaction involves four irreversible thermodynamic processes, related to the mass diffusion of species $A$ and $B$, the heat diffusion and the chemical reaction. The thermodynamic parameters of the diffusion-reaction process are the mass diffusion coefficients $L_A$ and $L_B$, the thermal conductivity coefficient $\lambda$ and the stoichiometric coefficients $\bar{\nu}_A = -1$ and $\bar{\nu}_B = 1$. The state vector is in this case $x = [c_A, c_B]^\top$ and $s$, and according to Proposition 1 the BC-IPHS formulation of (18) is

$$\frac{\partial}{\partial t}\begin{bmatrix} c_A \\ c_B \\ s\end{bmatrix} = \begin{bmatrix} 0 & 0 & \frac{r}{T} \\ 0 & 0 & -\frac{r}{T} \\ -\frac{r}{T} & \frac{r}{T} & 0\end{bmatrix}\begin{bmatrix} \mu_A \\ \mu_B \\ T\end{bmatrix} +$$
$$\begin{bmatrix} 0 & 0 & \frac{\partial}{\partial z}\left(\frac{L_A}{T}\frac{\partial\mu_A}{\partial z}(\cdot)\right) \\ 0 & 0 & \frac{\partial}{\partial z}\left(\frac{L_B}{T}\frac{\partial\mu_A}{\partial z}(\cdot)\right) \\ \frac{L_A}{T}\frac{\partial}{\partial z}(\cdot) & \frac{L_B}{T}\frac{\partial}{\partial z}(\cdot) & \frac{\lambda}{T^2}\left(\frac{\partial T}{\partial z}\right)\frac{\partial(\cdot)}{\partial z} + \frac{\partial}{\partial z}\left(\frac{\lambda}{T^2}\frac{\partial T}{\partial z}(\cdot)\right)\end{bmatrix}\begin{bmatrix} \mu_A \\ \mu_B \\ T\end{bmatrix}$$

The conjugated inputs and outputs are, respectively,

$$v = \begin{bmatrix} L_A\frac{\partial\mu_A}{\partial z}(t,a) \\ L_B\frac{\partial\mu_B}{\partial z}(t,a) \\ \frac{\lambda}{T}\frac{\partial T}{\partial z}(t,a) \\ L_A\frac{\partial\mu_A}{\partial z}(t,b) \\ L_B\frac{\partial\mu_B}{\partial z}(t,b) \\ \frac{\lambda}{T}\frac{\partial T}{\partial z}(t,b)\end{bmatrix}, \qquad y = \begin{bmatrix} -\mu_A(t,b) \\ -\mu_B(t,b) \\ -T(t,b) \\ \mu_A(t,a) \\ \mu_B(t,a) \\ T(t,a)\end{bmatrix}$$

i.e., the incoming and outgoing flows of matter and entropy evaluated at the boundaries and the intensive variables evaluated at the boundaries. From Lemma 1 the energy balance is given by

$$\begin{aligned}\dot{U} &= y^\top v \\ &= \left(L_A \frac{\partial \mu_A}{\partial z}\mu_A(b) - L_A \frac{\partial \mu_A}{\partial z}\mu_A(a)\right) \\ &+ \left(L_B \frac{\partial \mu_B}{\partial z}\mu_B(b) - L_B \frac{\partial \mu_B}{\partial z}\mu_B(a)\right) \\ &+ \left(\frac{\lambda}{T}\frac{\partial T}{\partial z}T(b) - \frac{\lambda}{T}\frac{\partial T}{\partial z}T(a)\right),\end{aligned}$$

while by Lemma 2 the entropy balance is

$$\begin{aligned}\dot{S} &= \\ &\int_a^b \frac{\lambda}{T^2}\left(\frac{\partial T}{\partial z}\right)^2 + \frac{L_A}{T}\left(\frac{\partial \mu_A}{\partial z}\right)^2 + \frac{L_B}{T}\left(\frac{\partial \mu_B}{\partial z}\right)^2 + \frac{r}{T}\mathcal{A}\, dz \\ &\qquad + \left(\frac{\lambda}{T}\frac{\partial T}{\partial z}(b) - \frac{\lambda}{T}\frac{\partial T}{\partial z}(a)\right)\end{aligned}$$

We observe that the total internal entropy production is

$$\sigma = \int_a^b \frac{\lambda}{T^2}\left(\frac{\partial T}{\partial z}\right)^2 + \frac{L_A}{T}\left(\frac{\partial \mu_A}{\partial z}\right)^2 + \frac{L_B}{T}\left(\frac{\partial \mu_B}{\partial z}\right)^2 + \frac{r}{T}\mathcal{A}\, dz$$

Furthermore, the pseudo-brackets $\{S|G_1(:,1)\frac{\partial}{\partial z}|U\} = \frac{\partial \mu_A}{\partial z}$, $\{S|G_1(:,2)\frac{\partial}{\partial z}|U\} = \frac{\partial \mu_B}{\partial z}$, $\{S|U\} = \frac{\partial T}{\partial z}$ and $\{S|G_0(:,i)|U\} = \mathcal{A}$, correspond, respectively, to the thermodynamic driving forces of mass and heat diffusion and chemical reactions. The diffusion-reaction process is hence given by the composition of the IPHS formulation of the diffusion process and the chemical reaction together with the mass and heat flows.

## 6. Conclusion

Boundary Controlled Irreversible Port-Hamiltonian Systems (BC-IPHS) defined on a 1-dimensional spatial domain have been defined (Definition 1 and 2) by extending the formulation of reversible BC-PHS to irreversible thermodynamic systems controlled at the boundaries of their spatial domain. The structure of BC-IPHS has clear physical interpretation, characterizing the coupling between energy storing and energy dissipating elements, furthermore, the irreversible nature of the model is precisely expressed by the thermodynamic driving forces. By extending the definition of boundary port variables of BC-PHS to deal with the irreversible dissipation of the energy, a set of boundary port variables have been defined such that BC-IPHS are passive with respect to a given set of conjugated inputs and outputs. It is interesting to notice that when no irreversible phenomena is present, and thus the entropy coordinate is not considered, Definition 1 and 2 define a BC-PHS. As for finite dimensional IPHS, the first and second laws of Thermodynamics are satisfied (Lemmas 1 and 2) as a structural property of the system. The proposed formulation has been illustrated on the examples of an isentropic fluid, with and without dissipation, heat conduction and a diffusion-reaction process. Future work will study the extension of passivity based boundary control design methods to BC-IPHS.

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