

# An irreversible port-Hamiltonian formulation of distributed diffusion processes

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**Abstract:** An infinite dimensional formulation of IPHS is proposed for a general class of mass and heat diffusion processes. The structure of the system is derived from the expression of the internal entropy creation, and just as for the lumped case the IPHS structure is expressed as a function of the distributed thermodynamic driving forces and a positive definite function containing the thermodynamic parameters of the different diffusion processes. The distributed thermodynamic driving forces are expressed as the evaluation of the internal energy density and entropy density on a pseudo-Poisson bracket defined by the skew-adjoint differential operator defining the coupling between the different energy domains. This is analogous to the case of lumped IPHS, where the pseudo-Poisson bracket is defined not by differential operators but by constant (canonical) skew-symmetric matrices.

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

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## 1. INTRODUCTION

Irreversible port-Hamiltonian system (IPHS) were proposed in Ramirez et al. (2013a) as an extension of port-Hamiltonian systems (PHS) (Maschke and van der Schaft, 1992; Maschke et al., 1992) towards the structural representation of irreversible thermodynamics. For processes described by lumped models it has been shown that the formalism encompasses a large and general class of irreversible thermodynamic systems, such as heat-exchangers, chemical reactions, chemical reaction networks and coupled mechanic-thermodynamic systems such as the gaspiston (Ramirez et al., 2013b). Different to representations which seek to encode the dynamics of irreversible thermodynamic systems by a differential geometric structure, such as GENERIC (Grmela and Öttinger, 1997; Öttinger and Grmela, 1997) or contact systems (Hermann, 1973; Mrugala et al., 1991; Mrugala, 1993; Eberard et al., 2007), the aim of the IPH formulation is to encode the dynamics with a pseudo-PH *control* structure. Indeed, using the definition of the availability function (Keenan, 1951; Alonso and Ydstie, 2001; Alonso et al., 2002) the IPHS structure has recently been employed to exploit the thermodynamic properties of irreversible processes to derive non-linear passivity based controllers (Ramirez et al., 2016).

This paper presents the first extension of IPHS towards irreversible thermodynamic processes modeled as infinite dimensional systems. More specifically the process of non-isothermal mass diffusion, i.e., simultaneous diffusion of

heat and mass, is considered and an infinite dimensional IPH representation is proposed. To this end a pseudo-PH structure constructed from the expression of the internal entropy creation and the distributed thermodynamic force is derived. It is shown that this structure is similar to the lumped case, begin the main difference that the pseudo-Poisson brackets defining the distributed thermodynamic driving forces are defined by skew-adjoint differential operators. The paper is organized as follows. In Section 2 the definition and main properties of IPHS are presented and the finite dimensional IPH models of the heat and mass diffusion processes are derived. In Section 3 the infinite dimensional IPHS modeling the heat equation and the complete diffusion process is presented. Finally in Section we give some concluding remarks and comments on future work.

## 2. IRREVERSIBLE PORT-HAMILTONIAN SYSTEMS

Irreversible port-Hamiltonian systems (IPHS) have been defined in Ramirez et al. (2013a) as an extension of port-Hamiltonian systems (PHS) for the purpose of representing not only the energy balance but also the entropy balance, essential in thermodynamic systems.

*Definition 1.* (Ramirez et al., 2013a) An input affine IPHS is defined by the dynamic equation and output relation

$$\begin{aligned} \dot{x} &= R \left( x, \frac{\partial U}{\partial x} \right) J \frac{\partial U}{\partial x} (x) + g \left( x, \frac{\partial U}{\partial x} \right) v, \\ y &= g^\top \left( x, \frac{\partial U}{\partial x} \right) \frac{\partial U}{\partial x} (x) \end{aligned} \quad (1)$$

where  $x(t) \in \mathbb{R}^n$  is the state vector, the smooth functions  $U(x) : \mathbb{R}^n \rightarrow \mathbb{R}$  and  $S(x) : \mathbb{R}^n \rightarrow \mathbb{R}$  represent,

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\* This work was supported by French sponsored project Labex ACTION under reference code ANR-11-LABX-0001- 01

respectively, the internal energy (the Hamiltonian) and the entropy functions,  $J \in \mathbb{R}^{n \times n}$  is a constant skew-symmetric structure (interconnection) matrix of the Poisson bracket (Maschke et al., 1992) acting on any two smooth functions  $Z$  and  $G$  as:

$$\{Z, G\}_J = \frac{\partial Z^\top}{\partial x}(x) J \frac{\partial G}{\partial x}(x). \quad (2)$$

The real function  $R = R(x, \frac{\partial U}{\partial x})$  is composed by the product of a positive definite function  $\gamma$  and the Poisson bracket between the entropy and the energy functions:

$$R(x, \frac{\partial U}{\partial x}) = \gamma(x, \frac{\partial U}{\partial x}) \{S, U\}_J,$$

with  $\gamma(x, \frac{\partial U}{\partial x}) : \mathbb{R}^n \rightarrow \mathbb{R}$ ,  $\gamma \geq 0$ , a non-linear positive function. The input map is defined by  $g(x, \frac{\partial U}{\partial x}) \in \mathbb{R}^{n \times m}$  with the input  $v(t) \in \mathbb{R}^m$  a time dependent function.

The drift dynamic in (1) is defined by a non-linear relation between the time derivative  $\dot{x}$  of the state (extensive) variables and  $\frac{\partial U}{\partial x}$ , characterized by the modulating function  $R(x, \frac{\partial U}{\partial x})$ , which explicitly depends on the co-energy (intensive) variables  $\frac{\partial U}{\partial x}$ . The balance equations of the total energy and entropy functions of IPHS express the first and second principles of irreversible Thermodynamics: the conservation of energy and the irreversible creation of entropy due to irreversible phenomena. By skew-symmetry of  $J$ , the balance equation of the internal energy, which is a convex function,

$$\frac{dU}{dt} = y^\top v, \quad (3)$$

expresses that the system (1) is a lossless dissipative systems with (energy) supply rate  $y^\top v$  (Willems, 1972). The balance equation of the entropy function is given by

$$\begin{aligned} \frac{dS}{dt} &= R(x, \frac{\partial U}{\partial x}, \frac{\partial S}{\partial x}) \frac{\partial S^\top}{\partial x} J(x) \frac{\partial U}{\partial x} + \frac{\partial S^\top}{\partial x} g(x, \frac{\partial U}{\partial x}) v \\ &= \gamma(x, \frac{\partial U}{\partial x}) \{S, U\}_J^2 + \left( g^\top(x, \frac{\partial U}{\partial x}) \frac{\partial S}{\partial U} \frac{\partial U}{\partial x} \right)^\top v. \\ &= \gamma(x, \frac{\partial U}{\partial x}) \{S, U\}_J^2 + y_s^\top v. \end{aligned} \quad (4)$$

where  $y_s = \frac{\partial S}{\partial U} y$  is an entropy conjugated output. By Definition 1 the first term is positive:  $\gamma(x, \frac{\partial U}{\partial x}) \{S, U\}_J^2 = \sigma(x, \frac{\partial U}{\partial x}) \geq 0$ . For irreversible thermodynamic systems, this term represents the *internal entropy production* and its positivity expresses the second principle of Thermodynamics. The second term in (4) corresponds to the definition of an entropy supply rate. For further details on IPHS and its thermodynamic interpretation we refer the reader to Ramirez et al. (2013a).

We shall first introduce the two fundamental phenomena that describe non-isothermal mass diffusion: namely the diffusion of heat and mass. These processes are described as *exchangers* of heat, respectively mass. We shall in a first instance consider them separately and investigate their IPH representation in finite dimensions.

### 2.1 The heat exchanger

Consider two simple thermodynamic systems, indexed by 1 and 2 (for instance two ideal gases), which may interact only through a conducting wall. The dynamic of this system is given by the following equation

$$\begin{bmatrix} \dot{S}_1 \\ \dot{S}_2 \end{bmatrix} = \lambda \begin{bmatrix} T_2(S_2) \\ T_1(S_1) \\ T_1(S_1) \\ T_2(S_2) \end{bmatrix} - 1 + \lambda_e \begin{bmatrix} 0 \\ T_e(t) \\ T_2(S_2) \end{bmatrix} - 1 \quad (5)$$

where  $S_1$  and  $S_2$  (resp.  $T_1$  and  $T_2$ ) are the entropies (resp. the temperatures) of subsystem 1 and 2,  $T_e(t)$  is the time dependent (controlled) temperature of the environment and  $\lambda > 0$  (resp.  $\lambda_e > 0$ ) denotes Fourier's heat conduction coefficient of the heat conducting wall between the two compartments (resp. between compartment 2 and the environment). This system may be written as

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \end{bmatrix} = \lambda \begin{pmatrix} 1 & -1 \\ \frac{\partial U}{\partial x_2} & -\frac{\partial U}{\partial x_1} \end{pmatrix} \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} \frac{\partial U}{\partial x_1} \\ \frac{\partial U}{\partial x_2} \end{bmatrix} + \lambda_e \begin{bmatrix} 0 \\ \frac{1}{\frac{\partial U}{\partial x_2}} - \frac{1}{u} \end{bmatrix} u,$$

where  $x = [S_1, S_2]$ ,  $U(x_1, x_2) = U_1(x_1) + U_2(x_2)$  is the internal energy of the overall system, sum of the internal energies of each subsystem,  $u(t)$  the controlled input that corresponds to the external temperature  $T_e(t)$  with  $\frac{\partial U}{\partial x_i} = T_i(x_i)$ . The system admits a IPH representation, which is given by (Ramirez et al., 2013a)

$$\dot{x} = R(x, T) J T(x) + g(T, u(t)) u(t), \quad (6)$$

with

$$R(x, T(x)) = \lambda \left( \frac{1}{T_2} - \frac{1}{T_1} \right), \quad (7)$$

$J = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}$  (where, for the sake of keeping a physical interpretation we denote  $\frac{\partial U}{\partial x} = T(x) = [T_1(x_1), T_2(x_2)]^T$ ) and with input map defined by  $g = \lambda_e \begin{bmatrix} 0 \\ \frac{1}{\frac{\partial U}{\partial x_2}} - \frac{1}{u} \end{bmatrix}$ . The

system (6) indeed fulfils the Definition 1. The total entropy of the system is given by the sum of the entropies of each compartments  $S(x) = x_1 + x_2$ . The Poisson bracket  $\{S, U\}_J$  is then simply the difference of temperatures between the compartments

$$\{S, U\}_J = \frac{\partial S^\top}{\partial x} J \frac{\partial U}{\partial x} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}^\top \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} T_1 \\ T_2 \end{bmatrix} = T_1 - T_2.$$

It may be noted immediately that the bracket is indeed the driving force of the heat conduction. Then one may identify the expression of the modulating function (7) and obtain

$$\gamma = \frac{\lambda}{T_1 T_2}.$$

Since the heat conduction coefficient satisfy  $\lambda > 0$ , as well as the temperatures  $T_1 > 0$  and  $T_2 > 0$ , then the condition  $\gamma > 0$  is also satisfied. The term  $g(T)u$  defines the entropy flow generated by the interaction of subsystem 2 and the external heat source and depends on the heat conduction coefficient  $\lambda_e$  between them.

### 2.2 The mass exchanger

Let us now consider a closed system consisting of two compartments,  $a$  and  $b$ , of equal temperature  $T$ , one with chemical potential  $\mu_a$  and mole number  $n_a$ , and the other with chemical potential  $\mu_b$  and mole number  $n_b$ . They are connected through a permeable wall with diffusion coefficient  $L$ . The flow of particles from one part to the other is given by the balance equation (Kondepudi and Prigogine, 1998)

$$\frac{dn_a}{dt} = -\frac{dn_b}{dt}$$

The change of moles goes from the part with highest chemical potential to the one with lowest, i.e., the thermodynamic force which drives the diffusion process is the chemical potential difference  $\mu_b - \mu_a$ , hence the flux is given by  $f_n = \frac{L}{T}(\mu_b - \mu_a)$  and the dynamic of the mole number balance is

$$\begin{aligned}\frac{dn_a}{dt} &= \frac{L}{T}(\mu_b - \mu_a) \\ \frac{dn_b}{dt} &= -\frac{L}{T}(\mu_b - \mu_a)\end{aligned}$$

The system dynamic is completed with the entropy balance, which is given by the internal entropy production due to the diffusion (Kondepudi and Prigogine, 1998)

$$\frac{dS}{dt} = \sigma = -\frac{1}{T} \sum_{a,b} f_n(\mu_b - \mu_a) = \frac{L}{T^2}(\mu_b - \mu_a)^2.$$

We may identify the IPHS structure from the entropy production. Indeed, since the the modulating term  $R_n$  is composed by a positive definite function  $\gamma_n$  and the thermodynamic driving force  $\mu_b - \mu_a$ , we have  $R_n = \frac{L}{T^2}(\mu_b - \mu_a)$  with  $\{S, U\}_J = (\mu_b - \mu_a)$  and  $\gamma = \frac{L}{T^2} > 0$ , which implies

$$J_n = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & -1 \\ -1 & 1 & 0 \end{bmatrix}.$$

Hence, by defining as state vector  $x = [n_a, n_b, S]$ , and as Hamiltonian the internal energy such that  $\frac{\partial U}{\partial x} = [\mu_a, \mu_b, T]^\top$ , we have the following IPHS representation of the discrete diffusion process,

$$\dot{x} = R_n J_n \frac{\partial U}{\partial x}.$$

### 3. THE DIFFUSION PROCESS AS A DISTRIBUTED IPHS

In this section we extend the IPH formulation of finite dimensional thermodynamic systems (1) to boundary controlled port Hamiltonian systems defined on a 1D spatial domain *i.e.*  $z \in (a, b)$ . The  $n$  state variables are now defined on real Hilbert spaces and the internal energy  $u(x)$  and the entropy  $s(x)$  are smooth functions of the state variables. We denote by  $x \in X((a, b), \mathbb{R}^n)$  the vector of state variables,  $U(t) = \int_a^b u(z, t) dz$  the total internal energy and  $S(t) = \int_a^b s(z, t) dz$  the total entropy functions. The co-state variables  $e(z, t)$  are derived from the internal energy considering the variational derivative as defined in Maschke and van der Schaft (2005), *i.e.*,

$$e(z, t) = \frac{\delta U}{\delta x} = \frac{\partial u}{\partial x},$$

this equality being valid as  $u$  is a function of  $x$  only. Let  $J$  now be a formally skew adjoint differential operator. We generalize the Poisson bracket (2) to infinite dimensional systems by defining a pseudo Poisson bracket as in () for any smooth functions  $Z$  and  $G$  as:

$$\{Z, G\}_J = \frac{\delta Z^\top}{\delta x}(x) J \left( \frac{\delta G}{\delta x}(x) \right) = \frac{\partial Z^\top}{\partial x}(x) J \left( \frac{\partial G}{\partial x}(x) \right)$$

We shall frequently omit arguments in the function when they are obvious for the sake of simplifying the presentation.

#### 3.1 The heat equation

We shall follow Duindam et al. (2009) and assume that the heat diffusion is over a 1D spatial domain and in a first instance consider only one physical domain, the thermal and its dynamics. The conserved quantity is the density of internal energy, denoted by  $u(t, z)$ , an extensive thermodynamic variable which satisfies the conservation law

$$\frac{\partial u}{\partial t} = -\frac{\partial}{\partial z} f_Q \quad (8)$$

where  $f_Q(t, z)$  is the flux variable, here the heat flux across the section at  $z$ . The heat flux itself arises from the thermodynamic non-equilibrium and is defined by some phenomenological law, for instance defined according to Fourier's law by

$$f_Q(t, z) = -\lambda(u, z) \frac{\partial}{\partial z} T(u, z) \quad (9)$$

where  $\lambda(u, z)$  denotes the heat conduction coefficient and  $T$  denotes the temperature of the medium, the intensive thermodynamic variable of the thermal domain. Actually the axioms of the Irreversible Thermodynamics near equilibrium, decompose the preceding relation by saying that the flux variable is a function of the thermodynamic driving force  $F(t, z) = \frac{\partial}{\partial z} T(t, z)$  which characterizes the non-equilibrium condition. The conservation law (8) and the constitutive relation (9) are completed by taking into account the thermodynamic properties of the medium, which provides a relation between the driving force  $F$  and the conserved quantity  $u$ . The thermodynamic properties are given by Gibbs relation which (Kondepudi and Prigogine, 1998), under the assumption that there is no exchange of matter and that the volume of the medium is constant, reduces to  $du = T ds$ , where  $s$  is the entropy of the medium which is also an extensive variable. Due to the irreversibility of thermodynamic processes, the temperature is strictly positive (Kondepudi and Prigogine, 1998) in such a way that one may choose equivalently the internal energy or the entropy as thermodynamical potential. Just as for the lumped case, we shall consider the internal energy  $u = u(s)$  as thermodynamic potential function, and in this case Gibbs relation defines the temperature as intensive variable conjugated to the (extensive variable) entropy by:  $T = \frac{du}{ds}(s)$ . This leads to write the following entropy balance equation (Duindam et al., 2009)

$$\begin{aligned}\frac{\partial s}{\partial t} &= -\frac{1}{T} \frac{\partial}{\partial z} f_Q = -\frac{\partial}{\partial z} f_S + \sigma \\ \frac{\partial s}{\partial t} &= \frac{\partial}{\partial z} \left( \frac{\lambda}{T} \frac{\partial T}{\partial z} \right) + \frac{\lambda}{T^2} \left( \frac{\partial T}{\partial z} \right)^2\end{aligned} \quad (10)$$

where  $f_S$  denotes the flux of entropy through the section at the point  $z$

$$f_S = \frac{1}{T} f_Q = -\lambda \frac{1}{T} \frac{\partial}{\partial z} T \quad (11)$$

and  $\sigma$  denotes the irreversible entropy creation and is given by

$$\sigma = -\frac{1}{T} \frac{\partial T}{\partial z} f_S = \frac{\lambda}{T^2} \left( \frac{\partial T}{\partial z} \right)^2 \quad (12)$$

Finally the flux of entropy may be written as a function characterizing the irreversible phenomenon of heat conduction  $f_S = -\frac{\lambda}{T} F$  in terms of the generating force  $F = \frac{\partial T}{\partial z} \frac{du}{ds}(s)$ , which itself depends on the differential of

the internal energy function characterizing the thermodynamic properties of the medium.

Let us look at (10) in some more details. The first term in (10) is related to the entropy flux through the boundaries of the system, hence it is related to the boundary variables, i.e., with the inputs and outputs of the system. The second term, the internal irreversible entropy production  $\sigma$ , is related with the internal dynamics, i.e., the drift dynamics. Hence, as just as in the finite dimensional case it is possible to identify (12) with a modulating function and a bracket defining the thermodynamic driving force.

*Proposition 2.* The distributed heat equation can be written as the distributed IPHS

$$\frac{\partial s}{\partial t} = R_s J_s \frac{\partial u}{\partial s} + \frac{\partial}{\partial z} \left( R_s \frac{\partial u}{\partial s} \right) \quad (13)$$

where

$$R_s = \gamma_s \left( s, \frac{\partial u}{\partial s}, z \right) \{S, U\}_{J_s}$$

with  $J_s = \frac{\partial}{\partial z}$ ,  $\gamma_s = \frac{1}{T^2} \lambda \left( s, \frac{\partial u}{\partial s}, z \right)$  and  $\{S, U\}_{J_s} = \frac{\partial T}{\partial z}$ . The input and output of the system are defined, respectively as

$$v = \begin{bmatrix} \left( R_s \frac{\partial u}{\partial s} \right) (t, b) \\ \left( R_s \frac{\partial u}{\partial s} \right) (t, a) \end{bmatrix}, \quad y = \begin{bmatrix} \frac{\partial u}{\partial s} (t, b) \\ -\frac{\partial u}{\partial s} (t, a) \end{bmatrix} \quad (14)$$

*Proof:* By direction inspection it is observed that (13) is equivalent to the entropy balance (10). It is direct to verify that (12) is equal to  $R_s \{S, U\}_{J_s}^2$  and that  $f_s = -\frac{\partial}{\partial z} \left( -\frac{\lambda}{T} \frac{\partial T}{\partial z} \right) = \frac{\partial}{\partial z} \left( R_s \frac{\partial u}{\partial s} \right)$ . The overall energy balance can be derived using the local entropy balance,

$$\begin{aligned} \frac{dU}{dt} &= \int_a^b \frac{du}{dt} dz \\ &= \int_a^b \left( \frac{\partial u}{\partial s} \right)^\top \left( \frac{\partial s}{\partial t} \right) dz \\ &= \int_a^b \left( \frac{\partial u}{\partial s} \right)^\top \left( R_s(T, z) J \frac{\partial u}{\partial s} + \frac{\partial}{\partial z} \left( R_s \frac{\partial u}{\partial s} \right) \right) dz, \end{aligned}$$

an integrating by parts this can be written as

$$\begin{aligned} \frac{dU}{dt} &= \int_a^b \frac{\partial}{\partial z} \left( \left( \frac{\partial u}{\partial s} \right)^\top R_s \frac{\partial u}{\partial s} \right) dz \\ &= y^\top v \end{aligned}$$

where (14) has been used. Hence, convexity of the internal energy function  $U$ , the system is a lossless dissipative system.  $\square$

Having derived an IPH formulation of the heat equation we shall now proceed to propose a formulation of simultaneous diffusion of mass and heat as IPHS.

### 3.2 The complete diffusion process

Let us now consider a distributed diffusion process of one component. The number of mole balance is characterized by the diffusion process, while the internal entropy creation is due to the irreversible diffusion process and heat conduction. The number of moles and entropy balances are given by (Kondepudi and Prigogine, 1998)

$$\begin{aligned} \frac{\partial n}{\partial t} &= -\frac{\partial}{\partial z} (f_n) \\ \frac{\partial s}{\partial t} &= -\frac{\partial}{\partial z} (f_s) + \sigma_s + \sigma_n \end{aligned} \quad (15)$$

where  $f_n = -\frac{L}{T} \frac{\partial \mu}{\partial z}$  corresponds to the number of mole flux,  $f_s = -\frac{\lambda}{T} \frac{\partial T}{\partial z}$  to the entropy flux,  $\sigma_s$  the internal entropy production due to heat conduction and  $\sigma_n$  the internal entropy production due to irreversible diffusion. The entropy production terms are defined respectively as

$$\sigma_s = -\frac{1}{T} f_s \frac{\partial T}{\partial z} = \frac{\lambda}{T^2} \left( \frac{\partial T}{\partial z} \right)^2 \quad (16)$$

$$\sigma_n = -\frac{1}{T} f_n \frac{\partial \mu}{\partial z} = \frac{L}{T^2} \left( \frac{\partial \mu}{\partial z} \right)^2 \quad (17)$$

Since there are two internal entropy production terms, each due to a different thermodynamic driving force, we expect to have two different modulating functions  $R \left( x, \frac{\partial U}{\partial x} \right)$  in the IPHS representation. This is for instance the case of coupled chemical reaction networks (Ramirez et al., 2014) where each individual reaction contributes with an entropy creation term. From the entropy creation terms we may identify

$$R_s = \gamma_s \{S, U\}_{J_s} = \frac{\lambda}{T^2} \left( \frac{\partial T}{\partial z} \right) \quad (18)$$

$$R_n = \gamma_n \{S, U\}_{J_n} = \frac{L}{T^2} \left( \frac{\partial \mu}{\partial z} \right) \quad (19)$$

As for the lumped case we may identify the functions  $\gamma_s$  and  $\gamma_n$  and the matrices  $J_s$  and  $J_n$  since the thermodynamic driving forces are respectively  $\{S, U\}_{J_s} = \frac{\partial T}{\partial z}$  and  $\{S, U\}_{J_n} = \frac{\partial \mu}{\partial z}$ . Hence we have

$$\begin{aligned} \gamma_s &= \frac{\lambda}{T^2} & J_s &= \begin{bmatrix} \alpha(x) & 0 \\ 0 & 1 \end{bmatrix} \frac{\partial}{\partial z} \\ \gamma_n &= \frac{L}{T^2} & J_n &= \begin{bmatrix} \beta(x) & 1 \\ 1 & 0 \end{bmatrix} \frac{\partial}{\partial z} \end{aligned}$$

with  $\alpha(x)$  and  $\beta(x)$  state dependent functions which do not affect the evaluation of the brackets  $\{S, U\}_{J_s}$  and  $\{S, U\}_{J_n}$  since  $\frac{\partial S}{\partial x} = [0 \ 1]^\top$ . Notice that if  $\alpha$  and  $\beta$  are constants then the brackets are Poisson brackets, if  $\alpha$  and  $\beta$  are state dependent then the brackets are possible pseudo-Poisson brackets. The functions  $\alpha$  and  $\beta$  can however not depend on the co-energy variables since that would destroy the linearity of the brackets. The dynamic equations (15) can be written as

$$\begin{aligned} \dot{x} &= \\ &= \frac{\lambda}{T^2} \frac{\partial T}{\partial z} \begin{bmatrix} -\frac{L}{\lambda} & 0 \\ 0 & 1 \end{bmatrix} \frac{\partial}{\partial z} \frac{\partial U}{\partial x} + \frac{L}{T^2} \frac{\partial \mu}{\partial z} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \frac{\partial}{\partial z} \frac{\partial U}{\partial x} \\ &\quad - \frac{\partial}{\partial z} \begin{bmatrix} -f_n \\ -f_s \end{bmatrix}, \end{aligned} \quad (20)$$

Hence we identify  $\alpha = -\frac{L}{\lambda}$  and  $\beta = 0$ . Now, from (17) and (16) we may make the following identification

$$\sigma_s = -\frac{1}{T} f_s \frac{\partial T}{\partial z} = R_s \frac{\partial T}{\partial z} \quad (21)$$

$$\sigma_n = -\frac{1}{T} f_n \frac{\partial \mu}{\partial z} = R_n \frac{\partial \mu}{\partial z} \quad (22)$$

which imply, since  $R_s$  and  $R_n$  are scalars, that

$$f_s = -R_s T = -R_s \frac{\partial u}{\partial s} \quad (23)$$

$$f_n = -R_n T = -R_n \frac{\partial u}{\partial s}. \quad (24)$$

Hence, the system (20) may be written as the IPHS

$$\dot{x} = (R_s J_s + R_n J_n) \frac{\partial u}{\partial x} + \frac{\partial}{\partial z} \left( \begin{bmatrix} R_n \\ R_s \end{bmatrix} \frac{\partial u}{\partial s} \right).$$

We observe, in analogy to the finite dimensional case, that the IPHS structure accounts for the irreversible entropy creation. The transport phenomena, which are related to the boundary values of the PDE, are also related to the IPHS structure. This is expected in the infinite dimensional case since the transport phenomena not only relate to the boundary values but also to the transport within the domain. Before generalizing this model to  $m$  species we assume the following.

*Assumption 3.* Assume that the heat conduction coefficient  $\lambda$  and that the diffusion coefficients of each species  $L_i$ , where  $i$  denotes a specie, are only functions of the states, i.e., of the entropy or the mole number of each specie.

The previous assumption establish that the  $\lambda$  and  $L_i$  do not depend explicitly on the co-energy variables, i.e., on the intensive variables. We generalize the IPH formulation in the following Proposition.

*Proposition 4.* Consider a diffusion process involving  $m$  species, described by the following set of equations

$$\begin{aligned} \frac{\partial n_i}{\partial t} &= -\frac{\partial}{\partial z} (f_{n_i}), \quad i = 1, \dots, m \\ \frac{\partial s}{\partial t} &= -\frac{\partial}{\partial z} (f_s) + \sigma_s + \sum_{i=1}^m \sigma_{n_i}. \end{aligned} \quad (25)$$

Define as state vector  $x = [n_1, \dots, n_m, s]$ , as inputs the extensive variables evaluated at the boundaries and as outputs the incoming and outgoing flows of matter and entropy evaluated at the boundaries, respectively,

$$v = \begin{bmatrix} \frac{\partial u}{\partial x}(t, a) \\ \frac{\partial u}{\partial x}(t, b) \end{bmatrix}, \quad y = \begin{bmatrix} \mathbf{f}_n(t, a) \\ -\mathbf{f}_n(t, b) \end{bmatrix} \quad (26)$$

with  $\mathbf{f}_n = [f_{n_1}, \dots, f_{n_m}, f_s]^\top$ . Then the diffusion process can be written as the infinite dimensional IPHS

$$\frac{\partial x}{\partial t} = \left( R_s J_s + \sum_{i=1}^m R_{n_i} J_{n_i} \right) \frac{\partial U}{\partial x} + \frac{\partial}{\partial z} \left( \mathbf{R} \frac{\partial u}{\partial s} \right) \quad (27)$$

where  $R_{n_i} = \gamma_{n_i} \{S, U\}_{J_{n_i}}$ ,  $\gamma_{n_i} = \frac{L_i}{T^2}$ ,

$$J_{n_1} = \begin{bmatrix} 0 & \dots & 1 \\ 0 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 1 & \dots & 0 \end{bmatrix} \frac{\partial}{\partial z}, \quad J_{n_2} = \begin{bmatrix} 0 & \dots & \dots & 0 \\ 0 & \ddots & \dots & 1 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 1 & \dots & 0 \end{bmatrix} \frac{\partial}{\partial z},$$

$$J_{n_3}, \dots, J_{n_{m-1}}, \quad J_{n_m} = \begin{bmatrix} 0 & \dots & \dots & 0 \\ 0 & \ddots & \vdots & \vdots \\ \vdots & \vdots & \ddots & 1 \\ 0 & \dots & 1 & 0 \end{bmatrix} \frac{\partial}{\partial z},$$

$R_s = \gamma_s \{S, U\}_{J_s}$ , with  $\gamma_s = \frac{\lambda}{T^2}$ ,

$$J_s = \begin{bmatrix} -\frac{L_1}{\lambda} & 0 & \dots & \dots & 0 \\ 0 & -\frac{L_2}{\lambda} & \vdots & \vdots & \vdots \\ \vdots & \vdots & \ddots & \vdots & 0 \\ \vdots & \vdots & \dots & -\frac{L_m}{\lambda} & 0 \\ 0 & \dots & \dots & 0 & 1 \end{bmatrix} \frac{\partial}{\partial z},$$

and  $\mathbf{R} \in \mathbb{R}^m$ ,  $\mathbf{R} = [R_{n_1} \dots R_{n_m} R_s]^\top$  a vector containing all the modulating functions. Furthermore, the system is conservative with respect to the total internal energy  $U = \int_a^b u(x, z) dz$  and the set of inputs and outputs (26).

*Proof:* It is straightforward to verify that (27) is equivalent to (25). Indeed, by noting that  $\frac{\partial u}{\partial x} = [\mu_1, \dots, \mu_m, T]^\top$  and developing the first term in (27) we have

$$\begin{aligned} \left( R_s J_s + \sum_{i=1}^m R_{n_i} J_{n_i} \right) \frac{\partial U}{\partial x} &= \\ &= \begin{bmatrix} 0 \\ \sum_{i=1}^m R_{n_i} \{s, u\}_{J_{n_i}} + R_s \{s, u\}_{J_s} \\ 0 \end{bmatrix} = \\ &= \begin{bmatrix} 0 \\ \sum_{i=1}^m \gamma_{n_i} \{s, u\}_{J_{n_i}}^2 + \gamma_s \{s, u\}_{J_s}^2 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ \sum_{i=1}^m \sigma_{n_i} + \sigma_s \\ 0 \end{bmatrix}, \end{aligned} \quad (28)$$

which together with the second term in (27) gives (25). From (28) it is also observed that the total internal entropy production  $\sigma = \sum_{i=1}^m \sigma_{n_i} + \sigma_s$  is completely determined by the IPHS structure. The diffusion coefficients  $L_i$  and the thermal conductivity coefficient  $\lambda$  are by assumption constant or state dependent, i.e., non co-state dependent, thus the operators  $J_{n_i}(\cdot)$  and  $J_s(\cdot)$  are formally skew-symmetric, and hence the brackets  $\{s, u\}_{J_{n_i}}$  and  $\{s, u\}_{J_s}$  define (pseudo)-Poisson brackets. Furthermore,  $\{s, u\}_{J_{n_i}} = \frac{\partial \mu_i}{\partial z}$  and  $\{s, u\}_{J_s} = \frac{\partial T}{\partial z}$ , which correspond, respectively, to the thermodynamic driving forces of the mass diffusions and the heat diffusion. Since  $L_i > 0$  and  $\lambda > 0$  the functions  $\gamma_{n_i} > 0$  and  $\gamma_s > 0$ , hence the modulating functions  $R_{n_i}$  and  $R_s$  are defined accordingly to the Definition 1. The total variation of entropy with respect to time is given by

$$\begin{aligned} \dot{S} &= \int_a^b \frac{\partial s}{\partial t} dz = \int_a^b \sigma dz + \int_a^b \frac{\partial}{\partial z} \left( R_s \frac{\partial u}{\partial s} \right) dz \\ &= \int_a^b \sigma dz + \left( R_s \frac{\partial u}{\partial s}(b, t) - R_s \frac{\partial u}{\partial s}(a, t) \right) \\ &= \int_a^b \sigma dz + \left( \frac{\lambda(t, b)}{T(t, b)} \frac{\partial T}{\partial z}(b, t) - \frac{\lambda(t, a)}{T(t, a)} \frac{\partial T}{\partial z}(a, t) \right). \end{aligned}$$

The variation of the total energy with respect to time is

$$\begin{aligned} \dot{U} &= \int_a^b \frac{\partial u}{\partial t} dz = \int_a^b \frac{\partial u}{\partial x}^\top \frac{\partial x}{\partial t} dz \\ &= \int_a^b \frac{\partial u}{\partial x}^\top \left[ \sum_{i=1}^m R_{n_i} \frac{\partial \mu_i}{\partial z} + R_s \frac{\partial T}{\partial z} \right] + \frac{\partial u}{\partial x}^\top \frac{\partial}{\partial z} \left( \mathbf{R} \frac{\partial u}{\partial s} \right) dz \end{aligned}$$

where we have used (28). Since in the first term of the integral only the last term of  $\frac{\partial u}{\partial x}$  is not multiplied by zero, the previous equation can be written as

$$\begin{aligned}\dot{U} &= \int_a^b \frac{\partial u}{\partial s} \mathbf{R}^\top \frac{\partial}{\partial z} \left( \frac{\partial u}{\partial x} \right) + \frac{\partial u}{\partial x}^\top \frac{\partial}{\partial z} \left( \mathbf{R} \frac{\partial u}{\partial s} \right) dz \\ &= \int_a^b \frac{\partial}{\partial z} \left( \frac{\partial u}{\partial x}^\top \mathbf{R} \frac{\partial u}{\partial s} \right) dz \\ &= \frac{\partial u}{\partial x}^\top \mathbf{R} \frac{\partial u}{\partial s}(t, b) - \frac{\partial u}{\partial x}^\top \mathbf{R} \frac{\partial u}{\partial s}(t, a)\end{aligned}$$

where we have used integration by parts. Using the definition of the inputs and outputs (26) and noticing that

$$y = \begin{bmatrix} \mathbf{f}_n(t, a) \\ -\mathbf{f}_n(t, b) \end{bmatrix} = \begin{bmatrix} -\mathbf{R} \frac{\partial u}{\partial s}(t, a) \\ \mathbf{R} \frac{\partial u}{\partial s}(t, b) \end{bmatrix}.$$

the total energy balance is finally given by

$$\dot{u} = y^\top v,$$

and by convexity of the internal energy  $U$ , is a lossless dissipative systems with (energy) supply rate  $y^\top v$ .  $\square$

#### 4. CONCLUSION

An infinite dimensional formulation of IPHS has been proposed for a general class of mass and heat diffusion processes. The structure of the system is derived from the expression of the internal entropy creation, and just as for the lumped case the IPHS structure is expressed as a function of the distributed thermodynamic driving forces and a positive definite function containing the thermodynamic parameters of the different diffusion processes. It is interesting to remark that the distributed thermodynamic driving forces are expressed as the evaluation of the internal energy density and entropy density on a pseudo-Poisson bracket defined by the skew-adjoint differential operator defining the coupling between the different energy domains. This is analogous to the case of lumped IPHS, where pseudo-Poisson bracket is not defined by differential operators but by constant (canonical) skew-symmetric matrices. Future work will study the incorporation of convection and reaction phenomena and the extension of passivity based control techniques to infinite dimensional IPHS.

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