

# On GENERIC formalisms for complex fluids

Yukihito Suzuki\*

Organization for University Research Initiatives,  
Waseda University

## Abstract

The General Equation for Non-Equilibrium Reversible-Irreversible Coupling (GENERIC), proposed by Grmela and Öttinger[1, 2], serves as a general framework for the thermodynamically consistent modeling of continua, wherein the conservative and dissipative mechanisms are clearly distinguished. The conservative mechanism is formulated as a Hamiltonian system using the Poisson bracket, whereas the dissipative mechanism is formulated using a dissipative bracket acting on the entropy functional. Barotropic fluids, Korteweg-type fluids, and complex fluids with complicated micro-structures that necessitate introducing additional structural variables, are all formulated within the GENERIC formalism.

In the GENERIC formalism for Korteweg-type fluids, the spatial gradient of the mass density is included in the constitutive relation concerning the internal energy from which the Korteweg stress is derived. The interstitial working proposed by Dunn and Serrin[3] appears in the energy equation. Indeed, the GENERIC formalism provides a fairly simple derivation of the interstitial working, which was derived employing a Coleman–Noll type procedure[4] in an elaborate analysis. The GENERIC formalism also shows that the Korteweg stress and interstitial working are isentropic. This is in contrast with Cahn–Hilliard type models, which are intrinsically dissipative in nature as apparent from their bracket formulations[5].

Complex fluids can also be formulated within the GENERIC formalism[2, 6]. An additional structural variable, called the conformation tensor, can be introduced to model viscoelastic microstructures. The conformation tensor is assumed to be contravariant, similar to the left Cauchy–Green tensor of the deformation, and the time evolution along the flow, which is naturally represented by the Lie derivative of the tensor, is prescribed by the Poisson bracket in the GENERIC formalism. Additional terms in the Poisson bracket are purely kinematic, as long as the entropy function does not explicitly depend on the conformation tensor. It is advantageous to adopt the internal energy density as a state variable instead of the entropy density when constructing a dissipative bracket that models dissipation due to the microstructure.

## 1 GENERIC formalism

We define a state space  $\mathfrak{X}$ , each point of which uniquely determines the state of the isolated thermomechanical system<sup>1)</sup> considered. We also define functionals of the total energy  $E : \mathfrak{X} \rightarrow \mathbb{R}$  and the total entropy  $S : \mathfrak{X} \rightarrow \mathbb{R}$  of the system defined on the state space  $\mathfrak{X}$ . A Poisson bracket  $\{\cdot, \cdot\} : \mathcal{F}(\mathfrak{X}) \times \mathcal{F}(\mathfrak{X}) \rightarrow \mathcal{F}(\mathfrak{X})$ , which is a skew-symmetric bilinear mapping, and a dissipative bracket  $[\cdot, \cdot] : \mathcal{F}(\mathfrak{X}) \times \mathcal{F}(\mathfrak{X}) \rightarrow \mathcal{F}(\mathfrak{X})$ , which is a symmetric and positive semi-definite bilinear mapping, are also defined, where  $\mathcal{F}(\mathfrak{X})$  is a set of functionals defined on  $\mathfrak{X}$ . The Poisson bracket satisfies the Jacobi identity:

$$\{A, \{B, C\}\} + \{B, \{C, A\}\} + \{C, \{A, B\}\} = 0, \quad (1)$$

and the derivation property (or Leibniz rule):

$$\{AB, C\} = B\{A, C\} + A\{B, C\}, \quad (2)$$

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\*y\_suzuki@aoni.waseda.jp

<sup>1)</sup>Here, we have assumed the system to be isolated to simplify the discussion.

for all  $A, B, C \in \mathcal{F}(\mathfrak{X})$ , and is assumed to specify the conservative mechanism of the system. The dissipative bracket satisfies the derivation property:

$$[AB, C] = B[A, C] + A[B, C], \quad (3)$$

for all  $A, B, C \in \mathcal{F}(\mathfrak{X})$ , and is assumed to specify the dissipative mechanism of the system. The Poisson and dissipative brackets degenerate in the sense that

$$\{F, S\} = 0 \quad \text{and} \quad [F, E] = 0 \quad (4)$$

for all  $F \in \mathcal{F}(\mathfrak{X})$ .

Under the above settings, we can describe the time evolution of the system considered. Specifically, the time evolution of any functional  $F \in \mathcal{F}(\mathfrak{X})$  along any trajectory  $x : \mathbb{R} \rightarrow \mathfrak{X}$  in the state space is described<sup>2)</sup> as

$$\frac{dF}{dt}(x(t)) \left( := \frac{d}{dt}F(x(t)) \right) = \{F, E\}(x(t)) + [F, S](x(t)), \quad t \in \mathbb{R}. \quad (5)$$

Then, the laws of energy conservation and increasing entropy (i.e., the first and second laws of thermodynamics),

$$\frac{dE}{dt} = \{E, E\} + [E, S] = 0 \quad \text{and} \quad \frac{dS}{dt} = \{S, E\} + [S, S] = [S, S] \geq 0, \quad (6)$$

hold, due to the skew-symmetric property of the Poisson bracket combined with the degeneracy of the dissipative bracket and the degeneracy of the Poisson bracket combined with the positive semi-definiteness of the dissipative bracket, respectively.

According to the derivation property of the Poisson bracket, the linear functional  $\{\cdot, E\}(x) : \mathcal{F}(\mathfrak{X}) \rightarrow \mathbb{R}$  may be identified with a "tangent vector"<sup>3)</sup> of the Hamiltonian vector field with the Hamiltonian  $E$  at  $x \in \mathfrak{X}$ . This is tangential to both the isoenergetic and isentropic hypersurfaces, which are guaranteed by the skew-symmetric property and degeneracy of the Poisson bracket. This tangent vector determines the velocity of the isentropic trajectory in the state space. In this sense, the Poisson bracket governs the isentropic process of the system. Similarly, according to the derivation property of the dissipative bracket, the linear functional  $[\cdot, S](x) : \mathcal{F}(\mathfrak{X}) \rightarrow \mathbb{R}$  may be identified with a "tangent vector" at  $x \in \mathfrak{X}$ , which is tangential to the isoenergetic hypersurface and points in the direction of increasing entropy. The tangency of the vector to the isoenergetic hypersurface is guaranteed by the degeneracy, whereas the entropy ascending direction of the vector is guaranteed by the positive semi-definiteness of the dissipative bracket. This tangent vector determines the velocity of the dissipating (i.e., entropy increasing) trajectory in the state space. In this sense, the dissipative bracket governs the irreversible processes of the system.

## 2 Korteweg-type fluids

In this section, we give an outline of the GENERIC formalism for Korteweg-type fluids. Details will be reported in [7, 8].

### 2.1 State space

For an isolated system of Korteweg-type fluid in a bounded domain  $\Omega \subset E$  of a three-dimensional Euclidean space  $E$  with piecewise smooth boundaries, we choose the state space

$$\mathfrak{X}_s = \{(\rho, \mathbf{m}, s) \mid \rho \in C^\infty(\Omega, \mathbb{R}_{>0}), \mathbf{m} \in C^\infty(\Omega, V), s \in C^\infty(\Omega, \mathbb{R})\} \quad (7)$$

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<sup>2)</sup>The differentiability of the function  $F \circ x : \mathbb{R} \rightarrow \mathbb{R}$  is assumed to be guaranteed in some manner. Note that a state of the system  $x \in \mathfrak{X}$  itself can be interpreted as a functional on  $\mathfrak{X}$  in a distributional sense.

<sup>3)</sup>Here, we are thinking of a naive infinite dimensional analogy of tangent spaces on a finite dimensional manifold.

composed of the mass density  $\rho$ , the momentum density  $\mathbf{m}$ , and the entropy density  $s$ .  $V$  is the translation space of  $E$ . We can also choose the state space

$$\mathfrak{X}_e = \{(\rho, \mathbf{m}, e) | \rho \in C^\infty(\Omega, \mathbb{R}_{>0}), \mathbf{m} \in C^\infty(\Omega, V), e \in C^\infty(\Omega, \mathbb{R})\}, \quad (8)$$

which contains the internal energy density  $e$  as a state variable instead of the entropy density.

## 2.2 Energy and entropy

We choose the total energy and total entropy functionals defined on the state space  $\mathfrak{X}_s$  such that

$$\mathbf{E}_s(\rho, \mathbf{m}, s) = \int_{\Omega} \left[ \frac{|\mathbf{m}|^2}{2\rho} + \rho \epsilon \left( \rho, \frac{s}{\rho}, \nabla \rho \right) \right] dv \quad \text{and} \quad \mathbf{S}_s(\rho, \mathbf{m}, s) = \int_{\Omega} s dv, \quad (9)$$

where  $\epsilon : \mathbb{R}_{>0} \times \mathbb{R} \times \mathbb{R}^3 \rightarrow \mathbb{R}$  is the specific internal energy function and  $\nabla \rho$  is the spatial gradient of the density. However, if we choose the state space  $\mathfrak{X}_e$ , the total energy and total entropy functionals are defined as

$$\mathbf{E}_e(\rho, \mathbf{m}, e) = \int_{\Omega} \left[ \frac{|\mathbf{m}|^2}{2\rho} + e \right] dv \quad \text{and} \quad \mathbf{S}_e(\rho, \mathbf{m}, e) = \int_{\Omega} \rho \eta \left( \rho, \frac{e}{\rho}, \nabla \rho \right) dv, \quad (10)$$

where  $\eta : \mathbb{R}_{>0} \times \mathbb{R} \times \mathbb{R}^3 \rightarrow \mathbb{R}$  is the specific entropy function, which is an implicit function obtained by solving the specific internal energy function  $\epsilon = \epsilon(\rho, \eta, \nabla \rho)$  with respect to the specific entropy.

Here we assume a dependence of the internal energy on the gradient of the density to obtain the Korteweg stress.

## 2.3 Poisson bracket

The Poisson bracket on the state space  $\mathfrak{X}_s$  is defined as

$$\begin{aligned} \{F, G\}_s &= \int_{\Omega} \rho \left( \frac{\delta G}{\delta \mathbf{m}} \cdot \nabla \frac{\delta F}{\delta \rho} - \frac{\delta F}{\delta \mathbf{m}} \cdot \nabla \frac{\delta G}{\delta \rho} \right) dv + \int_{\Omega} \mathbf{m} \cdot \left[ \left( \frac{\delta G}{\delta \mathbf{m}} \cdot \nabla \right) \frac{\delta F}{\delta \mathbf{m}} - \left( \frac{\delta F}{\delta \mathbf{m}} \cdot \nabla \right) \frac{G}{\delta \mathbf{m}} \right] dv \\ &+ \int_{\Omega} s \left( \frac{\delta G}{\delta \mathbf{m}} \cdot \nabla \frac{\delta F}{\delta s} - \frac{\delta F}{\delta \mathbf{m}} \cdot \nabla \frac{\delta G}{\delta s} \right) dv \end{aligned} \quad (11)$$

for  $F, G \in \mathcal{F}(\mathfrak{X}_s)$ . Note that the Poisson bracket contains only the state variables and functionals, and therefore it does not depend on the material properties. This Poisson bracket is the same as that used for usual fluids described by the Euler equations. If we choose the state space  $\mathfrak{X}_e$ , the Poisson bracket for a Korteweg-type fluid is defined as

$$\begin{aligned} \{F, G\}_e &= \int_{\Omega} \rho \left( \frac{\delta G}{\delta \mathbf{m}} \cdot \nabla \frac{\delta F}{\delta \rho} - \frac{\delta F}{\delta \mathbf{m}} \cdot \nabla \frac{\delta G}{\delta \rho} \right) dv + \int_{\Omega} \mathbf{m} \cdot \left[ \left( \frac{\delta G}{\delta \mathbf{m}} \cdot \nabla \right) \frac{\delta F}{\delta \mathbf{m}} - \left( \frac{\delta F}{\delta \mathbf{m}} \cdot \nabla \right) \frac{G}{\delta \mathbf{m}} \right] dv \\ &+ \int_{\Omega} \left\{ \frac{\delta G}{\delta \mathbf{m}} \cdot \left[ e \nabla \frac{\delta F}{\delta e} + \nabla \left( p \frac{\delta F}{\delta e} \right) \right] - \frac{\delta F}{\delta \mathbf{m}} \cdot \left[ e \nabla \frac{\delta G}{\delta e} + \nabla \left( p \frac{\delta G}{\delta e} \right) \right] \right\} dv \\ &+ \int_{\Omega} [(\nabla^2 \rho) \boldsymbol{\xi}] \cdot \left( \frac{\delta F}{\delta e} \frac{\delta G}{\delta \mathbf{m}} - \frac{\delta G}{\delta e} \frac{\delta F}{\delta \mathbf{m}} \right) dv - \int_{\Omega} \rho \left[ \left( \frac{\delta G}{\delta \mathbf{m}} \cdot \nabla \right) \nabla \cdot \left( \frac{\delta F}{\delta e} \boldsymbol{\xi} \right) - \left( \frac{\delta F}{\delta \mathbf{m}} \cdot \nabla \right) \nabla \cdot \left( \frac{\delta G}{\delta e} \boldsymbol{\xi} \right) \right] dv \end{aligned} \quad (12)$$

for  $F, G \in \mathcal{F}(\mathfrak{X}_e)$ , where

$$p = \rho^2 \frac{\partial \epsilon}{\partial \rho} \quad \text{and} \quad \boldsymbol{\xi} = \rho \frac{\partial \epsilon}{\partial \nabla \rho} \quad (13)$$

are the pressure and a vector related to the Korteweg stress, respectively, and are defined using the derivatives of the specific internal energy function with respect to  $\rho$  and  $\nabla \rho$ , which depend on the constitutive relations. This means that this bracket explicitly depends on the material properties, unlike

the bracket (11) on the state space  $\mathfrak{X}_s$ . In the case of usual fluids described by the Euler equations, the last two terms in (12) are absent.

The two brackets defined above are apparently skew-symmetric and satisfy the degenerate conditions:

$$\{\mathbf{F}, \mathbf{S}_s\}_s = 0, \quad \forall \mathbf{F} \in \mathcal{F}(\mathfrak{X}_s) \quad \text{and} \quad \{\mathbf{F}, \mathbf{S}_e\}_e = 0, \quad \forall \mathbf{F} \in \mathcal{F}(\mathfrak{X}_e), \quad (14)$$

which are easily confirmed via direct computations using the following functional derivatives:

$$\frac{\delta \mathbf{S}_s}{\delta \rho} = 0, \quad \frac{\delta \mathbf{S}_s}{\delta \mathbf{m}} = \mathbf{0}, \quad \text{and} \quad \frac{\delta \mathbf{S}_s}{\delta s} = 1 \quad (15)$$

and

$$\frac{\delta \mathbf{S}_e}{\delta \rho} = -\frac{g}{\theta} + \nabla \cdot \frac{\boldsymbol{\xi}}{\theta}, \quad \frac{\delta \mathbf{S}_e}{\delta \mathbf{m}} = \mathbf{0}, \quad \text{and} \quad \frac{\delta \mathbf{S}_e}{\delta e} = \frac{1}{\theta}, \quad (16)$$

where  $\theta = \partial \epsilon / \partial \eta$  is the temperature and  $g = \epsilon - \theta \eta + p / \rho$  is the specific Gibbs free energy<sup>4</sup>.

Incidentally, the Poisson brackets defined above can be derived from the canonical Hamiltonian formulation in Lagrangian coordinates. Let  $\boldsymbol{\chi}_t : B \rightarrow \Omega$  be the deformation of the fluid from a reference configuration  $B$  to the current configuration  $\Omega$  at time  $t$ , and let  $\mathbf{p}_t : B \rightarrow V$  be the momentum conjugate to  $\boldsymbol{\chi}_t$  defined on the reference configuration. The Hamiltonian is defined as

$$\mathbf{H}(\boldsymbol{\chi}, \mathbf{p}; \eta_R) = \int_B \left[ \frac{|\mathbf{p}|^2}{2\rho_R} + \rho_R \epsilon(\rho(\boldsymbol{\chi}), \eta_R, \nabla \rho(\boldsymbol{\chi})) \right] dV, \quad (17)$$

where  $\rho(\boldsymbol{\chi}) = \rho_R / \det(\partial \boldsymbol{\chi} / \partial \mathbf{X})$  is the density on the current configuration determined by a deformation,  $\boldsymbol{\chi} : B \rightarrow \Omega$ , and  $\rho_R$  and  $\eta_R$  are the reference density and entropy, respectively, on the reference configuration. The canonical Poisson bracket is defined as

$$\{\mathbf{F}, \mathbf{G}\} = \int_B \left( \frac{\delta \mathbf{F}}{\delta \boldsymbol{\chi}} \cdot \frac{\delta \mathbf{G}}{\delta \mathbf{p}} - \frac{\delta \mathbf{G}}{\delta \boldsymbol{\chi}} \cdot \frac{\delta \mathbf{F}}{\delta \mathbf{p}} \right) dV. \quad (18)$$

Then, the canonical equations of motion for the Hamiltonian system become the momentum equations of an inviscid fluid with the Korteweg stress

$$\begin{aligned} \dot{\boldsymbol{\chi}}_t &= \mathbf{p}_t / \rho_R, \\ \dot{\mathbf{p}}_t &= (\det \mathbf{F}_t) \nabla \cdot \{ [-p_t + \rho_t \nabla \cdot (c \rho_t \nabla \rho_t)] \mathbf{1} - c \rho_t \nabla \rho_t \otimes \nabla \rho_t \}, \end{aligned} \quad (19)$$

where a dot above the variables denotes a time derivative,  $\mathbf{F} = \partial \boldsymbol{\chi} / \partial \mathbf{X}$  is the deformation gradient,  $p = \rho^2 \partial \epsilon / \partial \rho$  is the pressure, and the subscript  $t$  denotes the variable at time  $t$ .

The formulation outlined above in Lagrangian coordinates can be formally transformed to Eulerian coordinates using the following relations:

$$\begin{aligned} \rho_t(\mathbf{x}) &= \Phi_\rho(\boldsymbol{\chi}_t)(\mathbf{x}) = \int_B \rho_R(\mathbf{X}) \delta(\mathbf{x} - \boldsymbol{\chi}_t(\mathbf{X})) dV, \\ \mathbf{m}_t(\mathbf{x}) &= \Phi_{\mathbf{m}}(\boldsymbol{\chi}_t, \mathbf{p}_t)(\mathbf{x}) = \int_B \mathbf{p}_t(\mathbf{X}) \delta(\mathbf{x} - \boldsymbol{\chi}_t(\mathbf{X})) dV, \\ s_t(\mathbf{x}) &= \Phi_s(\boldsymbol{\chi}_t)(\mathbf{x}) = \int_B \rho_R(\mathbf{X}) \eta_R(\mathbf{X}) \delta(\mathbf{x} - \boldsymbol{\chi}_t(\mathbf{X})) dV, \end{aligned} \quad (20)$$

and

$$e_t(\mathbf{X}) = \Phi_e(\boldsymbol{\chi}_t)(\mathbf{x}) = \rho_t(\mathbf{x}) = \rho_t \epsilon \left( \rho_t(\mathbf{x}), \frac{s_t(\mathbf{x})}{\rho_t(\mathbf{x})}, \nabla \rho_t(\mathbf{x}) \right), \quad (21)$$

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<sup>4</sup>Note that these definitions and (13) are needed only if we choose the state space  $\mathfrak{X}_e$ . If we choose  $\mathfrak{X}_s$  instead, we do not have to give a concrete form for the specific internal energy function  $\epsilon$  or assume local thermodynamic equilibrium.

which provide transformations  $\Phi = (\Phi_\rho, \Phi_{\mathbf{m}}, \Phi_s)$  and  $\tilde{\Phi} = (\Phi_\rho, \Phi_{\mathbf{m}}, \Phi_e)$  from the Lagrangian variables  $(\boldsymbol{\chi}, \mathbf{p})$  to the Eulerian variables  $(\rho, \mathbf{m}, s)$  and  $(\rho, \mathbf{m}, e)$ . Indeed, the Poisson brackets  $\{\cdot, \cdot\}_s$  and  $\{\cdot, \cdot\}_e$  on the previously defined Eulerian variables are obtained from

$$\Phi^*\{F, G\}_s = \{\Phi^*F, \Phi^*G\} \quad \text{for } F, G \in \mathcal{F}(\mathfrak{X}_s) \quad (22)$$

and

$$\tilde{\Phi}^*\{F, G\}_e = \{\tilde{\Phi}^*F, \tilde{\Phi}^*G\} \quad \text{for } F, G \in \mathcal{F}(\mathfrak{X}_e), \quad (23)$$

where  $\Phi^*$  and  $\tilde{\Phi}^*$  are pull-back operators defined such that

$$\Phi^*F(\boldsymbol{\chi}, \mathbf{p}) = F(\Phi_\rho(\boldsymbol{\chi}), \Phi_{\mathbf{m}}(\boldsymbol{\chi}, \mathbf{p}), \Phi_s(\boldsymbol{\chi})) \quad \text{for } F \in \mathcal{F}(\mathfrak{X}_s) \quad (24)$$

and

$$\tilde{\Phi}^*F(\boldsymbol{\chi}, \mathbf{p}) = F(\Phi_\rho(\boldsymbol{\chi}), \Phi_{\mathbf{m}}(\boldsymbol{\chi}, \mathbf{p}), \Phi_e(\boldsymbol{\chi})) \quad \text{for } F \in \mathcal{F}(\mathfrak{X}_e). \quad (25)$$

The Hamiltonian functional  $H$  on the Lagrangian variables defined above is the pull-back of the total energy functional  $E_s$  or  $E_e$  on the Eulerian variables defined in the previous section, that is,  $H = \Phi^*E_s = \tilde{\Phi}^*E_e$ .

## 2.4 Dissipative bracket

The dissipative bracket on the state space  $\mathfrak{X}_s$  is defined as

$$\begin{aligned} [F, G]_s &= \int_{\Omega} 2\mu\theta \left( \left\langle \nabla \frac{\delta F}{\delta \mathbf{m}} \right\rangle - \frac{1}{\theta} \frac{\delta F}{\delta s} \langle \nabla \mathbf{v} \rangle \right) \cdot \left( \left\langle \nabla \frac{\delta G}{\delta \mathbf{m}} \right\rangle - \frac{1}{\theta} \frac{\delta G}{\delta s} \langle \nabla \mathbf{v} \rangle \right) dv \\ &\quad + \int_{\Omega} \lambda\theta \left( \nabla \cdot \frac{\delta F}{\delta \mathbf{m}} - \frac{1}{\theta} \frac{\delta F}{\delta s} \nabla \cdot \mathbf{v} \right) \left( \nabla \cdot \frac{\delta G}{\delta \mathbf{m}} - \frac{1}{\theta} \frac{\delta G}{\delta s} \nabla \cdot \mathbf{v} \right) dv + \int_{\Omega} \kappa\theta^2 \nabla \left( \frac{1}{\theta} \frac{\delta F}{\delta s} \right) \cdot \nabla \left( \frac{1}{\theta} \frac{\delta G}{\delta s} \right) dv, \end{aligned} \quad (26)$$

for  $F, G \in \mathcal{F}(\mathfrak{X}_s)$ , where

$$\langle \mathbf{T} \rangle = \frac{1}{2} (\mathbf{T} + \mathbf{T}^T) - \frac{1}{3} (\text{tr} \mathbf{T}) \mathbf{1}$$

is the projection of the second-order tensor  $\mathbf{T}$  onto a symmetric deviatoric tensor,  $\mathbf{T}^T$  and  $\text{tr} \mathbf{T}$  denote the transpose and trace of  $\mathbf{T}$ , respectively,  $\mathbf{1}$  is the unit tensor,  $\mu$  and  $\lambda$  are the shear and bulk viscosity coefficients, respectively, and  $\kappa$  is the thermal conductivity. If we choose the state space  $\mathfrak{X}_e$ , the dissipative bracket is defined as

$$\begin{aligned} [F, G]_e &= \int_{\Omega} 2\mu\theta \left( \left\langle \nabla \frac{\delta F}{\delta \mathbf{m}} \right\rangle - \frac{\delta F}{\delta e} \langle \nabla \mathbf{v} \rangle \right) \cdot \left( \left\langle \nabla \frac{\delta G}{\delta \mathbf{m}} \right\rangle - \frac{\delta G}{\delta e} \langle \nabla \mathbf{v} \rangle \right) dv \\ &\quad + \int_{\Omega} \lambda\theta \left( \nabla \cdot \frac{\delta F}{\delta \mathbf{m}} - \frac{\delta F}{\delta e} \nabla \cdot \mathbf{v} \right) \left( \nabla \cdot \frac{\delta G}{\delta \mathbf{m}} - \frac{\delta G}{\delta e} \nabla \cdot \mathbf{v} \right) dv + \int_{\Omega} \kappa\theta^2 \left( \nabla \frac{\delta F}{\delta e} \right) \cdot \left( \nabla \frac{\delta G}{\delta e} \right) dv \end{aligned} \quad (27)$$

for  $F, G \in \mathcal{F}(\mathfrak{X}_e)$ . In these brackets, (26) and (27),

$$\mathbf{v} = \frac{\delta E_s}{\delta \mathbf{m}} = \frac{\delta E_e}{\delta \mathbf{m}} \quad \text{and} \quad \theta = \frac{\delta E_s}{\delta s} = \left( \frac{\delta S_e}{\delta e} \right)^{-1} > 0, \quad (28)$$

are the velocity and temperature of the fluid<sup>5)</sup>, respectively. The functional derivative of the total energy with respect to the entropy density needs to be positive due to the thermodynamic stability.

<sup>5)</sup>The temperature is already defined in (16). We do not need to use it, however, if we choose the state space  $\mathfrak{X}_s$ . In that case, we can define the velocity and temperature as functional derivatives of the total energy (which is given as an ingredient of GENERIC) as in (28) and then the dissipative bracket is (26) without any further assumptions, in particular, the assumption of local thermodynamic equilibrium.

The dissipative brackets defined above are symmetric and positive semi-definite as long as the transport coefficients are all positive:

$$\mu \geq 0, \quad \lambda \geq 0, \quad \text{and} \quad \kappa \geq 0, \quad (29)$$

and satisfy the degenerate conditions:

$$[\mathbf{F}, \mathbf{E}_s]_s = 0, \quad \forall \mathbf{F} \in \mathcal{F}(\mathfrak{X}_s), \quad \text{and} \quad [\mathbf{F}, \mathbf{E}_e]_e = 0, \quad \forall \mathbf{F} \in \mathcal{F}(\mathfrak{X}_e), \quad (30)$$

which can be confirmed via direct computations using the following functional derivatives<sup>6)</sup>:

$$\frac{\delta \mathbf{E}_s}{\delta \rho} = -\frac{|\mathbf{m}|^2}{2\rho^2} + g - \nabla \cdot \boldsymbol{\xi}, \quad \frac{\delta \mathbf{E}_s}{\delta \mathbf{m}} = \frac{\mathbf{m}}{\rho}, \quad \frac{\delta \mathbf{E}_s}{\delta s} = \theta, \quad (31)$$

and

$$\frac{\delta \mathbf{E}_e}{\delta \rho} = -\frac{|\mathbf{m}|^2}{2\rho^2}, \quad \frac{\delta \mathbf{E}_e}{\delta \mathbf{m}} = \frac{\mathbf{m}}{\rho}, \quad \frac{\delta \mathbf{E}_e}{\delta e} = 1. \quad (32)$$

## 2.5 Time evolution

In the GENERIC formalism, the time evolution of any functional  $\mathbf{F} \in \mathcal{F}(\mathfrak{X}_s)$  is prescribed such that

$$\frac{d\mathbf{F}}{dt} = \{\mathbf{F}, \mathbf{E}_s\}_s + [\mathbf{F}, \mathbf{S}_s]_s. \quad (33)$$

If we take a functional  $\mathbf{F}$  on  $\mathfrak{X}_s$  in the form

$$\mathbf{F}(\rho, \mathbf{m}, s) = \int_{\Omega} (\phi \rho + \boldsymbol{\zeta} \cdot \mathbf{m} + \psi s) dv \quad (34)$$

for arbitrary functions  $\phi, \psi \in C_0^\infty(\Omega, \mathbb{R})$  and  $\boldsymbol{\zeta} \in C_0^\infty(\Omega, V)$ , we obtain the following local balance equations for the mass, momentum, and entropy:

$$\begin{aligned} \frac{\partial \rho}{\partial t} &= -\nabla \cdot \mathbf{m}, \\ \frac{\partial \mathbf{m}}{\partial t} &= -\nabla \cdot \left( \mathbf{m} \otimes \frac{\mathbf{m}}{\rho} \right) + \nabla \cdot [(\rho \nabla \cdot \boldsymbol{\xi} - p)\mathbf{1} - \nabla \rho \otimes \boldsymbol{\xi}] + \nabla \cdot [2\mu \langle \nabla \mathbf{v} \rangle + \lambda(\nabla \cdot \mathbf{v})\mathbf{1}], \\ \frac{\partial s}{\partial t} &= -\nabla \cdot \left( s \frac{\mathbf{m}}{\rho} - \frac{\kappa \nabla \theta}{\theta} \right) + \frac{1}{\theta} \left[ 2\mu \langle \nabla \mathbf{v} \rangle \cdot \langle \nabla \mathbf{v} \rangle + \lambda(\nabla \cdot \mathbf{v})^2 + \frac{\kappa}{\theta} |\nabla \theta|^2 \right], \end{aligned} \quad (35)$$

at least if the solution is sufficiently smooth. The terms in the momentum equation that contain  $\boldsymbol{\xi}$  represent the Korteweg stress. The Korteweg stress models the surface tension acting on the diffuse interface and comes from the Poisson bracket; therefore, it has nothing to do with the dissipation.

If we choose the state space  $\mathfrak{X}_e$ , the time evolution of any functional  $\mathbf{F} \in \mathcal{F}(\mathfrak{X}_e)$  is described by

$$\frac{d\mathbf{F}}{dt} = \{\mathbf{F}, \mathbf{E}_e\}_e + [\mathbf{F}, \mathbf{S}_e]_e. \quad (36)$$

If we take a functional  $\mathbf{F}$  on  $\mathfrak{X}_e$  in the form

$$\mathbf{F}(\rho, \mathbf{m}, e) = \int_{\Omega} (\phi \rho + \boldsymbol{\zeta} \cdot \mathbf{m} + \psi e) dv \quad (37)$$

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<sup>6)</sup>Here, we have assumed local thermodynamic equilibrium and have employed standard relations in equilibrium thermodynamics to compute the concrete form of the functional derivatives of  $\mathbf{E}_s$ .

for arbitrary functions  $\phi, \psi \in C_0^\infty(\Omega, \mathbb{R})$  and  $\zeta \in C_0^\infty(\Omega, V)$ , we obtain the following local balance equations for the mass, momentum, and internal energy:

$$\begin{aligned}\frac{\partial \rho}{\partial t} &= -\nabla \cdot \mathbf{m}, \\ \frac{\partial \mathbf{m}}{\partial t} &= -\nabla \cdot \left( \mathbf{m} \otimes \frac{\mathbf{m}}{\rho} \right) + \nabla \cdot [(\rho \nabla \cdot \boldsymbol{\xi} - p)\mathbf{1} - \nabla \rho \otimes \boldsymbol{\xi}] + \nabla \cdot [2\mu \langle \nabla \mathbf{v} \rangle + \lambda(\nabla \cdot \mathbf{v})\mathbf{1}], \\ \frac{\partial e}{\partial t} &= -\nabla \cdot \left[ e \frac{\mathbf{m}}{\rho} + \rho(\nabla \cdot \mathbf{v})\boldsymbol{\xi} - \kappa \nabla \theta \right] + (\nabla \mathbf{v}) \cdot [(\rho \nabla \cdot \boldsymbol{\xi} - p)\mathbf{1} - \nabla \rho \otimes \boldsymbol{\xi}] + 2\mu \langle \nabla \mathbf{v} \rangle \cdot \langle \nabla \mathbf{v} \rangle + \lambda(\nabla \cdot \mathbf{v})^2,\end{aligned}\tag{38}$$

at least if the solution is sufficiently smooth. The balance equations for the mass and momentum are the same as before, and the Korteweg stress, which comes from the Poisson bracket, is contained in the momentum equation. The internal energy equation includes the interstitial work flux, which was first derived by Dunn and Serrin[3], in the first term on the right-hand side, in addition to the work done by the Korteweg stress in the second term. The interstitial work flux also comes from the Poisson bracket, and therefore the additional terms, that is, the Korteweg stress and interstitial work flux in this system of equations, are purely isentropic.

This is in contrast to Cahn–Hilliard type models, where the terms included to model two-phase flows are intrinsically dissipative. Indeed, the state space for the incompressible Navier–Stokes/Cahn–Hilliard equations can be written as

$$\mathfrak{X} = \{(\boldsymbol{\omega}, \varphi) | \boldsymbol{\omega} \in C^\infty(\Omega, V), \varphi \in C^\infty(\Omega, \mathbb{R})\};\tag{39}$$

the two functionals are the energy and enstrophy:

$$\mathbb{H} = \int_{\Omega} \frac{1}{2} |\mathbf{v}|^2 dv + \Psi \quad \text{and} \quad \mathbb{Z} = \int_{\Omega} \frac{1}{2} |\boldsymbol{\omega}|^2 dv + m\Psi,\tag{40}$$

where

$$\Psi = \int_{\Omega} \frac{1}{\varepsilon} \left[ f(\varphi) + \frac{\hat{\sigma}}{2} \varepsilon^2 |\nabla \varphi|^2 \right] dv\tag{41}$$

is the free energy of a diffuse interface,  $m$  is the mobility of the Cahn–Hilliard diffusion,  $\varepsilon$  is a measure of the thickness of the diffuse interface, and  $\hat{\sigma}$  is a measure of the surface energy; the Poisson and dissipative brackets are defined as

$$\{F, G\} = \int_{\Omega} \begin{pmatrix} \delta F / \delta \boldsymbol{\omega} & \delta F / \delta \varphi \end{pmatrix} \begin{pmatrix} \mathcal{L}_{11} & \mathcal{L}_{12} \\ \mathcal{L}_{21} & O \end{pmatrix} \begin{pmatrix} \delta G / \delta \boldsymbol{\omega} \\ \delta G / \delta \varphi \end{pmatrix} dv,\tag{42}$$

where

$$\mathcal{L}_{11} = -\nabla \times [\boldsymbol{\omega} \times (\nabla \times \cdot)], \quad \mathcal{L}_{12} = \nabla \times (\cdot \nabla \varphi), \quad \mathcal{L}_{21} = -\nabla \varphi \cdot (\nabla \times \cdot),$$

and

$$[F, G] = \int_{\Omega} \begin{pmatrix} \delta F / \delta \boldsymbol{\omega} & \delta F / \delta \varphi \end{pmatrix} \begin{pmatrix} \mathcal{M}_{11} & O \\ O & \mathcal{M}_{22} \end{pmatrix} \begin{pmatrix} \delta G / \delta \boldsymbol{\omega} \\ \delta G / \delta \varphi \end{pmatrix} dv,\tag{43}$$

where

$$\mathcal{M}_{11} = \nu \Delta \quad \text{and} \quad \mathcal{M}_{22} = \Delta,$$

which are skew-symmetric and symmetric positive semi-definite, respectively. Then, we obtain the vorticity and Cahn–Hilliard equations:

$$\begin{aligned}\frac{\partial \boldsymbol{\omega}}{\partial t} &= -\nabla \times (\boldsymbol{\omega} \times \mathbf{v}) - \varepsilon \hat{\sigma} \nabla \times (\Delta \varphi \nabla \varphi) + \nu \Delta \boldsymbol{\omega}, \\ \frac{\partial \varphi}{\partial t} &= -\mathbf{v} \cdot \nabla \varphi + m \Delta \left[ \frac{1}{\varepsilon} f'(\varphi) - \varepsilon \hat{\sigma} \Delta \varphi \right].\end{aligned}\tag{44}$$

The last terms on the right-hand sides of the two above equations come from the dissipative bracket, and therefore we see that the main part of the Cahn–Hilliard equation is purely dissipative.

Any solution of the balance equations (35) or (38) derived above satisfies the first and second laws of thermodynamics, because the balance equations have the GENERIC structure. Specifically,

$$\frac{dE}{dt} = \{E, E\} + [E, S] = 0 \quad \text{and} \quad \frac{dS}{dt} = \{S, E\} + [S, S] = [S, S] \geq 0 \quad (45)$$

are satisfied for the total energy and entropy functionals defined so far, irrespective of the state space  $\mathfrak{X}_s$  or  $\mathfrak{X}_e$ . Therefore, we obtain a thermodynamically consistent system of governing equations for Korteweg-type fluids.

### 3 Complex fluids

In this section, we give an outline of the GENERIC formalism for complex fluids. Details will be reported in [9].

#### 3.1 State space

For an isolated system of complex fluid in a bounded domain  $\Omega \subset E$  with piecewise smooth boundaries, we choose the state space

$$\mathfrak{X}_e = \{(\rho, \mathbf{m}, e, \mathbf{C}) \mid \rho \in C^\infty(\Omega, \mathbb{R}_{>0}), \mathbf{m} \in C^\infty(\Omega, V), e \in C^\infty(\Omega, \mathbb{R}), \mathbf{C} \in C^\infty(\Omega, \text{Sym})\} \quad (46)$$

composed of the mass density  $\rho$ , the momentum density  $\mathbf{m}$ , the internal energy density  $e$ , and the conformation tensor  $\mathbf{C}$ , where Sym is the set of all second-order symmetric tensors. The conformation tensor models viscoelastic microstructures, and is assumed to be symmetric and contravariant, similar to the left Cauchy–Green tensor  $\mathbf{B} = \mathbf{F}\mathbf{F}^T$  of the deformation  $\chi : B \rightarrow \Omega$ . A contravariant symmetric tensor induces an inner product in a cotangent space, and the left Cauchy–Green tensor can be interpreted as a change in the metric on the cotangent spaces caused by the deformation. Indeed, the left Cauchy–Green tensor is the push-forward of the unit tensor  $\mathbf{1}$  by the deformation, that is,  $\chi_* : \mathbf{1} \mapsto \mathbf{F}\mathbf{F}^T$ , because

$$(\chi_*\mathbf{1})(\alpha, \beta) = \mathbf{1}(\chi^*\alpha, \chi^*\beta) = (\mathbf{F}^T\alpha) \cdot \mathbf{1}(\mathbf{F}^T\beta) = \alpha \cdot \mathbf{F}\mathbf{1}\mathbf{F}^T\beta = (\mathbf{F}\mathbf{F}^T)(\alpha, \beta) \quad (47)$$

for all  $\alpha, \beta \in T_{\mathbf{x}}^*\Omega$ , where we have used the fact that a cotangent vector  $\alpha \in T_{\mathbf{x}}^*\Omega$  at a point  $\mathbf{x}$  in the current configuration  $\Omega$  is pulled back by the deformation  $\chi$  to  $\chi^*\alpha = \mathbf{F}^T\alpha \in T_{\chi^{-1}(\mathbf{x})}^*B$  at the corresponding point  $\chi^{-1}(\mathbf{x})$  in the reference configuration  $B$ . Similar to the left Cauchy–Green tensor, the conformation tensor is a contravariant symmetric tensor defined on the current configuration and is pulled back to the reference configuration as  $\chi^*\mathbf{C} = \mathbf{F}^{-1}\mathbf{C}\mathbf{F}^{-T}$  because

$$(\chi^*\mathbf{C})(\xi, \eta) = \mathbf{C}(\chi_*\xi, \chi_*\eta) = (\mathbf{F}^{-T}\xi) \cdot \mathbf{C}(\mathbf{F}^{-T}\eta) = \xi \cdot \mathbf{F}^{-1}\mathbf{C}\mathbf{F}^{-T}\eta = (\mathbf{F}^{-1}\mathbf{C}\mathbf{F}^{-T})(\xi, \eta) \quad (48)$$

for all  $\xi, \eta \in T_{\mathbf{X}}^*B$ , where we have used the fact that a cotangent vector  $\xi \in T_{\mathbf{X}}^*B$  at a point  $\mathbf{X}$  in the reference configuration  $B$  is pushed forward to  $\chi_*\xi = \mathbf{F}^{-T}\xi \in T_{\chi(\mathbf{X})}^*\Omega$  at the corresponding point  $\chi(\mathbf{X})$  in the current configuration  $\Omega$  by the deformation  $\chi$ . The time evolution of the conformation tensor along the motion is naturally given by the Lie derivative<sup>7)</sup>:

$$\begin{aligned} \mathcal{L}_{\mathbf{v}}\mathbf{C} &= \chi_{t*}(D_t(\chi_t^*\mathbf{C})) = \mathbf{F}(D_t(\mathbf{F}^{-1}\mathbf{C}\mathbf{F}^{-T}))\mathbf{F}^T \\ &= \mathbf{F}[(D_t\mathbf{F}^{-1})\mathbf{C}\mathbf{F}^{-T} + \mathbf{F}^{-1}(D_t\mathbf{C})\mathbf{F}^{-T} + \mathbf{F}^{-1}\mathbf{C}(D_t\mathbf{F}^{-T})]\mathbf{F}^T \\ &= \mathbf{F}\left[(-\mathbf{F}^{-1}\nabla\mathbf{v})\mathbf{C}\mathbf{F}^{-T} + \mathbf{F}^{-1}(D_t\mathbf{C})\mathbf{F}^{-T} + \mathbf{F}^{-1}\mathbf{C}(-\mathbf{F}^{-1}\nabla\mathbf{v})^T\right]\mathbf{F}^T \\ &= \frac{\partial\mathbf{C}}{\partial t} + (\mathbf{v} \cdot \nabla)\mathbf{C} - (\nabla\mathbf{v})\mathbf{C} - \mathbf{C}(\nabla\mathbf{v})^T, \end{aligned} \quad (49)$$

along the velocity field  $\mathbf{v} = d\chi_t/dt$  of the motion  $t \mapsto \chi_t$ , where  $D_t$  denotes the material time derivative, which is a time differentiation holding the material point fixed.

<sup>7)</sup>The Lie derivative is defined as  $\mathcal{L}_{\mathbf{v}}\mathbf{C}(\chi_t(\mathbf{X}), t) = \lim_{h \rightarrow 0}(1/h) \left[ (\chi_{-t}^* \circ \chi_{t+h}^*)\mathbf{C}(\chi_{t+h}(\mathbf{X}), t+h) - \mathbf{C}(\chi_t(\mathbf{X}), t) \right] = (d/d\tau) \left[ (\chi_{-t}^* \circ \chi_\tau^*)\mathbf{C}(\chi_\tau(\mathbf{X}), \tau) \right] \Big|_{\tau=t} = \chi_{-t}^* \left[ (d/d\tau) (\chi_\tau^*\mathbf{C})(\mathbf{X}, \tau) \Big|_{\tau=t} \right]$ , where  $\mathbf{X} = \chi_t^{-1}(\mathbf{x})$ .



### 3.2 Energy and entropy

We choose the total energy and total entropy functionals defined on the state space  $\mathfrak{X}_e$  such that

$$E_e(\rho, \mathbf{m}, e, \mathbf{C}) = \int_{\Omega} \left[ \frac{|\mathbf{m}|^2}{2\rho} + e + e_c(\rho, \mathbf{C}) \right] dv \quad \text{and} \quad S_e(\rho, \mathbf{m}, e, \mathbf{C}) = \int_{\Omega} \left[ \rho\eta \left( \rho, \frac{e}{\rho} \right) + \rho\eta_c(\mathbf{C}) \right] dv, \quad (50)$$

where  $e_c : \mathbb{R}_{>0} \times \text{Sym} \rightarrow \mathbb{R}$  is the internal energy density and  $\eta_c : \text{Sym} \rightarrow \mathbb{R}$  is the specific entropy due to the microstructure of the complex fluid. We chose these specific forms of additional energy and entropy to make the simplification easier, as shown later.

### 3.3 Poisson bracket

The Poisson bracket on the state space  $\mathfrak{X}_e$  for complex fluids is defined such that

$$\begin{aligned} \{F, G\}_e &= \int_{\Omega} \rho \left( \frac{\delta G}{\delta \mathbf{m}} \cdot \nabla \frac{\delta F}{\delta \rho} - \frac{\delta F}{\delta \mathbf{m}} \cdot \nabla \frac{\delta G}{\delta \rho} \right) dv + \int_{\Omega} \mathbf{m} \cdot \left[ \left( \frac{\delta G}{\delta \mathbf{m}} \cdot \nabla \right) \frac{\delta F}{\delta \mathbf{m}} - \left( \frac{\delta F}{\delta \mathbf{m}} \cdot \nabla \right) \frac{G}{\delta \mathbf{m}} \right] dv \\ &\quad + \int_{\Omega} \left\{ \frac{\delta G}{\delta \mathbf{m}} \cdot \left[ e \nabla \frac{\delta F}{\delta e} + \nabla \left( p \frac{\delta F}{\delta e} \right) \right] - \frac{\delta F}{\delta \mathbf{m}} \cdot \left[ e \nabla \frac{\delta G}{\delta e} + \nabla \left( p \frac{\delta G}{\delta e} \right) \right] \right\} dv \\ &\quad - 2 \int_{\Omega} \rho \theta \mathbf{C} \frac{\partial \eta_c}{\partial \mathbf{C}} \cdot \left[ \frac{\delta F}{\delta e} \left( \nabla \frac{\delta G}{\delta \mathbf{m}} \right)^T - \frac{\delta G}{\delta e} \left( \nabla \frac{\delta F}{\delta \mathbf{m}} \right)^T \right] dv \\ &\quad + \int_{\Omega} \mathbf{C} \cdot \left[ \nabla \cdot \left( \frac{\delta F}{\delta \mathbf{C}} \otimes \frac{\delta G}{\delta \mathbf{m}} - \frac{\delta G}{\delta \mathbf{C}} \otimes \frac{\delta F}{\delta \mathbf{m}} \right) \right. \\ &\quad \left. + \left( \nabla \frac{\delta G}{\delta \mathbf{m}} \right)^T \frac{\delta F}{\delta \mathbf{C}} - \left( \nabla \frac{\delta F}{\delta \mathbf{m}} \right)^T \frac{\delta G}{\delta \mathbf{C}} + \frac{\delta F}{\delta \mathbf{C}} \left( \nabla \frac{\delta G}{\delta \mathbf{m}} \right) - \frac{\delta G}{\delta \mathbf{C}} \left( \nabla \frac{\delta F}{\delta \mathbf{m}} \right) \right] dv \end{aligned} \quad (51)$$

for functionals  $F, G \in \mathcal{F}(\mathfrak{X}_e)$ . If the last two terms, which contain the conformation tensor, are absent, the formulation reduces to that for simple fluids governed by the Euler equations.

The Poisson bracket defined above is apparently skew-symmetric and satisfies the degenerate condition:  $\{F, S_e\}_e = 0$ , for all functionals  $F \in \mathcal{F}(\mathfrak{X}_e)$ . This can be confirmed via direct computations using the following functional derivatives:

$$\frac{\delta S_e}{\delta \rho} = -\frac{g}{\theta} + \eta_c, \quad \frac{\delta S_e}{\delta \mathbf{m}} = \mathbf{0}, \quad \frac{\delta S_e}{\delta e} = \frac{1}{\theta}, \quad \text{and} \quad \frac{\delta S_e}{\delta \mathbf{C}} = \rho \frac{\partial \eta_c}{\partial \mathbf{C}}. \quad (52)$$

The fourth term of the Poisson bracket (51), which is necessary to satisfy the degenerate condition as long as the additional entropy  $\eta_c$  depends on the conformation tensor, includes  $\theta = (\delta S_e / \delta e)^{-1} = (\partial \eta / \partial \epsilon)^{-1}$  and  $\partial \eta_c / \partial \mathbf{C}$  and therefore depends on the constitutive relations. This is also true for the Poisson bracket:

$$\begin{aligned} \{F, G\}_s &= \int_{\Omega} \rho \left( \frac{\delta G}{\delta \mathbf{m}} \cdot \nabla \frac{\delta F}{\delta \rho} - \frac{\delta F}{\delta \mathbf{m}} \cdot \nabla \frac{\delta G}{\delta \rho} \right) dv + \int_{\Omega} \mathbf{m} \cdot \left[ \left( \frac{\delta G}{\delta \mathbf{m}} \cdot \nabla \right) \frac{\delta F}{\delta \mathbf{m}} - \left( \frac{\delta F}{\delta \mathbf{m}} \cdot \nabla \right) \frac{G}{\delta \mathbf{m}} \right] dv \\ &\quad + \int_{\Omega} s \left( \frac{\delta G}{\delta \mathbf{m}} \cdot \nabla \frac{\delta F}{\delta s} - \frac{\delta F}{\delta \mathbf{m}} \cdot \nabla \frac{\delta G}{\delta s} \right) dv \\ &\quad - 2 \int_{\Omega} \rho \theta \mathbf{C} \frac{\partial \eta_c}{\partial \mathbf{C}} \cdot \left[ \frac{\delta F}{\delta e} \left( \nabla \frac{\delta G}{\delta \mathbf{m}} \right)^T - \frac{\delta G}{\delta e} \left( \nabla \frac{\delta F}{\delta \mathbf{m}} \right)^T \right] dv \\ &\quad + \int_{\Omega} \mathbf{C} \cdot \left[ \nabla \cdot \left( \frac{\delta F}{\delta \mathbf{C}} \otimes \frac{\delta G}{\delta \mathbf{m}} - \frac{\delta G}{\delta \mathbf{C}} \otimes \frac{\delta F}{\delta \mathbf{m}} \right) \right. \\ &\quad \left. + \left( \nabla \frac{\delta G}{\delta \mathbf{m}} \right)^T \frac{\delta F}{\delta \mathbf{C}} - \left( \nabla \frac{\delta F}{\delta \mathbf{m}} \right)^T \frac{\delta G}{\delta \mathbf{C}} + \frac{\delta F}{\delta \mathbf{C}} \left( \nabla \frac{\delta G}{\delta \mathbf{m}} \right) - \frac{\delta G}{\delta \mathbf{C}} \left( \nabla \frac{\delta F}{\delta \mathbf{m}} \right) \right] dv \end{aligned} \quad (53)$$

on the state space  $\mathfrak{X}_s = \{(\rho, \mathbf{m}, s, \mathbf{C}) | \rho \in C^\infty(\Omega, \mathbb{R}_{>0}), \mathbf{m} \in C^\infty(\Omega, V), s \in C^\infty(\Omega, \mathbb{R}), \mathbf{C} \in C^\infty(\Omega, \text{Sym})\}$ , which otherwise does not explicitly contain any information concerning the material. The material properties enter the Poisson bracket if the entropy depends on the conformation tensor.

### 3.4 Dissipative bracket

The dissipative bracket for a complex fluid on the state space  $\mathfrak{X}_e$  is defined such that

$$\begin{aligned} [\mathbf{F}, \mathbf{G}]_e &= \int_{\Omega} \begin{pmatrix} \delta\mathbf{F}/\delta e & \delta\mathbf{F}/\delta\mathbf{C} \\ -\mathcal{R}(\partial e_c/\partial\mathbf{C}) & \mathcal{R} \end{pmatrix} \begin{pmatrix} (\partial e_c/\partial\mathbf{C}) \cdot \mathcal{R}(\partial e_c/\partial\mathbf{C}) & -\mathcal{R}(\partial e_c/\partial\mathbf{C}) \\ \mathcal{R} & \mathcal{R} \end{pmatrix} \begin{pmatrix} \delta\mathbf{G}/\delta e \\ \delta\mathbf{G}/\delta\mathbf{C} \end{pmatrix} dv \\ &= \int_{\Omega} \left[ \frac{\delta\mathbf{F}}{\delta e} \left( \frac{\partial e_c}{\partial\mathbf{C}} \cdot \mathcal{R} \frac{\partial e_c}{\partial\mathbf{C}} \right) \frac{\delta\mathbf{G}}{\delta e} - \frac{\delta\mathbf{F}}{\delta e} \left( \frac{\partial e_c}{\partial\mathbf{C}} \cdot \mathcal{R} \frac{\delta\mathbf{G}}{\delta\mathbf{C}} \right) - \left( \frac{\delta\mathbf{F}}{\delta\mathbf{C}} \cdot \mathcal{R} \frac{\partial e_c}{\partial\mathbf{C}} \right) \frac{\delta\mathbf{G}}{\delta e} + \frac{\delta\mathbf{F}}{\delta\mathbf{C}} \cdot \mathcal{R} \frac{\delta\mathbf{G}}{\delta\mathbf{C}} \right] dv, \end{aligned} \quad (54)$$

for functionals  $\mathbf{F}, \mathbf{G} \in \mathcal{F}(\mathfrak{X}_e)$ , where  $\mathcal{R} : \text{Sym} \rightarrow \text{Sym}$  is a symmetric and positive semi-definite fourth-order tensor satisfying

$$\mathbf{A} \cdot \mathcal{R}\mathbf{B} = \mathcal{R}\mathbf{A} \cdot \mathbf{B} \quad \text{and} \quad \mathbf{A} \cdot \mathcal{R}\mathbf{A} \geq 0 \quad (55)$$

for all  $\mathbf{A}, \mathbf{B} \in \text{Sym}$ .

The dissipative bracket defined above is apparently symmetric and is positive semi-definite because

$$\begin{aligned} [\mathbf{F}, \mathbf{F}]_e &= \int_{\Omega} \left[ \frac{\delta\mathbf{F}}{\delta e} \left( \frac{\partial e_c}{\partial\mathbf{C}} \cdot \mathcal{R} \frac{\partial e_c}{\partial\mathbf{C}} \right) \frac{\delta\mathbf{F}}{\delta e} - \frac{\delta\mathbf{F}}{\delta e} \left( \mathcal{R} \frac{\partial e_c}{\partial\mathbf{C}} \cdot \frac{\delta\mathbf{F}}{\delta\mathbf{C}} \right) - \left( \mathcal{R} \frac{\delta\mathbf{F}}{\delta\mathbf{C}} \cdot \frac{\partial e_c}{\partial\mathbf{C}} \right) \frac{\delta\mathbf{F}}{\delta e} + \frac{\delta\mathbf{F}}{\delta\mathbf{C}} \cdot \mathcal{R} \frac{\delta\mathbf{F}}{\delta\mathbf{C}} \right] dv \\ &= \int_{\Omega} \left( \frac{\delta\mathbf{F}}{\delta e} \frac{\partial e_c}{\partial\mathbf{C}} - \frac{\delta\mathbf{F}}{\delta\mathbf{C}} \right) \cdot \mathcal{R} \left( \frac{\delta\mathbf{F}}{\delta e} \frac{\partial e_c}{\partial\mathbf{C}} - \frac{\delta\mathbf{F}}{\delta\mathbf{C}} \right) dv \geq 0. \end{aligned} \quad (56)$$

for all  $\mathbf{F} \in \mathcal{F}(\mathfrak{X}_e)$ . It also satisfies the degenerate condition:  $[\mathbf{F}, \mathbf{E}_e]_e = 0$  for all  $\mathbf{F} \in \mathcal{F}(\mathfrak{X}_e)$ , which can be confirmed via direct computations using the functional derivatives:

$$\frac{\delta\mathbf{E}_e}{\delta\rho} = -\frac{|\mathbf{m}|^2}{2\rho^2} + \frac{\partial e_c}{\partial\rho}, \quad \frac{\delta\mathbf{E}_e}{\delta\mathbf{m}} = \frac{\mathbf{m}}{\rho}, \quad \frac{\delta\mathbf{E}_e}{\delta e} = 1, \quad \text{and} \quad \frac{\delta\mathbf{E}_e}{\delta\mathbf{C}} = \frac{\partial e_c}{\partial\mathbf{C}}. \quad (57)$$

Note that the dissipative bracket (54) represents the dissipation due to the microstructure. If there is heat conduction, for example, we need to add a corresponding term:  $\int_{\Omega} \kappa \theta^2 \nabla(\delta\mathbf{F}/\delta e) \cdot \nabla(\delta\mathbf{G}/\delta e) dv$ , which is the same as in the case of Korteweg-type fluids, as explained in the previous section.

We can also choose the state space  $\mathfrak{X}_s$ , which contains the entropy density instead of the internal energy density as a state variable, and define the Poisson bracket (53), as well as the total energy and entropy functionals on  $\mathfrak{X}_s$ . It appears difficult, however, to define the dissipative bracket on  $\mathfrak{X}_s$  transforming the bracket (54) on  $\mathfrak{X}_e$  to that on  $\mathfrak{X}_s$  while maintaining the degenerate condition:

$$[\mathbf{F}, \mathbf{E}_e]_e = \int_{\Omega} \left[ \frac{\delta\mathbf{F}}{\delta e} \left( \frac{\partial e_c}{\partial\mathbf{C}} \cdot \mathcal{R} \frac{\partial e_c}{\partial\mathbf{C}} \right) 1 - \frac{\delta\mathbf{F}}{\delta e} \left( \frac{\partial e_c}{\partial\mathbf{C}} \cdot \mathcal{R} \frac{\partial e_c}{\partial\mathbf{C}} \right) - \left( \frac{\delta\mathbf{F}}{\delta\mathbf{C}} \cdot \mathcal{R} \frac{\partial e_c}{\partial\mathbf{C}} \right) 1 + \frac{\delta\mathbf{F}}{\delta\mathbf{C}} \cdot \mathcal{R} \frac{\partial e_c}{\partial\mathbf{C}} \right] dv = 0. \quad (58)$$

This condition holds because  $\delta\mathbf{E}_e/\delta e = 1$  and  $\delta\mathbf{E}_e/\delta\mathbf{C} = \partial e_c/\partial\mathbf{C}$ . However, these functional derivatives will be replaced with  $\delta\mathbf{E}_s/\delta s$  and  $\delta\mathbf{E}_s/\delta\mathbf{C}$  in the dissipative bracket on  $\mathfrak{X}_s$  if we change the state space  $\mathfrak{X}_e$  to  $\mathfrak{X}_s$ . In that case, it will be difficult to satisfy the corresponding condition  $[\mathbf{F}, \mathbf{E}_s]_s = 0$  because  $\delta\mathbf{E}_s/\delta s$  necessarily contains the temperature  $\theta$ .

### 3.5 Time evolution

The time evolution of the functional defined on the state space  $\mathfrak{X}_e$  is prescribed such that

$$\frac{d\mathbf{F}}{dt} = \{\mathbf{F}, \mathbf{E}_e\}_e + [\mathbf{F}, \mathbf{S}_e]_e \quad (59)$$

for  $F \in \mathcal{F}(\mathfrak{X}_e)$ . If we take a functional  $F$  on  $\mathfrak{X}_e$  in the form

$$F(\rho, \mathbf{m}, e, \mathbf{C}) = \int_{\Omega} (\phi\rho + \boldsymbol{\zeta} \cdot \mathbf{m} + \psi e + \boldsymbol{\Sigma} \cdot \mathbf{C}) dv \quad (60)$$

for arbitrary functions  $\phi, \psi \in C_0^\infty(\Omega, \mathbb{R})$ ,  $\boldsymbol{\zeta} \in C_0^\infty(\Omega, V)$  and  $\boldsymbol{\Sigma} \in C_0^\infty(\Omega, \text{Sym})$ , we obtain the following local balance equations for the mass, momentum, internal energy, and conformation tensor:

$$\begin{aligned} \frac{\partial \rho}{\partial t} &= -\nabla \cdot \mathbf{m}, \\ \frac{\partial \mathbf{m}}{\partial t} &= -\nabla \cdot \left( \mathbf{m} \otimes \frac{\mathbf{m}}{\rho} \right) - \rho \nabla \frac{\partial e_c}{\partial \rho} - \nabla \cdot \left( p\mathbf{1} + 2\rho\theta \frac{\partial \eta_c}{\partial \mathbf{C}} \mathbf{C} \right) + \nabla \cdot \left( e_c \mathbf{1} + 2 \frac{\partial e_c}{\partial \mathbf{C}} \mathbf{C} \right), \\ \frac{\partial e}{\partial t} &= -\nabla \cdot \left( e \frac{\mathbf{m}}{\rho} \right) - \left( p\mathbf{1} + 2\rho\theta \frac{\partial \eta_c}{\partial \mathbf{C}} \mathbf{C} \right) \cdot \left( \nabla \frac{\mathbf{m}}{\rho} \right) + \frac{1}{\theta} \frac{\partial e_c}{\partial \mathbf{C}} \cdot \mathcal{R} \left( \frac{\partial e_c}{\partial \mathbf{C}} - \rho\theta \frac{\partial \eta_c}{\partial \mathbf{C}} \right), \\ \mathcal{L}_v \mathbf{C} &= -\frac{1}{\theta} \mathcal{R} \left( \frac{\partial e_c}{\partial \mathbf{C}} - \rho\theta \frac{\partial \eta_c}{\partial \mathbf{C}} \right), \end{aligned} \quad (61)$$

at least if the solution is sufficiently smooth. Note that  $\rho, \mathbf{m}$ , and  $e$  are densities, which are quantities to integrate over a spatial domain, and their time evolutions are described by partial derivatives with the spatial coordinates held fixed. Conversely,  $\mathbf{C}$  represents a local quantity, which is a microstructure of the fluid and advects with the flow.

If we assume the following constitutive relations:

$$e_c(\rho, \mathbf{C}) = \frac{1}{2} \text{tr} [(\mathbf{C} - \mathbf{1})^2], \quad \eta_c(\mathbf{C}) = \text{const.}, \quad \text{and} \quad \mathcal{R} = \frac{\theta}{\tau} \mathcal{I}, \quad (62)$$

where  $\mathcal{I}$  is a fourth-order unit tensor and  $\tau$  is the time scale of dissipation, we obtain a standard model for complex fluids as follows:

$$\begin{aligned} \frac{\partial \rho}{\partial t} &= -\nabla \cdot \mathbf{m}, \\ \frac{\partial \mathbf{m}}{\partial t} &= -\nabla \cdot \left( \mathbf{m} \otimes \frac{\mathbf{m}}{\rho} \right) - \nabla p + \nabla \cdot \left\{ \frac{1}{2} |\mathbf{C} - \mathbf{1}|^2 \mathbf{1} + 2(\mathbf{C} - \mathbf{1})\mathbf{C} \right\}, \\ \frac{\partial e}{\partial t} &= -\nabla \cdot \left( e \frac{\mathbf{m}}{\rho} \right) - p \left( \nabla \cdot \frac{\mathbf{m}}{\rho} \right) + \frac{1}{\tau} |\mathbf{C} - \mathbf{1}|^2, \\ \mathcal{L}_v \mathbf{C} &= -\frac{1}{\tau} (\mathbf{C} - \mathbf{1}), \end{aligned} \quad (63)$$

where we computed the partial derivatives of the constitutive relations as follows:

$$\frac{\partial e_c}{\partial \rho} = 0, \quad \frac{\partial e_c}{\partial \mathbf{C}} = \mathbf{C} - \mathbf{1}, \quad \text{and} \quad \frac{\partial \eta_c}{\partial \mathbf{C}} = \mathbf{0}. \quad (64)$$

The assumed form of the additional internal energy satisfies the objectivity requirement of continuum mechanics because it can be written using the principal invariants of the contravariant tensor  $\hat{\mathbf{C}} = \mathbf{C} - \mathbf{1}$  defined on the current configuration. Indeed,

$$e_c(\rho, \mathbf{C}) = \frac{1}{2} \text{tr} \hat{\mathbf{C}}^2 = \frac{1}{2} (\text{tr} \hat{\mathbf{C}})^2 - \frac{1}{2} \left[ (\text{tr} \hat{\mathbf{C}})^2 - \text{tr} \hat{\mathbf{C}}^2 \right] = \frac{1}{2} \text{I}_{\hat{\mathbf{C}}}^2 - \text{II}_{\hat{\mathbf{C}}}, \quad (65)$$

where  $\text{I}_{\hat{\mathbf{C}}} = \text{tr} \hat{\mathbf{C}}$  and  $\text{II}_{\hat{\mathbf{C}}} = (1/2)[(\text{tr} \hat{\mathbf{C}})^2 - \text{tr} \hat{\mathbf{C}}^2]$  are the first and second invariants of the second-order tensor  $\hat{\mathbf{C}}$ , respectively. Note that, if tensor  $\mathbf{C}$  is a unit tensor, this additional energy vanishes and all terms concerning the conformation tensor in the balance equations also vanish. The assumed form of the additional energy guarantees that the Poisson bracket (53) on the state space  $\mathfrak{X}_s$  does not explicitly depend on the material properties because  $\partial \eta_c / \partial \mathbf{C} = \mathbf{0}$ , and therefore the fourth term of the Poisson bracket (53) also vanishes; the remaining terms contain only state variables and derivatives of functionals with respect to the state variables.

Any solution of the balance equations, (61) or (63) derived above, satisfies the first and second laws of thermodynamics because the balance equations have the GENERIC structure. Specifically,

$$\frac{dE_e}{dt} = \{E_e, E_e\}_e + [E_e, S_e]_e = 0 \quad \text{and} \quad \frac{dS_e}{dt} = \{S_e, E_e\}_e + [S_e, S_e]_e = [S_e, S_e]_e \geq 0 \quad (66)$$

hold for the total energy and entropy functionals defined in (50). Therefore, we obtain a thermodynamically consistent system of governing equations for complex fluids.

## 4 Concluding remarks

Thermodynamically consistent governing equations for Korteweg-type fluids and complex fluids are derived in the GENERIC formalism, where the conservation of the total energy and the condition of increasing total entropy are always satisfied. Conservative and dissipative terms in the governing equations are clearly distinguished, which is a one of prominent features of the GENERIC formalism.

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