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Abstract: In this paper we suggest a Port Hamiltonian model of the solidification process of water, using the phase field approach. Firstly, the Port Hamiltonian formulation of the dynamics of the phase field variable, governed by the Allen-Cahn equation, is recalled. It is based on adding to the phase field variable, its gradient, and extending the system with its dynamics. Secondly, the model is completed by the energy balance equation for the heat conduction and the complete Port Hamiltonian model is derived. Thirdly a Algebro-differential Port Hamiltonian representation is suggested, where the Port Hamiltonian system is defined on a Lagrangian submanifold, allowing to use directly the variables defining the thermodynamical data.

Keywords: Port Hamiltonian systems on Lagrange subspaces, Phase Field, Diffuse interface, Solidification process, Thermodynamical properties

1. INTRODUCTION

The deterioration of the environment through the discharge of wastewater, harmful to the flora and the fauna, leads also to the shortage of clean water ressources. In this context, the green processes development like melt crystallization of water may provide a low energy solution and simultaneously enables the minimization of use of hazardous material (Yin et al. (2017)). In this paper, we suggest a structured Port Hamiltonian model of the solidification process in order to provide numerical models suitable for the simulation, design and control of such a processes. The companion paper of (Bendimerad-Hohl et al. (2022)) gives the procedure to derive a finite-dimensional discretized model preserving the Port Hamiltonian structure. The main challenge to establish this solidification model is the moving interface between the solid and the liquid phase.

Two approaches are possible. The first one, called *thin interface approach*, consists in describing the interface as the boundary of the spatial domains of each phase, using for instance their characteristic functions. The second one called *diffuse interface approach*, consists in introducing a function called *phase field* that is a smooth approximation of the characteristic function of the domain. The boundary is replaced by a narrow interface layer corresponding to intermediate values of the phase field variable.

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In this paper we suggest a Dissipative Port-Hamiltonian formulation of a solidification process. Port-Hamiltonian systems are a modelling framework, allowing the thermodynamically consistent representation of open physical systems (Duindam et al. (2009); van der Schaft and Jeltsema (2014)) and well-suited for representing open thermodynamical processes (Ramirez et al. (2013b,a); Favache et al. (2010)).

The Port-Hamiltonian formulation of systems with moving interface has been proposed following both approaches, considering sharp interfaces in (Diagne and Maschke (2013)) and diffuse interfaces (Vincent et al. (2020)). In this paper we shall elaborate on the phase field approach and extend the model Port Hamiltonian formulation of the Allen-Cahn equation formulated by Vincent et al. (2020) by coupling it to the heat diffusion to an extended Port Hamiltonian system. In the section 2, we shall recall the definition of Port Hamiltonian systems and recall the Port Hamiltonian formulation of the phase field variable dynamics described by the Allen-Cahn equation (Vincent et al. (2020)) and finish with its extension to the complete process of solidification. In the section 3, we shall recall the thermodynamical properties of the water and ice and their extension to a biphasic model with diffuse interface, including the phase field variable. In the section 4, we shall reformulate the Port Hamiltonian model of section 2, using the entropy as generating function, but using an formulation as a Differential-Algebraic Partial Differential Equation system, or a Implicit Port Hamiltonian System (Maschke and van der Schaft (2020); van der Schaft and Maschke (2021)), thereby expressing the dynamics in terms of intensive rather than extensive variables.

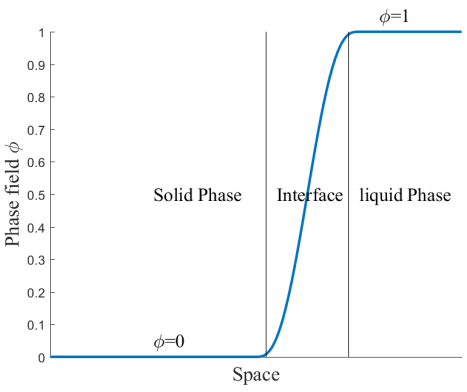

Fig. 1. Liquid/Solid interface : Phase field representation

2. PORT HAMILTONIAN FORMULATION OF SOLIDIFICATION PROCESS

In this section, we present a Port Hamiltonian formulation of the phase field model of a solidification process, following the thermodynamic approach of (Wang et al. (1993)). This model consists in coupling the energy balance equation with the Allen-Cahn equation, taking the entropic form of the Gibbs' equation. This leads to extend the Port Hamiltonian formulation of the Allen Cahn equation of (Vincent et al. (2020)) by coupling it to the Port Hamiltonian model of heat diffusion model.

2.1 Reminder of the solidification model

Following the phase field approach, (Wang et al. (1993)) present a model of a solidification process, consisting in a closed system of volume V in which a pure material undergoes a phase transition between solid and liquid.

Thermodynamic model This model corresponds to the diffuse interface model of bi-phasic systems where the spatial localization of the two phases is represented by the continuous *phase field variable* ϕ. ϕ takes values in the interval [0, 1], taking value 0 for the solid state, 1 for the liquid state and intermediate value at the diffuse interface (see the figure 1). The authors write the entropy balance equation and use *Gibbs' equation in the entropy form* [1] :

$$ds = \left(\frac{\partial s}{\partial \phi}\right) d\phi + \tau du \tag{1}$$

where s denotes the entropy density, u the internal energy density and τ the reciprocal temperature $\tau = \left(\frac{\partial s}{\partial e}\right)_\phi = \left(\frac{1}{T}\right)$.

The total entropy functional of the bi-phasic system is expressed by the *Landau-Ginzburg* entropy functional:

$$S(\phi, u) = \int_V \left(s(\phi, u) - \frac{1}{2}\epsilon^2 (grad\,\phi)^2 \right) dv, \tag{2}$$

where the quadratic term accounts for the entropy of the diffuse interface, ϵ is a constant related to the thickness of the interface (see Boettinger et al. (2002); Kobayashi (1993)) and $s(\phi, u)$ is the entropy density function associated with Gibbs' equation (1).

[1] In this paper, we make the usual assumption that the mass density is uniform Wang et al. (1993).

Dynamic equations The dynamical model consists first in the energy balance equation:

$$\frac{\partial u}{\partial t} = -div\, q \tag{3}$$

where q denotes the heat flux

$$q = M_\tau \bar{F} \tag{4}$$

and $\bar{F}$ the driving force

$$\bar{F} = -grad(\tau) \tag{5}$$

where $M_\tau = \frac{\lambda(\frac{1}{\tau}, \phi)}{\tau^2}$, λ being the thermal conductivity [2]. It is coupled to the relaxation dynamics of the phase field variable ϕ, the gradient system called *Allen Cahn equation*:

$$\eta \frac{\partial \phi}{\partial t} = \frac{\partial s}{\partial \phi}(\phi) + div(\epsilon^2 grad\,\phi) = -\frac{\delta(-S)}{\delta \phi}, \tag{6}$$

where η is the positive interface mobility and $\frac{\delta S}{\delta \phi}$ denotes the variational derivative of the functional S with respect to ϕ.

2.2 Reminder on the dissipative Port Hamiltonian Systems

Consider the following dissipative systems :

$$\frac{\partial x}{\partial t}(t, z) = \left(-\mathcal{G}_R \mathcal{R} \mathcal{G}_R^*\right) \frac{\delta \mathcal{H}}{\delta x}, \tag{7}$$

where $x(t, z) \in \mathbb{R}^n$ is the state variable defined on the spatial domain V and a time interval in $\mathbb{R}_+$, $\mathcal{H}$ is the Hamiltonian functional, $\mathcal{R}$ is a positive, coercive matrix operator and $\mathcal{G}_R$ is a matrix differential operator ($\mathcal{G}_R^*$ denoting its formal adjoint).

Its Port Hamiltonian formulation is the defined by considering the Hamiltonian matrix differential operator

$$\mathcal{J}_e = \begin{bmatrix} 0 & \mathcal{G}_R \\ -\mathcal{G}_R^* & 0 \end{bmatrix}, \tag{8}$$

and decomposing the system (7) into

$$\begin{pmatrix} \frac{\partial x}{\partial t} \\ F \end{pmatrix} = \mathcal{J}_e \begin{pmatrix} \frac{\delta \mathcal{H}}{\delta x} \\ Q \end{pmatrix} \tag{9}$$

where the driving force F and the flux Q variable are related by the *dissipative relation* :

$$Q = \mathcal{R}\, F \tag{10}$$

The Port Hamiltonian system is then obtained by augmenting the system with *boundary port variables* (the interface variables of the system at its boundary) associated with the *Stokes-Dirac structure* defined by the Hamiltonian operator $\mathcal{J}_e$ (van der Schaft and Maschke (2002)). These boundary port variables are by linear functions of the *trace* of the vector $\begin{pmatrix} \frac{\delta \mathcal{H}}{\delta x} & Q \end{pmatrix}^\perp$.

[2] The thermal conductivity of ice ($\phi = 0$) and water ($\phi = 1$) can be found in Yen (1981); IAPWS (2009b)

Example: the heat conduction The energy balance equation (3) and the definition of the driving force (5) leads to the Dissipative Port Hamiltonian formulation (9) (10) with $\mathcal{G}_R = -div$ and $\mathcal{R} = M_\tau$:

$$\begin{pmatrix} \dfrac{\partial u}{\partial t} \\ \bar{F} \end{pmatrix} = \begin{pmatrix} 0 & -div \\ -grad & 0 \end{pmatrix} \begin{pmatrix} \dfrac{\partial s}{\partial u} \\ q \end{pmatrix} \tag{11}$$

The associated pair of boundary port variables is :

$$\begin{pmatrix} f_\partial \\ e_\partial \end{pmatrix} = \overline{\mathcal{W}}\, e = \begin{pmatrix} \gamma_0 \dfrac{\delta s}{\delta u} \\ -\gamma_\perp q \end{pmatrix} \tag{12}$$

where the boundary operator $\overline{\mathcal{W}}$ is defined as:

$$\overline{\mathcal{W}} = \begin{pmatrix} \gamma_0 & 0 \\ 0 & -\gamma_\perp \end{pmatrix} \tag{13}$$

and γ_0 is the *Dirichlet trace map* and $\gamma_\perp$ is the *normal trace map*, (Kurula and Zwart (2012)).

2.3 Port Hamiltonian formulation of the Allen-Cahn equation

We briefly recall now the dissipative Hamiltonian formulation of the Allen-Cahn equation as suggested by (Vincent et al. (2020)). The state space representation is augmented with the new state :

$$\psi = grad\, \phi \tag{14}$$

leading to define the extended state vector : (ϕ, ψ, u). The Landau-Ginzburg entropy functional (2) is then written :

$$\bar{S}(\phi, \psi, u) = \int_\Omega s(\phi, u) - \frac{1}{2}\epsilon^2 \psi^2 \, dV \tag{15}$$

Let us now compute the variational derivative $\frac{\delta S}{\delta \phi}$ in (6) in terms of $\bar{S}(\phi, \psi, u)$:

$$\frac{\delta S}{\delta \phi} = \frac{\delta \bar{S}}{\delta \phi} - div \frac{\partial \bar{S}}{\partial \psi} := F_{\phi\psi} \tag{16}$$

Defining

$$E_{\phi\psi} = -\frac{\partial \phi}{\partial t} \tag{17}$$

the gradient dynamics (6) is expressed by the following dissipative constitutive relation

$$E_{\phi\psi} = 1/\eta F_{\phi\psi} \tag{18}$$

The dynamics of the added state variable ψ is then easily obtained by permutation of the spatial and time derivatives :

$$\frac{\partial \psi}{\partial t} = \frac{\partial}{\partial t} grad \phi = grad \frac{\partial \phi}{\partial t} = -grad\, E_{\phi\psi} \tag{19}$$

Hence the Allen-Cahn equation augmented with the dynamics of the added variable ψ admits the Dissipative Port Hamiltonian formulation (9) (10):

$$\begin{pmatrix} \dfrac{\partial \phi}{\partial t} \\ \dfrac{\partial \psi}{\partial t} \\ F_{\phi\psi} \end{pmatrix} = \begin{pmatrix} 0 & 0 & -1 \\ 0 & 0 & -grad \\ 1 & -div & 0 \end{pmatrix} \begin{pmatrix} \dfrac{\delta(-\bar{S})}{\delta \phi} \\ \dfrac{\delta(-\bar{S})}{\delta \psi} \\ E_{\phi\psi} \end{pmatrix} \tag{20}$$

with $\mathcal{G}_R = \begin{pmatrix} -1 \\ -grad \end{pmatrix}$ and $\mathcal{R} = \eta$.

Once again with the aid of (Kurula and Zwart (2012)), the boundary port variables of the Port Hamiltonian formulation of the Allen-Cahn equation are :

$$\begin{pmatrix} f_\partial^{\phi\psi} \\ e_\partial^{\phi\psi} \end{pmatrix} = \mathcal{W}\, e_{\phi\psi} = \begin{pmatrix} -\gamma_\perp \dfrac{\delta(-\bar{S})}{\delta \psi} \\ \gamma_0\, E_{\phi\psi} \end{pmatrix} \tag{21}$$

with the boundary operator $\mathcal{W}$:

$$\mathcal{W} = \begin{pmatrix} 0 & -\gamma_\perp & 0 \\ 0 & 0 & \gamma_0 \end{pmatrix} \tag{22}$$

2.4 Port Hamiltonian formulation of the solidification process

Recalling that

$$\frac{\delta \bar{S}}{\delta u} = \frac{\partial s}{\partial u} = \tau \tag{23}$$

the Dissipative Port Hamiltonian formulation of solidification process is obtained by assembling (11) and (20)

$$\begin{pmatrix} \dfrac{\partial \phi}{\partial t} \\ \dfrac{\partial \psi}{\partial t} \\ F_{\phi\psi} \\ \dfrac{\partial u}{\partial t} \\ \bar{F} \end{pmatrix} = \mathcal{J} \begin{pmatrix} -\dfrac{\partial s}{\partial \phi}(\phi, u) \\ \epsilon^2 \psi \\ E_{\phi\psi} \\ -\tau \\ q \end{pmatrix} \tag{24}$$

with Hamiltonian matrix differential operator

$$\mathcal{J} = \begin{pmatrix} 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & -grad & 0 & 0 \\ 1 & -div & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -div \\ 0 & 0 & 0 & -grad & 0 \end{pmatrix} \tag{25}$$

and Hamiltonian functional $-\bar{S}$ defined in (15), completed with the two dissipative relation (4) and (18).

The associated boundary operator $\widetilde{\mathcal{W}}$ are also obtained by assembling the boundary operators of the heat conduction and the augmented Allen-Cahn equation :

$$\widetilde{\mathcal{W}} = \begin{pmatrix} 0 & -\gamma_\perp & 0 & 0 & 0 & 0 \\ 0 & 0 & \gamma_0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \gamma_0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\gamma_\perp \end{pmatrix} \tag{26}$$

and the extended pair of boundary port variables is :

$$\begin{pmatrix} f_\partial^{\phi\psi} \\ e_\partial^{\phi\psi} \\ f_\partial \\ e_\partial \end{pmatrix} = \widetilde{\mathcal{W}} \begin{pmatrix} -\dfrac{\partial s}{\partial \phi}(\phi, u) \\ \epsilon^2 \psi \\ F_{\phi\psi} \\ -\tau \\ q \end{pmatrix} = \begin{pmatrix} -\gamma_\perp(\epsilon^2 \psi) \\ \gamma_0\,(1/\eta E_{\phi\psi}) \\ \gamma_0 \tau \\ -\gamma_\perp M_\tau(-grad(\tau)) \end{pmatrix} \tag{27}$$

It may be shown, from (Vincent et al. (2020); Kurula and Zwart (2012)), that the operator $\mathcal{J}$ in (25) and the boundary operator $\widetilde{\mathcal{W}}$ in (26) define a Stokes-Dirac structure van der Schaft and Maschke (2002).

From the properties of a Stokes-Dirac structure, one may deduce the neg-entropy balance equation :

$$\frac{d(-\bar{S})}{dt} = -\int_V E_{\phi\psi} F_{\phi\psi} dV - \int_V q\bar{F} dV - \int_{\partial V} \tilde{e}_\partial \tilde{f}_\partial \, dS \quad (28)$$

which becomes, by means of the dissipation relations (4) and (18)

$$\frac{d(-\bar{S})}{dt} = -\int_V \eta F_{\phi\psi}^2 dV - \int_V M_\tau \bar{F}^2 dV + \int_{\partial V} \tilde{e}_\partial \tilde{f}_\partial \, dS \quad (29)$$

where the two first terms corresponds to the irreversible entropy production due to the gradient dynamics of the phase field and the heat conduction and the third one corresponds to the external entropy flow flowing into the system.

3. THERMODYNAMIC PROPERTIES USING PHASE FIELD

The objective of this section is to present how to compute extended thermodynamic properties from the thermodynamics properties of the liquid water and ice.

3.1 Thermodynamic properties of liquid water and ice

Thermodynamics properties of the liquid water and ice are practically found in literature (IAPWS (2009a)) and (IAPWS (2009b)). The provided thermodynamic potential is the Gibbs energy expressed as a function of temperature and pressure. The expression of the specific Gibbs energy of the liquid phase is as follows:

$$g_{liq}(T,p)/g^* = \sum_{j=0}^{7}\sum_{k=0}^{6} g_{jk}\tau^i\pi^k \quad (30)$$

with the reduced temperature $\tau = (T - T_0)/T^*$ and the reduced pressure $\pi = (p - p_0)/p^*$. The constants T_0, p_0, T^*, p^*, g^* and the g_{jk} are given in (IAPWS (2009b)). In a same way the expression of the specific Gibbs energy of the solid phase is as follows:

$$g_{sol}\ (T,p) = g_0(p) - s_0 T_t \tau + T_t Re\left(\sum_{k=1}^{2} r_k\Big[(t_k - \tau) \ln(t_k - \tau) + (t_k + \tau)\ln(t_k + \tau) - 2t_k \ln(t_k) - \frac{\tau^2}{t_k}\Big]\right) \quad (31)$$

with $g_0(p) = \sum_{k=0}^{4} g_{0k}(\pi - \pi_0)^k$ and $r_2(p) = \sum_{k=0}^{2} r_{2k}(\pi - \pi_0)^k$, $\tau = T/T_t$, $\pi = p/p_t$, and $\pi_0 = p_0/p_t$. All The constants T_t, p_t, p_0, s_0, g_0, r_1 as well as the g_{ok}, r_{2k}, t_k are given in (IAPWS (2009a)). From the expression of these state equations, other specific thermodynamic quantities as entropy, Helmotz energy and density for each phase can be derived from standard thermodynamic computations (see IAPWS (2009a), IAPWS (2009b) and Callen (1991)). As an example the specific Helmotz energy $f_\star$, the specific entropy $s_\star$ as a function of temperature and pressure and the density $\rho_\star$ as well as the heat capacity $c_{p_\star}$ can be deduced from $g_\star$ for $\star = sol, liq$ by the formulas:

$$f_\star(T,p) = g - p\frac{\partial g_\star}{\partial p} \quad (32)$$

$$s_\star(T,p) = -\frac{\partial g_\star}{\partial T} \quad (33)$$

$$\rho_\star(T,p) = \Big(\frac{\partial g_\star}{\partial p}\Big)^{-1} \quad (34)$$

$$c_{p_\star}(T,p) = -T\frac{\partial^2 g_\star}{\partial T^2} \quad (35)$$

Finally we give some values of these properties at the melting temperature (273.15K) at atmospheric pressure.

Table 1. Values of some thermodynamic properties at the melting temperature

$\star$	$g_\star$	$f_\star$	$s_\star$	$\rho_\star$	$c_{p_\star}$
liq	101.343	0.0018	–0.1476	999.843	4219.41
sol	101.343	– 9.1870	– 1220.769	916.721	2096.71

3.2 The extended Equation of State

For sake of brevity, we restrict our attention to the extended specific entropy s assuming constant density. The stability principle of thermodynamics when two phases are present requires (see Callen (1991)):

$$\left.\frac{\partial s}{\partial \phi}\right|_{\phi=0} = \left.\frac{\partial s}{\partial \phi}\right|_{\phi=1} \text{ and } \left.\frac{\partial^2 s}{\partial \phi^2}\right|_{\phi=0,1} < 0. \quad (36)$$

From the constraint that at equilibrium the variational derivative of the Landau-Ginzburg entropy functional: must be equal to 0 in each phase ($grad\,\phi = 0$), we have (see Wang et al. (1993); Boettinger et al. (2002)):

$$\left.\frac{\partial s}{\partial \phi}\right|_{\phi=0,1} = 0 \text{ and } \left.\frac{\partial^2 s}{\partial \phi^2}\right|_{\phi=0,1} < 0. \quad (37)$$

Let us follow the method proposed in Boettinger et al. (2002) to obtain the extended specific entropy function:

$$s(\phi,T) = s_{sol}(T) + p_i(\phi)[s_{liq}(T) - s_{sol}(T)] + wp_w(\phi) \quad (38)$$

with $p_i(\phi) = \phi^3(6\phi^2 - 15\phi + 10)$, $p_w(\phi) = -\phi^2(1-\phi)^2$ where s_{liq}, s_{sol} represent the specific entropy of pure water and of pure ice respectively. $p_w(\phi)$ is the double-well polynomial and $p_i(\phi)$ is the interpolating polynomial. This choice of p_i ensures that $\left.\frac{\partial s}{\partial \phi}\right|_{\phi=0,1} = 0$. w gives the tuning of the hollow between the two local maximum (see Boettinger et al. (2002)). w must be positive in order to check $\frac{\partial^2 s}{\partial \phi^2}\frac{\partial^2 s}{\partial u^2} - \Big(\frac{\partial^2 s}{\partial \phi \partial u}\Big)^2 > 0$ (see Callen (1991)). Figure 2 shows the extended entropy for water and ice.

4. IMPLICIT PORT HAMILTONIAN SYSTEM

In the Port Hamiltonian formulation of the section 2, the Hamiltonian function is the entropy functional (2) which depends on the internal energy u and the phase field variable ϕ and its gradient ψ. In the section 3, the practical

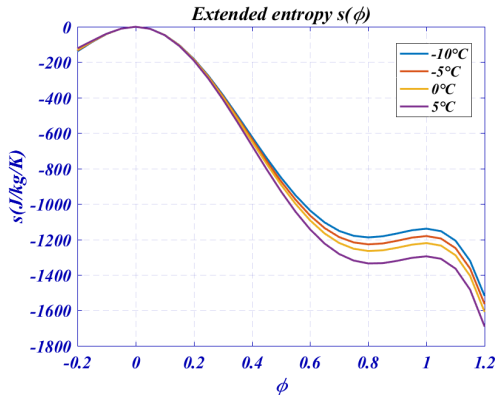

Fig. 2. Extended specific entropy with $w = 18\ 10^3$

definition of the thermodynamic properties of the bi-phasic water-ice system has been given, leading to the expressions of the entropy density (38) depending on the temperature rather than the internal energy. That means that we need to change a coordinate of the state space from the internal energy u, an extensive variable, to the temperature T, an intensive variable.

In this section, we reformulate the Port Hamiltonian model from Section 2, through the definition of the Implicit Port Hamiltonian formulation. For these systems, the energy function is actually not defined explicitly but rather by a set of constitutive relations between the extensive and intensive variables, satisfying the Maxwell reciprocity conditions. The graph of these relations have a geometrical interpretation as Lagrangian submanifolds which allow the definition of reciprocal constitutive equations in a coordinate free way (van der Schaft and Maschke (2018); van der Schaft and Maschke (2020)) and may be adapted to distributed parameter systems (Maschke and van der Schaft (2020); van der Schaft and Maschke (2021)).

Consider Gibbs' equation (1) associated with the entropy density function $s(\phi, u)$; it gives rise to the following Lagrangian submanifold defined by the graph of $s(\phi, u)$

$$L_s = \left\{ (x,e) \in \mathbb{R}^2 \times \mathbb{R}^2 : \ e = \begin{pmatrix} \frac{\partial s}{\partial \phi}(\phi,u) \\ \frac{\partial s}{\partial u}(\phi,u) \end{pmatrix} ; \ x = \begin{pmatrix} \phi \\ u \end{pmatrix} \right\} \tag{39}$$

In order to perform the change of coordinates, let us consider the Legendre transform of the entropy density $s(\phi, u)$ with respect to u

$$s^*(\phi, \tau) = \tau\, u - s(\phi, u) \tag{40}$$

where the internal energy u is considered to be a function of the phase field variable ϕ and the reciprocal temperature obtained by partial inversion of $\tau = \frac{\partial s}{\partial u}(\phi, u)$with respect to u [3]. Then the Legendre submanifold (39) can be defined as follows

[3] The invertibility is actually insured by the strict concavity of $s(\phi, u)$ due to the strict concavity of the entropy functions s_{sol} and s_{liq} of the solid and liquid phases and its definition (38).

$$L_s = \left\{ (x,e) \in \mathbb{R}^2 \times \mathbb{R}^2 \ / \right.$$
$$\left. x = \begin{pmatrix} \phi \\ \frac{\partial s^*}{\partial \tau}(\phi,\tau) \end{pmatrix} ; \ e = \begin{pmatrix} \frac{\partial s^*}{\partial \phi}(\phi,\tau) \\ \tau \end{pmatrix} ; \ \begin{pmatrix} \phi \\ \tau \end{pmatrix} \in \mathbb{R}^2 \right\} \tag{41}$$

The dynamics of the solidification process can then be expressed as follows. First, considering the extended entropy functional (15), one have the associated Legendre submanifold:

$$L_{(-\bar{s})} = \left\{ \left(\begin{pmatrix} x \\ \psi \end{pmatrix}, \begin{pmatrix} e \\ e_\psi \end{pmatrix} \right) \in \mathbb{R}^3 \times \mathbb{R}^3 \ / \right.$$
$$\left. (x, -e) \in L_s;\ e_\psi = \epsilon^2 \psi;\ \psi \in \mathbb{R} \right\} \tag{42}$$

Now let us write the Port Hamiltonian system, *in coordinates*. First compute the time derivative of the vector x, with its expression in the definition (41) of the Lagrange submanifold L_s:

$$\begin{aligned} \frac{\partial}{\partial t}\begin{pmatrix} \phi \\ u \end{pmatrix} &= \frac{\partial}{\partial t}\begin{pmatrix} \phi \\ \frac{\partial s^*}{\partial u}(\phi,\tau) \end{pmatrix} \\ &= \begin{pmatrix} 1 & 0 \\ \frac{\partial s^*}{\partial \phi \partial \tau}(\phi,\tau) & \frac{\partial^2 s^*}{\partial \tau^2}(\phi,\tau) \end{pmatrix} \frac{\partial}{\partial t}\begin{pmatrix} \phi \\ \tau \end{pmatrix} \end{aligned} \tag{43}$$

with $\frac{\partial^2 s^*}{\partial \tau^2} = -c_p - \tau \frac{\partial c_p}{\partial \tau}$ where $c_p(\phi, \tau)$ is the extended heat capacity and $\frac{\partial s^*}{\partial \phi \partial \tau} = -\tau \frac{\partial c_p}{\partial \phi}$.

The thermal conductivity becomes:

$$\lambda = \lambda_{sol} + p_i(\phi)\Big[\lambda_{liq} - \lambda_{sol}\Big]. \tag{44}$$

The Port Hamiltonian System (24), using (43) in the right-hand side term and the parametrization of the extensive variables e in (41), leads to the following implicit PDE:

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ \frac{\partial s^*}{\partial \phi \partial \tau} & 0 & 0 & \frac{\partial^2 s^*}{\partial \tau^2} & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \frac{\partial \phi}{\partial t} \\ \frac{\partial \psi}{\partial t} \\ F_{\phi\psi} \\ \frac{\partial \tau}{\partial t} \\ F \end{pmatrix} = \mathcal{J} \begin{pmatrix} -\frac{\partial s^*}{\partial \phi}(\phi,\tau) \\ \epsilon^2 \psi \\ E_{\phi\psi} \\ -\tau \\ q \end{pmatrix}. \tag{45}$$

This PDE, augmented with the dissipative relations (18) and (4) and with the boundary port variables (27), defines a Dissipative Boundary Port Hamiltonian System.

It is remarkable that the dynamics of phase field models of solidification processes often lead to implicit formulations of the dynamics. For instance (Wang et al. (1993)) and (Boettinger et al. (2002)) begin their paper using the entropy as thermodynamical potential, in order to ensure the irreversible entropy creation of the phase field dynamics. However, they use the Helmhotz free energy density $f(\phi, T)$ as a generating function of Thermodynamic properties of the bi-phasic system. Yet, even with f, these authors finally obtain an implicit dynamic system (see for instance equations (54) to (58) in Wang et al. (1993)).

5. CONCLUSION

In this contribution, we have proposed a Boundary Port Hamiltonian representation of the solidification of water or any other pure substance using the diffuse interface approach and using a phase field variable. Therefore, we have augmented the Port Hamiltonian representation suggested by (Vincent et al. (2020)) of the Allen-Cahn equation, representing the dynamics of a non-conserved phase field variable, to a Port Hamiltonian system including the heat transport. Finally we have suggested a DAE-PDE Port Hamiltonian formulation of the system, that allow to change in a consistent way the coordinates on which the dynamics is expressed. In the given case we have expressed the energy balance equation in terms of the reciprocal temperature instead of the internal energy, enabling to use the experimental datas of thermodynamic properties of water and ice.

Forthcoming work will consist in modifying this model by adding the pollutant in the thermodynamics functional and in the conservation equations in order to provide a model of the melt crystallisation process as well as relaxing the assumption of uniform mass density. Furthermore the control of the process will be considered, using passivity-based control methods, taking account of the energy balance and entropy balance equations (Ramirez et al. (2016)).

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