

NON-LOCAL THERMODYNAMIC MODELS FOR INHOMOGENEOUS SOLIDS

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ABSTRACT

Introduction

The purpose of the current work is the formulation of thermodynamic models for chemically and structurally inhomogeneous solids undergoing finite deformation. In particular, these models are based on both "standard" non-equilibrium thermodynamics [SNET: 1,2] and on the General Equation for Non-Equilibrium Reversible-Irreversible Coupling [GENERIC: 3]. In particular, model formulations are obtained in this context in [4] for non-isothermal generalizations of standard isothermal conservative (e.g., Cahn-Hilliard) and non-conservative (e.g., Allen-Cahn) diffuse interface or "phase-field" models for multicomponent, multiphase solids. In the isothermal context, isothermal models for geometrically non-linear gradient solids with microstructure have recently been formulated in [5]. The current treatment is consistent with and subsumes previous work on non-isothermal systems [e.g., 6]. In the context of no-flux boundary conditions, the SNET- and GENERIC-based approaches are shown to be completely consistent with each other and result in equivalent temperature evolution relations. For more details, the reader is referred to [4,5].

For simplicity, attention is restricted here to the (simplest) case of a solid mixture consisting of two chemical components and two thermoelastic solid phases. In this work, (three-dimensional) Euclidean vectors are represented by lower-case bold italic characters $\mathbf{a}, \mathbf{b}, \dots$. Second-order tensors are represented by upper-case bold italic characters $\mathbf{A}, \mathbf{B}, \dots$, with \mathbf{I} the second-order identity. The notation $A \cdot B := A_{i\dots} B_{i\dots}$ (sum on repeated indices) represents the scalar product of two tensors A and B of any order. Additional notation will be introduced as needed.

SNET-based formulation

In the formulation to follow, all fields are defined on the mixture reference configuration R with boundary ∂R and outward unit normal \mathbf{n} . For simplicity, assume that the two components do not react chemically. As well, all supplies of mass, momentum and energy are assumed negligible. Let ρ_1 and ρ_2 represent the mass densities of the two components. Again for simplicity, assume that the mixture mass density $\rho = \rho_1 + \rho_2$ is constant. In what follows, let $\rho \equiv \rho_1$ and $\mathbf{j} \equiv \mathbf{j}_1$, where \mathbf{j} represents the component mass flux density. Adapting next the approach of [1] to the current referential or Lagrangian setting relevant to geometrically non-linear solids, the balance relations

$$\dot{\rho} = -\operatorname{div} \mathbf{j}, \quad \dot{\mathbf{m}} = \operatorname{div} \mathbf{P}, \quad \dot{\varepsilon} = \mathbf{P} \cdot \nabla \dot{\boldsymbol{\chi}} - \operatorname{div} \mathbf{q}, \quad (1)$$

on R hold for component mass, mixture linear momentum, and mixture internal energy, balance, respectively. In these relations, $\mathbf{m} = \rho \dot{\boldsymbol{\chi}}$ and ε represent the mixture momentum and internal energy densities, respectively, with $\boldsymbol{\chi}$ the mixture motion. Further, \mathbf{P} is the momentum flux density, and \mathbf{q} represents the heat flux density. Assuming for simplicity that R is closed with respect to mass and momentum, the boundary conditions

$$\mathbf{j}|_{\partial R} \cdot \mathbf{n} = 0, \quad \mathbf{P}|_{\partial R} \mathbf{n} = \mathbf{0}, \quad \mathbf{q}|_{\partial R} \cdot \mathbf{n} = q_{\partial R}, \quad (2)$$

hold on ∂R . Besides (1), the mixture entropy balance $\dot{\eta} = \pi - \operatorname{div} \boldsymbol{\phi}$ is relevant to the current SNET-based formulation. In this relation, η represents the entropy density, π the entropy production-rate density, and $\boldsymbol{\phi}$ the entropy flux density. Let θ represent the (absolute) temperature and $\vartheta := \theta^{-1}$. In the current context of mass and heat diffusion [1], $\boldsymbol{\phi} = \check{\mathbf{q}} - \check{\mu} \mathbf{j}$ in terms of the chemical potential μ and notation $\check{f} := \vartheta f$. Combining this with the entropy balance and (1)_{1,3} yields the generalized Gibbs relation $\pi = \mathbf{q} \cdot \nabla \vartheta - \mathbf{j} \cdot \nabla \check{\mu} + \check{\mathbf{P}} \cdot \nabla \dot{\boldsymbol{\chi}} + \check{\mu} \dot{\rho} + \varepsilon \dot{\vartheta} - \check{\Psi}$ based on the (negative) free entropy density $\check{\Psi} := \check{\varepsilon} - \eta = \vartheta \psi$, with $\psi := \varepsilon - \theta \eta$ the free energy density as usual. For the current class of two-component, two-phase, inhomogeneous thermoelastic solids, the (entropic) constitutive forms

$$\check{\Psi} = \check{\Psi}(\vartheta, \nabla \boldsymbol{\chi}, \rho, \nabla \rho, \phi, \nabla \phi), \quad \varepsilon = \partial_{\vartheta} \check{\Psi}, \quad \check{\mathbf{P}} = \partial_{\nabla \boldsymbol{\chi}} \check{\Psi}, \quad \check{\mu} = \delta_{\rho} \check{\Psi}, \quad (3)$$

hold in the context of the generalized Gibbs relation above. Here, ϕ represents the (non-conservative) structural order parameter, and $\delta_x a := \partial_x a - \operatorname{div} \partial_{\nabla_x} a$ is the variational derivative of the density a with respect to x . In the simplest case, the no-flux boundary conditions

$$\partial_{\nabla \rho} \varepsilon|_{\partial R} \cdot \mathbf{n} = 0, \quad \partial_{\nabla \rho} \eta|_{\partial R} \cdot \mathbf{n} = 0, \quad \partial_{\nabla \phi} \varepsilon|_{\partial R} \cdot \mathbf{n} = 0, \quad \partial_{\nabla \phi} \eta|_{\partial R} \cdot \mathbf{n} = 0, \quad (4)$$

and integrand continuity result in the "residual" form $\pi = \mathbf{q} \cdot \nabla \vartheta - \mathbf{j} \cdot \nabla \check{\mu} - \dot{\phi} \delta_{\phi} \check{\Psi}$ for π . As usual, this motivates (in the simplest case) "diagonal" flux-force relations

$$\mathbf{q} = \theta^2 \mathbf{K} \nabla \vartheta, \quad \mathbf{j} = -\theta \mathbf{D} \nabla \check{\mu}, \quad \dot{\phi} = -\theta m \delta_{\phi} \check{\Psi}; \quad (5)$$

symmetry and non-negativity of the thermal conductivity \mathbf{K} and mass diffusivity \mathbf{D} , as well as non-negativity of the phase mobility m , are then sufficient for non-negative entropy production $\pi = (\nabla \vartheta) \cdot \theta^2 \mathbf{K} (\nabla \vartheta) + (\nabla \check{\mu}) \cdot \theta \mathbf{D} (\nabla \check{\mu}) + (\delta_{\phi} \check{\Psi}) \theta m (\delta_{\phi} \check{\Psi}) \geq 0$.

In summary, (1), (3), (4), and (5) result in the system

$$\dot{\rho} = \text{div } \theta \mathbf{D} \nabla \delta_\rho \check{\psi}, \quad \dot{\mathbf{m}} = \text{div } \partial_{\nabla \chi} \psi, \quad c \dot{\theta} = \varpi + \text{div } \mathbf{K} \nabla \theta, \quad \dot{\phi} = -\theta m \delta_\phi \check{\psi}, \quad (6)$$

of evolution-field relations for $(\rho, \mathbf{m}, \theta, \phi)$ and boundary conditions

$$\theta \mathbf{D} \nabla \delta_\rho \check{\psi}|_{\partial R} \cdot \mathbf{n} = 0, \quad \partial_{\nabla \chi} \varepsilon|_{\partial R} \mathbf{n} = \mathbf{0}, \quad \partial_{\nabla \chi} \eta|_{\partial R} \mathbf{n} = \mathbf{0}, \quad -\mathbf{K} \nabla \theta|_{\partial R} \cdot \mathbf{n} = q_{\partial R}, \quad (7)$$

from (2) via (3)₃ and (5)₁. In particular, (6)₃ for $\dot{\theta}$ follows from (1)₃, (3)₁₋₃, and (5)₁ in terms of the heat capacity $c = -\partial^2 \delta_\theta \varepsilon \equiv \partial_\theta \varepsilon$ and the volumetric heating rate density $\varpi = \varpi_{\text{ene}} + \varpi_{\text{dis}}$, with

$$\varpi_{\text{ene}} := -\theta (d_\chi \eta) \diamond \chi, \quad \varpi_{\text{dis}} := -(d_\rho \varepsilon) \diamond \dot{\rho} - (d_\phi \varepsilon) \diamond \dot{\phi}, \quad (8)$$

its energetic and dissipative parts, respectively. In these relations, the operator notation

$$(d_s a) \diamond f := (\partial_s a) f + (\partial_{\nabla_s} a) \cdot \nabla f, \quad (d_v a) \diamond \mathbf{f} := (\partial_v a) \cdot \mathbf{f} + (\partial_{\nabla_v} a) \cdot \nabla \mathbf{f}, \quad (9)$$

has been introduced in terms of scalar s, f and vector \mathbf{v}, \mathbf{f} quantities. The alternative forms

$$\begin{aligned} \varpi_{\text{dis}} &= -(\delta_\rho \varepsilon) \dot{\rho} - (\delta_\phi \varepsilon) \dot{\phi} = -(\delta_\rho \varepsilon) \text{div } \theta \mathbf{D} \nabla \delta_\rho \check{\psi} + (\delta_\phi \varepsilon) \theta m \delta_\phi \check{\psi} \\ &= (\nabla \delta_\rho \varepsilon) \cdot \theta \mathbf{D} (\nabla \delta_\rho \check{\psi}) + (\delta_\phi \varepsilon) \theta m (\delta_\phi \check{\psi}) \end{aligned} \quad (10)$$

also hold for ϖ_{dis} from (2)₁, (4)_{1,3}, and (6)_{1,4} via integration by parts and the divergence theorem. As will be seen below, the forms (8) for ϖ_{ene} and ϖ_{dis} also arise directly in the GENERIC-based model formulation, to which we now turn.

GENERIC-based formulation

The GENERIC [3]

$$\dot{\mathbf{x}} = \dot{\mathbf{x}}|_{\text{rev}} + \dot{\mathbf{x}}|_{\text{irr}}, \quad \dot{\mathbf{x}}|_{\text{rev}} = \mathcal{L} \mathcal{D}_x E, \quad \dot{\mathbf{x}}|_{\text{irr}} = \mathcal{M} \mathcal{D}_x S, \quad (11)$$

is a general formalism for the reversible (rev) and irreversible (irr) evolution of thermodynamic state variables \mathbf{x} driven by energy $\mathcal{D}_x E$ and entropy $\mathcal{D}_x S$ gradients mediated by the Poisson \mathcal{L} and friction \mathcal{M} operators. With respect to the scalar product $\langle \mathcal{D}_x A, \mathcal{D}_x B \rangle$ on functionals A, B and definition $\langle \mathcal{D}_x B, \mathcal{O}^T \mathcal{D}_x A \rangle := \langle \mathcal{D}_x A, \mathcal{O} \mathcal{D}_x B \rangle$ of the operator transpose, \mathcal{L} is (symplectic) skew-symmetric (i.e., $\mathcal{L}^T = -\mathcal{L}$), and \mathcal{M} (Onsager-Casimir) symmetric, non-negative definite (i.e., $\mathcal{M}^T = \mathcal{M}$ and $\langle \mathcal{D}_x A, \mathcal{M} \mathcal{D}_x A \rangle \geq 0$). These properties determine in turn those of the induced Poisson $\{A, B\} := \langle \mathcal{D}_x A, \mathcal{L} \mathcal{D}_x B \rangle$ and dissipation $[A, B] := \langle \mathcal{D}_x A, \mathcal{M} \mathcal{D}_x B \rangle$ brackets. In terms of these brackets, $\dot{A} = \{A, E\} + [A, S]$ models the evolution of any A . In this context, the orthogonality conditions $\mathcal{L} \mathcal{D}_x S = 0$ and $\mathcal{M} \mathcal{D}_x E = 0$ enforce energy conservation $\dot{E} = \{E, E\} = 0$, and non-negative entropy production $\dot{S} = [S, S] \geq 0$. For more details, the reader is referred to [3]. As already done tacitly in the last section, in the relations to follow, operators such as ∇ , $\text{div} \equiv \nabla \cdot$, \mathcal{L} , and \mathcal{M} , operate on everything to their right (unless otherwise indicated).

Consider now the application of the GENERIC to the formulation of a NET model for the two-component, two-phase solid mixture from the last section. For this material class, we have $\mathbf{x} = (\chi, \mathbf{m}, \theta, \rho, \phi)$ and

$$E[\mathbf{x}] = \int_R e(\mathbf{m}, \theta, \nabla \chi, \rho, \nabla \rho, \phi, \nabla \phi) dv, \quad e(\mathbf{m}, \theta, \nabla \chi, \rho, \nabla \rho, \phi, \nabla \phi) = \frac{1}{2\rho} \mathbf{m} \cdot \mathbf{m} + \varepsilon(\theta, \nabla \chi, \rho, \nabla \rho, \phi, \nabla \phi), \quad S[\mathbf{x}] = \int_R \eta(\theta, \nabla \chi, \rho, \nabla \rho, \phi, \nabla \phi) dv. \quad (12)$$

These forms for $E[\mathbf{x}]$ and $S[\mathbf{x}]$ induce those $\mathcal{D}_x A|_R = \partial_x a$ ($x \in \{\mathbf{m}, \theta\}$) and $\mathcal{D}_x A|_R = \delta_x a$ ($x \in \{\chi, \rho, \phi\}$) for the GENERIC gradient of $A = E, S$ ($a = e, \eta$) in R , and that $\mathcal{D}_x A|_{\partial R} = \partial_{\nabla_x} a|_{\partial R} \mathbf{n} = 0$ ($x \in \{\chi, \rho, \phi\}$) on ∂R via (4) and (7)_{2,3}. In addition, $\langle \mathcal{D}_x A, \mathcal{D}_x B \rangle := \int_R \mathcal{D}_x A \cdot \mathcal{D}_x B dv$. The operator relations $(\delta_s a) * g := g(\partial_s a) - \nabla \cdot g(\partial_{\nabla_s} a)$ and $(\delta_v a) * g := g(\partial_v a) - \nabla \cdot g(\partial_{\nabla_v} a)$ [e.g., 7, §4.1] are "adjoint" or "dual" to (9) in the sense that $\int_R f \{(\delta_s a) * g\} dv = \int_R g \{(d_s a) \diamond f\} dv$ and $\int_R \mathbf{f} \cdot \{(\delta_v a) * g\} dv = \int_R g \{(d_v a) \diamond \mathbf{f}\} dv$ hold via the divergence theorem and the GENERIC gradients.

Since momentum flux (stress) (3)₃ is purely energetic (thermoelastic), χ and \mathbf{m} are modeled as purely reversible. Consequently, $\dot{\chi}|_{\text{irr}} = \mathbf{0}$ and $\dot{\mathbf{m}}|_{\text{irr}} = \mathbf{0}$. On the other hand, mass diffusion and structural relaxation are modeled as purely irreversible; then $\dot{\rho}|_{\text{rev}} = 0$ and $\dot{\phi}|_{\text{rev}} = 0$. Lastly, the evolution of θ is general (e.g., thermal expansion, heat conduction). In this case, the reversible part $\dot{\mathbf{x}}|_{\text{rev}} = \mathcal{L} \mathcal{D}_x E$ of (11) reduces to

$$\left[\begin{array}{c} \dot{\chi} \\ \dot{\mathbf{m}} \\ \dot{\theta} \end{array} \right] \Big|_{\text{rev}} = \left[\begin{array}{ccc} 0 & L_{\chi \mathbf{m}} & L_{\chi \theta} \\ L_{\mathbf{m} \chi} & 0 & L_{\mathbf{m} \theta} \\ L_{\theta \chi} & L_{\theta \mathbf{m}} & 0 \end{array} \right] \left[\begin{array}{c} \delta_\chi e \\ \delta_{\mathbf{m}} e \\ \delta_\theta e \end{array} \right]. \quad (13)$$

Orthogonality $\mathcal{L} \mathcal{D}_x S = 0$ and skew-symmetry $\mathcal{L}^T = -\mathcal{L}$ imply in particular $L_{\chi \theta} = \mathbf{0}$, $L_{\theta \chi} = -L_{\chi \theta}^T = \mathbf{0}$, and $L_{\mathbf{m} \theta} = -L_{\mathbf{m} \chi} (\delta_\chi \eta) * (\partial_\theta \eta)^{-1}$. Then $\dot{\chi} = L_{\chi \mathbf{m}} \delta_{\mathbf{m}} e + L_{\chi \theta} \delta_\theta e = \frac{\mathbf{m}}{\rho}$, $\dot{\mathbf{m}} = L_{\mathbf{m} \chi} \delta_\chi e + L_{\mathbf{m} \theta} \delta_\theta e = \nabla \cdot \partial_{\nabla \chi} \psi$, we then obtain $L_{\theta \mathbf{m}} = -L_{\mathbf{m} \theta}^T = -(\partial_\theta \eta)^{-1} (d_\chi \eta) \diamond$. In summary,

$$\begin{aligned} \dot{\chi}|_{\text{rev}} &= L_{\chi \mathbf{m}} \delta_{\mathbf{m}} e + L_{\chi \theta} \delta_\theta e = \frac{\mathbf{m}}{\rho}, \\ \dot{\mathbf{m}}|_{\text{rev}} &= L_{\mathbf{m} \chi} \delta_\chi e + L_{\mathbf{m} \theta} \delta_\theta e = \nabla \cdot \partial_{\nabla \chi} \psi, \\ \dot{\theta}|_{\text{rev}} &= L_{\theta \chi} \delta_\chi e + L_{\theta \mathbf{m}} \delta_{\mathbf{m}} e = \frac{1}{c} \varpi_{\text{ene}}, \end{aligned} \quad (14)$$

via (8)₂, (13), $\theta = \partial_\theta \varepsilon / \partial_\theta \eta$, $\psi = \varepsilon - \theta \eta$, and $c = \partial_\theta \varepsilon$.

Consider next the irreversible part $\dot{\mathbf{x}}|_{\text{irr}} = \mathcal{M} \mathcal{D}_x S$ of (11). Assuming no coupling between ρ and ϕ , this reduces to

$$\left[\begin{array}{c} \dot{\theta} \\ \dot{\rho} \\ \dot{\phi} \end{array} \right] \Big|_{\text{irr}} = \left[\begin{array}{ccc} M_{\theta \theta} & M_{\theta \rho} & M_{\theta \phi} \\ M_{\rho \theta} & M_{\rho \rho} & 0 \\ M_{\phi \theta} & 0 & M_{\phi \phi} \end{array} \right] \left[\begin{array}{c} \delta_\theta \eta \\ \delta_\rho \eta \\ \delta_\phi \eta \end{array} \right]. \quad (15)$$

Orthogonality $\mathcal{M} \mathcal{D}_x E = 0$ implies in particular $M_{\rho\theta} = -M_{\rho\rho} (\delta_\rho \varepsilon) * (\partial_\theta \varepsilon)^{-1}$ and $M_{\theta\theta} = -M_{\theta\phi} (\delta_\phi \varepsilon) * (\partial_\theta \varepsilon)^{-1}$, resulting in

$$\dot{\rho}|_{\text{irr}} = M_{\rho\theta} \delta_\theta \eta + M_{\rho\rho} \delta_\rho \eta = -M_{\rho\rho} \delta_\rho \psi, \quad \dot{\phi}|_{\text{irr}} = M_{\theta\theta} \delta_\theta \eta + M_{\theta\phi} \delta_\phi \eta = -M_{\theta\phi} \delta_\phi \psi. \quad (16)$$

Given then $M_{\rho\rho} = -\nabla \cdot \theta \mathbf{D} \nabla$ and $M_{\theta\phi} = \theta m$ consistent with (5)_{2,3}, $M_{\rho\theta} = \nabla \cdot \theta \mathbf{D} \nabla (\delta_\rho \varepsilon) * \frac{1}{c}$ and $M_{\theta\theta} = -\theta m (\delta_\phi \varepsilon) * \frac{1}{c}$ follow. These together with the symmetry relations $\langle \mathcal{D}_\theta B, M_{\theta\rho} \mathcal{D}_\rho A \rangle = \langle \mathcal{D}_\rho A, M_{\rho\theta} \mathcal{D}_\theta B \rangle$ and $\langle \mathcal{D}_\theta B, M_{\theta\phi} \mathcal{D}_\phi A \rangle = \langle \mathcal{D}_\phi A, M_{\phi\theta} \mathcal{D}_\theta B \rangle$ imply

$$M_{\theta\rho} = M_{\rho\theta}^T = \frac{1}{c} (d_\rho \varepsilon) \diamond \nabla \cdot \theta \mathbf{D} \nabla, \quad M_{\theta\theta} = M_{\theta\phi}^T = -\frac{1}{c} (d_\phi \varepsilon) \diamond \theta m, \quad (17)$$

via integration by parts, the divergence theorem, and the GENERIC gradients. Assuming next that heat conduction affects only the evolution of θ , the split

$$M_{\theta\theta} = M_{C\theta\theta} + M_{N\theta\theta}, \quad M_{C\theta\theta} = -\frac{1}{c} \nabla \cdot \theta^2 \mathbf{K} \nabla \frac{1}{c}, \quad (18)$$

of $M_{\theta\theta}$ into conduction $M_{C\theta\theta}$ and non-conduction $M_{N\theta\theta}$ parts is relevant. Then

$$\begin{aligned} M_{C\theta\theta} \delta_\theta \eta &= -\frac{1}{c} \nabla \cdot \theta^2 \mathbf{K} \nabla \frac{\delta_\theta \eta}{c} = \frac{1}{c} \nabla \cdot \mathbf{K} \nabla \theta, \\ M_{C\theta\theta} \delta_\theta \varepsilon &= -\frac{1}{c} \nabla \cdot \theta^2 \mathbf{K} \nabla \frac{\varepsilon}{c} = 0. \end{aligned} \quad (19)$$

The second of these combined with orthogonality $\mathcal{M} \mathcal{D}_x E = 0$ yields

$$\begin{aligned} M_{N\theta\theta} &= -M_{\theta\rho} (\delta_\rho \varepsilon) * \frac{1}{c} - M_{\theta\phi} (\delta_\phi \varepsilon) * \frac{1}{c} \\ &= -\frac{1}{c} (d_\rho \varepsilon) \diamond \nabla \cdot \theta \mathbf{D} \nabla (\delta_\rho \varepsilon) * \frac{1}{c} + \frac{1}{c} (d_\phi \varepsilon) \diamond \theta m (\delta_\phi \varepsilon) * \frac{1}{c} \end{aligned} \quad (20)$$

for $M_{N\theta\theta}$ via (17), and so

$$M_{N\theta\theta} \delta_\theta \eta + M_{\theta\rho} \delta_\rho \eta + M_{\theta\phi} \delta_\phi \eta = -M_{\theta\rho} \delta_\rho \psi - M_{\theta\phi} \delta_\phi \psi = \frac{1}{c} \varpi_{\text{dis}} \quad (21)$$

via the fact that $\dot{\rho}$ and $\dot{\phi}$ are purely irreversible, and (8)₂. Besides being symmetric, note that \mathcal{M} is positive semi-definite. With all component of \mathcal{M} now determined, the reduced form

$$\begin{aligned} \dot{\rho}|_{\text{irr}} &= M_{\rho\theta} \delta_\theta \eta + M_{\rho\rho} \delta_\rho \eta + 0 = \nabla \cdot \theta \mathbf{D} \nabla \delta_\rho \psi, \\ \dot{\phi}|_{\text{irr}} &= M_{\theta\theta} \delta_\theta \eta + 0 + M_{\theta\phi} \delta_\phi \eta = -\theta m \delta_\phi \psi, \\ \dot{\theta}|_{\text{irr}} &= M_{\theta\theta} \delta_\theta \eta + M_{\theta\rho} \delta_\rho \eta + M_{\theta\phi} \delta_\phi \eta = \frac{1}{c} \varpi_{\text{dis}} + \frac{1}{c} \nabla \cdot \mathbf{K} \nabla \theta, \end{aligned} \quad (22)$$

of (15) is obtained.

In summary, combination of (14) and (22) leads to the GENERIC-based system

$$\dot{\rho} = \nabla \cdot \theta \mathbf{D} \nabla \delta_\rho \psi, \quad \dot{\mathbf{m}} = \nabla \cdot \partial_{\nabla \mathbf{x}} \psi, \quad c \dot{\theta} = \varpi + \nabla \cdot \mathbf{K} \nabla \theta, \quad \dot{\phi} = -\theta m \delta_\phi \psi, \quad (23)$$

for $(\rho, \mathbf{m}, \theta, \phi)$ via (8) and (10), in complete agreement with the corresponding SNET-based system (6).

Discussion

The current SNET- and GENERIC-based model formulations represent non-isothermal generalizations of the original isothermal formulations of Cahn-Hilliard and Allen-Cahn in the spirit of [6]. They are also consistent with more recently GENERIC-based non-isothermal generalization of the Ginzburg-Landau equation [e.g., 7]. As shown by the current SNET-based formulation, non-standard and higher-order gradients and fluxes postulated on purely formal grounds [e.g., 8, 9] are completely superfluous. This is due in particular to the treatment of boundary conditions in the current approach as part of the physical model formulation. Indeed, the choice of these has a direct influence on model behavior and predictions (i.e., via solution of the evolution / field relations), especially in the non-local case.

For more details, the reader is referred to [4,5].

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