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Generalized Stefan Models Accounting for Discontinuous Temperature Field

Alexandre Danescu*

Abstract

In this paper we construct a class of generalized Stefan models able to account for discontinuous temperature field across a nonmaterial mouving interface. The resulting theory introduces a constitutive scalar interfacial field, denoted $\overline{\theta}$ and called the equivalent temperature of the interface. A classical procedure, based on the interfacial dissipation inequality, relates the interfacial energy release to the interfacial mass flux and restrict the equivalent temperature of the interface. We show that previously proposed theories are obtained as particular cases when $\overline{\theta} = \langle\theta\rangle$ or $\overline{\theta} = \langle\frac{1}{\theta}\rangle^{-1}$ or, more generally, $\overline{\theta} = \langle\theta^r\rangle\langle\frac{1}{\theta^{1-r}}\rangle^{-1}$ for $0 \leq r \leq 1$. We study in a particular constitutive framework the solidification of an under-cooled liquid and the melting of a super-cooled solid and we are able to obtain necessary and sufficient conditions for a unique travelling wave solution. These conditions involve the superficial field $\overline{\theta}$, the given data and the material parameters, providing in this way a method for the identification of the constitutive function $\overline{\theta}$.

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1 Introduction

Classical sharp interface theory in thermoelastic materials [1], [2] concerns structured or unstructured nonmaterial interfaces along which the displacement and temperature fields are continuous. Several extensions of this framework to include incoherent motions or discontinuous temperature fields were proposed by [3], [4], [5].

In a recent paper Fried and Shen [3] propose a generalization of the Stefan model that allows for both velocity and temperature jumps. Such situations, when temperature and velocity experience sharp changes may appear for example in combustion theory [6]. Fried and Shen [3] discuss the constitutive aspects of the resulting theory and as an illustration study the solidification of a pure substance in the absence of the flow, in a specific constitutive framework. Their result provides *sufficient conditions* for the existence of a unique travelling wave solution.

The fundamental result in [3] is the interfacial dissipation inequality obtained without using a priori neither the coherence of the motion nor the continuity of the temperature field. Following a classical procedure of Coleman and Noll [7] the interfacial dissipation inequality is then used to render constitutive relations compatible with the interfacial version of the imbalance of entropy. The particular form of the interfacial dissipation inequality used in in [3] introduces naturally a scalar interfacial field called the *scaled temperature jump*. In order to account for discontinuous temperature field across nonmaterial interfaces, a different version of the interfacial dissipation inequality was presented [8] and a natural question concerns the relation between the resulting theories.

We show in this paper that as long as the temperature field suffers a discontinuity across a nonmaterial surface, the specific form of the interfacial dissipation inequality is based on a *constitutive choice* of a interfacial scalar field which we call **equivalent temperature of the interface**. To this end, we shall review the arguments leading to the interfacial dissipation inequality from two different points of view:

- A revisited form of the dissipation inequality proposed in [3];
- The use of (a slightly modified version of) the theory of structured interfaces based on the balance of configurational forces as presented in the recent book [1], followed by neglecting interfacial structure.

We show that both lines of thinking lead to the *same interfacial dissipation inequality based on the equivalent temperature of the interface* which in turn has to be regarded as prescribed by *a constitutive function.*

Our results show that the theory proposed by Fried and Shen [3] is obtained as a special case of the general theory developed here, when the equivalent temperature for the interface, denoted in the following $\overline{\theta}$ is prescribed as $\overline{\theta} = \langle \frac{1}{\theta} \rangle^{-1}$, where $\langle a \rangle$ denotes the mean value of a. Other constitutive choices for $\overline{\theta}$, like $\overline{\theta} = \langle \theta \rangle$, or $\overline{\theta} = \sqrt{\theta^+\theta^-}$, or $\overline{\theta} = \max(\theta^-, \theta^+)$ are possible, leading to different models. As previously noted, the interfacial version of the dissipation inequality is used to restrict constitutive relations. Following this classical procedure we derive supplemental relations at the interface in the general setting. In a motionless body they involve restrictions on the interfacial energy release and on the equivalent temperature of the interface.

We recall that in classical sharp interface theory when the temperature field is continuous across the nonmaterial interface, the interfacial energy release equals the jump across the interface of the free energy [1]. As a consequence, the single source of dissipation at the nonmaterial interface for thermoelastic materials is the motion of the interface, which in turn, is related to the jump of the free energy (the driving force) by a supplemental constitutive relation [?], [?], [11]. For discontinuous temperature fields this is no longer valid, and the interfacial energy release contains also a contribution of the entropy. The additional term is

$$[\![\eta(\theta - \overline{\theta})]\!]$$

and vanishes if the temperature is continuous, under the mild assumption $\overline{\theta} \in [\min(\theta^-, \theta^+), \max(\theta^-, \theta^+)]$. This weak constitutive restriction also reduces the present theory to the classical one [1] when the temperature field is continuous across the nonmaterial interface.

To focus on thermal implications of the model, following Fried and Shen [3], we treat as an application the solidification of a under-cooled liquid and the solidification of a super-heated solid of a motionless body. In a classical constitutive context our supplemental constitutive relations at the interface lead to the **unicity** of a travelling wave solution of the free-boundary problem.

2 Interfacial versions of balance and imbalance laws

For completeness, following Fried and Shen [3], we recall in this section the basic balance laws for thermoelastic materials under the general assumption that both constitutive variables, the deformation gradient and the temperature field may be discontinuous across a nonmaterial propagating surface.

We denote by $\mathcal{D}(t)$ the region occupied by the material body at time t, and by $\mathcal{S}(t)$ the nonmaterial surface across which the velocity $\boldsymbol{v}$ and the temperature θ may experience finite jump discontinuities. We denote by $\boldsymbol{n}(\boldsymbol{x}, t)$ the unit normal to $\mathcal{S}(t)$ in $\boldsymbol{x} \in \mathcal{S}(t)$ and by $V(\boldsymbol{x}, t)$ the scalar normal velocity of $\mathcal{S}(t)$ at $\boldsymbol{x} \in \mathcal{S}(t)$, respectively. If a is a field on $\mathcal{D}(t)$, discontinuous across $\mathcal{S}(t)$, for we denote by $a^{\pm}$ the limits

$$a^{\pm}(\boldsymbol{x}, t) = \lim_{h \to 0} a(\boldsymbol{x} \pm h\boldsymbol{n}(\boldsymbol{x}, t), t)). \tag{1}$$

We use $[\![a]\!]$ and $\langle a \rangle$ for the jump and the mean value of a across $\mathcal{S}(t)$, and we recall the following algebraic identity

$$[\![ab]\!] = [\![a]\!]\langle b \rangle + \langle a \rangle [\![b]\!]. \tag{2}$$

Following Fried and Shen [3], we denote by a superposed dot the material time differentiation and by an accent the spatial time differentiation, so that for a smooth field a we have

$$\dot{a}(\boldsymbol{x}, t) = a'(\boldsymbol{x}, t) + a_{,k}(\boldsymbol{x}, t) v_k(\boldsymbol{x}, t), \tag{3}$$

where $a_{,k}$ stands for the partial derivative of a with respect to x_k.

2.1 Mass balance and mass flux

We denote by ρ the mass density, and we assume the bulk field equation for the mass balance in the form

$$\dot{\rho} + \rho \mathrm{div} \boldsymbol{v} = 0, \tag{4}$$

and the associated interface counterpart

$$[\![\rho(\boldsymbol{\nu} - \boldsymbol{v})]\!] \cdot \boldsymbol{n} = 0, \tag{5}$$

where $\boldsymbol{\nu}$ denotes the interface velocity. Following [3], we define the *mass flux* across $\mathcal{S}$ through

$$\mathsf{m} = \langle \rho(\boldsymbol{\nu} - \boldsymbol{v}) \rangle \cdot \boldsymbol{n} \tag{6}$$

2.2 Momentum balance

If $\boldsymbol{T}$ denotes the Cauchy stress tensor, in the absence of body forces, the balance of momentum at regular points in the bulk is assumed to hold in the form

$$\rho \dot{\boldsymbol{v}} = \mathrm{div} \boldsymbol{T}, \tag{7}$$

while it's counterpart across $\mathcal{S}$ is

$$[\![\rho \boldsymbol{v} \otimes (\boldsymbol{\nu} - \boldsymbol{v})]\!] \boldsymbol{n} + [\![\boldsymbol{T}]\!] \boldsymbol{n} = 0, \tag{8}$$

and taking into account (5) and (6) we obtain

$$\mathsf{m} [\![\boldsymbol{v}]\!] + [\![\boldsymbol{T}]\!] \boldsymbol{n} = 0. \tag{9}$$

2.3 Energy balance

In the absence of supplies, if we denote by e the internal energy density and $\boldsymbol{q}$ the heat flux, at regular points in the bulk the conservation of energy reads

$$\frac{d}{dt} \left[\rho e + \frac{\rho}{2} \boldsymbol{v} \cdot \boldsymbol{v} \right] = \mathrm{div}(\boldsymbol{T} \boldsymbol{v}) - \mathrm{div} \boldsymbol{q}, \tag{10}$$

while across $\mathcal{S}$, the associated jump condition is

$$[\![(\rho e + \frac{1}{2} \rho \boldsymbol{v} \cdot \boldsymbol{v})(\boldsymbol{\nu} - \boldsymbol{v})]\!] \cdot \boldsymbol{n} + [\![\boldsymbol{T} \boldsymbol{v}]\!] \cdot \boldsymbol{n} - [\![\boldsymbol{q}]\!] \cdot \boldsymbol{n} = 0. \tag{11}$$

Using the mass conservation (5) and formula (2) we obtain

$$\mathsf{m} [\![e]\!] + \langle \boldsymbol{T} \boldsymbol{n} \rangle \cdot [\![\boldsymbol{v}]\!] - [\![\boldsymbol{q}]\!] \cdot \boldsymbol{n} = 0. \tag{12}$$

The velocity jump can be decomposed into a normal part and a superficial part as

$$[\![\boldsymbol{v}]\!] = [\![\boldsymbol{v} \cdot \boldsymbol{n}]\!]\boldsymbol{n} + \mathsf{P}[\![\boldsymbol{v}]\!], \tag{13}$$

where $\mathsf{P} = \boldsymbol{I} - \boldsymbol{n} \otimes \boldsymbol{n}$ denotes the interfacial projector. If $\mathsf{s} = \mathsf{P}[\![\boldsymbol{v}]\!]$ denotes the *interfacial velocity slip* and $\mathsf{t} = \mathsf{P}\langle \boldsymbol{T}\boldsymbol{n}\rangle$ the *interfacial friction*, we obtain the equivalent form of (12)

$$\mathsf{m}[\![e]\!] + \langle \boldsymbol{T}\boldsymbol{n}\rangle \cdot [\![\boldsymbol{v} \cdot \boldsymbol{n}]\!]\boldsymbol{n} + \mathsf{t} \cdot \mathsf{s} - [\![\boldsymbol{q}]\!] \cdot \boldsymbol{n} = 0. \tag{14}$$

Finally, the sequence of identities:

$$\langle \boldsymbol{T}\boldsymbol{n} \cdot \boldsymbol{n}\rangle \cdot [\![\boldsymbol{v} \cdot \boldsymbol{n}]\!] = -\mathsf{m}\langle \boldsymbol{T}\boldsymbol{n} \cdot \boldsymbol{n}\rangle [\![\frac{1}{\rho}]\!] = -\mathsf{m}[\![\frac{1}{\rho}\boldsymbol{T}\boldsymbol{n} \cdot \boldsymbol{n}]\!] + \mathsf{m}[\![\boldsymbol{T}\boldsymbol{n} \cdot \boldsymbol{n}]\!]\langle \frac{1}{\rho}\rangle =$$

$$= \mathsf{m}[\![-\frac{1}{\rho}\boldsymbol{T}\boldsymbol{n} \cdot \boldsymbol{n} + \frac{1}{2}(\boldsymbol{\nu} \cdot \boldsymbol{n} - \boldsymbol{v} \cdot \boldsymbol{n})^2]\!] \tag{15}$$

gives another version of the interfacial balance of energy (14), in the form:

$$\mathsf{m}[\![e - \frac{1}{\rho}\boldsymbol{T}\boldsymbol{n} \cdot \boldsymbol{n} + \frac{1}{2}(\boldsymbol{\nu} \cdot \boldsymbol{n} - \boldsymbol{v} \cdot \boldsymbol{n})^2]\!] + \mathsf{t} \cdot \mathsf{s} - [\![\boldsymbol{q}]\!] \cdot \boldsymbol{n} = 0. \tag{16}$$

2.4 Entropy inequality

At regular points in the bulk the entropy inequality is

$$\rho\dot{\eta} \geq -\mathrm{div}\left(\frac{\boldsymbol{q}}{\theta}\right) \tag{17}$$

and the associated jump condition is

$$[\![\rho\eta(\boldsymbol{\nu} - \boldsymbol{v})]\!] \cdot \boldsymbol{n} \leq [\![\frac{\boldsymbol{q}}{\theta} \cdot \boldsymbol{n}]\!]. \tag{18}$$

Using (5) and (6) we obtain

$$\mathsf{m}[\![\eta]\!] \leq [\![\frac{\boldsymbol{q}}{\theta} \cdot \boldsymbol{n}]\!], \tag{19}$$

and introducing the bulk free energy $\psi = e - \theta\eta$ we rewrite the balance of the energy across the interface (16) in the form

$$\mathsf{m}[\![\psi - \frac{1}{\rho}\boldsymbol{T}\boldsymbol{n} \cdot \boldsymbol{n} + \frac{1}{2}(\boldsymbol{\nu} \cdot \boldsymbol{n} - \boldsymbol{v} \cdot \boldsymbol{n})^2]\!] + \mathsf{t} \cdot \mathsf{s} + \mathsf{m}[\![\theta\eta]\!] = [\![\boldsymbol{q}]\!] \cdot \boldsymbol{n}. \tag{20}$$

3 Equivalent temperature of the interface

This section is devoted to a key ingredient for interfacial models allowing discontinuities of the temperature field across a nonmaterial interface. The first subsection recall the framework proposed in [3] based on the scaled temperature jump field . The version of the interfacial dissipation inequality obtained in [3] is then discussed and an alternative interpretation is proposed in subsection 3.2. This point of view leads us to a general form of the dissipation inequality based on the notion of *equivalent temperature of the interface*. The results of Fried and Shen [3] and Dascalu and Danescu [8] are recovered as special cases when the equivalent temperature of the interface is defined as $\langle\frac{1}{\theta}\rangle^{-1}$, and respectively, $\langle\theta\rangle$.

To underline the physical meaning of the equivalent temperature of the interface we discuss in section 3.4 the structured interface theory based on a balance of configurational forces as proposed by Gurtin in [1]. We slightly extend this theory to take into account discontinuous temperature fields and we show that in the absence of interfacial structure, the interfacial dissipation inequality obtained from the balance of configurational forces is identical to the one proposed in subsection 3.3. A crucial advantage of the is the fact that it introduces the equivalent temperature of the interface in relation to the entropy flow across the interface, identifying in this way the physical meaning of the concept.

3.1 Scaled temperature jump

Strating from relation (20), Fried and Shen introduced in [3] the *scaled temperature jump* defined through

$$\mathsf{j} = \frac{[\![\theta]\!]}{\langle\theta\rangle} = -\frac{[\![\frac{1}{\theta}]\!]}{\langle\frac{1}{\theta}\rangle} \tag{21}$$

and using the identities

$$[\![\boldsymbol{q}\cdot\boldsymbol{n}]\!] = \frac{1}{\langle\frac{1}{\theta}\rangle}[\![\frac{\boldsymbol{q}}{\theta}\cdot\boldsymbol{n}]\!] + \mathsf{j}\langle\boldsymbol{q}\cdot\boldsymbol{n}\rangle, \tag{22}$$

$$\mathsf{m}[\![\theta\eta]\!] = \frac{\mathsf{m}}{\langle\frac{1}{\theta}\rangle}[\![\eta]\!] + \mathsf{j}\mathsf{m}\langle\theta\eta\rangle, \tag{23}$$

rewrite (20) as

$$\mathsf{m}[\![\psi - \frac{1}{\rho}\boldsymbol{n}\cdot\boldsymbol{T}\boldsymbol{n} + \frac{1}{2}(\boldsymbol{\nu}\cdot\boldsymbol{n} - \boldsymbol{v}\cdot\boldsymbol{n})^2]\!] + \mathsf{s}\cdot\mathsf{t} + \mathsf{j}\,[\mathsf{m}\langle\theta\eta\rangle - \langle\boldsymbol{q}\cdot\boldsymbol{n}\rangle] =$$

$$\langle \frac{1}{\theta} \rangle^{-1} ([\![\frac{\boldsymbol{q}}{\theta} \cdot \boldsymbol{n}]\!] - \mathsf{m} [\![\eta]\!]). \tag{24}$$

The right hand side above is the product between two positive factors, i.e., $\langle \frac{1}{\theta} \rangle^{-1}$ and $[\![\frac{\boldsymbol{q}}{\theta} \cdot \boldsymbol{n}]\!] - \mathsf{m}[\![\eta]\!]$. Thus the the entropy imbalance (19) holds if and only if

$$\mathsf{m}[\![\psi - \frac{1}{\rho} \boldsymbol{n} \cdot \boldsymbol{T} \boldsymbol{n} + \frac{1}{2} (\boldsymbol{\nu} \cdot \boldsymbol{n} - \boldsymbol{v} \cdot \boldsymbol{n})^2]\!] + \mathsf{s} \cdot \mathsf{t} + \mathsf{j} [\mathsf{m} \langle \theta \eta \rangle - \langle \boldsymbol{q} \cdot \boldsymbol{n} \rangle] \geq 0. \tag{25}$$

For Fried and Shen [3] the various terms in (25), represent:

- $\hat{\mathsf{e}} = [\![\psi - \frac{1}{\rho} \boldsymbol{n} \cdot \boldsymbol{T} \boldsymbol{n} + \frac{1}{2} (\boldsymbol{\nu} \cdot \boldsymbol{n} - \boldsymbol{v} \cdot \boldsymbol{n})^2]\!]$ – the *interfacial energy release*,
- t – the interfacial friction and
- $\hat{\mathsf{h}} = \mathsf{m} \langle \theta \eta \rangle - \langle \boldsymbol{q} \cdot \boldsymbol{n} \rangle$ – the *interfacial heating.*

Rewriting (25) as

$$\hat{\mathsf{e}} \mathsf{m} + \mathsf{t} \mathsf{s} + \hat{\mathsf{j}} \mathsf{h} \geq 0. \tag{26}$$

shows that $\hat{\mathsf{e}}$, t and $\hat{\mathsf{h}}$ are *objects conjugate, in the sense of the energy dissipation, to the interfacial mass flux* m, *the slip velocity* s *and the scaled temperature jump* j.

3.2 Alternative form of the dissipation inequality

We propose an alternative interpretation of formula (25) which seems to be more relevant. The departure point is the term $\mathsf{j}\mathsf{m}\langle \theta \eta \rangle$ which may be considered either as a part of the heating conjugated to the scaled temperature jump j (as already done in [3]) *or as an interfacial energy* conjugated to interfacial mass flux m. As stated at the beginning of this section, this second choice is more relevant and will lead us to a more general setting. To argue this statement we present two arguments:

1. We show that our interpretation leading to relation (28) is a special case of a larger class of theories based on an additional constitutive concept we shall call here *the equivalent temperature of the interface.* This is the subject of the next subsection.

2. A second argument is presented, for convenience, in the purely thermal setting. We shall derive the same version of the dissipation inequality (relation (28)) using the theory of structured interfaces based on a balance of configurational forces following a line of thinking developed by Gurtin in [1]. This will be the subject of the section 4.

Using in (25), the sequence of identities

$$\mathsf{jm}\langle\theta\eta\rangle = \mathsf{m}\frac{[\![\theta]\!]}{\langle\theta\rangle}\langle\theta\eta\rangle = \mathsf{m}[\![\eta(\theta - \langle\frac{1}{\theta}\rangle^{-1})]\!], \tag{27}$$

we obtain an alternative form of the dissipation inequality:

$$\mathsf{m}[\![\psi - \frac{1}{\rho}\boldsymbol{n}\cdot\boldsymbol{T}\boldsymbol{n} + \frac{1}{2}(\boldsymbol{\nu}\cdot\boldsymbol{n} - \boldsymbol{v}\cdot\boldsymbol{n})^2 + \eta(\theta - \langle\frac{1}{\theta}\rangle^{-1})]\!] +$$

$$+ \mathsf{s}\cdot\mathsf{t} - \mathsf{j}\langle\boldsymbol{q}\cdot\boldsymbol{n}\rangle) \geq 0. \tag{28}$$

With respect to (25) the interfacial energy release e and the interfacial heating h are now respectively

- $\mathsf{e} = [\![\psi - \frac{1}{\rho}\boldsymbol{n}\cdot\boldsymbol{T}\boldsymbol{n} + \frac{1}{2}(\boldsymbol{\nu}\cdot\boldsymbol{n} - \boldsymbol{v}\cdot\boldsymbol{n})^2 + \eta(\theta - \langle\frac{1}{\theta}\rangle^{-1})]\!]$,
- $\mathsf{h} = -\langle\boldsymbol{q}\cdot\boldsymbol{n}\rangle$,

but remain *objects conjugate, in the sense of the energy dissipation, to the interfacial mass flux* m *and the scaled temperature jump* j. The interfacial form of the dissipation inequality is formally the same as (26), i.e.,

$$\mathsf{em} + \mathsf{ts} + \mathsf{jh} \geq 0. \tag{29}$$

The expression of the last term of e is the departure point for a more general approach of the dissipation inequality on a nonmaterial interface.

3.3 General dissipation inequality

Using (27) in (24) we obtain an equivalent form of the interfacial energy balance

$$\mathsf{m}[\![\psi - \frac{1}{\rho}\boldsymbol{n}\cdot\boldsymbol{T}\boldsymbol{n} + \frac{1}{2}(\boldsymbol{\nu}\cdot\boldsymbol{n} - \boldsymbol{v}\cdot\boldsymbol{n})^2 + \eta(\theta - \langle\frac{1}{\theta}\rangle^{-1})]\!] + \mathsf{s}\cdot\mathsf{t} - \mathsf{j}\langle\boldsymbol{q}\cdot\boldsymbol{n}\rangle =$$

$$\langle\frac{1}{\theta}\rangle^{-1}([\![\frac{\boldsymbol{q}}{\theta}\cdot\boldsymbol{n}]\!] - \mathsf{m}[\![\eta]\!]). \tag{30}$$

and using sing the identity

$$[\![\boldsymbol{q}\cdot\boldsymbol{n}(1 - \frac{1}{\theta}\langle\frac{1}{\theta}\rangle^{-1})]\!] = [\![\boldsymbol{q}\cdot\boldsymbol{n}]\!]\langle 1 - \langle\frac{1}{\theta}\rangle\langle\frac{1}{\theta}\rangle^{-1}\rangle - \langle\boldsymbol{q}\cdot\boldsymbol{n}\rangle[\![\frac{1}{\theta}]\!]/\langle\frac{1}{\theta}\rangle = \mathsf{j}\langle\boldsymbol{q}\cdot\boldsymbol{n}\rangle, \tag{31}$$

we get

$$\mathsf{m}[\![\psi - \frac{1}{\rho}\boldsymbol{n}\cdot\boldsymbol{T}\boldsymbol{n} + \frac{1}{2}(\boldsymbol{\nu}\cdot\boldsymbol{n} - \boldsymbol{v}\cdot\boldsymbol{n})^2 + \eta(\theta - \langle\frac{1}{\theta}\rangle^{-1})]\!] + \mathsf{s}\cdot\mathsf{t} -$$

$$-[\![\frac{q}{\theta}(\theta-\langle\frac{1}{\theta}\rangle^{-1})\cdot n]\!] = \langle\frac{1}{\theta}\rangle^{-1}([\![\frac{q}{\theta}\cdot n]\!] - \mathsf{m}[\![\eta]\!]). \tag{32}$$

By inspection in (32) we note that both terms containing the difference $\theta - \langle\frac{1}{\theta}\rangle^{-1}$ in the left hand side appear as a consequence of the particular choice of Fried and Shen [3] to write the right hand side in the form:

$$\langle\frac{1}{\theta}\rangle^{-1}([\![\frac{q}{\theta}\cdot n]\!] - \mathsf{m}[\![\eta]\!]).$$

It is interesting to note here that a result obtained in [8] is the interfacial balance of energy in the form

$$\mathsf{m}[\![\psi - \frac{1}{\rho}n\cdot Tn + \frac{1}{2}(\nu\cdot n - v\cdot n)^2 + \eta(\theta-\langle\theta\rangle)]\!] + \mathsf{s}\cdot\mathsf{t} -$$
$$-[\![\frac{q}{\theta}(\theta-\langle\theta\rangle)\cdot n]\!] = \langle\theta\rangle([\![\frac{q}{\theta}\cdot n]\!] - \mathsf{m}[\![\eta]\!]),$$

which is (formally) obtained using $\langle\theta\rangle$ instead of $\langle\frac{1}{\theta}\rangle^{-1}$ in (32). This remark leads to a more general result. A straightforward computation shows that the balance of energy (16) is equivalent with the general identity

$$\mathsf{m}[\![\psi - \frac{1}{\rho}n\cdot Tn + \frac{1}{2}(\nu\cdot n - v\cdot n)^2 + \eta(\theta-\overline{\theta})]\!] + \mathsf{s}\cdot\mathsf{t} -$$
$$-[\![\frac{q}{\theta}(\theta-\overline{\theta})\cdot n]\!] = \overline{\theta}([\![\frac{q}{\theta}\cdot n]\!] - \mathsf{m}[\![\eta]\!]), \tag{33}$$

which introduces a **positive interfacial field** $\overline{\theta}$. We call $\overline{\theta}$ **the equivalent temperature of the interface** and we regard this concept as to be prescribed by a *constitutive function*. Using (33), (19) and the fact that $\overline{\theta}$ is positive we obtain the general form of the interfacial dissipation inequality when the temperature field is discontinuous in the form

$$\mathsf{m}[\![\psi - \frac{1}{\rho}n\cdot Tn + \frac{1}{2}(\nu\cdot n - v\cdot n)^2 + \eta(\theta-\overline{\theta})]\!] + \mathsf{s}\cdot\mathsf{t} - [\![\frac{q}{\theta}(\theta-\overline{\theta})\cdot n]\!] \geq 0. \tag{34}$$

It is now clear that (32) is a particular case of (33) when the constitutive choice for $\overline{\theta}$ is

$$\overline{\theta} = \langle\frac{1}{\theta}\rangle^{-1}.$$

Other choices are possible and we shall develop this issue later on. The next section presents another derivation of (33) based on a slightly extension of the theory of structured interfaces as developed in [1]. This approach is based on a configurational force balance and highlights the physical meaning of $\overline{\theta}$.

3.4 Physical meaning of $\overline{\theta}$ using the structured interface theory and the balance of configurational forces

For a classical background concerning configurational forces and applications, including solidification with surface structure, we send the reader to the recent reference [1]. According to the notations introduced in [1] we shall use an overbar to denote superficial fields, and for convenience, as in previous sections, we shall ignore supplies and external fields. In this subsection we slightly extend the theory of Gurtin ([1], chap. 24) in order to account for situations where **the temperature field is discontinuous across the nonmaterial interface**. While the previous sections use the spatial description and includes the motion, in the present subsection, following the point of view of Gurtin, we use the material description. However, for simplicity, we discuss here only a pure thermal problem so that the two points of view are identical.

Following Gurtin [1], we consider a migrating control volume $\mathcal{P}$ that contains a part of an interface $\mathcal{S}$. We denote by $\mathcal{G}$ the subsurface $\mathcal{S} \cap \mathcal{P}$, we use $\boldsymbol{m}$ for the normal field to $\partial\mathcal{P}$, $\boldsymbol{n}$ for the normal field to $\mathcal{G}$, V for the normal velocity of $\mathcal{G}$ and $V_{\partial\mathcal{G}}$ for the velocity of $\partial\mathcal{G}$ in the direction n, normal to $\partial\mathcal{G}$ in the tangent plane to $\mathcal{G}$. The basic laws for a migrating control volume are the balance of energy and the imbalance of entropy are assumed in the form

$$\frac{d}{dt}\left[\int_{\mathcal{P}} e dv + \int_{\mathcal{G}} \overline{e} da\right] = -\int_{\partial\mathcal{P}} \boldsymbol{q}\cdot\boldsymbol{m} da + \int_{\partial\mathcal{P}} QU da + \int_{\partial\mathcal{G}} \overline{Q} V_{\partial\mathcal{G}} ds + W(\mathcal{P}), \tag{35}$$

$$\frac{d}{dt}\left[\int_{\mathcal{P}} \eta dv + \int_{\mathcal{G}} \overline{\eta} da\right] \geq -\int_{\partial\mathcal{P}} \frac{\boldsymbol{q}}{\theta}\cdot\boldsymbol{m} da + \int_{\partial\mathcal{P}} \frac{Q}{\theta} U da + \int_{\partial\mathcal{G}} \frac{\overline{Q}}{\overline{\theta}} V_{\partial\mathcal{G}} ds. \tag{36}$$

We also assume the balance of configurational forces in the form

$$\int_{\partial\mathcal{P}} \boldsymbol{C}\boldsymbol{m} da + \int_{\mathcal{P}} \boldsymbol{g} dv + \int_{\partial\mathcal{G}} \mathsf{C}\mathsf{n} ds + \int_{\mathcal{G}} \boldsymbol{g}^{S} da = 0. \tag{37}$$

In (37), $\boldsymbol{g}$ is the internal bulk force and $\boldsymbol{g}^S$ is the superficial bulk force while $\boldsymbol{C}$ and C are the bulk stress and interfacial stress tensors, respectively. The second terms in the right-hand side of (35) and (36) represent the flow of heat and entropy into $\mathcal{P}$ associated with the transfer of material across $\partial\mathcal{P}$, while the third terms in the right-hand side of (35) and (36) represent flow of heat and entropy into $\mathcal{G}$ associated with the transfer of material across $\partial\mathcal{G}$.

We note that when the temperature field is continuous the flow of entropy across $\partial\mathcal{G}$ is (as in [1], chap. 24) $\int_{\partial\mathcal{G}} \overline{Q}/\theta ds$ since the temperature of the interface is well-defined. When the temperature field is discontinuous across $\mathcal{G}$ we introduce a scalar superficial field, the *equivalent temperature of the interface* in order to define the entropy flow and denote this field by $\overline{\theta}$.

The form of the working $W(\mathcal{P})$ in the right hand side of (35) is

$$W(\mathcal{P}) = \int_{\partial\mathcal{P}} \boldsymbol{C}\boldsymbol{n} \cdot \boldsymbol{w}_{\partial\mathcal{P}} + \int_{\partial\mathcal{G}} \mathsf{C}\mathsf{n} \cdot \boldsymbol{w}_{\partial\mathcal{G}}, \tag{38}$$

where $\boldsymbol{w}_{\partial\mathcal{P}}$ and $\boldsymbol{w}_{\partial\mathcal{G}}$ are velocity fields for $\partial\mathcal{P}$ and $\partial\mathcal{G}$, respectively.

We recall briefly the main consequences of (35-38) as obtained in [1]:

1. Invariance of the working reduces $\boldsymbol{C}$ to a bulk tension, i.e., $\boldsymbol{C} = \pi\boldsymbol{I}$.

2. The interfacial stress has the form

$$\mathsf{C} = \sigma\mathsf{P} + \boldsymbol{n} \otimes \boldsymbol{\tau}, \tag{39}$$

   where σ is the surface tension and $\boldsymbol{\tau}$ the surface shear.

3. The interfacial force balance is

$$[\![\boldsymbol{C}]\!]\boldsymbol{n} + \boldsymbol{g}^{\mathcal{S}} + \mathrm{div}_{\mathcal{S}}\mathsf{C} = \boldsymbol{0}, \tag{40}$$

   and its normal component gives:

$$\sigma K + \mathrm{div}_{\mathcal{S}}\boldsymbol{\tau} + [\![\pi]\!] + g^{\mathcal{S}} = 0, \tag{41}$$

   where $K = -\mathrm{div}\boldsymbol{n}$ is the mean curvature.

4. The working (38) can be rewritten as

$$W(\mathcal{P}) = -\int_{\mathcal{G}} [\sigma KV + \boldsymbol{\tau} \cdot \boldsymbol{n}^{\circ} + ([\![\pi]\!] + g^{\mathcal{G}})V] + \int_{\partial\mathcal{G}} \sigma V_{\partial\mathcal{G}} ds + \int_{\partial\mathcal{P}} \pi U da, \tag{42}$$

   where a° denotes the normal time derivative following the motion of $\mathcal{S}$.

Using (42), a transport theorem and an invariance argument applied to (35) we get

$$e = Q + \pi, \qquad \overline{e} = \overline{Q} + \sigma, \tag{43}$$

and a similar argument in (36) leads to

$$\eta = Q/\theta, \qquad \overline{\eta} = \overline{Q}/\overline{\theta}. \tag{44}$$

We define the bulk free energy $\psi = e - \theta\eta$ and the superficial free energy $\overline{\psi} = \overline{e} - \overline{\theta}\overline{\eta}$, and conclude that

$$\pi = \psi, \qquad \sigma = \overline{\psi}, \tag{45}$$

so that the normal component of the interfacial force balance becomes

$$\overline{\psi}K + \mathrm{div}_{\mathcal{S}}\boldsymbol{\tau} + [\![\psi]\!] + g^{\mathcal{S}} = 0. \tag{46}$$

Finally, the interfacial forms of the balance of energy and imbalance of entropy are

$$[\![\theta\eta]\!]V = [\![\boldsymbol{q}\cdot\boldsymbol{n}]\!] + \overline{e}^{\circ} - \overline{\theta}\overline{\eta}KV + \boldsymbol{\tau}\cdot\mathbf{n}^{\circ} + g^{\mathcal{S}}V, \tag{47}$$

$$[\![\eta]\!]V \leq \overline{\eta}^{\circ} - \overline{\eta}KV + [\![\frac{\boldsymbol{q}}{\theta}\cdot\boldsymbol{n}]\!]. \tag{48}$$

We remark that without additional constitutive assumptions, in the absence of the superficial structure (i.e. when $\overline{e} = \overline{\eta} = 0$) and without superficial shear, i.e., $\boldsymbol{\tau} = 0$, using (46), relation (47) reduces to the purely thermal version of (20). Under the same assumptions (48) reduces to (19), so that at this point the equivalent temperature of the interface plays no particular role, as expected.

The next step is to deduce the interfacial form of the dissipation inequality from (47) and (48). Multiplying (48) by $\overline{\theta}$ and combining with (47) we obtain

$$\overline{\psi}^{\circ} + \overline{\eta}\overline{\theta}^{\circ} + \boldsymbol{\tau}\cdot\boldsymbol{n}^{\circ} + g^{\mathcal{S}}V + [\![\boldsymbol{q}(1 - \frac{\overline{\theta}}{\theta})\cdot\boldsymbol{n}]\!] - [\![\eta(\theta - \overline{\theta})]\!]V \leq 0. \tag{49}$$

When we compare this result with the standard derivation in [1], obtained when the temperature field is continuous, we note two additional terms. In order to obtain the physical significance of different terms we rearrange (49) as

$$\overline{\psi}^{\circ} + \overline{\eta}\overline{\theta}^{\circ} + \boldsymbol{\tau}\cdot\boldsymbol{n}^{\circ} + (g^{\mathcal{S}} - [\![\eta(\theta - \overline{\theta})]\!])V + [\![\mathbf{q}(1 - \frac{\overline{\theta}}{\theta})\cdot\boldsymbol{n}]\!] \leq 0, \tag{50}$$

and note that in the purely thermal setting without interface structure and without interfacial shear[1], i.e. when $\overline{\psi} = \overline{\eta} = 0$ the normal component of the configurational forces balance reduces to

$$-g^{\mathcal{S}} = [\![\psi]\!], \tag{51}$$

[1]With additional constitutive assumptions it follows from the work of Gurtin [1] that the interfacial shear is the derivative of the surface free energy with respect to the orientation so that using additional constitutive assumptions without interfacial structure the interfacial shear vanishes.

which substituted in (50) gives

$$V[\![\psi + \eta(\theta - \overline{\theta})]\!] - [\![\frac{\boldsymbol{q}}{\theta}(\theta - \overline{\theta}) \cdot \boldsymbol{n}]\!] \geq 0. \tag{52}$$

This is exactly the material form of the purely thermal version of (34), where V is substituted[2] by ρV.

This derivation shows clearly that the interfacial dissipation inequality, which is obtained here combining (47) and (48), makes use of the equivalent temperature of the interface $\overline{\theta}$, which is uniquely defined when the temperature is continuous, but has to be prescribed by a constitutive function when the temperature field is discontinuous.

4 Constitutive relations at the interface; special theories

In this section we shall discuss only the pure thermal setting in motionless bodies, but our main results can be generalized straightforward following the line of [3] to include both the motion and the interfacial slip and friction. In the purely thermal setting the interfacial energy release and the entropy imbalance are

$$\mathsf{e} = [\![\psi + \eta(\theta - \overline{\theta})]\!], \qquad \mathsf{me} - [\![\frac{\boldsymbol{q}}{\theta}(\theta - \overline{\theta}) \cdot \boldsymbol{n}]\!] \geq 0, \tag{53}$$

We now assume that the interfacial energy release and the equivalent temperature of the interface are given by the following constitutive functions

$$\overline{\theta} = \tilde{\theta}(\theta^-, \theta^+), \qquad \mathsf{e} = \tilde{\mathsf{e}}(\theta^-, \theta^+, \mathsf{m}). \tag{54}$$

Compatibility with (53) imposes

$$\tilde{\mathsf{e}}(\theta^-, \theta^+, \mathsf{m}) = \alpha(\theta^-, \theta^+, \mathsf{m})\mathsf{m}, \tag{55}$$

with α positive and

$$[\![\frac{\boldsymbol{q}}{\theta} \cdot \boldsymbol{n}]\!] \geq \frac{1}{\tilde{\theta}}[\![\boldsymbol{q} \cdot \boldsymbol{n}]\!]. \tag{56}$$

Moreover, we assume that the constitutive function $\tilde{\theta}$ is such that

$$\min(\theta^-, \theta^+) \leq \tilde{\theta} \leq \max(\theta^-, \theta^+). \tag{57}$$

This additional assumption has two important consequences:

[2] This is a consequence of the convention of Gurtin in [1] which use volume densities.

1. It is sufficient to fix $\overline{\theta} = \theta$ when the temperature is continuous[3], in which case relation (55) gives the classical formula

$$[\![\Psi]\!] = \alpha \mathsf{m},$$

so that (56) holds obviously. In fact (57) renders the present theory consistent with classical Stefan model.

2. In a classical simplified constitutive context, which is the subject of the next section, (57) is sufficient to insure (56).

Two special choices of the constitutive function $\overline{\theta}$ were already proposed in the literature leading to different theories. They are discussed in the following two paragraphs and generalized below.

Theory based on: $\overline{\theta} = \langle \frac{1}{\theta} \rangle^{-1}$ This assumption has been made by Fried and Shen [3] although the form of the interfacial energy release and interfacial heating are those from subsection 3.1. In the pure thermal setting the inequality (56) becomes

$$\langle \frac{1}{\theta} \rangle^{-1} [\![\frac{\boldsymbol{q}}{\theta} \cdot \boldsymbol{n}]\!] \geq [\![\boldsymbol{q} \cdot \boldsymbol{n}]\!], \tag{58}$$

or equivalently

$$\langle \boldsymbol{q} \cdot \boldsymbol{n} \rangle \mathsf{j} \leq 0. \tag{59}$$

This is satisfied by a supplemental constitutive choice

$$\langle \boldsymbol{q} \cdot \boldsymbol{n} \rangle = -\gamma \mathsf{j} \tag{60}$$

for some function $\gamma \geq 0$.

Theory based on: $\overline{\theta} = \langle \theta \rangle$ This choice was used in [8] and (56) becomes

$$\langle \theta \rangle [\![\frac{\boldsymbol{q}}{\theta} \cdot \boldsymbol{n}]\!] \geq [\![\boldsymbol{q} \cdot \boldsymbol{n}]\!], \tag{61}$$

or equivalently,

$$\langle \frac{\boldsymbol{q}}{\theta} \rangle \cdot \boldsymbol{n} [\![\theta]\!] \leq 0. \tag{62}$$

In this case a supplemental constitutive choice is usually

$$\langle \frac{\boldsymbol{q}}{\theta} \rangle \cdot \boldsymbol{n} = -\gamma \mathsf{j} \tag{63}$$

for some positive function γ.

[3] This is only a technical assumption and we found it useful for applications presented in the last section. Of course, one may use a weaker version like $\theta^+ = \theta^- \Rightarrow \overline{\theta} = \theta^+ = \theta^-$.

Theory based on: $\overline{\theta} = \langle \theta^r \rangle \langle \frac{1}{\theta^{1-r}} \rangle^{-1}$ This class includes the two previous examples for $r = 0$ and $r = 1$. It contains also for $r = 1/2$ the choice $\overline{\theta} = \sqrt{\theta^+ \theta^-}$. In this case (56) becomes successively

$$\langle \theta^r \rangle \langle \frac{1}{\theta^{1-r}} \rangle^{-1} [\![\frac{\boldsymbol{q}}{\theta}]\!] \cdot \boldsymbol{n} \geq [\![\boldsymbol{q}]\!] \cdot \boldsymbol{n} \Longleftrightarrow \tag{64}$$

$$\langle \frac{1}{\theta^{1-r}} \rangle^{-1} [\![\frac{\boldsymbol{q}}{\theta^r} \frac{1}{\theta^{1-r}}]\!] \cdot \boldsymbol{n} \geq \frac{1}{\langle \theta^r \rangle} [\![\boldsymbol{q}]\!] \cdot \boldsymbol{n} \Longleftrightarrow \tag{65}$$

$$\langle \frac{1}{\theta^{1-r}} \rangle^{-1} \left[[\![\frac{\boldsymbol{q}}{\theta^r}]\!] \cdot \boldsymbol{n} \langle \frac{1}{\theta^{1-r}} \rangle + \langle \frac{\boldsymbol{q}}{\theta^r} \rangle \cdot \boldsymbol{n} [\![\frac{1}{\theta^{1-r}}]\!] \right] \geq \frac{1}{\langle \theta^r \rangle} [\![\frac{\boldsymbol{q}}{\theta^r} \theta^r]\!] \cdot \boldsymbol{n} \Longleftrightarrow \tag{66}$$

$$\langle \frac{\boldsymbol{q}}{\theta^r} \rangle \cdot \boldsymbol{n} \frac{[\![\frac{1}{\theta^{1-r}}]\!]}{\langle \frac{1}{\theta^{1-r}} \rangle} \geq \langle \frac{\boldsymbol{q}}{\theta^r} \rangle \cdot \boldsymbol{n} \frac{[\![\theta^r]\!]}{\langle \theta^r \rangle}. \tag{67}$$

Using the identity

$$\frac{[\![\theta^r]\!]}{\langle \theta^r \rangle} = -\frac{[\![\frac{1}{\theta^r}]\!]}{\langle \frac{1}{\theta^r} \rangle}, \tag{68}$$

we obtain finally

$$\langle \frac{\boldsymbol{q}}{\theta^r} \rangle \cdot \boldsymbol{n} \left[\frac{[\![\theta^r]\!]}{\langle \theta^r \rangle} + \frac{[\![\theta^{1-r}]\!]}{\langle \theta^{1-r} \rangle} \right] \leq 0 \tag{69}$$

which is satisfied by the choice

$$\langle \frac{\boldsymbol{q}}{\theta^r} \rangle \cdot \boldsymbol{n} = -\gamma \left[\frac{[\![\theta^r]\!]}{\langle \theta^r \rangle} + \frac{[\![\theta^{1-r}]\!]}{\langle \theta^{1-r} \rangle} \right], \tag{70}$$

for some positive function γ.

We can conclude that the generalized Stefan model in the pure thermal setting consists in the conservation of energy in the bulk (equation (10)), the interfacial condition (18), supplemented by two constitutive functions e and $\overline{\theta}$ compatible with (55) and (56). Supplemented by initial and boundary conditions they form a free-boundary problem the temperature field.

We end this section with a comment: it is not a priori obvious that a supplemental relation (see (70)) is necessary in order to satisfy (56). In agreement with a classical line of thinking (see [7]) we can regard (56) as a restriction on the constitutive function $\overline{\theta}$. The next section shows that in a particular constitutive context any choice of the constitutive function $\overline{\theta}$ compatible with (57) also satisfies (56).

5 Applications

The solidification of a pure substance in the absence of the mouvement was studied in a particular constitutive framework in [3] and *sufficient conditions* for the existence of a unique travelling wave solution were obtained.

To demonstrate the role of the equivalent temperature of the interface and that of the supplemental relations on the interface we shall study both the solidification of a under-cooled liquid and the melt of a super-heated solid in the constitutive framework provided in section 4.

The assumptions on the free-energies of the liquid and solid phases are classic so that we shall focus on travelling waves solutions of the free boundary problem. Our main result of this section gives necessary and sufficient conditions for the existence of travelling wave solutions.

5.1 Field equations and jump conditions

The mass density is supposed constant over the whole body and the motion is neglected. In this case, the field equation is the *balance of energy*

$$\rho\dot{e} = -\mathrm{div}\boldsymbol{q}, \tag{71}$$

and the associated interface balance is

$$\rho V[\![e]\!] = [\![q]\!], \tag{72}$$

where $V = \boldsymbol{\nu}\cdot\boldsymbol{n}$. In the general setting according to (55) and (56) the supplemental constitutive relations for the interfacial energy release is

$$[\![\Psi + \eta(\theta - \overline{\theta})]\!] = \alpha\rho V, \tag{73}$$

where α is a positive constant and $\overline{\theta}$ is a positive constitutive function compatible with

$$\min(\theta^+,\theta^-) \le \overline{\theta} \le \max(\theta^+,\theta^-), \qquad \overline{\theta}[\![\frac{q}{\theta}]\!]\cdot\boldsymbol{n} \ge [\![q]\!]\cdot\boldsymbol{n}. \tag{74}$$

5.2 Constitutive assumptions

Following Fried and Shen [3] we use the subscripts l and s for the liquid and respectively solid phases and we assume the free-energy density in the form:

$$\Psi(\theta) = \begin{cases} c_s\theta(1-\ln(\theta/\theta_s)) & \text{in the solid phase,} \\ c_l\theta(1-\ln(\theta/\theta_l)) + l & \text{in the liquid phase,} \end{cases} \tag{75}$$

where c_s, c_l, θ_s, θ_l and l are positive constants. As a consequence of the imbalance of entropy in the bulk we obtain

$$\eta(\theta) = -\Psi'(\theta) = \begin{cases} c_s \ln(\theta/\theta_s) & \text{in the solid phase,} \\ c_l \ln(\theta/\theta_l) & \text{in the liquid phase,} \end{cases} \tag{76}$$

and

$$e(\theta) = \Psi(\theta) - \theta\eta(\theta) = \begin{cases} c_s\theta & \text{in the solid phase,} \\ c_l\theta + l & \text{in the liquid phase.} \end{cases} \tag{77}$$

We assume the heat flux $\boldsymbol{q}$ in the classical form

$$\boldsymbol{q} = \begin{cases} -k_s \mathrm{grad}\theta & \text{in the solid phase,} \\ -k_l \mathrm{grad}\theta & \text{in the liquid phase,} \end{cases} \tag{78}$$

for k_s and k_l positive.

Following an assumption of Fried and Shen [3] we suppose moreover that there exists a unique *transition temperature* $\theta_l < \theta_\star < \theta_s$ such that

$$\Psi_s(\theta_\star) = \Psi_l(\theta_\star). \tag{79}$$

5.3 Travelling waves solutions

We investigate a special class of solutions in the whole space in the case where the phase interface $\mathcal{S}_t$ is a plane that propagates with an unknown but constant scalar velocity $V > 0$. Thus we study the existence of solutions

$$\theta(\boldsymbol{x}, t) = \hat{\theta}(\xi), \tag{80}$$

where $\xi = \boldsymbol{x} \cdot \boldsymbol{n} - Vt$, having a constant profile in a mouving frame.

Solidification of a under-cooled liquid: We shall assume that the solid phase is located in the half-space $\xi < 0$ and the liquid phase in the half-space $\xi > 0$ and we look for solutions with $V > 0$. For the solidification of a under-cooled liquid we shall assume that in the liquid phase the far-field temperature, denoted θ_∞, is such that:

$$\theta_\infty \leq \theta^+ \leq \theta^- \leq \theta_\star. \tag{81}$$

A straightforward computation shows that there is a temperature field compatible with the bulk equations and the jump condition (72) in the form

$$\theta(\boldsymbol{x}, t) = \begin{cases} \theta^- & \text{if } \xi < 0, \\ \theta_\infty + (\theta^+ - \theta_\infty)\exp\left(-c_l V \rho \xi / k_l\right)) & \text{if } \xi > 0, \end{cases} \tag{82}$$

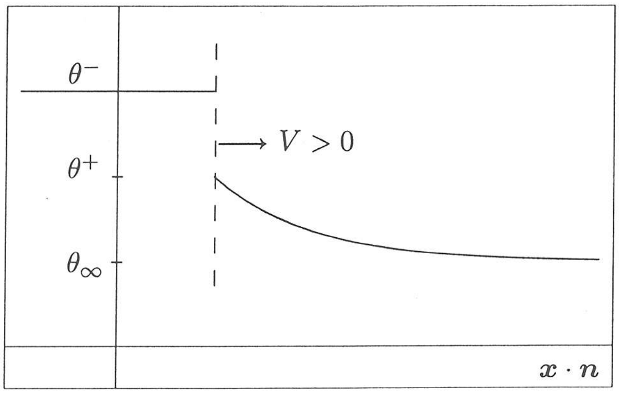

Figure 1: Travelling wave profile for $V > 0$ in a fixed frame; the dashed line is the wave front. In the right part $\xi = \boldsymbol{x} \cdot \boldsymbol{n} - Vt > 0$ while on the left $\xi < 0$.

with

$$\theta^- = \frac{c_l \theta_\infty + l}{c_s}. \tag{83}$$

It remains to verify when this solution is compatible with (73) and (74.2) under the assumption (74.1). First, we prove that for any choice of $\overline{\theta}$ compatible with (74.1), the general solution (82) satisfies (74.2). The computation of $\boldsymbol{q} \cdot \boldsymbol{n}$ gives

$$\boldsymbol{q} \cdot \boldsymbol{n} = \begin{cases} 0 & \text{for } \xi < 0, \\ \rho c_l V(\theta^+ - \theta_\infty) & \text{for } \xi > 0. \end{cases} \tag{84}$$

We have $(\boldsymbol{q} \cdot \boldsymbol{n})^- = 0$ and $(\boldsymbol{q} \cdot \boldsymbol{n})^+ > 0$ so that relation (74.2) is equivalent to

$$\overline{\theta} \geq \theta^+, \tag{85}$$

which is implied by the constitutive assumption (74.1).

The last supplemental condition (73) can be rewritten as

$$[\![e]\!] - \overline{\theta}[\![\eta]\!] = \rho \alpha V, \tag{86}$$

and taking into account (76), (77) and (83) we obtain

$$c_l(\theta^+ - \theta_\infty) - \overline{\theta}\left[c_l \ln(\theta^+/\theta_l) - c_s \ln\left(\frac{c_l\theta_\infty + l}{c_s\theta_s}\right)\right] = \rho\alpha V. \tag{87}$$

We conclude that a *unique travelling wave solution exists if and only if the material coefficients* $(c_l, c_s, \theta_l, \theta_s, l)$ *and the given data* $(\theta^+, \theta_\infty)$ *satisfy*

$$c_l(\theta^+ - \theta_\infty) \geq \overline{\theta}\left[c_l \ln(\theta^+/\theta_l) - c_s \ln\left(\frac{c_l\theta_\infty + l}{c_s\theta_s}\right)\right]. \tag{88}$$

If θ^+ and θ_∞ are considered as given data relation (88) has to be regarded as a restriction on $\overline{\theta}$. Toward experimental evidence for $\overline{\theta}$ we note that a measure of V, for a given material $(c_l, c_s, \theta_l, \theta_s, l)$ and given data $(\theta^+, \theta_\infty)$ provides using (77) a value of $\overline{\theta}$.

Melting of a super-heated solid: We still consider the solid phase in the half-space $\xi < 0$ and the liquid phase in the half space $\xi > 0$ but we look for solutions with $V < 0$. The far-field in the super-heated solid equals θ_∞, and we suppose

$$\theta_\star \leq \theta^+ \leq \theta^- \leq \theta_\infty. \tag{89}$$

A travelling wave solution is now in the form

$$\theta(\boldsymbol{x}, t) = \begin{cases} \theta_\infty + (\theta^+ - \theta_\infty)\exp\left(c_s\rho\xi V/k_s\right) & \text{if } \xi > 0, \\ \theta^+ & \text{if } \xi < 0, \end{cases} \tag{90}$$

with

$$\theta^+ = \frac{c_s\theta_\infty - l}{c_l}. \tag{91}$$

In this case $(\boldsymbol{q}\cdot\boldsymbol{n})^+ = 0$ and $(\boldsymbol{q}\cdot\boldsymbol{n})^- = \rho c_s V(\theta_\infty - \theta^-) < 0$ so that (74.2) follows from (74.1). A unique travelling wave solution exists if and only if

$$c_s(\theta^- - \theta_\infty) \geq \overline{\theta}\left[c_s \ln(\theta^-/\theta_l) - c_l \ln\left(\frac{c_s\theta_\infty - l}{c_l\theta_l}\right)\right]. \tag{92}$$

We underline here that a supplemental constitutive relation similar to (70) is not needed and necessary and sufficient conditions are obtained for the existence of a unique travelling wave solutions in terms of the material parameters $(c_l, c_s, \theta_l, \theta_s, l)$ and given data $(\theta^+, \theta_\infty)$ if $\overline{\theta}$ is given. Otherwise, a measure of V for fixed material parameters and given data gives $\overline{\theta}$ as in (87).

6 Conclusions

We propose in this paper a generalized Stefan model allowing for jumps in the temperature field across a nonmaterial evolving interface. We show that the general form of the interfacial dissipation inequality is based on an additional superficial field, denoted here $\overline{\theta}$, and we regard it as to be prescribed by a constitutive function. We argue in this direction using two different points of view:

- We derive a general form of the interfacial balance of energy that combined with the imbalance of entropy provides the interfacial dissipation inequality (34).
- In section 4, we start with a slightly modified version of a theory based on a balance of configurational forces for structured interfaces and recover the interfacial dissipation inequality obtained following this line of thinking. The use of a theory based on configurational force balance on structured interfaces highlights the physical significance of the equivalent temperature of the interface, as it introduces this concept in relation to the flow of entropy. We recover, as particular cases, two approaches proposed in the literature, when $\overline{\theta} = \langle \frac{1}{\theta} \rangle^{-1}$, and $\overline{\theta} = \langle \theta \rangle$.

It is interesting to note here that for structured interfaces, the interfacial dissipation inequality (49) involves $\overline{\theta}$ even if the surface structure is absent. On the other hand, in the absence of surface structure the balance of energy (47) and the imbalance of entropy (48) do not involve the scalar field $\overline{\theta}$. This may explain previous particular choices presented in Fried and Shen [3] and Dascalu and Danescu [8].

For simplicity, to discuss the constitutive relations we focus on a pure thermal problem and we use the interfacial dissipation inequality in order to obtain restrictions on the interfacial energy release and the equivalent temperature of the interface. We only assume that

$$\min(\theta^-, \theta^+) \leq \overline{\theta} \leq \max(\theta^-, \theta^+) \tag{93}$$

and render the theory consistent with the classical Stefan model (in which case the temperature is continuous).

As an illustration of the model we study in a simplified constitutive context the existence of travelling waves solutions for two problems: the solidification of an under-cooled liquid and the melting of an super-heated solid. Without constitutive specifications for $\overline{\theta}$, using only (93) we are able to give necessary and sufficient conditions for the existence of a unique travelling wave solution (relations (88) and (92)) involving only material parameters and given data.

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