

A deformational and configurational framework for geometrically non-linear continuum thermomechanics coupled to diffusion

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ABSTRACT

A general framework encompassing both the (conventional) deformational and configurational settings of continuum mechanics is presented. A systematic application of balance principles over a migrating control volume in the undeformed configuration of the continuum body yields the system of governing equations in the bulk, on the surface and on a coherent interface within the continuum. The equations governing the response of the bulk agree with those of the conventional deformational approach. The localised balance equations are expressed in the configurational setting using a pull-back operator and reformulated in terms of the Eshelby stress. The configurational expression of the dissipation elucidates the energy loss associated with configurational changes. The general framework is introduced by considering the problem of coupled deformation, heat conduction and species diffusion within a geometrically non-linear continuum body intersected by a coherent interface. The nature of the coupling is emphasised throughout the presentation and via an example.

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1. Introduction

The theoretical underpinnings of the configurational setting of mechanics have been vigorously developed over the last half-century since the seminal work by Eshelby [1,2] with important contributions by Gurtin [3], Gurtin and Podio-Guidugli [4], Kienzler and Herrmann [5], Maugin [6–8], among others. Our own contributions include [9–12].²

Configurational mechanics describes the energetic (configurational) changes that accompany a variation of the undeformed (initial) configuration of a continuum. Configurational forces arise due to the response of the undeformed continuum to variations in the material placement of particles with respect to the ambient material. Configurational mechanics is thus ideally suited to describe the role of defects such as dislocations, inhomogeneities, inclusions, interfaces, cracks, etc. (see the collection [14] and [3,5–7,9–11,13,15–19], among others).

This contribution considers the coupled problem of heat conduction and species diffusion within an inelastic continuum intersected by a coherent interface undergoing finite deformations.

While a considerable amount of literature exists on the configurational setting for heat conduction and, separately, for diffusion, there is relatively little work concerning both.

Configurational mechanics, for instance, has been used as a framework for investigating classical and non-classical heat conduction. The configurational setting of classical thermoelasticity (also termed type I) has been explored in [10,20–22], among others. Non-classical wave-like heat conduction (type III) within a geometrically non-linear setting is investigated in [23], while type II heat conduction is investigated in [24–27].

Various approaches are adopted to derive the equations governing thermoelasticity in the configurational setting. Dasgupta and Maugin [24] derive the governing equations from energy-release considerations. Kalpadike and Dasgupta [25] formulate the configurational force balance by exploiting the invariance requirements of the configurational working. Problems of type II are expressible within a variational formulation as they possess the unusual property that the formulation may be purely energetic (i.e. without dissipation). As a consequence, in addition to the well-known relations of hyper-thermoelasticity, the Helmholtz energy acts as a potential for the entropy flux—a result which is impossible within the classical type I model.

In a less restrictive approach, adopted in [20] for type I heat conduction, for example, configurational forces are viewed as a basis for classical dissipative thermoelastic continua. Furthermore, the governing configurational equations are obtained by applying a pull-back operator to their spatial counterparts [10,22,23].

The coupling of diffusion and mechanical deformation is considered in [28,29] to describe the chemically induced swelling

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² The widely used designation “configurational mechanics” is due to Gurtin [3,13]; others include “mechanics in material spaces” [5] and “Eshelbian mechanics” [7].

of hydrogels. The case of thermally induced swelling is considered independently in [30]. The recent comprehensive treatise on configurational mechanics by Maugin [8] considers heat conduction and species diffusion, among other phenomena.

The first comprehensive, purely mechanical description of material surfaces which accounts for surface stress in an elastic medium is due to Gurtin and Murdoch [31]. The kinematics and the balance laws are derived and the tensorial nature of surface tension established. This work was extended by Gurtin and co-workers to include thermal effects [32–34]. Furthermore, Knowles [35] demonstrated that a surface of discontinuity in the deformation gradient causes dissipation in a hyper-elastic system.

A key extension of the surface theory in [31] to describe propagating interfaces within a solid undergoing infinitesimal deformations is due to Gurtin and Voorhees [36]. Configurational forces provide an elegant and powerful description of the role of surfaces separating distinct phases [3,12,13,34,36]. Gurtin [3,13] assigns an equivalent status to the configurational force balance as is reserved for the conventional momentum balance in deformational mechanics. He derives the relations for interfaces using a configurational (non-standard) observer, invariance-based argument; the conventional approach invokes the invariance of a spatial observer. Central to the theory is a configurational interfacial balance which contains both the standard force and mass balances in the bulk phases and across the interface. Simha and Bhattacharya [37,38] generalised this approach to the junctions of interfaces. Singular surfaces in a configurational thermomechanics framework are studied by Dascalu and Danescu [39]. Further related work by Maugin and Berezovski [21] considers the thermal conditions at interfaces in a thermoelastic composite using the concept of a configurational thermal force.

One contribution of the work presented here is a general framework for the deformational and configurational mechanics description of geometrically non-linear deformation coupled to diffusion and heat conduction. A systematic application of balance principles over the undeformed configuration of the continuum body and an identification of the associated fluxes yields the system of governing equations. The time rate of change of various conserved quantities is measured relative to a reference state that plays the role of an independent observer. The integral balances are then localised to general points in the bulk, on the surface and on the coherent interface. The governing equations in the bulk, so obtained, agree with those of the conventional deformational approach. The localised balance equations are then recast into the configurational setting using a pull-back operator. The configurational setting elucidates the role of inhomogeneities and the energy dissipation associated with changes in the undeformed configuration. The nature of the coupling of the various fields is emphasised throughout.

The inverse-motion problem is intimately related to the aforementioned developments. Thereby, the inverse-motion problem and its duality with the direct-motion problem, in particular the duality of the Cauchy stress and the Eshelby stress, has been studied by Shield [40], Chadwick [41], Ogden [42,43], Golebiewska-Herrmann [44], among others.

In [45] the conventional deformational framework for geometrically non-linear thermomechanics coupled to standard and case II type diffusion in polymeric solids is discussed (see [46] for a review of various mathematical models for case II diffusion and a description of the phenomenon). This approach is extended in [47] to account for surfaces that possess their own energies. As a continuation of these works, this contribution develops the configurational framework for thermomechanics coupled to diffusion in a very general manner.

The outline of this paper is as follows. The basic notation and key concepts are introduced in Section 2. Next, the governing

equations are systematically derived by considering the conservation of several key properties, namely solid mass, diffusing species mass, linear and angular momentum, internal energy and entropy over a migrating control volume in the undeformed configuration. The governing equations are reformulated in the configurational setting in Section 4. Key aspects of the configurational setting are emphasised with the aid of an example in Section 5. We conclude and discuss further work in Section 6.

2. Preliminaries: notation and basic concepts

The purpose of this preliminary section is to summarise certain key concepts in non-linear continuum mechanics and to introduce the notation adopted here. Detailed expositions on non-linear continuum mechanics can be found in [48–51], among others.³

2.1. Motion and deformation

We denote by the open set $\mathcal{B}_0 \subset \mathbb{R}^3$ the undeformed configuration of a continuum body, as depicted in Fig. 1, with material particles labelled $\mathbf{X} \in \mathcal{B}_0$. The surface of \mathcal{B}_0 , assumed smooth, is denoted $\partial\mathcal{B}_0$. The unit normal to $\partial\mathcal{B}_0$ is denoted \mathbf{N} . The continuum body is composed of two phases occupying closed, complementary subregions, denoted \mathcal{B}_0^- and \mathcal{B}_0^+ , where $\mathcal{B}_0 = \mathcal{B}_0^- \cup \mathcal{B}_0^+$. The subregions are separated by an interface $\mathcal{S}_0 := \mathcal{B}_0^- \cap \mathcal{B}_0^+$ with the outward unit normal relative to the region \mathcal{B}_0^- denoted \mathbf{M} . The outward unit normals to the regions \mathcal{B}_0^+ and \mathcal{B}_0^- are denoted \mathbf{M}^+ and $\mathbf{M}^- = \mathbf{M}$, respectively, with $\mathbf{M}^+ = -\mathbf{M}^-$.

Let $T = [0, T^{\text{end}}] \subset \mathbb{R}_+$ denote the time domain. Here time simply provides a history parameter to order the sequence of events and quasi-static conditions are assumed henceforth. We denote by the orientation preserving spatial deformation map $\boldsymbol{\varphi} : \mathcal{B}_0 \rightarrow \mathbb{R}^3$, a smooth motion of the undeformed configuration \mathcal{B}_0 for a time $t \in T$. The placement of the body at time t associated with the motion $\boldsymbol{\varphi}$ is denoted $\mathcal{B}_t = \boldsymbol{\varphi}(\mathcal{B}_0, t)$, with particles designated as $\mathbf{x} = \boldsymbol{\varphi}(\mathbf{X}, t) \in \mathcal{B}_t$. The material (inverse) deformation map from the deformed to the undeformed configuration is denoted $\boldsymbol{\Phi}(\mathbf{x}, t) = \boldsymbol{\varphi}^{-1}(\mathbf{x}, t)$. It proves convenient to define a stationary reference state \mathcal{B}_\square from where the relative motions are observed. The reference state plays the role of an observer and does not constitute an actual configuration; nonetheless, in order to facilitate the presentation, “particles” in the reference state are labelled \mathbf{Y} . The material map $\boldsymbol{\Xi} : \mathcal{B}_\square \rightarrow \mathbb{R}^3$ describes the motion of the undeformed configuration \mathcal{B}_0 relative to the reference state. The spatial map $\boldsymbol{\xi} : \mathcal{B}_\square \rightarrow \mathbb{R}^3$ describes the motion of the deformed configuration \mathcal{B}_t relative to the reference state. Thus, in summary:

$$\mathbf{X} = \boldsymbol{\Phi}(\mathbf{x}, t) = \boldsymbol{\Xi}(\mathbf{Y}, t) \circ \boldsymbol{\xi}^{-1} \quad \text{and} \quad \mathbf{x} = \boldsymbol{\varphi}(\mathbf{X}, t) = \boldsymbol{\xi}(\mathbf{Y}, t) \circ \boldsymbol{\Xi}^{-1},$$

where $f \circ g$ denotes the composition of two functions f and g , respectively.

The temporal rates of change of a quantity $\{\bullet\}$ relative to the reference state \mathcal{B}_\square , the undeformed configuration \mathcal{B}_0 and the

³ Direct notation is used throughout. In addition, occasional use is made of index notation. Upper and lower case Roman indices refer to tensor components defined on the undeformed and deformed configurations, respectively. The scalar product of two vectors \mathbf{a} and \mathbf{b} is denoted $\mathbf{a} \cdot \mathbf{b} = a_i b_i$. The scalar product of two second-order tensors \mathbf{A} and \mathbf{B} is denoted $\mathbf{A} : \mathbf{B} = A_{ij} B_{ij}$. The action of a second-order tensor \mathbf{A} on a vector \mathbf{b} is represented as $\mathbf{A} \cdot \mathbf{b}$, and in index notation as $A_{ij} b_j$. The action of a third-order tensor \mathbf{A} on a first-order tensor \mathbf{b} is represented as $\mathbf{A} \cdot \mathbf{b}$ with components $A_{ijk} b_k$. The tensor product $\mathbf{a} \otimes \mathbf{b}$ of two vectors \mathbf{a} and \mathbf{b} is a second-order tensor defined by the relation $(\mathbf{a} \otimes \mathbf{b}) \cdot \mathbf{c} = [\mathbf{b} \cdot \mathbf{c}] \mathbf{a} \forall$ vectors \mathbf{c} and is expressed in index notation as $d_{ij} = a_i b_j$. The non-standard tensor product of a second-order tensor \mathbf{A} and a vector \mathbf{b} , denoted $\mathbf{A} \otimes \mathbf{b}$, is a third-order tensor with components $A_{ij} b_k$. The non-standard tensor product of a vector \mathbf{a} and a second-order tensor \mathbf{B} , denoted $\mathbf{a} \otimes \mathbf{B}$, is a third-order tensor with components $a_i B_{jk}$. Blackboard bold font is used for constitutive tensors (of any order) and projection operators.

deformed configuration \mathcal{B}_t are respectively defined by

$$\dot{\{\bullet\}} := \partial_t \{\bullet\}|_Y, \quad D_t \{\bullet\} := \partial_t \{\bullet\}|_X, \quad d_t \{\bullet\} := \partial_t \{\bullet\}|_x.$$

Accordingly, the spatial velocity $\mathbf{v} := D_t \boldsymbol{\varphi}$ is defined as the material time derivative of the spatial motion $\boldsymbol{\varphi}$, and the material velocity $\mathbf{V} := d_t \boldsymbol{\Phi}$ as the spatial time derivative of the material motion $\boldsymbol{\Phi}$. The total material and spatial velocities are defined relative to the reference state \mathcal{B}_\square by $\mathbf{U} := \dot{\boldsymbol{\Xi}}$ and $\mathbf{u} := \dot{\boldsymbol{\xi}}$, respectively.

The invertible linear tangent map $\mathbf{F}: T\mathcal{B}_0 \rightarrow T\mathcal{B}_t$ (that is, the deformation gradient) maps a line element $d\mathbf{X} \in T\mathcal{B}_0$ in the undeformed configuration to a line element $d\mathbf{x} \in T\mathcal{B}_t$ in the deformed configuration and is defined as the derivative of the spatial motion with respect to the material placement; that is,

$$\mathbf{F}(\mathbf{X}, t) := \nabla_{\mathbf{X}} \boldsymbol{\varphi}(\mathbf{X}, t),$$

where $\nabla_{\mathbf{X}} \{\bullet\} := \partial \{\bullet\} / \partial \mathbf{X}$ is the gradient operator with respect to the reference placement. The notation $T\mathcal{B}_{\{\bullet\}}$ denotes the tangent space to $\mathcal{B}_{\{\bullet\}}$. The action of the gradient operator with respect to the current placement is denoted $\nabla_{\mathbf{x}} \{\bullet\} := \partial \{\bullet\} / \partial \mathbf{x}$. The Jacobian determinant of the deformation gradient is denoted $J(\mathbf{X}, t) := \det(\mathbf{F}(\mathbf{X}, t)) > 0$. The inverse of the deformation gradient is denoted $\mathbf{f} := \mathbf{F}^{-1}$ with an associated inverse Jacobian determinant $j := \det \mathbf{f} = 1/J > 0$. The Jacobian determinants are (invertible) volume maps that relate the spatial and material volume elements, dv and dV respectively, as

$$dv = J dV \quad \text{and} \quad dV = j dv. \quad (1)$$

The right and left Cauchy–Green tensors, measures of the stretch, are defined by $\mathbf{C} := \mathbf{F}^t \cdot \mathbf{F}$ and $\mathbf{c} := \mathbf{f}^t \cdot \mathbf{f}$, respectively.

The total material and spatial velocities, i.e. those measured relative to the reference state \mathcal{B}_\square , are related as follows (see Fig. 1):

$$\mathbf{U} := \dot{\boldsymbol{\Xi}} = \mathbf{V} + \mathbf{f} \cdot \mathbf{u} \quad \text{and} \quad \mathbf{u} := \dot{\boldsymbol{\xi}} = \mathbf{v} + \mathbf{F} \cdot \mathbf{U}. \quad (2)$$

As a direct consequence of the above relations, the material and spatial velocities are simply related via the deformation gradients as

$$\mathbf{V} = -\mathbf{f} \cdot \mathbf{v} \quad \text{and} \quad \mathbf{v} = -\mathbf{F} \cdot \mathbf{V}. \quad (3)$$

The interface S_0 is assumed to be coherent: the total material and spatial velocities are continuous across the interface, smooth away from the interface, and smooth up to the interface from either side (see [13]), as depicted schematically in Fig. 2. The following relations thus hold on the interface:

$$\mathbf{U} = \mathbf{U} \cdot [\mathbf{M} \otimes \mathbf{M}] \quad \text{on } S_0 \quad \text{and} \quad \mathbf{u} = \mathbf{u} \cdot [\mathbf{m} \otimes \mathbf{m}] \quad \text{on } S_t, \quad (4)$$

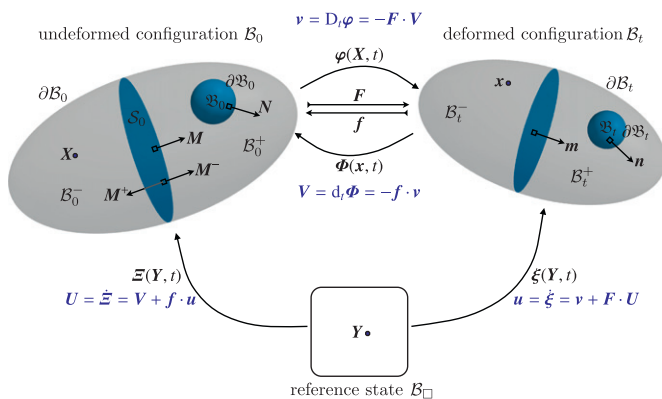


Fig. 1. The forward and backward motions, $\boldsymbol{\varphi}$ and $\boldsymbol{\Phi}$ respectively, of a continuum body intersected by a coherent interface S_0 to the deformed configuration \mathcal{B}_t , and vice versa. The migrating control volume $\mathcal{B}_0 \subset \mathcal{B}_0$ is shown. The reference state \mathcal{B}_\square provides a relative reference frame for the forward and backward motions. The total material and spatial velocities, \mathbf{U} and \mathbf{u} , are defined relative to the reference state.

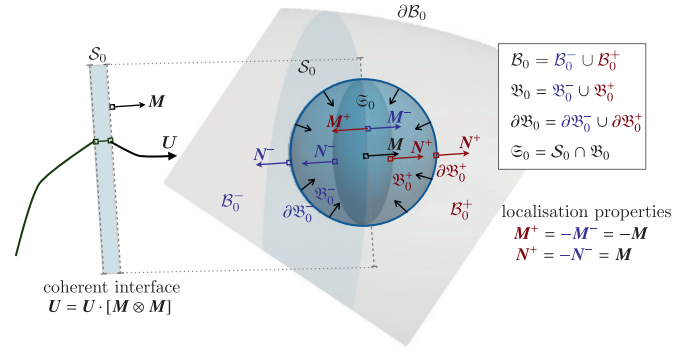


Fig. 2. A portion of the undeformed domain \mathcal{B}_0 containing a control volume \mathcal{B}_0 intersected by a coherent interface S_0 . The directions of the various unit normals are illustrated. Also indicated are the localisation properties that hold on the interface $\Xi_0 := S_0 \cap \mathcal{B}_0$.

where S_t is the interface in the deformed configuration \mathcal{B}_t and \mathbf{m} is the unit outward normal to S_t . The assumption of a coherent interface yields the first compatibility condition [13] on the jump in the spatial velocity \mathbf{v}

$$[\![\mathbf{v}]\!] = [\![-\mathbf{F} \cdot \mathbf{V}]\!] = [\![-\mathbf{F} \cdot (\mathbf{U} - \mathbf{f} \cdot \mathbf{u})]\!] = -[\![\mathbf{F}]\!] \cdot \mathbf{U}, \quad (5)$$

where the jump and average operators for an arbitrary field $\{\bullet\}$ across an interface S_0 are respectively defined by

$$[\![\bullet]\!] := \{\bullet\}^+ - \{\bullet\}^- \quad \text{and} \quad \{\!\!\{\bullet\}\!\!\} := \frac{1}{2}(\{\bullet\}^+ + \{\bullet\}^-).$$

The following identity relates the jump of the scalar product of two quantities, denoted \mathbf{a} and \mathbf{b} , to the products of their jumps and averages:

$$[\![\mathbf{a} \cdot \mathbf{b}]\!] = [\![\mathbf{a}]\!] \cdot \{\!\!\{\mathbf{b}\}\!\!\} + \{\!\!\{\mathbf{a}\}\!\!\} \cdot [\![\mathbf{b}]\!]. \quad (6)$$

2.2. Integral relations

Let $\mathcal{B}_0 = \mathcal{B}_0(t)$ be a (smoothly) migrating control volume with boundary $\partial\mathcal{B}_0$ and outward unit normal \mathbf{N} , as depicted in Figs. 1 and 2. The potentially empty intersection of the interface S_0 with the control volume \mathcal{B}_0 is denoted Ξ_0 . The migration of the control volume \mathcal{B}_0 in the undeformed configuration \mathcal{B}_0 results in the flux of material across the boundary $\partial\mathcal{B}_0$.

Gauss's theorem, in its extended form, relates the material divergence of a quantity over the volume \mathcal{B}_0 to the flux of the quantity over the boundary $\partial\mathcal{B}_0$, and the jump of the flux in the quantity over the interface Ξ_0 . Gauss's theorem for material scalars a_0 , and vectors and second-order tensors, collectively denoted \mathbf{a}_0 , is

$$\begin{aligned} \int_{\mathcal{B}_0} \nabla_{\mathbf{X}} a_0 dV &= \int_{\partial\mathcal{B}_0} a_0 \mathbf{N} dA - \int_{\Xi_0} [\![a_0]\!] \mathbf{M} dA, \\ \int_{\mathcal{B}_0} \text{Div } \mathbf{a}_0 dV &= \int_{\partial\mathcal{B}_0} \mathbf{a}_0 \cdot \mathbf{N} dA - \int_{\Xi_0} [\![\mathbf{a}_0]\!] \cdot \mathbf{M} dA. \end{aligned} \quad (7)$$

A modified form of Reynolds's transport theorem then gives the total time rate of change, i.e. as measured relative to the reference state \mathcal{B}_\square , of a material scalar a_0 , and vectors and second-order tensors, collectively denoted \mathbf{a}_0 , as

$$\begin{aligned} \dot{a} &= \int_{\mathcal{B}_0} D_t a_0 dV + \int_{\partial\mathcal{B}_0} a_0 \mathbf{U} \cdot \mathbf{N} dA - \int_{\Xi_0} [\![a_0]\!] \mathbf{U} \cdot \mathbf{M} dA, \\ \dot{\mathbf{a}} &= \int_{\mathcal{B}_0} D_t \mathbf{a}_0 dV + \int_{\partial\mathcal{B}_0} [\![\mathbf{a}_0 \otimes \mathbf{U}]\!] \cdot \mathbf{N} dA - \int_{\Xi_0} [\![\mathbf{a}_0]\!] \otimes \mathbf{U} \cdot \mathbf{M} dA. \end{aligned} \quad (8)$$

Remark. In the more common deformational setting, the balance equations are performed over a control volume in the deformed configuration and the undeformed and reference configurations

coincide. Here and henceforth, this approach shall be referred to as the “conventional approach”. The control volume $\mathfrak{B}_t \subset \mathcal{B}_t$ is obtained from a mapping via the motion φ of $\mathfrak{B}_0 \subset \mathcal{B}_0$ to the current configuration \mathcal{B}_t as $\mathfrak{B}_t = \varphi(\mathfrak{B}_0, t) \subset \mathcal{B}_t$. The smooth surface of \mathfrak{B}_t is denoted $\partial\mathfrak{B}_t$ with outward unit normal \mathbf{n} . \square

2.3. Implications of the total formulation for deformation gradient \mathbf{F}

The governing equations derived in Section 3 are constructed from balances over a migrating control volume wherein total rates of change are considered. The implications of the total formulation for the relation of the deformation gradient \mathbf{F} to the various descriptions of the velocity are now discussed.

Let \mathbf{F} denote the integral of the deformation gradient over the migrating control volume \mathfrak{B}_0 :

$$\mathbf{F} := \int_{\mathfrak{B}_0} \mathbf{F} dV.$$

The global rate of change of \mathbf{F} due to the movement of the control volume in the undeformed configuration is balanced by external fluxes, denoted \mathbf{F}^{ext} , acting on the boundary $\partial\mathfrak{B}_0$ and defined by

$$\mathbf{F}^{\text{ext}} := \int_{\partial\mathfrak{B}_0} \hat{\mathbf{v}} \otimes \mathbf{N} dA.$$

The spatial velocity on the boundary $\partial\mathfrak{B}_0$ is defined by $\hat{\mathbf{v}} := \mathbf{u}|_{\partial\mathfrak{B}_0}$; a verification of this statement will be given shortly. The expression for the rate of change of the deformation gradient thus follows as

$$\dot{\mathbf{F}} = \mathbf{F}^{\text{ext}},$$

and using Reynolds’s transport theorem (8) yields

$$\begin{aligned} & \int_{\mathfrak{B}_0} D_t \mathbf{F} dV + \int_{\partial\mathfrak{B}_0} [\mathbf{F} \otimes \mathbf{U}] \cdot \mathbf{N} dA - \int_{\mathfrak{E}_0} [[\mathbf{F}]] \otimes \mathbf{U} \cdot \mathbf{M} dA \\ &= \int_{\partial\mathfrak{B}_0} \hat{\mathbf{v}} \otimes \mathbf{N} dA \\ &\leftrightarrow \int_{\mathfrak{B}_0} D_t \mathbf{F} dV + \int_{\partial\mathfrak{B}_0} \underbrace{[\mathbf{F} \otimes \mathbf{U} - \hat{\mathbf{v}} \otimes \mathbf{I}]}_{-\mathbf{v} \otimes \mathbf{I}} \cdot \mathbf{N} dA \\ &\quad - \int_{\mathfrak{E}_0} [[\mathbf{F}]] \otimes \mathbf{U} \cdot \mathbf{M} dA = 0, \end{aligned} \quad (9)$$

where \mathbf{v} is the spatial velocity and \mathbf{I} is the ordinary, mixed, second-order unit tensor of the three-dimensional embedding Euclidean space.

Consider first the situation where the control volume is not intersected by an interface, i.e. $\mathfrak{E}_0 = \emptyset$. Using Gauss’s theorem (7) to transform the surface integral in Eq. (9) to a volume integral yields⁴

$$\int_{\mathfrak{B}_0} [D_t \mathbf{F} - \underbrace{\text{Div}(\mathbf{v} \otimes \mathbf{I})}_{\nabla_{\mathbf{x}} \mathbf{v}}] dV = 0$$

and by localising to a regular point in the domain

$$D_t \mathbf{F} - \nabla_{\mathbf{x}} \mathbf{v} = 0 \quad \text{in } \mathfrak{B}_0. \quad (10)$$

The preceding definition of the material rate of change of the deformation gradient \mathbf{F} is standard.

For a regular point on the surface $\partial\mathfrak{B}_0$ the following relation holds

$$[\mathbf{F} \otimes \mathbf{U} + \mathbf{v} \otimes \mathbf{I}] \cdot \mathbf{N} = \hat{\mathbf{v}} \otimes \mathbf{N} \quad \text{on } \partial\mathfrak{B}_0. \quad (11)$$

Consider now a control volume $\mathfrak{B}_0 \subset \mathcal{B}_0$ intersected by a coherent interface S_0 as depicted in Fig. 2. The portion of the interface within the control volume is defined by $\mathfrak{E}_0 := S_0 \cap \mathfrak{B}_0$. The interface \mathfrak{E}_0 partitions the control volume into two

complementary subregions, denoted \mathfrak{B}_0^- and \mathfrak{B}_0^+ , where $\mathfrak{B}_0 = \mathfrak{B}_0^- \cup \mathfrak{B}_0^+$. The outer surfaces of \mathfrak{B}_0^- and \mathfrak{B}_0^+ are denoted $\partial\mathfrak{B}_0^-$ and $\partial\mathfrak{B}_0^+$ respectively, where $\partial\mathfrak{B}_0 = \partial\mathfrak{B}_0^- \cup \partial\mathfrak{B}_0^+$. The outward unit normals to $\partial\mathfrak{B}_0^-$ and $\partial\mathfrak{B}_0^+$ are denoted \mathbf{N}^- and \mathbf{N}^+ , respectively.

The process of localising an integral expression to a singular point on the interface S_0 is depicted in Fig. 2. Conceptually, the volume of the control volume \mathfrak{B}_0 is decreased to zero such that the surfaces $\partial\mathfrak{B}_0^-$ and $\partial\mathfrak{B}_0^+$ coincide with \mathfrak{E}_0 and $-\mathbf{N}^- = \mathbf{N}^+ = \mathbf{M}$. Hence all terms involving integrals over the volume \mathfrak{B}_0 vanish. The remaining terms are then localised to a point on the surface \mathfrak{E}_0 in the standard manner.

Localising Eq. (9) to a singular point on the interface S_0 yields

$$\begin{aligned} 0 &= -\mathbf{v}^+ \otimes \mathbf{N}^+ - \mathbf{v}^- \otimes \mathbf{N}^- - [[\mathbf{F}]] \otimes \mathbf{U} \cdot \mathbf{M} \\ &= [[\mathbf{F}]] \otimes \mathbf{U} + [[\mathbf{v}]] \otimes \mathbf{I} \cdot \mathbf{M} \quad \text{on } S_0. \end{aligned} \quad (12)$$

The significance of the localised version of the deformation balance on the interface is made apparent by substituting the restriction on the total material velocity \mathbf{U} on the interface S_0 imposed by the first compatibility condition (5) into Eq. (12), and rearranging to obtain

$$[[\mathbf{F}]] \cdot \underbrace{[\mathbf{I} - \mathbf{M} \otimes \mathbf{M}]}_{\mathbb{P}_0} = 0 \quad \text{on } S_0, \quad (13)$$

where \mathbb{P}_0 is the projection operator in the undeformed configuration which maps an arbitrary vector in \mathbb{R}^3 tangent to the surface with normal \mathbf{M} . The result (13) thus states that the action of \mathbf{F} on vectors in the plane S_0 (i.e. tangent vectors) is continuous across the interface. The results (5) and (13) are known collectively as the interface compatibility conditions. The second compatibility condition (13) thus arises directly from the balance of the deformation gradient over a singular surface.

Remark. The spatial velocity at the surface $\partial\mathfrak{B}_0$ was previously defined by $\hat{\mathbf{v}} := \mathbf{u}|_{\partial\mathfrak{B}_0}$. A proof thereof is as follows. Contracting both sides of Eq. (11) with the normal \mathbf{N} and using the coherency of the total material velocity across the surface $\partial\mathfrak{B}_0$ given in Eq. (4) yields

$$[[\mathbf{F} \otimes \mathbf{U} + \mathbf{v} \otimes \mathbf{I}]] \cdot \mathbf{N} = [\hat{\mathbf{v}} \otimes \mathbf{N}] \cdot \mathbf{N} \leftrightarrow \mathbf{F} \cdot \mathbf{U} = \hat{\mathbf{v}} - \mathbf{v}$$

and using the definition of the total spatial velocity \mathbf{u} in Eq. (2)₂ yields

$$\hat{\mathbf{v}} = \mathbf{u} \quad \text{on } \partial\mathfrak{B}_0. \quad \square$$

Remark. The continuity of the velocity $\hat{\mathbf{v}}$ across the interface can be deduced by considering the interface as a two-sided surface and restricting the result given in Eq. (11) to the surface:

$$\begin{aligned} \hat{\mathbf{v}}^+ \otimes \mathbf{M}^+ + \hat{\mathbf{v}}^- \otimes \mathbf{M}^- &= [\mathbf{F}^+ \otimes \mathbf{U} + \mathbf{v}^+ \otimes \mathbf{I}] \cdot \mathbf{M}^+ \\ &\quad + [\mathbf{F}^- \otimes \mathbf{U} + \mathbf{v}^- \otimes \mathbf{I}] \cdot \mathbf{M}^- \end{aligned}$$

$$\begin{aligned} -[[\hat{\mathbf{v}}]] \otimes \mathbf{M} &= -[[\mathbf{F}]] \otimes \mathbf{U} + [[\mathbf{v}]] \otimes \mathbf{I} \cdot \mathbf{M} \\ &= 0 \quad (\text{from Eq. (12)}). \quad \square \end{aligned}$$

3. Governing equations

The objective of this section is to introduce the general framework for deformational and configurational mechanics by deriving the equations governing the response of an inelastic continuum subject to the influence of heat and diffusion. The governing equations are systematically derived by considering the conservation of several key properties, namely solid mass, diffusing species mass, linear and angular momentum, internal energy and entropy over a migrating control volume \mathfrak{B}_0 in the undeformed configuration \mathcal{B}_0 . By contrast, in the conventional approach the undeformed configuration is taken as the reference

⁴ The material divergence of a third-order tensor is defined using index notation by $\mathbf{A} = \text{Div } \mathbf{A} \Rightarrow A_{ij} = \partial A_{ijk} / \partial X_k$.

configuration. The time rate of change of all quantities is expressed relative to the reference state \mathcal{B}_0 , as depicted in Fig. 1. The integral form of the governing balance equations are stated in a manner that allows them to be localised to a point in the bulk \mathcal{B}_0 , on the surface $\partial\mathcal{B}_0$ or on the interface \mathcal{S}_0 by applying the procedures discussed in Section 2 and elaborated upon further in this section. The Clausius–Duhem form of the second law of thermodynamics and the resulting local dissipation inequality suggest a form for the constitutive relations. The restrictions that arise from the reduced dissipation inequality stipulate the thermodynamically consistent form for the remaining evolution equations.

3.1. Conservation of solid mass

Consider the migrating material control volume \mathfrak{B}_0 shown in Figs. 1 and 2. The bulk density of the solid in the undeformed configuration \mathcal{B}_0 is denoted ρ_0 [kg/m³]. The integral of the bulk density over the control volume (i.e. the mass of the control volume) is

$$R := \int_{\mathfrak{B}_0} \rho_0 \, dV.$$

Sources of mass within the bulk attributed to external agencies, and physical mass flux over the boundary of the control volume are collectively defined by

$$R^{\text{ext}} := \int_{\mathfrak{B}_0} \bar{m}_0 \, dV + \int_{\partial\mathfrak{B}_0} \hat{m}_0 \, dA.$$

The sources of mass (e.g. due to nutrition [52,53]) per unit volume of \mathfrak{B}_0 are denoted \bar{m}_0 . The mass contribution per unit area of the undeformed configuration due to physical flux over the surface $\partial\mathfrak{B}_0$ is denoted \hat{m}_0 . The expression for the balance of solid mass is

$$\dot{R} = R^{\text{ext}}$$

and using Reynolds's transport theorem (8) yields

$$\begin{aligned} & \int_{\mathfrak{B}_0} D_t \rho_0 \, dV + \int_{\partial\mathfrak{B}_0} \rho_0 \mathbf{U} \cdot \mathbf{N} \, dA - \int_{\mathfrak{E}_0} [\rho_0] \mathbf{U} \cdot \mathbf{M} \, dA \\ &= \int_{\mathfrak{B}_0} \bar{m}_0 \, dV + \int_{\partial\mathfrak{B}_0} \hat{m}_0 \, dA \\ &\leftrightarrow \int_{\mathfrak{B}_0} [D_t \rho_0 - \bar{m}_0] \, dV + \int_{\partial\mathfrak{B}_0} \underbrace{[\rho_0 \mathbf{U} \cdot \mathbf{N} - \hat{m}_0]}_{-m_0 = \mathbf{R} \cdot \mathbf{N}} \, dA \\ &\quad - \int_{\mathfrak{E}_0} [\rho_0] \mathbf{U} \cdot \mathbf{M} \, dA = 0, \end{aligned} \quad (14)$$

where m_0 denotes the net mass flux and \mathbf{R} is the associated net mass flux vector.⁵ The net mass flux m_0 includes contributions from the physical flux of mass over the boundary $\partial\mathfrak{B}_0$ (i.e. the term \hat{m}_0) and convective flux due to the motion of the migrating control volume in the undeformed configuration (i.e. the term $\rho_0 \mathbf{U} \cdot \mathbf{N}$).

Using Gauss's theorem (7) to transform the surface integral in the global mass balance (14) to a volume integral yields

$$\int_{\mathfrak{B}_0} [D_t \rho_0 - \bar{m}_0 + \text{Div } \mathbf{R}] \, dV = 0$$

⁵ The sign convention for the net flux and the associated net flux vector adopted henceforth, unless stated otherwise, is based on a system centric perspective wherein the addition of a quantity results in a positive flux. The net flux is thus defined as the scalar product of the net flux vector with the negative of the outward normal to the control volume. Furthermore, in the absence of a convective flux, an increase or decrease in the physical flux must correspond to an increase or decrease in the net flux.

and by localising to a regular point in the domain

$$D_t \rho_0 + \text{Div } \mathbf{R} = \bar{m}_0 \quad \text{in } \mathcal{B}_0. \quad (15)$$

For a regular point on the boundary $\partial\mathcal{B}_0$ the following relation holds:

$$[\rho_0 \mathbf{U} - \mathbf{R}] \cdot \mathbf{N} = \hat{m}_0 \quad \text{on } \partial\mathcal{B}_0. \quad (16)$$

Localising Eq. (14) to a singular point on the interface \mathcal{S}_0 yields

$$\begin{aligned} 0 &= \mathbf{R}^+ \cdot \mathbf{N}^+ + \mathbf{R}^- \cdot \mathbf{N}^- - [\rho_0] \mathbf{U} \cdot \mathbf{M} \\ &= [[\mathbf{R}]] - [\rho_0] \mathbf{U} \cdot \mathbf{M} \quad \text{on } \mathcal{S}_0. \end{aligned} \quad (17)$$

Remark. The balance of the physical mass flux \hat{m}_0 across the interface \mathcal{S}_0 can be deduced by considering the interface as a two-sided surface. From Eq. (16) one obtains

$$\begin{aligned} \hat{m}_0^+ + \hat{m}_0^- &= [\rho_0^+ \mathbf{U}^+ - \mathbf{R}^+] \cdot \mathbf{M}^+ + [\rho_0^- \mathbf{U}^- - \mathbf{R}^-] \cdot \mathbf{M}^- \\ &= [[\mathbf{R}]] - [\rho_0] \mathbf{U} \cdot \mathbf{M} \\ &= 0 \quad (\text{from Eq. (17)}). \end{aligned}$$

The physical mass fluxes acting on either side of the interface thus cancel one another. \square

Remark. In a typical solid mechanics application there would be zero net mass flux, i.e. $m_0 := -\mathbf{R} \cdot \mathbf{N} = 0$, and no sources of mass production, i.e. $\bar{m}_0 = 0$. There would, however, be a physical mass flux \hat{m}_0 which would be cancelled by the convective mass flux $\rho_0 \mathbf{U} \cdot \mathbf{N}$. In the conventional approach, the mass balance is performed over a material control volume in the deformed configuration. The definition of a material control volume precludes solid mass flux over the boundary of the control volume. \square

3.2. Conservation of diffusing species

The mass of the diffusing species per unit volume of the undeformed solid is denoted ρ_0^* [kg/m³]. The concentration of the diffusing species per unit volume of the undeformed solid, denoted c_0 [mol/m³], is related to the diffusing species density ρ_0^* via the inverse of the diffusing species molar mass c [mol/kg] as $c_0 = c \rho_0^*$ [mol/m³] = [mol/kg][kg/m³].

Consider the migrating control volume \mathfrak{B}_0 . Bulk sources of species generation are denoted \bar{w}_0 [mol/m³ s], while \hat{w}_0 [mol/m² s] denotes the physical diffusion flux over the surface $\partial\mathfrak{B}_0$. The integral of the diffusing species concentration field over the control volume (i.e. the amount of diffusing species in the control volume) is denoted by

$$W := \int_{\mathfrak{B}_0} c_0 \, dV$$

and the integral of the external sources of species by

$$W^{\text{ext}} := \int_{\mathfrak{B}_0} \bar{w}_0 \, dV + \int_{\partial\mathfrak{B}_0} \hat{w}_0 \, dA.$$

The expression for the balance of the diffusing species is

$$\dot{W} = W^{\text{ext}}$$

$$\begin{aligned} & \int_{\mathfrak{B}_0} D_t c_0 \, dV + \int_{\partial\mathfrak{B}_0} c_0 \mathbf{U} \cdot \mathbf{N} \, dA - \int_{\mathfrak{E}_0} [c_0] \mathbf{U} \cdot \mathbf{M} \, dA \\ &= \int_{\mathfrak{B}_0} \bar{w}_0 \, dV + \int_{\partial\mathfrak{B}_0} \hat{w}_0 \, dA \\ &\leftrightarrow \int_{\mathfrak{B}_0} [D_t c_0 - \bar{w}_0] \, dV + \int_{\partial\mathfrak{B}_0} \underbrace{[c_0 \mathbf{U} \cdot \mathbf{N} - \hat{w}_0]}_{-w_0 = \mathbf{W} \cdot \mathbf{N}} \, dA \\ &\quad - \int_{\mathfrak{E}_0} [c_0] \mathbf{U} \cdot \mathbf{M} \, dA = 0, \end{aligned} \quad (18)$$

where w_0 denotes the net concentration flux and \mathbf{W} is the associated net concentration flux vector. The net concentration flux includes contributions from the physical flux of species over the boundary $\partial\mathfrak{B}_0$ (i.e. the term \hat{w}_0) and the convective flux due to the motion of the migrating control volume in the undeformed configuration (i.e. the term $c_0 \mathbf{U} \cdot \mathbf{N}$).

The localisation of Eq. (18) to regular points in the bulk \mathfrak{B}_0 , onto the surface $\partial\mathfrak{B}_0$ and onto the interface S_0 follows in a near identical manner to that for the solid mass presented in Section 3.1. Using Gauss's theorem (7) to transform the surface integral in the global diffusing species balance given by Eq. (18) to a volume integral yields

$$\int_{\mathfrak{B}_0} [\mathbf{D}_t c_0 - \bar{w}_0 + \text{Div } \mathbf{W}] dV = 0$$

and by localising to a regular point in the domain one obtains Fick's second law:

$$\mathbf{D}_t c_0 + \text{Div } \mathbf{W} = \bar{w}_0 \quad \text{in } \mathfrak{B}_0. \quad (19)$$

For regular points on the boundary the following relation holds:

$$[c_0 \mathbf{U} - \mathbf{W}] \cdot \mathbf{N} = \hat{w}_0 \quad \text{on } \partial\mathfrak{B}_0. \quad (20)$$

Using the relations summarised in Fig. 2 to localise Eq. (18) to a singular point on the interface yields

$$\begin{aligned} 0 &= \mathbf{W}^+ \cdot \mathbf{N}^+ + \mathbf{W}^- \cdot \mathbf{N}^- - [c_0] \mathbf{U} \cdot \mathbf{M} \\ &= [[\mathbf{W}]] - [c_0] \mathbf{U} \cdot \mathbf{M} \quad \text{on } S_0. \end{aligned} \quad (21)$$

Remark. Conservation of the physical concentration flux \hat{w}_0 across the interface S_0 is demonstrated by applying Eq. (20) to either side of the interface to obtain

$$\begin{aligned} \hat{w}_0^+ + \hat{w}_0^- &= [c_0^+ \mathbf{U} - \mathbf{W}^+] \cdot \mathbf{M}^+ + [c_0^- \mathbf{U} - \mathbf{W}^-] \cdot \mathbf{M}^- \\ &= [[\mathbf{W}]] - [c_0] \mathbf{U} \cdot \mathbf{M} \\ &= 0 \quad (\text{from Eq. (21)}). \end{aligned}$$

The physical concentration fluxes acting on either side of the interface thus cancel one another. \square

3.3. Balance of linear momentum (force balance)

For the sake of simplicity, inertial forces are not considered. The Piola stress tensor is denoted \mathbf{P} with components P_{ij} . The (net) traction vector acting on a surface with normal \mathbf{N} is defined by $\mathbf{s}_0 := \mathbf{P} \cdot \mathbf{N}$.

The balance of linear momentum, or rather the statement of equilibrium, over the control volume \mathfrak{B}_0 stipulates that the net force, denoted \mathbf{P}^{ext} , acting on the system is zero. That is,

$$\mathbf{P}^{\text{ext}} := \int_{\mathfrak{B}_0} \bar{\mathbf{s}}_0 dV + \int_{\partial\mathfrak{B}_0} \underbrace{\hat{\mathbf{s}}_0}_{\mathbf{s}_0 := \mathbf{P} \cdot \mathbf{N}} dA = \mathbf{0}, \quad (22)$$

where $\bar{\mathbf{s}}_0$ are the body forces in \mathfrak{B}_0 and $\hat{\mathbf{s}}_0 = \mathbf{s}_0 := \mathbf{P} \cdot \mathbf{N}$ is the traction acting on the surface $\partial\mathfrak{B}_0$.

Localising Eq. (22) to a regular point in the bulk yields

$$\text{Div } \mathbf{P} = -\bar{\mathbf{s}}_0 \quad \text{in } \mathfrak{B}_0. \quad (23)$$

The following relationship defining the traction holds on the surface $\partial\mathfrak{B}_0$:

$$\mathbf{P} \cdot \mathbf{N} = \hat{\mathbf{s}}_0 = \mathbf{s}_0 \quad \text{on } \partial\mathfrak{B}_0. \quad (24)$$

Implicit in the statement of equilibrium (22) is the conventional force balance for a regular point on the interface:

$$[[\mathbf{P}]] \cdot \mathbf{M} = \mathbf{0} \quad \text{on } S_0. \quad (25)$$

Remark. The conservation of the traction vector $\hat{\mathbf{s}}_0$ over the interface S_0 follows from applying Eq. (24) to both sides of the

interface:

$$\begin{aligned} \mathbf{s}_0^+ + \mathbf{s}_0^- &= \mathbf{P}^+ \cdot \mathbf{M}^+ + \mathbf{P}^- \cdot \mathbf{M}^- \\ &= -[[\mathbf{P}]] \cdot \mathbf{M} \\ &= \mathbf{0} \quad (\text{from Eq. (25)}). \end{aligned}$$

The traction vectors acting on either side of the interface thus cancel one another. \square

3.4. Balance of angular momentum (moment balance)

We assume a non-polar continuum from the onset. The balance of angular momentum over the control volume \mathfrak{B}_0 stipulates that the total external angular momentum \mathbf{L}^{ext} , i.e. the angular momentum due to sources in \mathfrak{B}_0 and flux contributions on the boundary $\partial\mathfrak{B}_0$, is zero:

$$\mathbf{L}^{\text{ext}} = \int_{\mathfrak{B}_0} \underbrace{[\mathbf{r} \times \bar{\mathbf{s}}_0]}_{\bar{\mathbf{m}}_0} dV + \int_{\partial\mathfrak{B}_0} \underbrace{[\mathbf{r} \times \hat{\mathbf{s}}_0]}_{\mathbf{m}_0 := \mathbf{L} \cdot \mathbf{N} = \hat{\mathbf{m}}_0} dA = \mathbf{0}, \quad (26)$$

where \mathbf{r} is an arbitrary vector and \mathbf{L} is the second-order moment stress.

Localising Eq. (26) to a regular point in the bulk yields

$$-\text{Div } \mathbf{L} = \bar{\mathbf{m}}_0 \quad \text{in } \mathfrak{B}_0. \quad (27)$$

The following relationship holds on the surface:

$$\mathbf{L} \cdot \mathbf{N} = \hat{\mathbf{m}}_0 = \mathbf{m}_0 \quad \text{on } \partial\mathfrak{B}_0. \quad (28)$$

Implicit in the statement (26) is the moment balance for a regular point on the interface:

$$[[\mathbf{L}]] \cdot \mathbf{M} = \mathbf{0} \quad \text{on } S_0. \quad (29)$$

Remark. The conservation of the moment vector \mathbf{m}_0 over the interface S_0 follows from applying Eq. (28) to both sides of the interface:

$$\begin{aligned} \mathbf{m}_0^+ + \mathbf{m}_0^- &= \mathbf{L}^+ \cdot \mathbf{M}^+ + \mathbf{L}^- \cdot \mathbf{M}^- \\ &= -[[\mathbf{L}]] \cdot \mathbf{M} \\ &= \mathbf{0} \quad (\text{from Eq. (29)}). \quad \square \end{aligned}$$

Remark. The important symmetry property in the bulk $[\mathbf{P} \cdot \mathbf{F}^t]^{\text{skw}} = \mathbf{0}$ is obtained by substituting the definition of the traction $\hat{\mathbf{s}}_0$ in Eq. (24) into the integral version of the balance of angular momentum (26), using Gauss's theorem (7) and simplifying using the localised equilibrium statement (23). \square

3.5. Balance of internal energy

The enthalpy of the diffusing species per unit volume of the undeformed solid φ_0 [N m/m³] that contributes to the internal energy is related to the diffusing species concentration in the bulk c_0 as

$$\varphi_0 = \varphi c_0 \quad [\text{N m/m}^3] = [\text{N m/mol}][\text{mol/m}^3],$$

where φ [N m/mol] is the enthalpy of diffusing species per unit amount of diffusing species.

The total energy density per unit volume of the undeformed solid due to deformation, heat and the diffusing species is denoted ε_0 and the integral thereof as

$$E := \int_{\mathfrak{B}_0} \varepsilon_0 dV.$$

The energy input due to sources in \mathfrak{B}_0 and the various fluxes over $\partial\mathfrak{B}_0$ is denoted E^{ext} and consists of the deformational, thermal and diffusional power, that is:

$$E^{\text{ext}} := \underbrace{\int_{\mathfrak{B}_0} [\mathbf{v} \cdot \bar{\mathbf{s}}_0 + \bar{h}_0 + \varphi \bar{w}_0] dV}_{\bar{e}_0^{\text{eff}}} + \underbrace{\int_{\partial\mathfrak{B}_0} [\mathbf{v} \cdot \hat{\mathbf{s}}_0 + \hat{h}_0 + \varphi \hat{w}_0] dA}_{\hat{e}_0^{\text{eff}}}.$$

The effective energy source term is denoted \bar{e}_0^{eff} and the effective physical energy flux as \hat{e}_0^{eff} . Thermal sources in the bulk are denoted h_0 and the physical thermal flux as \hat{h}_0 . The contribution of the diffusing species sources in the bulk to the energy is $\varphi\bar{w}_0$ and that due to the physical flux of species over the surface is $\varphi\hat{w}_0$.

The expression for the balance of energy over the migrating control volume \mathfrak{B}_0 follows as

$$\dot{E} = E^{\text{ext}}$$

$$\begin{aligned} & \int_{\mathfrak{B}_0} D_t \varepsilon_0 \, dV + \int_{\partial\mathfrak{B}_0} \varepsilon_0 \mathbf{U} \cdot \mathbf{N} \, dA - \int_{\Xi_0} [\varepsilon_0] \mathbf{U} \cdot \mathbf{M} \, dA \\ &= \int_{\mathfrak{B}_0} \bar{e}_0^{\text{eff}} \, dV + \int_{\partial\mathfrak{B}_0} \hat{e}_0^{\text{eff}} \, dA \\ &\leftrightarrow \int_{\mathfrak{B}_0} [D_t \varepsilon_0 - \bar{e}_0^{\text{eff}}] \, dV + \int_{\partial\mathfrak{B}_0} \underbrace{[\varepsilon_0 \mathbf{U} \cdot \mathbf{N} - \hat{e}_0^{\text{eff}}]}_{-\mathbf{e}_0^{\text{eff}} \cdot \mathbf{N}} \, dA \\ &\quad - \int_{\Xi_0} [\varepsilon_0] \mathbf{U} \cdot \mathbf{M} \, dA = 0, \end{aligned} \quad (30)$$

where $\mathbf{e}_0^{\text{eff}}$ denotes the net effective energy flux and \mathbf{E}^{eff} is the associated net effective energy flux vector. The net effective energy flux $\mathbf{e}_0^{\text{eff}}$ and the net effective energy flux vector \mathbf{E}^{eff} contain contributions from deformation, heat conduction and the energy associated with the diffusing species:

$$\mathbf{e}_0^{\text{eff}} := \underbrace{[\mathbf{v} \cdot \mathbf{P} - \mathbf{H} - \varphi \mathbf{W}]}_{-\mathbf{E}^{\text{eff}}}, \mathbf{N},$$

where \mathbf{H} and \mathbf{W} are the heat and diffusion flux vectors, respectively.

Using Gauss's theorem (7) to transform the surface integral in the global energy balance (30) to a volume integral yields

$$\int_{\mathfrak{B}_0} [D_t \varepsilon_0 - \bar{e}_0^{\text{eff}} + \text{Div } \mathbf{E}^{\text{eff}}] \, dV = 0 \quad (31)$$

and by localising to a regular point in the domain

$$D_t \varepsilon_0 + \text{Div } \mathbf{E}^{\text{eff}} = \bar{e}_0^{\text{eff}} \quad \text{in } \mathcal{B}_0. \quad (32)$$

The following relation holds for regular points on the boundary:

$$[\varepsilon_0 \mathbf{U} - \mathbf{E}^{\text{eff}}] \cdot \mathbf{N} = \hat{e}_0^{\text{eff}} \quad \text{on } \partial\mathcal{B}_0. \quad (33)$$

Further insight into the net effective energy flux vector \mathbf{E}^{eff} and its relation to the heat flux vector \mathbf{H} and the diffusion flux vector \mathbf{W} is obtained by restating Eq. (33) as

$$\underbrace{-\mathbf{E}^{\text{eff}} \cdot \mathbf{N}}_{\mathbf{e}_0^{\text{eff}}} = \hat{e}_0^{\text{eff}} - \varepsilon_0 \mathbf{U} \cdot \mathbf{N} = [\mathbf{v} \cdot \mathbf{P} - \mathbf{H} - \varphi \mathbf{W}] \cdot \mathbf{N}.$$

If the effective physical energy flux \hat{e}_0^{eff} is positive then energy is entering the body; conversely if the term is negative, energy is leaving the body. The second term on the right-hand side of the middle equation $-\varepsilon_0 \mathbf{U} \cdot \mathbf{N}$ is the diffusive energy flux due to the motion of the control volume in the undeformed configuration. It is important to note that, in accordance with standard convention, the net effective energy flux vector \mathbf{E}^{eff} acts in the same direction as the heat and diffusion flux vectors, \mathbf{H} and \mathbf{W} .

Localising Eq. (30) to a regular point on the interface yields

$$\begin{aligned} 0 &= \mathbf{E}^{\text{eff},-} \cdot \mathbf{N}^- + \mathbf{E}^{\text{eff},+} \cdot \mathbf{N}^+ - [\varepsilon_0] \mathbf{U} \cdot \mathbf{M} \\ &= [[\mathbf{E}^{\text{eff}}]] - [\varepsilon_0] \mathbf{U} \cdot \mathbf{M} \quad \text{on } \mathcal{S}_0. \end{aligned} \quad (34)$$

Remark. The conservation of the effective energy flux \bar{e}_0^{eff} over the interface \mathcal{S}_0 is demonstrated by applying Eq. (33) to both sides of \mathcal{S}_0 :

$$\hat{e}_0^{\text{eff},+} + \hat{e}_0^{\text{eff},-} = [\varepsilon_0^+ \mathbf{U} - \mathbf{E}^{\text{eff},+}] \cdot \mathbf{M}^+ + [\varepsilon_0^- \mathbf{U} - \mathbf{E}^{\text{eff},-}] \cdot \mathbf{M}^-$$

$$\begin{aligned} &= [[\mathbf{E}^{\text{eff}}]] - [\varepsilon_0] \mathbf{U} \cdot \mathbf{M} \\ &= 0 \quad (\text{from Eq. (34)}). \end{aligned}$$

The physical effective energy fluxes acting on either side of the interface thus cancel one another. That is, the energy that enters from one side of the interface leaves from the opposite side. \square

3.6. Balance of entropy

The entropy density of the diffusing species in the undeformed configuration \mathcal{B}_0 is denoted ς_0 [N m/K m³] and is related to the diffusing species concentration c_0 via the entropy of the diffusing species per amount of diffusing species ς [N m/K mol] as

$$\varsigma_0 = \varsigma c_0 \quad [\text{N m/K m}^3] = [\text{N m/K mol}][\text{mol/m}^3].$$

The total entropy density is denoted σ_0 and the integral thereof over the control volume as

$$S = \int_{\mathfrak{B}_0} \sigma_0 \, dV.$$

The second law of thermodynamics imposes the physical restriction that the entropy production S^{pro} is non-negative. The (total) rate of change of the total entropy in a body is thus not less than the total entropy supplied to the body S^{ext} . The entropy balance is thus

$$\dot{S} = \underbrace{\int_{\mathfrak{B}_0} \bar{n}_0^{\text{eff}} \, dV + \int_{\partial\mathfrak{B}_0} \hat{n}_0^{\text{eff}} \, dA}_{S^{\text{ext}}} + \underbrace{\int_{\mathfrak{B}_0} \bar{\pi}_0 \, dV + \int_{\partial\mathfrak{B}_0} \hat{\pi}_0 \, dA + \int_{\Xi_0} \tilde{\pi}_0 \, dA}_{S^{\text{pro}} \geq 0},$$

where \bar{n}_0^{eff} is the effective physical entropy density due to sources (i.e. heat and the entropy associated with the diffusing species) and \hat{n}_0^{eff} is the effective physical entropy flux over the surface $\partial\mathfrak{B}_0$. The effective entropy source is composed of contributions from heat sources \bar{n}_0 and diffusing species sources $\varsigma\bar{w}_0$. Similarly, the effective entropy flux has contributions from heat \hat{n}_0 and the diffusing species $\varsigma\hat{w}_0$. That is,

$$\bar{n}_0^{\text{eff}} := \bar{n}_0 + \varsigma\bar{w}_0 \quad \text{and} \quad \hat{n}_0^{\text{eff}} := \hat{n}_0 + \varsigma\hat{w}_0. \quad (35)$$

The non-negative entropy production density in the bulk, on the surface and on the interface are denoted $\bar{\pi}_0 \geq 0$, $\hat{\pi}_0 \geq 0$ and $\tilde{\pi}_0 \geq 0$, respectively, and the integrals thereof as $S^{\text{pro}} \geq 0$.

The expression for the balance of entropy over the migrating control volume is

$$\dot{S} = S^{\text{ext}} + S^{\text{pro}},$$

$$\begin{aligned} & \int_{\mathfrak{B}_0} D_t \sigma_0 \, dV + \int_{\partial\mathfrak{B}_0} \sigma_0 \mathbf{U} \cdot \mathbf{N} \, dA - \int_{\Xi_0} [\sigma_0] \mathbf{U} \cdot \mathbf{M} \, dA \\ &= \int_{\mathfrak{B}_0} [\bar{n}_0^{\text{eff}} + \bar{\pi}_0] \, dV + \int_{\partial\mathfrak{B}_0} [\hat{n}_0^{\text{eff}} + \hat{\pi}_0] \, dA + \int_{\Xi_0} \tilde{\pi}_0 \, dA \\ &\leftrightarrow \int_{\mathfrak{B}_0} [D_t \sigma_0 - \bar{n}_0^{\text{eff}} - \bar{\pi}_0] \, dV + \int_{\partial\mathfrak{B}_0} \underbrace{[\sigma_0 \mathbf{U} \cdot \mathbf{N} - \hat{n}_0^{\text{eff}} - \hat{\pi}_0]}_{-\bar{n}_0^{\text{eff}} \cdot \mathbf{N}} \, dA \\ &\quad - \int_{\Xi_0} [[\sigma_0] \mathbf{U} \cdot \mathbf{M} + \tilde{\pi}_0] \, dA = 0, \end{aligned} \quad (36)$$

where \bar{n}_0^{eff} denotes the net effective entropy flux and \mathbf{S}^{eff} is the associated net effective entropy flux vector.

Using Gauss's theorem (7) to transform the surface integral in the global entropy balance given in Eq. (36) to a volume integral produces

$$\int_{\mathfrak{B}_0} [D_t \sigma_0 - \bar{n}_0^{\text{eff}} - \bar{\pi}_0 + \text{Div } \mathbf{S}^{\text{eff}}] \, dV = 0$$

and localising to a regular point in the domain yields

$$D_t \sigma_0 + \text{Div } \mathbf{S}^{\text{eff}} = \bar{n}_0^{\text{eff}} + \bar{\pi}_0 \quad \text{in } \mathcal{B}_0. \quad (37)$$

The following relation holds for regular points on the boundary:

$$[\sigma_0 \mathbf{U} - \mathbf{S}^{\text{eff}}] \cdot \mathbf{N} = \hat{n}_0^{\text{eff}} + \hat{\pi}_0 \quad \text{on } \partial B_0. \quad (38)$$

The definition of the effective entropy flux vector \mathbf{S}^{eff} and the sign convention adopted mimics that of the effective energy flux vector \mathbf{E}^{eff} (see Eq. (33) and the discussion directly thereafter).

Localising the entropy balance equation (36) to a regular point on the interface S_0 gives

$$\begin{aligned} 0 &= \mathbf{S}^{\text{eff},-} \cdot \mathbf{N}^- + \mathbf{S}^{\text{eff},+} \cdot \mathbf{N}^+ - [\llbracket \sigma_0 \rrbracket \mathbf{U} \cdot \mathbf{M} + \hat{\pi}_0] \\ &= [\llbracket \mathbf{S}^{\text{eff}} \rrbracket - \llbracket \sigma_0 \rrbracket \mathbf{U}] \cdot \mathbf{M} - \hat{\pi}_0 \end{aligned}$$

$$\leftrightarrow \hat{\pi}_0 = [\llbracket \mathbf{S}^{\text{eff}} \rrbracket - \llbracket \sigma_0 \rrbracket \mathbf{U}] \cdot \mathbf{M} \quad \text{on } S_0. \quad (39)$$

Remark. The conservation of the entropy flux \hat{n}_0 and an interpretation of the entropy production on the interface $\hat{\pi}_0$ is obtained by applying Eq. (38) to both sides of the interface S_0 :

$$\begin{aligned} [\hat{n}_0^{\text{eff},+} + \hat{\pi}_0^+] + [\hat{n}_0^{\text{eff},-} + \hat{\pi}_0^-] &= [\sigma_0^+ \mathbf{U} - \mathbf{S}^{\text{eff},+}] \cdot \mathbf{M}^+ + [\sigma_0^- \mathbf{U} - \mathbf{S}^{\text{eff},-}] \cdot \mathbf{M}^- \\ &= [\llbracket \mathbf{S}^{\text{eff}} \rrbracket - \llbracket \sigma_0 \rrbracket \mathbf{U}] \cdot \mathbf{M} \\ &= \hat{\pi}_0 \quad (\text{from Eq. (39)}). \end{aligned}$$

The entropy production and the entropy sources are independent, and since the entropy production terms are constrained to be non-negative, i.e. $\hat{\pi}_0^\pm \geq 0$, it obviously follows that $\hat{n}_0^{\text{eff},-} + \hat{n}_0^{\text{eff},+} = 0$ and $\hat{\pi}_0 = \hat{\pi}_0^- + \hat{\pi}_0^+$. \square

3.7. Dissipation inequality

As is customary in solid mechanics we choose to work with the Helmholtz energy ψ_0 and the chemical potential μ , as defined via Legendre transforms (see e.g. [54]) as

$$\psi_0 := \varepsilon_0 - \theta \sigma_0 \quad \text{and} \quad \mu := \varphi - \theta \zeta. \quad (40)$$

The functional form of the Helmholtz energy density is chosen as⁶

$$\psi_0 = \psi_0(\mathbf{F}, \theta, c_0, \boldsymbol{\alpha}_0; \mathbf{X}), \quad (41)$$

where $\theta > 0$ [K] is the absolute temperature, c_0 is the concentration of the diffusing species expressed in the undeformed configuration, and $\boldsymbol{\alpha}_0$ is the set of internal variables (most generally scalars or second-order tensors) that describe the inelastic response of the solid associated with dissipative phenomena such as damage, plasticity, viscosity, etc.⁷ The argument of the Helmholtz energy density in the second slot denotes the parameterisation in terms of position \mathbf{X} . We shall generally omit the reference to the explicit dependence of the Helmholtz energy on the position henceforth for the sake of brevity.

As in [28,58], for example, we assume from the onset that the temperature θ and the chemical potential μ are continuous across the interface,⁸ that is

$$[\llbracket \theta \rrbracket] = 0 \quad \text{and} \quad [\llbracket \mu \rrbracket] = 0 \quad \text{on } S_0,$$

⁶ Note that in order to satisfy the principle of material objectivity [48] the dependence of the Helmholtz energy ψ_0 on the deformation gradients \mathbf{F} is required to be via the right Cauchy–Green tensor \mathbf{C} . For the sake of clarity, however, we indicate the dependence of the Helmholtz energy explicitly in terms of the deformation gradient \mathbf{F} , with the implicit understanding that this dependence is via the right Cauchy–Green tensor \mathbf{C} .

⁷ For an overview of thermodynamics with internal variables the reader is referred to [55,56], among others. In order to account for non-locality of the internal variable (required, for example, in gradient theories of plasticity [57]) the gradient of the internal variable could also be included in the Helmholtz energy.

⁸ Continuity of the temperature and chemical potential across the interface need not be assumed a priori. As shown in [47], the continuity assumptions are logical constraints that arise from the reduced dissipation inequality in order to satisfy thermodynamic consistency.

and hence

$$[\llbracket \psi_0 \rrbracket] = [\llbracket \varepsilon_0 \rrbracket] - \theta [\llbracket \sigma_0 \rrbracket] \quad \text{and} \quad [\llbracket \varphi \rrbracket] = \theta [\llbracket \zeta \rrbracket] \quad \text{on } S_0. \quad (42)$$

The effective physical entropy source and flux, denoted \hat{n}_0^{eff} and \hat{n}_0^{eff} and defined in Eq. (35)₁₋₂, contain contributions from heat conduction and the diffusing species. We adopt the commonly made Clausius–Duhem assumption (see e.g. [59]) that the heat source \bar{h}_0 and the heat flux \bar{h}_0 are proportional to the entropy source \bar{n}_0 and the entropy flux \hat{n}_0 , respectively, as

$$\hat{n}_0 := \theta^{-1} \bar{h}_0 \quad \text{and} \quad \bar{n}_0 := \theta^{-1} \bar{h}_0.$$

The effective physical entropy flux vector \mathbf{S}^{eff} , first introduced in Eq. (36) as $\mathbf{n}_0^{\text{eff}} := -\mathbf{S}^{\text{eff}} \cdot \mathbf{N}$, contains contributions from heat conduction and the diffusing species. From the Clausius–Duhem assumption the contribution to the effective physical entropy flux vector \mathbf{S}^{eff} from heat only, denoted \mathbf{S} , is defined by

$$-n_0 := \mathbf{S} \cdot \mathbf{N} = \theta^{-1} \mathbf{H} \cdot \mathbf{N}.$$

The contribution to the effective physical entropy flux vector from species diffusion is $\zeta \mathbf{W}$. Thus, the effective physical entropy flux and associated vector are defined by

$$-n_0^{\text{eff}} := \mathbf{S}^{\text{eff}} \cdot \mathbf{N} = [\theta^{-1} \mathbf{H} + \zeta \mathbf{W}] \cdot \mathbf{N}.$$

We respectively define the density of the dissipation power in the bulk B_0 , on the surface ∂B_0 and on the interface S_0 by

$$\bar{\delta}_0 := \theta \bar{\pi}_0, \quad \hat{\delta}_0 := \theta \hat{\pi}_0 \quad \text{and} \quad \tilde{\delta}_0 := \theta \tilde{\pi}_0.$$

Multiplying the expression for the balance of entropy for a regular point in the domain (37) by the absolute temperature θ , and using the definition of the Helmholtz energy given in Eq. (40)₁ yields

$$\begin{aligned} \theta [\underbrace{\theta^{-1} \bar{h}_0 + \zeta \bar{w}_0}_{\bar{n}_0^{\text{eff}}}] + \theta \bar{\pi}_0 &= \underbrace{[-\sigma_0 D_t \theta + D_t (\varepsilon_0 - \psi_0)]}_{\theta D_t \sigma_0} + \theta \text{Div}(\underbrace{\theta^{-1} \mathbf{H} + \zeta \mathbf{W}}_{\mathbf{S}^{\text{eff}}}) \\ \leftrightarrow \bar{\delta}_0 &= -\sigma_0 D_t \theta + D_t (\varepsilon_0 - \psi_0) + \text{Div} \mathbf{H} + \text{Div}(\theta \zeta \mathbf{W}) \\ &\quad - \mathbf{S}^{\text{eff}} \cdot \nabla_{\mathbf{X}} \theta - [\bar{h}_0 + \theta \zeta \bar{w}_0] \geq 0 \quad \text{in } B_0. \end{aligned} \quad (43)$$

Multiplying the local expression for the balance of entropy for a regular point on the surface ∂B_0 (38) by the absolute temperature θ and making use of the definition of the Helmholtz energy given in Eq. (40)₁ yields

$$\begin{aligned} \theta [\underbrace{\theta^{-1} \hat{h}_0 + \zeta \hat{w}_0}_{\hat{n}_0^{\text{eff}}}] + \theta \hat{\pi}_0 &= [\underbrace{[\varepsilon_0 - \psi_0]}_{\theta \sigma_0} \mathbf{U} - \underbrace{\theta [\theta^{-1} \mathbf{H} + \zeta \mathbf{W}]}_{\mathbf{S}^{\text{eff}}}] \cdot \mathbf{N} \\ \leftrightarrow \hat{\delta}_0 &= [\varepsilon_0 - \psi_0] \mathbf{U} \cdot \mathbf{H} - \theta \zeta \mathbf{W} \cdot \mathbf{N} - [\hat{h}_0 + \theta \zeta \hat{w}_0] \geq 0 \quad \text{on } \partial B_0. \end{aligned} \quad (44)$$

Multiplying the local expression for the balance of entropy for a regular point on the interface (39) by the absolute temperature $\theta = \llbracket \theta \rrbracket$ and making use of the relationships given in Eq. (42) yields

$$\begin{aligned} \theta \hat{\pi}_0 &= \theta [\llbracket \mathbf{S}^{\text{eff}} \rrbracket - \llbracket \sigma_0 \rrbracket \mathbf{U}] \cdot \mathbf{M}, \\ \tilde{\delta}_0 &= \theta [\llbracket \theta^{-1} \mathbf{H} + \zeta \mathbf{W} \rrbracket \cdot \mathbf{M}] - \theta [\llbracket \sigma_0 \rrbracket \mathbf{U} \cdot \mathbf{M} \\ &\quad - \llbracket [\varepsilon_0 - \psi_0] \mathbf{U} - \llbracket \mathbf{H} \rrbracket - \theta [\zeta \mathbf{W}] \rrbracket \cdot \mathbf{M} \quad \text{on } S_0. \end{aligned} \quad (45)$$

The dissipation inequalities are obtained by substituting the equations for the balance of energy in Eqs. (32)–(34) into Eqs. (43)–(45) and making use of the definitions of the Helmholtz energy ψ_0 and the chemical potential μ given in Eq. (40) and the resulting relations given in Eq. (42).

Substituting Eq. (32) into Eq. (43) yields the dissipation inequality for a regular point in the domain as

$$\begin{aligned} \bar{\delta}_0 &= -\sigma_0 D_t \theta - D_t \psi_0 + \underbrace{[\bar{\varepsilon}_0^{\text{eff}} - \text{Div} \mathbf{E}^{\text{eff}}]}_{D_t \varepsilon_0} + \text{Div} \mathbf{H} + \text{Div}(\theta \zeta \mathbf{W}) \\ &\quad - \mathbf{S}^{\text{eff}} \cdot \nabla_{\mathbf{X}} \theta - \bar{h}_0 - \theta \zeta \bar{w}_0 \end{aligned}$$

$$= -\sigma_0 D_t \theta - D_t \psi_0 + \text{Div}(\underbrace{\mathbf{v} \cdot \mathbf{P} - \mathbf{H} - \varphi \mathbf{W}}_{-\mathbf{E}^{\text{eff}}}) + \underbrace{[\mathbf{v} \cdot \hat{\mathbf{s}}_0 + \bar{h}_0 + \varphi \bar{w}_0]}_{\bar{e}_0^{\text{eff}}} \\ + \text{Div} \mathbf{H} + \text{Div}(\theta \zeta \mathbf{W}) - \mathbf{S}^{\text{eff}} \cdot \nabla_X \theta - \bar{h}_0 - \theta \zeta \bar{w}_0$$

and using the relation $[\text{Div}(\mathbf{v} \cdot \mathbf{P}) = \nabla_X \mathbf{v} : \mathbf{P} + \mathbf{v} \cdot \text{Div} \mathbf{P}]$ and the equilibrium equation (23), i.e. $[\text{Div} \mathbf{P} + \bar{\mathbf{s}}_0 = \mathbf{0}]$, yields

$$= \nabla_X \mathbf{v} : \mathbf{P} - D_t \psi_0 - \sigma_0 D_t \theta + \mu D_t c_0 - \mu \text{Div} \mathbf{W} - \mathbf{W} \cdot \nabla_X \mu - \mathbf{S}^{\text{eff}} \cdot \nabla_X \theta$$

and from the relation $\text{Div} \mathbf{W} = \bar{w}_0 - D_t c_0$ obtained from the expression for the conservation of solvent mass (19)

$$= \nabla_X \mathbf{v} : \mathbf{P} - D_t \psi_0 - \sigma_0 D_t \theta + \mu D_t c_0 - \mathbf{W} \cdot \nabla_X \mu - \mathbf{S}^{\text{eff}} \cdot \nabla_X \theta \geq 0 \quad \text{in } B_0. \quad (46)$$

The dissipation inequality for the bulk is identical to that obtained using the conventional approach (cf. [47]).

Substituting Eq. (33) into Eq. (44) yields the dissipation inequality for a regular point on the surface as

$$\hat{\delta}_0 = \underbrace{[\bar{e}_0^{\text{eff}} + \mathbf{E}^{\text{eff}} \cdot \mathbf{N}]}_{\varepsilon_0 \mathbf{U} \cdot \mathbf{N}} - [\psi_0 \mathbf{U} + \mathbf{H} + \theta \zeta \mathbf{W}] \cdot \mathbf{N} - \hat{h}_0 - \theta \zeta \hat{w}_0 \\ = \underbrace{[\mathbf{v} \cdot \hat{\mathbf{s}}_0 + \hat{h}_0 + \varphi \hat{w}_0]}_{\bar{e}_0^{\text{eff}}} - \underbrace{[\mathbf{v} \cdot \mathbf{P} - \mathbf{H} - \varphi \mathbf{W}]}_{-\mathbf{E}^{\text{eff}}} \cdot \mathbf{N} \\ - [\psi_0 \mathbf{U} + \mathbf{H} + \theta \zeta \mathbf{W}] \cdot \mathbf{N} - \hat{h}_0 - \theta \zeta \hat{w}_0$$

and from the relation $\hat{\mathbf{s}}_0 \cdot \mathbf{P} \cdot \mathbf{N} = \mathbf{0}$ given in the equilibrium equation on the surface (24)

$$= \mu \hat{w}_0 + [\mu \mathbf{W} - \psi_0 \mathbf{U}] \cdot \mathbf{N}.$$

Using the expression $\mathbf{W} \cdot \mathbf{N} = c_0 \mathbf{U} \cdot \mathbf{N} - \hat{w}_0$ obtained from the conservation of solvent mass (20) yields

$$\hat{\delta}_0 = \underbrace{[-\psi_0 + \mu c_0]}_{-\phi_0} \mathbf{U} \cdot \mathbf{N} \geq 0 \quad \text{on } \partial B_0. \quad (47)$$

The dissipation inequality for the surface is interpreted as follows. The term $-\phi_0 := -\psi_0 + \mu c_0$ expresses the transformation of the Helmholtz energy ψ_0 as a function of the concentration c_0 into one that is a function of the chemical potential μ , denoted by ϕ_0 , via a Legendre transform. The conjugacy of the chemical potential and the concentration shall be demonstrated shortly when developing the constitutive relations in Section 3.8. The energy ϕ_0 is non-negative, i.e. $\phi_0 \geq 0$. The reduced dissipation $-\phi_0 \mathbf{U} \cdot \mathbf{N} \geq 0$ expresses that the only admissible material velocity \mathbf{U} relative to the surface ∂B_0 of the undeformed configuration is a contraction, that is $\mathbf{U} \cdot \mathbf{N} \leq 0$ as depicted in Fig. 3(a).

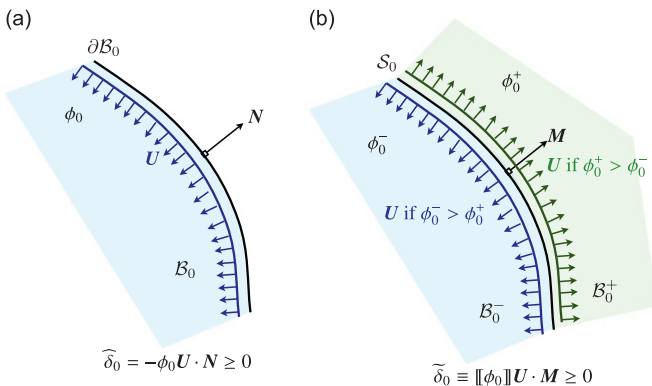


Fig. 3. The energetically feasible motions of (a) the boundary ∂B_0 and (b) the interface S_0 (for the case of a rigid, heat conducting diffuser).

Substituting Eq. (34) into Eq. (45) renders the dissipation inequality for a regular point on the interface as

$$\tilde{\delta}_0 = -[\varepsilon_0] \mathbf{U} \cdot \mathbf{M} + [[\psi_0] \mathbf{U} + [\mathbf{H}] + \theta [\zeta \mathbf{W}]] \cdot \mathbf{M} \\ = -[\mathbf{E}^{\text{eff}}] \cdot \mathbf{M} + [[\psi_0] \mathbf{U} + [\mathbf{H}] + \theta [\zeta \mathbf{W}]] \cdot \mathbf{M} \\ = [\mathbf{v} \cdot \mathbf{P} - \mathbf{H} - \varphi \mathbf{W}] \cdot \mathbf{M} + [[\psi_0] \mathbf{U} + [\mathbf{H}] + \theta [\zeta \mathbf{W}]] \cdot \mathbf{M}$$

and using Eq. (6) and the equilibrium equation for a point on the interface (25) whereby $[[\mathbf{P}]] \cdot \mathbf{M} = \mathbf{0}$

$$= [[\mathbf{v}]] \cdot [[\mathbf{P}]] - \mu [[\mathbf{W}]] + [[\psi_0]] \mathbf{U} \cdot \mathbf{M}$$

and using the expression $[[\mathbf{W}]] \cdot \mathbf{M} = [c_0] \mathbf{U} \cdot \mathbf{M}$ obtained from the conservation of solvent mass (21) yields

$$= [[\mathbf{v}]] \cdot [[\mathbf{P}]] + [[\psi_0]] - \mu [c_0] \mathbf{U} \cdot \mathbf{M} \\ = [[\mathbf{v}]] \cdot [[\mathbf{P}]] + [[\phi_0]] \mathbf{U} \cdot \mathbf{M} \geq 0 \quad \text{on } S_0. \quad (48)$$

3.8. Constitutive relations

The objective of the following section is to derive the constitutive relations for the bulk based on the thermodynamic constraints imposed by the dissipation inequality (46). Expanding the material time derivative of the Helmholtz energy in Eq. (46) gives

$$\tilde{\delta}_0 = -[\partial_F \psi_0 : D_t \mathbf{F} + \partial_\theta \psi_0 D_t \theta + \partial_{c_0} \psi_0 D_t c_0 + \partial_{\alpha_0} \psi_0 : D_t \alpha_0] \\ + \nabla_X \mathbf{v} : \mathbf{P} - \sigma_0 D_t \theta + \mu D_t c_0 - \mathbf{W} \cdot \nabla_X \mu - \mathbf{S}^{\text{eff}} \cdot \nabla_X \theta \geq 0,$$

and from the standard Coleman and Noll [60] argument:

$$\Rightarrow \mathbf{P} = \partial_F \psi_0, \quad \sigma_0 = -\partial_\theta \psi_0, \quad \mu = \partial_{c_0} \psi_0 \quad (49)$$

by which the dissipation inequality reduces to

$$\delta_0 = -\partial_{\alpha_0} \psi_0 : D_t \alpha_0 - \mathbf{W} \cdot \nabla_X \mu - \mathbf{S}^{\text{eff}} \cdot \nabla_X \theta \geq 0. \quad (50)$$

As mentioned previously (see the discussion following Eq. (47)), the conjugacy of the concentration c_0 and the chemical potential μ is clear from Eq. (49)₃.⁹ The coupling of heat conduction and species diffusion is clear. The non-standard effective entropy flux vector $\mathbf{S}^{\text{eff}} := [\theta^{-1} \mathbf{H} + \zeta \mathbf{W}]$ contains contributions due to thermal conduction and species diffusion, and is conjugate to the gradient of the temperature.

4. Formulation in terms of the Eshelby stress

The main objectives of this section are to reformulate the equilibrium equations (23)–(25) in terms of the Eshelby stress tensor [1,2] and to identify the role it plays in dissipating energy. The reformulation of the equilibrium equations is accomplished by a pull-back of the respective balance equations to the undeformed configuration. For an overview of the properties of the Eshelby stress tensor, the reader is referred to [61].

The Helmholtz energy based Eshelby stress tensor Σ^* is defined by

$$\Sigma^* = \psi_0 \mathbf{I} - \mathbf{F}^t \cdot \mathbf{P} \quad \leftrightarrow \quad \Sigma_{ij}^* = \psi_0 \delta_{ij} - F_{mi} P_{mj}. \quad (51)$$

The extension of the standard Eshelby stress tensor to account for diffusional effects is denoted Σ and defined by

$$\Sigma = \phi_0 \mathbf{I} - \mathbf{F}^t \cdot \mathbf{P}. \quad (52)$$

An interpretation of the energy ϕ_0 in Eq. (52) as a Legendre transform of the Helmholtz energy ψ_0 was given in the discussion following Eq. (47). The constitutive relations for the Piola stress \mathbf{P}

⁹ Remarks on the form of the constitutive relations for the diffusion flux vector \mathbf{W} and the effective entropy flux vector \mathbf{S}^{eff} , and the evolution equation for the inelastic internal variables α_0 are given in Appendix A.

and the total entropy density σ_0 given in Eq. (49)_{1–2} can be restated in terms of the energy ϕ_0 by simply interchanging ψ_0 and ϕ_0 . The explicit gradients of the energies ϕ_0 and ψ_0 are the same, that is $\partial_X \phi_0 = \partial_X \psi_0$.

4.1. Equilibrium equations in terms of the Eshelby stresses Σ^* and Σ

The counterparts of the equilibrium equations (23)–(25) in the bulk, and on the surface and the interface expressed in terms of the Eshelby stresses Σ^* and Σ are obtained via a pull-back of the equations to the undeformed configuration.

A pull-back of Eq. (23) for a regular point in the domain yields

$$\begin{aligned} \mathbf{0} &= -\mathbf{F}^t \cdot [-\text{Div } \mathbf{P} - \bar{\mathbf{S}}_0] \\ &= \text{Div}(\mathbf{F}^t \cdot \mathbf{P}) - \nabla_X \mathbf{F}^t : \mathbf{P} + \mathbf{F}^t \cdot \bar{\mathbf{S}}_0 \\ &= \text{Div}(\underbrace{-\psi_0 \mathbf{I} + \mathbf{F}^t \cdot \mathbf{P}}_{-\Sigma^*}) - \nabla_X \mathbf{F}^t : \mathbf{P} + \mathbf{F}^t \cdot \bar{\mathbf{S}}_0 + \nabla_X \psi_0 \\ &= -\text{Div } \Sigma^* - \nabla_X \mathbf{F}^t : \mathbf{P} + \mathbf{F}^t \cdot \bar{\mathbf{S}}_0 \\ &\quad + [\partial_F \psi_0 : \nabla_X \mathbf{F} + \partial_\theta \psi_0 \nabla_X \theta + \partial_{c_0} \psi_0 \nabla_X c_0 + \partial_{\alpha_0} \psi_0 : \nabla_X \alpha_0 + \partial_X \psi_0] \\ &= -\text{Div } \Sigma^* - [\sigma_0 \nabla_X \theta - \mu_0 \nabla_X c_0 + \mathbf{A}_0 : \nabla_X \alpha_0 - \partial_X \psi_0 - \mathbf{F}^t \cdot \bar{\mathbf{S}}_0] \\ &= -\text{Div } \Sigma - \underbrace{[\sigma_0 \nabla_X \theta + c_0 \nabla_X \mu + \mathbf{A}_0 : \nabla_X \alpha_0 - \partial_X \phi_0 - \mathbf{F}^t \cdot \bar{\mathbf{S}}_0]}_{\bar{\mathbf{S}}_0} \end{aligned} \quad (53)$$

where $\bar{\mathbf{S}}_0$ represents the inhomogeneity force. The following relation, which follows from the compatibility of the deformation gradient \mathbf{F} , was used in the above manipulation:

$$\nabla_X \mathbf{F}^t : \mathbf{P} = \mathbf{P} : \nabla_X \mathbf{F}.$$

The inhomogeneity force accounts for, among other things, the inhomogeneous distribution of the energy in the undeformed configuration.

For a regular point on the boundary one obtains

$$\begin{aligned} \mathbf{0} &= -\mathbf{F}^t \cdot [\mathbf{P} \cdot \mathbf{N}] + \underbrace{\mathbf{F}^t \cdot \hat{\mathbf{S}}_0}_{-\hat{\mathbf{S}}_0} \\ &= [\Sigma - \phi_0 \mathbf{I}] \cdot \mathbf{N} - \hat{\mathbf{S}}_0 \\ \Leftrightarrow \quad \Sigma \cdot \mathbf{N} &= \phi_0 \mathbf{N} + \hat{\mathbf{S}}_0 \quad \text{on } \partial B_0. \end{aligned} \quad (54)$$

Finally, for a regular point on the interface one obtains

$$\begin{aligned} \mathbf{0} &= -\llbracket \mathbf{F}^t \rrbracket \cdot \llbracket \mathbf{P} \rrbracket \cdot \mathbf{M} \\ &= -\llbracket \mathbf{F}^t \cdot \mathbf{P} \rrbracket - \llbracket \mathbf{F}^t \rrbracket \cdot \llbracket \mathbf{P} \rrbracket \cdot \mathbf{M} \\ &= -\llbracket \phi_0 \mathbf{I} - \Sigma \rrbracket - \llbracket \mathbf{F}^t \rrbracket \cdot \llbracket \mathbf{P} \rrbracket \cdot \mathbf{M} \\ &= \llbracket \Sigma \rrbracket - \llbracket \phi_0 \rrbracket \mathbf{I} \cdot \mathbf{M} + \underbrace{\llbracket \mathbf{F}^t \rrbracket \cdot \llbracket \mathbf{P} \rrbracket \cdot \mathbf{M}}_{\bar{\mathbf{S}}_0} \\ \Leftrightarrow \quad \llbracket \Sigma \rrbracket \cdot \mathbf{M} &= \llbracket \phi_0 \rrbracket \mathbf{M} - \underbrace{\llbracket \mathbf{F}^t \rrbracket \cdot \hat{\mathbf{S}}_0}_{-\bar{\mathbf{S}}_0} \quad \text{on } S_0. \end{aligned} \quad (55)$$

4.2. Dissipation in terms of the Eshelby stress

The following results are needed to rewrite the dissipation inequalities in terms of the Eshelby stress measures:

$$\begin{aligned} \nabla_X \mathbf{V} : \Sigma^* &= \nabla_X \mathbf{V} : [-\mathbf{F}^t \cdot \mathbf{P} + \psi_0 \mathbf{I}] \\ &= -\nabla_X \mathbf{V} : [\mathbf{F}^t \cdot \mathbf{P}] + \text{Div}(\psi_0 \mathbf{V}) - \mathbf{V} \cdot \nabla_X \psi_0 \\ &= -\nabla_X \mathbf{V} : [\mathbf{F}^t \cdot \mathbf{P}] + \text{Div}(\psi_0 \mathbf{V}) \\ &\quad - \mathbf{V} \cdot [\partial_X \psi_0 + \mathbf{P} : \nabla_X \mathbf{F} - \sigma_0 \nabla_X \theta + \mu \nabla_X c_0 - \mathbf{A}_0 : \nabla_X \alpha_0] \\ &= \nabla_X \mathbf{v} : \mathbf{P} + \text{Div}(\psi_0 \mathbf{V}) + \mathbf{V} \cdot \underbrace{[-\partial_X \psi_0 + \mathbf{A}_0 : \nabla_X \alpha_0]}_{\bar{\mathbf{S}}_0^{\text{loc}}} \\ &\quad - [\sigma_0 \nabla_X \theta - \mu \nabla_X c_0] \cdot \mathbf{v}, \end{aligned} \quad (56)$$

and

$$\begin{aligned} \nabla_X \mathbf{V} : \Sigma &= \nabla_X \mathbf{v} : \mathbf{P} + \text{Div}(\phi_0 \mathbf{V}) + \mathbf{V} \cdot \underbrace{[-\partial_X \phi_0 + \mathbf{A}_0 : \nabla_X \alpha_0]}_{\bar{\mathbf{S}}_0^{\text{loc}}} \\ &\quad - [\sigma_0 \nabla_X \theta - c_0 \nabla_X \mu] \cdot \mathbf{v}. \end{aligned} \quad (57)$$

Based on the constitutive assumptions on the form of the diffusion flux vector \mathbf{W} and the effective entropy flux vector \mathbf{S}^{eff} given in Eqs. (A.1) and (A.2), it proves convenient to decompose the dissipation power in the bulk $\bar{\delta}_0$ (46) into a local and a conduction–diffusion part, denoted $\bar{\delta}_0^{\text{loc}}$ and $\bar{\delta}_0^{\text{con-diff}}$ respectively, as follows:

$$\bar{\delta}_0 = \bar{\delta}_0^{\text{loc}} + \underbrace{[-\mathbf{W} \cdot \nabla_X \mu - \mathbf{S}^{\text{eff}} \cdot \nabla_X \theta]}_{\bar{\delta}_0^{\text{con-diff}}}. \quad (58)$$

Substituting the expression for $\nabla_X \mathbf{v} : \mathbf{P}$ obtained from Eq. (56) into the dissipation inequality for the bulk (46), and exploiting the relationships (see Eq. (3)):

$$D_t \psi_0 = J d_t \psi_t - \text{Div}(\psi_0 \mathbf{V}),$$

$$D_t \theta = d_t \theta - \nabla_X \theta \cdot \mathbf{V} \quad \text{and} \quad D_t c_0 = d_t c_0 - \nabla_X c_0 \cdot \mathbf{V},$$

yields

$$\begin{aligned} \bar{\delta}_0^{\text{loc}} &= \nabla_X \mathbf{v} : \mathbf{P} - D_t \psi_0 - \sigma_0 D_t \theta + \mu D_t c_0 \\ &= [\nabla_X \mathbf{V} : \Sigma^* - J d_t \psi_t - D_t \psi_0] - \mathbf{V} \cdot \bar{\mathbf{S}}_0^{\text{loc}} + [\sigma_0 \nabla_X \theta \cdot \mathbf{v} - \mu \nabla_X c_0 \cdot \mathbf{v}] \\ &\quad - D_t \psi_0 - \sigma_0 D_t \theta + \mu D_t c_0 \\ &= \nabla_X \mathbf{V} : \Sigma^* - J d_t \psi_t - \mathbf{V} \cdot \bar{\mathbf{S}}_0^{\text{loc}} - [\sigma_0 d_t \theta - \mu d_t c_0] \\ &= \nabla_X \mathbf{V} : \Sigma - J d_t \phi_t - \mathbf{V} \cdot \bar{\mathbf{S}}_0^{\text{loc}} - [\sigma_0 d_t \theta - c_0 d_t \mu] \geq 0 \quad \text{in } B_0. \end{aligned} \quad (59)$$

The dissipation due to inhomogeneities in the undeformed configuration, that is $\mathbf{V} \cdot \bar{\mathbf{S}}_0^{\text{loc}}$, is clear in the configurational setting of Eq. (59). It is absent in the conventional statement of dissipation in the bulk (46).

Substituting the definition of the Eshelby stress Σ^* into the reduced dissipation inequality on the surface (47) yields

$$\begin{aligned} \hat{\delta}_0 &= [-\psi_0 + \mu c_0] \mathbf{U} \cdot \mathbf{N} \\ &= -\mathbf{U} \cdot \llbracket \Sigma^* - \mu c_0 \mathbf{I} \rrbracket \cdot \mathbf{N} + \mathbf{F}^t \cdot \hat{\mathbf{S}}_0 \\ &= -\mathbf{U} \cdot \llbracket \Sigma \cdot \mathbf{N} - \hat{\mathbf{S}}_0 \rrbracket \geq 0 \quad \text{on } \partial B_0. \end{aligned} \quad (60)$$

The following relation incorporating Eqs. (5) and (25) is required to determine the form of the dissipation inequality for a point on the singular surface S_0 :

$$\llbracket \mathbf{v} \rrbracket \cdot \llbracket \mathbf{P} \rrbracket \cdot \mathbf{M} = -\mathbf{U} \cdot \llbracket \mathbf{F}^t \cdot \mathbf{P} \rrbracket \cdot \mathbf{M}.$$

Substituting the previous relation into the dissipation inequality for a point on the singular surface S_0 (48) yields

$$\begin{aligned} \tilde{\delta}_0 &= \llbracket \llbracket \mathbf{v} \rrbracket \cdot \llbracket \mathbf{P} \rrbracket + \llbracket \phi_0 \rrbracket \mathbf{U} \rrbracket \cdot \mathbf{M} \\ &= \mathbf{U} \cdot \llbracket \Sigma \rrbracket \cdot \mathbf{M} \geq 0 \quad \text{on } S_0, \end{aligned} \quad (61)$$

thereby identifying the Eshelby stress Σ expressed in terms of the Legendre transformed energy ϕ_0 as the driving force behind the movement of the interface in the reference configuration and the associated energy dissipated.

5. Example

The objective of this section is to elucidate the nature of configurational forces via a simple example. Inelastic effects and body forces are ignored here for the sake of simplicity.

Consider a rigid diffuser wherein heat conduction and species diffusion can occur, that is $\phi_0 = \phi_0(\theta, \mu, \mathbf{X})$. From the definition of rigidity, the energetic Piola stress is non-existent. The

Table 1Summary of the key relations in the domain \mathcal{B}_0 , on the surface $\partial\mathcal{B}_0$ and on the interface \mathcal{S}_0 .

	Domain \mathcal{B}_0	Surface $\partial\mathcal{B}_0$	Interface \mathcal{S}_0
Deformation gradient	$D_t \mathbf{F} - \nabla_{\mathbf{x}} \mathbf{v} = \mathbf{0}$	$[\mathbf{F} \otimes \mathbf{U} + \mathbf{v} \otimes \mathbf{I}] \cdot \mathbf{N} = \hat{\mathbf{v}} \otimes \mathbf{N}$	$[[\mathbf{F}]] \otimes \mathbf{U} + [[\mathbf{v}]] \otimes \mathbf{I} \cdot \mathbf{M} = \mathbf{0}$
Conservation of:			
Solid mass	$D_t \rho_0 + \text{Div } \mathbf{R} = \bar{m}_0$	$[\rho_0 \mathbf{U} - \mathbf{R}] \cdot \mathbf{N} = \hat{m}_0$	$[[\mathbf{R}]] - [[\rho_0]] \mathbf{U} \cdot \mathbf{M} = 0$
Species mass	$D_t c_0 + \text{Div } \mathbf{W} = \bar{w}_0$	$[c_0 \mathbf{U} - \mathbf{W}] \cdot \mathbf{N} = \hat{w}_0$	$[[\mathbf{W}]] - [[c_0]] \mathbf{U} \cdot \mathbf{M} = 0$
Momentum:			
Linear	$\text{Div } \mathbf{P} = -\bar{\mathbf{s}}_0$ $\text{Div } \boldsymbol{\Sigma} = -\bar{\mathbf{S}}_0$	$\mathbf{P} \cdot \mathbf{N} = \hat{\mathbf{s}}_0 = \mathbf{s}_0$ $\boldsymbol{\Sigma} \cdot \mathbf{N} = \phi_0 \mathbf{N} + \hat{\mathbf{S}}_0$	$[[\mathbf{P}]] \cdot \mathbf{M} = \mathbf{0}$ $[[\boldsymbol{\Sigma}]] \cdot \mathbf{M} = [[\phi_0]] \mathbf{M} + \hat{\mathbf{S}}_0$
Angular	$\text{Div } \mathbf{L} = -\bar{\mathbf{m}}_0$	$\mathbf{L} \cdot \mathbf{N} = \hat{\mathbf{m}}_0 = \mathbf{m}_0$	$[[\mathbf{L}]] \cdot \mathbf{M} = \mathbf{0}$
Internal energy	$D_t \varepsilon_0 + \text{Div } \mathbf{E}^{\text{eff}} = \bar{\varepsilon}_0^{\text{eff}}$ $\mathbf{E}^{\text{eff}} := -\mathbf{v} \cdot \mathbf{P} + \mathbf{H} + \varphi \mathbf{W}$ $\bar{\varepsilon}_0^{\text{eff}} := \mathbf{v} \cdot \bar{\mathbf{s}}_0 + \bar{h}_0 + \varphi \bar{w}_0$	$[\varepsilon_0 \mathbf{U} - \mathbf{E}^{\text{eff}}] \cdot \mathbf{N} = \hat{\varepsilon}_0^{\text{eff}}$ $\hat{\varepsilon}_0^{\text{eff}} := \mathbf{v} \cdot \hat{\mathbf{s}}_0 + \hat{h}_0 + \varphi \hat{w}_0$	$[[\mathbf{E}^{\text{eff}}]] - [[\varepsilon_0]] \mathbf{U} \cdot \mathbf{M} = 0$
Entropy	$D_t \sigma_0 + \text{Div } \mathbf{S}^{\text{eff}} = \bar{\sigma}_0^{\text{eff}} + \bar{\pi}_0$ $\mathbf{S}^{\text{eff}} := \theta^{-1} \mathbf{H} + \zeta \mathbf{W}$ $\bar{\sigma}_0^{\text{eff}} := \theta^{-1} \bar{h}_0 + \zeta \bar{w}_0$	$[\sigma_0 \mathbf{U} - \mathbf{S}^{\text{eff}}] \cdot \mathbf{N} = \hat{\sigma}_0^{\text{eff}} + \hat{\pi}_0$ $\hat{\sigma}_0^{\text{eff}} := \theta^{-1} \hat{h}_0 + \zeta \hat{w}_0$	$[[\mathbf{S}^{\text{eff}}]] - [[\sigma_0]] \mathbf{U} \cdot \mathbf{M} = \hat{\pi}_0$
Constitutive relations	$\mathbf{P} = \partial_{\mathbf{F}} \psi_0, \mu = \partial_{c_0} \psi_0, s_0 = -\partial_{\theta} \psi_0$	$\hat{\delta}_0 = [-\psi_0 + \mu c_0] \mathbf{U} \cdot \mathbf{N} \geq 0$ $\phi_0 := \psi_0 - \mu c_0$	$\tilde{\delta}_0 = [[\mathbf{v}]] \cdot [[\mathbf{P}]] + [[\phi_0]] \mathbf{U} \cdot \mathbf{M} \geq 0$
Dissipation inequalities	$\bar{\delta}_0^{\text{loc}} = \nabla_{\mathbf{x}} \mathbf{v} : \mathbf{P} - D_t \psi_0 - \sigma_0 D_t \theta + \mu D_t c_0 \geq 0$ $\bar{\delta}_0^{\text{loc}} = \nabla_{\mathbf{x}} \mathbf{V} : \boldsymbol{\Sigma} - J d_t \psi_t - \mathbf{V} \cdot \nabla_{\mathbf{x}} \psi_0 - [\sigma_0 d_t \theta - c_0 d_t \mu] \geq 0$	$\hat{\delta}_0 = -\mathbf{U} \cdot [\boldsymbol{\Sigma} \cdot \mathbf{N} - \hat{\mathbf{S}}_0] \geq 0$ $\phi_0 := \psi_0 - \mu c_0$	$\tilde{\delta}_0 = \mathbf{U} \cdot [[\boldsymbol{\Sigma}]] \cdot \mathbf{M} \geq 0$

conventional equilibrium statement (23) is trivially satisfied. The configurational statement of equilibrium in the bulk (53) reduces to

$$\text{Div } \boldsymbol{\Sigma} = -\sigma_0 \nabla_{\mathbf{x}} \theta - c_0 \nabla_{\mathbf{x}} \mu + \partial_{\mathbf{x}} \phi_0.$$

The first two terms on the right-hand side describe the energetic resistance to changes in temperature and chemical potential in the undeformed configuration. The quantity $\sigma_0 \nabla_{\mathbf{x}} \theta$ is termed the thermal configurational (material) force [20,62]. The third term is the (configurational) body force.

The expression for the energy dissipated in the bulk in (59), reduces to

$$\bar{\delta}_0^{\text{loc}} \equiv \nabla_{\mathbf{x}} \mathbf{V} : \boldsymbol{\Sigma}^* - J d_t \psi_t + \mathbf{V} \cdot \nabla_{\mathbf{x}} \psi_0 - [\sigma_0 d_t \theta - c_0 d_t \mu].$$

The last term on the right-hand side accounts for the energy dissipated in evolving the temperature θ and the chemical potential μ in the undeformed configuration \mathcal{B}_0 . For the current example $J \equiv 1$.

The dissipation inequality on the surface \mathcal{S}_0 (61) yields

$$\tilde{\delta}_0 = \mathbf{U} \cdot [[\boldsymbol{\Sigma}]] \cdot \mathbf{M} \equiv [[\phi_0]] \mathbf{U} \cdot \mathbf{M} \geq 0 \quad \text{on } \mathcal{S}_0.$$

The above is a thermodynamic constraint that the interface can only propagate in the direction of increasing energy ϕ_0 , as depicted in Fig. 3(b). Energy from the region with the higher energy is expended to propagate the interface and thereby increase the extent of the lower energy phase.

6. Discussion and conclusions

A general framework for both deformational and configurational mechanics has been presented. The governing equations were obtained by considering the balance of several key quantities over a migrating control volume in the undeformed configuration. The framework was applied to the coupled problem of heat conduction and species diffusion within an inelastic continuum (the governing equations are summarised in Table 1); however it could be readily extended to consider a range of other phenomena such as energetic surfaces and interfaces, electro-magneto-mechanics, growth, higher-order and micromorphic continua, etc. Our recent work [47,63], for example, provides

the necessary foundation upon which to apply the framework developed here to continua having a surface or interface possessing its own energy.

The governing equations were then reformulated in terms of the Eshelby stress tensor via a pull-back to the undeformed configuration. The role of the Eshelby stress (and a modification thereof to account for species diffusion) as the driving force behind the kinetics of defects (e.g. cracks, inclusions, phase boundaries, dislocations) is clear in the configurational setting. This additional insight is one of the key reasons for adopting a configurational description as compared to the conventional deformational one.

The benefit of adopting a configurational description is not limited to describing defects. Various energy-based r-adaptive schemes to improve the quality of a finite element discretisation based on ideas from configurational mechanics are discussed in [19] and references therein, for example. Numerical computations based on the finite element method that extend those presented by the authors and co-workers in, for e.g., [22,23] will be presented in a future work.

A further extension of the work presented here to consider non-coherent surfaces is planned.

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Appendix A. Remarks on the form of the constitutive relations

Remark. A relationship for the diffusion flux vector \mathbf{W} that satisfies Eq. (50) is obtained from a classical Stokes–Einstein type argument [64] wherein the molecular velocity is assumed proportional to the driving force (i.e. the gradient of the chemical potential μ) via the, potentially concentration, temperature and deformation dependent,

second-order, positive-definite mobility tensor \mathbb{B} ; that is

$$\mathbf{W} = -c_0 \mathbb{B}(\mathbf{C}, \theta, c_0) \cdot \mathbf{C}^{-1} \cdot \nabla_{\mathbf{x}} \mu. \quad (\text{A.1})$$

Note that, even for a constant mobility tensor \mathbb{B} , there is coupling between deformation and diffusion due to the presence of the Finger tensor \mathbf{C}^{-1} which is a measure of the stretch. \square

Remark. A relationship of the form suggested by Eq. (50) for the effective entropy flux vector \mathbf{S}^{eff} is given by a non-standard Fourier–Duhamel type law (cf. [65]) of the form

$$\mathbf{S}^{\text{eff}} := [\theta^{-1} \mathbf{H} + \zeta \mathbf{W}] = -\mathbb{K}(\mathbf{C}, \theta, c_0) \cdot \mathbf{C}^{-1} \cdot \nabla_{\mathbf{x}} \theta, \quad (\text{A.2})$$

where \mathbb{K} is the positive-definite, second-order conductivity-like tensor for the bulk. Note that, as in the constitutive relation for the diffusing species flux vector in Eq. (A.1), even for a constant conductivity-like tensor \mathbb{K} there is geometric coupling due to the presence of the Finger tensor \mathbf{C}^{-1} . Additional coupling arises as the non-standard effective entropy flux vector \mathbf{S}^{eff} contains contributions due to thermal conduction and species diffusion. \square

Remark. An evolution equation for the inelastic internal variables α_0 that satisfies the reduced dissipation inequality is required. By defining $\mathbf{A}_0 := -\partial \psi_0 / \partial \alpha_0$ as the non-equilibrium stress conjugate to the history variable α_0 , a suitable form for the evolution of the history variable is [66]:

$$\mathbf{D}_t \alpha_0 = \mathbb{F}(\mathbf{C}, \alpha_0, c_0, \theta) : \mathbf{A}_0, \quad (\text{A.3})$$

where \mathbb{F} is the positive-definite, fourth-order fluidity tensor for the bulk. For further details on the development of constitutive relations for viscoelastic solids the reader is referred to Simo and Hughes [66]. \square

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