Cancellation of vorticity in steady-state non-isentropic flows of complex fluids

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Abstract
In steady-state non-isentropic flows of perfect fluids, there is always thermodynamic generation of vorticity when the difference between the product of the temperature with the gradient of the entropy and the gradient of total enthalpy is different from zero. We note that this property does not hold in general for complex fluids for which the prominent influence of the material substructure on the gross motion may cancel the thermodynamic vorticity. We indicate the explicit condition for this cancellation (topological transition from vortex sheet to shear flow) for general complex fluids described by coarse-grained order parameters and extended forms of Ginzburg–Landau energies. As a prominent sample case we treat first Korteweg's fluid, used commonly as a model of capillary motion or phase transitions characterized by diffused interfaces. Then we discuss general complex fluids. We show also that, when the entropy and the total enthalpy are constant throughout the flow, vorticity may be generated by the inhomogeneous character of the distribution of material substructures, and indicate the explicit condition for such a generation. We discuss also some aspects of unsteady motion and show that in two-dimensional flows of incompressible perfect complex fluids the vorticity is in general not conserved, due to a mechanism of transfer of energy between different levels.

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1. Introduction and statement of the problem

For steady-state non-isentropic flows of perfect fluids, the following pointwise relation holds throughout the regular region $\mathcal{B}$ of the three-dimensional Euclidean point space $\mathcal{E}$ occupied by the fluid:

$$\omega \times \mathbf{v} = \vartheta \operatorname{grad} \eta - \operatorname{grad} H, \tag{1}$$

where **v** is the velocity of each material element ($\mathbf{v} = \tilde{\mathbf{v}}(\mathbf{x})$), $\boldsymbol{\omega}$ the vorticity ($\boldsymbol{\omega} = \mathrm{curl}\,\mathbf{v}$), ϑ the temperature, η the entropy density, H the total enthalpy density (grad and curl are calculated with respect to $\mathbf{x} \in \mathcal{B}$). Equation (1) is known as Crocco–Vaszony's theorem (see [1–3]). It states basically that we may observe thermodynamical generation of vorticity when

$$\vartheta\,\mathrm{grad}\,\eta - \mathrm{grad}\,H \neq 0. \tag{2}$$

For complex fluids, for which the gross behaviour is influenced by a prominent presence of material substructure, the condition (2) is no longer sufficient to assure vorticity and we may have situations in which the effects due to the substructure cancel the thermodynamic generation of vorticity, or may produce it even when the entropy and the total enthalpy are constant.

In what follows we give explicit conditions for the occurrence of such a topological transition, due to the complex structure of the fluid, from a vortex sheet to a shear flow and vice versa[1]. To fix basic ideas, we consider first the simplest case of complex fluid, the one of Korteweg, in which effects associated with the gradient of the specific volume are accounted for. Then, we treat a general case (following the unified theory in [4]) in which each material element at **x**, at time t, has an articulated morphology and can be considered as a 'system', described by a coarse-grained order parameter ν, taken here as an element of an 'abstract' differentiable manifold $\mathcal{M}$ to cover a class of complex fluids as large as possible. The possible non-uniform distribution of the order parameters influences the formation of vorticity during the flow. Finally, we discuss the unsteady case and show that in a two-dimensional flow of incompressible perfect complex fluids the vorticity is in general *not* conserved (as in simple perfect fluids) unless an explicit condition is satisfied. The influence of the material substructure, rendering not conserved the vorticity, is not of viscous nature: there is just a transfer of energy from the coarse-grained (macroscopic) level to the substructural one, altering the macroscopic energetic landscape of the vorticity (that may generate possible drag reduction in turbulent flows). This phenomenon implies the possibility that even in a two-dimensional flow of complex fluids a vortex may be destroyed and, possibly, reconnected in two or more subvortices.

For the sake of simplicity we do not consider applied external fields.

2. The case of Korteweg's fluid

Motivated by the work of van der Walls and previous ideas of Lord Rayleigh and Gibbs, to model at coarse scale the effects of interfacial tension in capillary phenomena, in 1901, Korteweg [5] introduced a model of fluid in which the energy depends on the gradient of the density. Experimental works have supported this approach [6–8] and the model has been source of analytical investigations [9, 10]. A detailed critical review about this topic can be found in [11]. The work of Korteweg has been the germ of a general modelling of 'materials of grade N' in which higher order deformation gradients up to grade N are involved in constitutive equations (see [12] for the general thermodynamic treatment). In 1993 Capriz [13] proved clearly that the constitutive dependence on higher order 'deformation' gradients is an indicator of the prominent presence of a complex material substructure which needs the introduction of some order parameter, under the assumption of the existence of an internal constraint linking the order parameter with the deformation (Korteweg's model follows as a special case). Our prominent interest in the present setting is not properly on capillary phenomena, the original motivation of Korteweg's model, rather it is focused on the circumstance that such a model

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[1] Such a kind of transition may occur in disparate circumstances, such as, e.g., geophysical flows [18].

is currently used to represent phase transitions on the basis of a *diffuse interface* approach (see [14] for a detailed review). In its simplest form, in fact, the free energy is of Cahn–Hilliard type: the gradient of the mass density account for the free energy excess of the interfacial region between phases. Such an excess of energy may influence the generation of vorticity in non-isentropic flows: it may cancel or produce vorticity.

2.1. The main result about Korteweg's fluids

Here we analyse the simplest case of complex fluid, i.e. the perfect Korteweg's one: a compressible perfect fluid characterized by the functional dependence of the potential ϕ on the gradient grad ι of the specific volume ι (being $\iota = \tilde{\iota}(\mathbf{x}) = \det \mathbf{g}(\mathbf{x})$, with $\mathbf{g}(\mathbf{x})$ the metric in space at $\mathbf{x} \in \mathcal{B}$, and grad is calculated with respect to $\mathbf{x}$) in addition to ι itself; in other words, we consider the case in which $\phi = \phi(\iota, \text{grad}\,\iota, \eta)$, with ϕ a sufficiently smooth function.

In the following, we write formally $\phi(\iota, \text{grad}\,\iota, \eta)$ being conscious that since ϕ is a scalar function depending on a vector (namely, grad ι), for reasons of objectivity (frame indifference under the action of $SO(3)$) ϕ must depend on the vector grad ι only through its amplitude $|\text{grad}\,\iota|$. The simplest choice of ϕ is Cahn–Hilliard's form: $\phi = f(\iota, \eta) + \frac{1}{2}\beta|\text{grad}\,\iota|^2$, with β some constant and f a function describing, e.g., a two-well energy; then ϕ may account for the spinodal decomposition. We also indicate with ρ the current density of mass of the fluid and consider the referential density ρ_0 equal to 1 so that $\iota = \rho^{-1}$. In general, the Lagrangian density of Korteweg's fluid is considered to be given by

$$\tfrac{1}{2}\rho|\mathbf{v}|^2 + \chi(\iota, i) - \rho\phi(\iota, \text{grad}\,\iota, \eta) \tag{3}$$

for non-isentropic flows, where χ is a sufficiently smooth function such that $\partial_{ii}^2\chi \neq 0$, $\chi(\iota, i) \geqslant 0$ and the equality sign holds when $i = 0$. The function χ accounts for possible substructural inertia effects that may generate gradient inertia. In other words, the appearance of the time derivative of ι, namely i, in (3) is *not* of viscous nature, rather it is of inertial nature and the physical dimensions of χ are those of a kinetic energy. Note that the kinetic energy is the partial Legendre transform with respect to i of χ which is called kinetic *co-energy*, following the terminology of [4]. The possible existence of gradient inertia effects in Korteweg's fluid has been pointed out in [13], however, these effects seem to be negligible unless the fluid oscillates at very high frequencies. In any case we formally account for the presence of χ in the following, because in the general setting treated below its effects may be sensible.

Hereafter, the dot indicates the scalar product associated with the natural dual pairing; moreover, we denote with ∂_y the partial derivative with respect to the argument y and, for different types of linear operators, with a superscript T we indicate the transposition rendered explicit by a subsequent detailed expression in components, when the meaning of the transposition is not immediately evident. For A and B tensors of the same order, $A \cdot B$ indicates scalar product.

The main result of the present section is summarized in the proposition and the corollaries below.

Proposition 1. *For a steady-state non-isentropic flow of a Korteweg's fluid, the following pointwise relation holds:*

$$\boldsymbol{\omega} \times \mathbf{v} = \vartheta \,\text{grad}\,\eta - \text{grad}\,h - \text{grad}(\iota^2 \,\text{div}\,\rho\partial_{\text{grad}\,\iota}\phi + \partial_{\text{grad}\,\iota}\phi \cdot \text{grad}\,\iota) + \iota \,\text{grad}\left(\frac{\text{d}}{\text{d}t}(\partial_i\chi) - \partial_\iota\chi\right). \tag{4}$$

In equation (4), h is the total enthalpy density of Korteweg's fluid and its explicit expression is given in section 2.3.

Corollary 1. *In a perfect Korteweg's fluid, the gradient effects cancel the thermodynamic generation of vorticity when*

$$\vartheta \operatorname{grad} \eta - \operatorname{grad} h = \operatorname{grad}(\iota^2 \operatorname{div} \rho \partial_{\operatorname{grad} \iota} \phi + \partial_{\operatorname{grad} \iota} \phi \cdot \operatorname{grad} \iota) - \iota \operatorname{grad} \left(\frac{\mathrm{d}}{\mathrm{d}t}(\partial_i \chi) - \partial_\iota \chi \right). \qquad (5)$$

Corollary 2. *In the case in which both the specific entropy and the total enthalpy are constant throughout the flow of a perfect Korteweg's fluid, the gradient effects may generate vorticity:*

$$\omega \times \mathbf{v} = -\operatorname{grad}(\iota^2 \operatorname{div} \rho \partial_{\operatorname{grad} \iota} \phi + \partial_{\operatorname{grad} \iota} \phi \cdot \operatorname{grad} \iota) + \iota \operatorname{grad} \left(\frac{\mathrm{d}}{\mathrm{d}t}(\partial_i \chi) - \partial_\iota \chi \right). \qquad (6)$$

2.2. Preliminaries to perfect Korteweg's fluids

2.2.1. Equilibrium. In the absence of body forces, the equilibrium of the fluid in $\mathcal{B}$ can be determined by evaluating the variation of the functional

$$\Phi = \int_{\mathcal{B}} \rho \phi(\iota, \operatorname{grad} \iota) \qquad (7)$$

and putting it equal to zero, i.e.

$$\hat{\delta} \int_{\mathcal{B}} \rho \phi(\iota, \operatorname{grad} \iota) = 0 \qquad (8)$$

for any choice of $\delta \mathbf{x}$, where $\hat{\delta}$ indicates the *total* variation (in the sense used in elementary treatises when one deals with 'total' time derivatives), so that we have (see [4], p 31)

$$\begin{aligned}
\hat{\delta} \int_{\mathcal{B}} \rho \phi &= \int_{\mathcal{B}} \delta(\rho \phi) + \int_{\partial \mathcal{B}} \rho \phi \mathbf{n} \cdot \delta \mathbf{x} \\
&= \int_{\mathcal{B}} (\delta(\rho \phi) + \operatorname{div}(\rho \phi \delta \mathbf{x})) \\
&= \int_{\mathcal{B}} \rho \hat{\delta} \phi \qquad (9)
\end{aligned}$$

where $\mathbf{n}$ is the outward unit normal to the boundary $\partial \mathcal{B}$ of $\mathcal{B}$.

We note that

$$\hat{\delta} \phi(\iota, \operatorname{grad} \iota) = \partial_\iota \phi \hat{\delta} \iota + \partial_{\operatorname{grad} \iota} \phi \hat{\delta} \operatorname{grad} \iota \qquad (10)$$

where $\hat{\delta} \iota$ and $\hat{\delta} \operatorname{grad} \iota$ are the total variations of the relevant arguments calculated taking into account that ι varies in space. We have in fact

$$\hat{\delta} \iota = \iota \operatorname{div} \delta \mathbf{x} \qquad (11)$$

as a consequence of the Euler formula, and by the chain rule

$$\hat{\delta} \operatorname{grad} \iota = \operatorname{grad} \hat{\delta} \iota - (\operatorname{grad} \delta \mathbf{x})^T \operatorname{grad} \iota \qquad (12)$$

(see [4] for other details). By developing the variation in (8), taking into account (10), (11) and using the Gauss theorem repeatedly, we recognize that the arbitrariness of $\delta \mathbf{x}$ implies in the bulk the pointwise balance

$$\operatorname{div} \mathbf{T} = \mathbf{0} \qquad (13)$$

(as the Euler–Lagrange equation) with

$$\mathbf{T} = -p\mathbf{I} - \mathbf{T}^E \tag{14}$$

where $\mathbf{I}$ is the second-order unit tensor, p is a non-standard pressure given by

$$p = -\rho\iota\partial_\iota\phi + \iota\,\mathrm{div}\,\rho\partial_{\mathrm{grad}\,\iota}\phi \tag{15}$$

and $\mathbf{T}^E$ is a *non-viscous* stress of Ericksen's type called in this context the Korteweg stress, i.e.

$$\mathbf{T}^E = \mathrm{grad}\,\iota \otimes \rho\partial_{\mathrm{grad}\,\iota}\phi. \tag{16}$$

2.2.2. Flows. Let us consider first isentropic flows. The dynamics of a Korteweg's fluid can be simply derived by making use of a Hamilton variational principle of the form

$$\hat{\delta}\int_0^{\bar{t}}\int_{\mathfrak{b}}\left(\frac{1}{2}|\mathbf{v}|^2 + \chi(\iota, i)\right) - \int_0^{\bar{t}}\hat{\delta}\int_{\mathfrak{b}}\rho\phi(\iota, \mathrm{grad}\,\iota) = 0 \tag{17}$$

where the time t runs in $[0, \bar{t}\,]$ and $\hat{\delta}$ means *total* variation as before. By developing (17), we realize that the arbitrariness of $\delta\mathbf{x}$ implies the standard balance

$$\rho\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = \mathrm{div}\,\mathbf{T}. \tag{18}$$

The stress tensor $\mathbf{T}$ is of the form

$$\mathbf{T} = -\bar{p}\mathbf{I} - \mathbf{T}^E \tag{19}$$

but now the non-standard pressure $\bar{p}$ accounts for kinetic pressure effects and is

$$\bar{p} = -\rho\iota\partial_\iota\phi + \iota\,\mathrm{div}\,\rho\partial_{\mathrm{grad}\,\iota}\phi - \rho\iota\frac{\mathrm{d}}{\mathrm{d}t}\partial_i\chi + \partial_\iota\chi \tag{20}$$

while $\mathbf{T}^E$ remains the same as (16).

2.3. Proof of proposition 1

We denote with q the amplitude of the velocity, i.e. $q = |\mathbf{v}|$. Then, by using the standard Lagrange formula

$$\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = \partial_t\mathbf{v} + (\mathrm{grad}\,\mathbf{v})\mathbf{v} = \partial_t\mathbf{v} + \omega \times \mathbf{v} + \frac{1}{2}\mathrm{grad}\,q^2. \tag{21}$$

We recognize that in the case of *steady motion*, i.e. when $\partial_t\mathbf{v} = \mathbf{0}$, the balance equation (18) can be written as

$$\omega \times \mathbf{v} = -\tfrac{1}{2}\mathrm{grad}\,q^2 - \iota\,\mathrm{grad}\,\bar{p} - \iota\,\mathrm{div}\,\mathbf{T}^E. \tag{22}$$

When the flow is not isentropic, we may identify the potential ϕ with the internal energy and write

$$\phi = \phi(\iota, \mathrm{grad}\,\iota, \eta) \tag{23}$$

η being the entropy density. From (23), we define the *specific enthalpy density* ξ as the opposite of the partial Legendre transform of ϕ with respect to the kinematic variables, so that we have

$$\xi = \phi - \iota\partial_\iota\phi - \partial_{\mathrm{grad}\,\iota}\phi \cdot \mathrm{grad}\,\iota \tag{24}$$

i.e. from (20),

$$\xi = \phi + \iota\bar{p} - \iota^2\,\mathrm{div}\,\rho\partial_{\mathrm{grad}\,\iota}\phi + \iota\check{p} - \partial_{\mathrm{grad}\,\iota}\phi \cdot \mathrm{grad}\,\iota \tag{25}$$

where

$$\check{p} = \rho \iota \frac{\mathrm{d}}{\mathrm{d}t}(\partial_i \chi) - \partial_\iota \chi \tag{26}$$

is the kinetic pressure due to possible gradient inertia effects. By indicating with ϑ the temperature given by $\partial_\eta \phi$, the calculation of the gradient of (25) allows us to obtain

$$-\iota \operatorname{grad} \bar{p} = \vartheta \operatorname{grad} \eta - \operatorname{grad} \xi + \iota \operatorname{grad} \check{p} - \iota^2 \operatorname{grad}(\operatorname{div} \rho \partial_{\operatorname{grad} \iota} \phi)$$
$$- (\operatorname{grad} \partial_{\operatorname{grad} \iota} \phi)^T \operatorname{grad} \iota - \iota(\operatorname{div} \rho \partial_{\operatorname{grad} \iota} \phi) \operatorname{grad} \iota. \tag{27}$$

By inserting (27) in (22), taking into account that

$$\operatorname{div} \mathbf{T}^E = (\operatorname{div} \rho \partial_{\operatorname{grad} \iota} \phi) \operatorname{grad} \iota + (\rho \partial_{\operatorname{grad} \iota} \phi) \operatorname{grad}^2 \iota \tag{28}$$

and defining the *total specific enthalpy h* of Korteweg's fluid as

$$h = \tfrac{1}{2}q^2 + \xi \tag{29}$$

we obtain (4) and proposition 1 is proved. The corollaries are immediate consequences.

3. General complex fluids

We follow here the unified setting proposed in [4] (and further discussed in [15] adding the treatment of singular surfaces) with the aim of encompassing a class of complex flows as large as possible. We then consider each material element as a subsystem collapsed into a place $\mathbf{x}$ and described by a coarse-grained order parameter ν. We do not specify ν; we require only that it belongs to a differentiable paracompact manifold $\mathcal{M}$ without boundary where we presume that physical circumstances induce a single choice of metric and of connection. We have then a sufficiently smooth mapping $\mathcal{B} \ni \mathbf{x} \overset{\tilde{\nu}}{\longmapsto} \nu = \tilde{\nu}(\mathbf{x}) \in \mathcal{M}$.

We account for gradient effects, i.e. we consider the interaction between neighbouring material elements under the suggestions of the results about Korteweg's fluid. These weakly non-local effects are the crucial mechanism altering the standard thermomechanical behaviour of the vorticity.

Under previous assumptions, the Lagrangian density of a general complex fluid can be written as

$$\tfrac{1}{2}\rho|\mathbf{v}|^2 + \chi(\nu, \dot{\nu}) - \rho\phi(\iota, \nu, \operatorname{grad} \nu, \eta) \tag{30}$$

where the substructural kinetic co-energy χ (if perceptible in experiments) depends now on ν and its rate, and the potential ϕ accounts for weak non-local gradient effects. The contemporary presence of ν and $\operatorname{grad} \nu$ in the constitutive list of entries of ϕ is not simply a matter of choice of generality in the modelling (due, say, to a principle of equipresence), rather it is of geometric origin. The manifold $\mathcal{M}$ is in general not trivial (in most cases of physical interest it is not a linear space); the pair $(\tilde{\nu}, \operatorname{grad} \tilde{\nu})$ collects the peculiar elements of the tangent mapping $T\tilde{\nu} : T\mathcal{B} \to T\mathcal{M}$ between the tangent bundle of $\mathcal{B}$ and the one of $\mathcal{M}$. In general, the two elements cannot be separated invariantly unless $\mathcal{M}$ is endowed with a parallelism. One asks also a physically significant parallelism. Even when $\mathcal{M}$ is Riemannian, there is no immediate physical reason, in principle, prescribing that the consequent Levi-Civita connection over $\mathcal{M}$ has a prevalent role even in exotic cases. Taking into account the possible articulated geometry of $\mathcal{M}$, in general we account for both ν and $\operatorname{grad} \nu$ as entries of ϕ when we decide to model interactions between neighbouring material elements.

We list just below some well-known special cases of our treatment to clarify the topic; other cases are collected at the end of this section.

(1) For nematic liquid crystals, ν is identified with a unit vector, say **n**, indicating the direction of the prevailing nematic order of stick molecules at **x**; $\mathcal{M}$ is the unit sphere with the identification of the antipodes and ϕ is the Oseen–Frank potential (see, e.g., [16]).

(2) For semi-dilute polymeric fluids, the material element is like a box containing a population of polymer chains described by end-to-end vectors **r** and ν is identified at each **x** with a second-order tensor, $\mathcal{R}$, precisely the second-order moment of the distribution of the **r** averaged over the population considered (see, e.g., [17]).

(3) The simplest reasonable form of ϕ is of Ginzburg–Landau's type, namely $\phi = \gamma(\iota, \nu, \eta) + \frac{1}{2}a\|\text{grad}\,\nu\|^2$, with a some appropriate constant and $\|\text{grad}\,\nu\|$ the norm of $\text{grad}\,\tilde{\nu}(x)$ in $\text{Hom}(T_\mathbf{x}\mathcal{B}, T_\nu\mathcal{M})$, the space of linear maps between the tangent space of $\mathcal{B}$ at **x** and the tangent space of $\mathcal{M}$ at $\nu = \tilde{\nu}(\mathbf{x})$.

Note that if we impose the internal constraint $\tilde{\iota}(\mathbf{x}) = \tilde{\nu}(\mathbf{x})$ we reduce the treatment to Korteweg's fluid.

3.1. The main result about complex fluids

By taking into account the structure (30) of the Lagrangian density, we may formulate the natural generalization of proposition 1.

Proposition 2. *For a steady-state non-isentropic flow of a general perfect complex fluid, the following pointwise relation holds:*

$$\boldsymbol{\omega} \times \mathbf{v} = \vartheta\,\text{grad}\,\eta - \text{grad}\,h_c - (\text{grad}\,\partial_{\text{grad}\,\nu}\phi)^T\,\text{grad}\,\nu$$
$$- \left(\text{grad}\left(\text{div}\,\partial_{\text{grad}\,\nu}\phi - \frac{\text{d}}{\text{d}t}(\partial_{\dot{\nu}}\chi) - \partial_\nu\chi\right)\right)^T \boldsymbol{\nu}$$
$$+ \iota(\text{grad}\,\nu)^T\,\text{div}\,\partial_{\text{grad}\,\nu}\phi + \iota(\partial_{\text{grad}\,\nu}\phi)^T\,\text{grad}\,\text{grad}\,\nu \tag{31}$$

where h_c is the total enthalpy of the complex fluid defined below.

By indicating with α components on some chart over $\mathcal{M}$ and with $i, j, \ldots$ the standard spatial components, (31) may be read as

$$(\boldsymbol{\omega} \times \mathbf{v})_i = \vartheta\,(\text{grad}\,\eta)_i - (\text{grad}\,h_c)_i - \left(\text{grad}\left(\text{div}\,\partial_{\text{grad}\,\nu}\phi - \frac{\text{d}}{\text{d}t}(\partial_{\dot{\nu}}\chi) - \partial_\nu\chi\right)\right)_{i\alpha} \nu^\alpha$$
$$- (\text{grad}\,\partial_{\text{grad}\,\nu}\phi)_{i\alpha}^j(\text{grad}\,\nu)_j^\alpha + \iota(\text{grad}\,\nu)_i^\alpha(\text{div}\,\partial_{\text{grad}\,\nu}\phi)_{\alpha j}^j$$
$$+ \iota(\partial_{\text{grad}\,\nu}\phi)_\alpha^j(\text{grad}\,\text{grad}\,\nu)_{ji}^\alpha. \tag{32}$$

Corollary 3. *In a perfect complex fluid, the presence of material substructure cancels the thermodynamic generation of vorticity when*

$$\vartheta\,\text{grad}\,\eta - \text{grad}\,h_c = (\text{grad}\,\partial_{\text{grad}\,\nu}\phi)^T\,\text{grad}\,\nu - \iota(\text{grad}\,\nu)^T\,\text{div}\partial_{\text{grad}\,\nu}\phi$$
$$+ \left(\text{grad}\left(\text{div}\,\partial_{\text{grad}\,\nu}\phi - \frac{\text{d}}{\text{d}t}(\partial_{\dot{\nu}}\chi) - \partial_\nu\chi\right)\right)^T \boldsymbol{\nu} - \iota(\partial_{\text{grad}\,\nu}\phi)^T\,\text{grad}\,\text{grad}\,\nu. \tag{33}$$

Corollary 4. *In the case in which both the specific entropy and the total enthalpy are constant throughout the flow of a perfect complex fluid, the presence of material substructure may generate vorticity:*

$$\boldsymbol{\omega} \times \mathbf{v} = -(\text{grad}\,\partial_{\text{grad}\,\nu}\phi)^T\,\text{grad}\,\nu + \iota(\text{grad}\,\nu)^T\,\text{div}\,\partial_{\text{grad}\,\nu}\phi + \iota(\partial_{\text{grad}\,\nu}\phi)^T\,\text{grad}\,\text{grad}\,\nu$$
$$- \left(\text{grad}\left(\text{div}\,\partial_{\text{grad}\,\nu}\phi - \frac{\text{d}}{\text{d}t}(\partial_{\dot{\nu}}\chi) - \partial_\nu\chi\right)\right)^T \boldsymbol{\nu}. \tag{34}$$

3.2. Proof of proposition 2

3.2.1. Flows of isentropic perfect complex fluids. To obtain the field equations for general complex fluids, we consider first the total Lagrangian

$$L = \int_{\mathcal{B}} \left(\frac{1}{2} \rho |\mathbf{v}|^2 + \chi(\nu, \dot{\nu}) - \rho \phi(\iota, \nu, \operatorname{grad} \nu) \right) \tag{35}$$

and set equal to zero the first total variation (in the sense of (10)) of its integral over the time interval $[0, \bar{t}]$, namely

$$\hat{\delta} \int_0^{\bar{t}} L = 0. \tag{36}$$

We consider also that

$$\hat{\delta} \nu = \delta \nu + (\operatorname{grad} \nu) \, \delta \mathbf{x} \tag{37}$$

in components

$$(\hat{\delta} \nu)^\alpha = (\delta \nu)^\alpha + (\operatorname{grad} \nu)_i^\alpha (\delta \mathbf{x})^i \tag{38}$$

and that

$$\int_{\mathcal{B}} \rho \hat{\delta} \phi = \int_{\mathcal{B}} \rho (\partial_\iota \phi \hat{\delta} \iota + \partial_\nu \phi \cdot \hat{\delta} \nu + \partial_{\operatorname{grad} \nu} \phi \cdot \hat{\delta} \operatorname{grad} \nu). \tag{39}$$

By using the Gauss theorem repeatedly, variations vanishing at the boundary of $\mathcal{B}$ and the guidelines of section 2.2.1 (see also [4], pp 30–34), we obtain the following balances:

$$\rho \frac{\mathrm{d} \mathbf{v}}{\mathrm{d} t} = \operatorname{div} \mathbf{T} \tag{40a}$$

$$\operatorname{div} \mathcal{S} - \mathbf{z} = \frac{\mathrm{d}}{\mathrm{d} t} \partial_{\dot{\nu}} \chi - \partial_\nu \chi \tag{40b}$$

where the stress tensor $\mathbf{T}$ has in this case the form

$$\mathbf{T} = \rho \iota \partial_\iota \phi \mathbf{I} - (\operatorname{grad} \nu)^T \partial_{\operatorname{grad} \nu} \phi \tag{41}$$

and we use $\mathcal{S}$ and $\mathbf{z}$ as

$$\mathcal{S} = \rho \partial_{\operatorname{grad} \nu} \phi \tag{42a}$$
$$\mathbf{z} = \rho \partial_\nu \phi \tag{42b}$$

calling them microstress and self-interaction, respectively. The pointwise balance of substructural interactions (40b) states that self-interactions $\mathbf{z}$ accrue within each material element (due to its substructure) to balance the 'contact' interactions $\mathcal{S}$ between neighbouring material elements (due to the relative change of substructure). At each $\mathbf{x}$, $\mathbf{z}$ is an element of the cotangent space $T_\nu^* \mathcal{M}$ while $\mathcal{S}$ belongs to $\operatorname{Hom}(T_\mathbf{x}^* \mathcal{B}, T_\nu^* \mathcal{M})$. As for the pair $(\nu, \operatorname{grad} \nu)$, even in this case the non-trivial structure of $\mathcal{M}$ does not allow us to separate invariantly the microstress from the self-interaction, in general. However, when an appropriate parallelism permits us to select an explicit form of ϕ depending on the sole $\operatorname{grad} \nu$ and substructural inertia effects are negligible, equation (40b) reduces to a divergence form. For example, such a situation happens in the special case of nematic liquid crystals when we select just the simplest Frank's potential and reduce ourselves to investigate only the physics described by harmonic maps taking values in S^2 [19].

As anticipated in discussing the special case of Korteweg's fluid, the kinetic co-energy $\chi(\nu, \dot{\nu})$ is such that its Legendre transform with respect to the rate $\dot{\nu}$ coincides with the

substructural kinetic energy $k(\boldsymbol{\nu}, \dot{\boldsymbol{\nu}})$, i.e. $k = \partial_{\dot{\nu}} \chi \cdot \dot{\boldsymbol{\nu}} - \chi$. Its contribution may be in general sensible. Note that, even when $k(\boldsymbol{\nu}, \dot{\boldsymbol{\nu}})$ is of the form $\frac{1}{2} \dot{\nu}^{\alpha} \Omega_{\alpha\beta} \dot{\nu}^{\beta}$, the explicit form of χ differs from k by an addendum of the type $\lambda_{\alpha} \dot{\nu}^{\alpha}$, which may be helpful to describe some prominent physical effects. For example, in the case of magnetizable fluids, if we select the magnetization vector as order parameter and constrain its rate to be of gyroscopic nature, we reduce (40b) to the equation of Gilbert.

3.2.2. Details about proposition 2. When the flow is not isentropic, the potential is of the form

$$\phi = \phi(\iota, \boldsymbol{\nu}, \operatorname{grad} \boldsymbol{\nu}, \eta) \tag{43}$$

and we define (as in (24)) the specific enthalpy density ξ_c of a complex fluid as the opposite of the partial Legendre transform with respect to the morphological descriptors, namely

$$\xi_c = \phi - \iota \partial_{\iota} \phi - \partial_{\nu} \phi \cdot \boldsymbol{\nu} - \partial_{\operatorname{grad} \nu} \phi \cdot \operatorname{grad} \boldsymbol{\nu}. \tag{44}$$

We may also rewrite the term $-\iota \partial_{\iota} \phi$ as $\iota \tilde{p}$, where $\tilde{p}$ is the pressure relevant for this case, given by $-\partial_{\iota} \phi$. Equation (22) becomes

$$\boldsymbol{\omega} \times \mathbf{v} = -\frac{1}{2} \operatorname{grad} q^2 - \iota \operatorname{grad} \tilde{p} - \iota \operatorname{div} \bar{\mathbf{T}}^E \tag{45}$$

with

$$\bar{\mathbf{T}}^E = (\operatorname{grad} \boldsymbol{\nu})^T \partial_{\operatorname{grad} \nu} \phi \qquad (\bar{\mathbf{T}}^E)_i^j = (\operatorname{grad} \boldsymbol{\nu})_i^{\alpha} (\partial_{\operatorname{grad} \nu} \phi)_{\alpha}^j. \tag{46}$$

Then we get

$$\operatorname{div} \bar{\mathbf{T}}^E = (\operatorname{grad} \boldsymbol{\nu})^T \operatorname{div} \partial_{\operatorname{grad} \nu} \phi + (\partial_{\operatorname{grad} \nu} \phi)^T \operatorname{grad} \operatorname{grad} \boldsymbol{\nu}. \tag{47}$$

The gradient of (44) allows us to write also

$$-\iota \operatorname{grad} \tilde{p} = \vartheta \operatorname{grad} \eta - \operatorname{grad} \xi_c - (\operatorname{grad} \partial_{\nu} \phi)^T \boldsymbol{\nu} - (\operatorname{grad} \partial_{\operatorname{grad} \nu} \phi)^T \operatorname{grad} \boldsymbol{\nu}. \tag{48}$$

By inserting (48) and (47) into (45) and taking into account (40b) and (42b), we get proposition 2 where

$$h_c = \frac{1}{2} q^2 + \xi_c. \tag{49}$$

The corollaries are immediate.

3.3. Further special cases

Well-known cases covered by our general modelling have been listed at the beginning of section 3, namely nematic liquid crystals and polymeric fluids, and we may also mention ferrofluids once, in the presence of external electric fields, we add to ϕ the electromagnetic energy and develop appropriate variations of the relevant fields.

We may also investigate more exotic cases by making use of the flexibility of the general unifying framework in which we act. Some examples are listed below, but they do not exhaust the range of possibilities.

(1) *Smectic-A liquid crystals.* In the smectic-A phase, liquid crystals appear organized in layers in which stick molecules tend to be aligned orthogonally to the layer interface. Within each layer the molecules flow freely; in the orthogonal direction (where the behaviour is basically that of a one-dimensional crystal) they may permeate from one layer into another. Linear [20] and non-linear [21–23] continuum models have been formulated to describe various aspects of the elasticity and hydrodynamics of the smectic-A phase, paying some attention to the behaviour of possible vortices there. Since the current

formulation of the hydrodynamics of smectic-A liquid crystals falls within the general setting discussed here, under the conditions of proposition 2 and subsequent corollaries, we could foresee formation or cancellation of vortices. In fact, natural ingredients for modelling the smectic-A phase are a vector $\mathbf{n} \in S^2$ at each $\mathbf{x} \in \mathcal{B}$ describing the local orientational order and a scalar function w parametrizing the layers. More precisely, we may write [23] $w(\mathbf{x}, t, a\lambda)$, with λ an appropriate length scale and a running in a set of integers, to account for possible unequal spacing of layers. However, at a (gross) coarse-grained scale, we may imagine that $w(\mathbf{x}, t, \cdot)$ is defined in a continuum approximation on an interval of the real line so that, as shown in [23], $|\mathrm{grad}\, w|^{-1}$ measures the current thickness of the layers. Then, we can select the order parameter as the pair $(\mathbf{n}, w)$; however, in the absence of tilt (a condition reasonable outside the defect core) we have strictly

$$\mathbf{n} = \frac{\mathrm{grad}\, w}{|\mathrm{grad}\, w|} \tag{50}$$

and the simplest choice for the potential ϕ in the compressible case is of the form (see [22])

$$\phi(\iota, w, \mathrm{grad}\, w) = \bar{\phi}(\iota) + \tfrac{1}{2}\gamma_1(|\mathrm{grad}\, w| - 1)^2 + \tfrac{1}{2}\gamma_2(\mathrm{div}\, \mathbf{n})^2 \tag{51}$$

with the identification (50) and with γ_1 and γ_2 material constants. In (51), the term $(|\mathrm{grad}\, w| - 1)^2$ accounts for the compression of layers while $(\mathrm{div}\, \mathbf{n})^2$ describes the nematic phase and is the first addendum of (three constant) Frank's potential (see [3], p 55). Inertial effects can be considered by putting $\chi = \tfrac{1}{2}\rho\alpha|\dot{\mathbf{n}}|^2$, with α a material constant [23]. The special counterparts of (31), (33) and (34), associated with (51), follow after straightforward calculations. To simplify the matter further, one may imagine having an incompressible flow, neglecting $\bar{\phi}(\iota)$, a circumstance not incompatible with the assumed compressibility of the layers. Taking into account the incompressible limit of (51), namely $\phi(w, \mathrm{grad}\, w)$, the application of proposition 2, in the absence of prominent substructural inertia of stick molecules in the smectic-A phase, leads to

$$\boldsymbol{\omega} \times \mathbf{v} = \vartheta \, \mathrm{grad}\, \eta - \mathrm{grad}\, h_c - (\mathrm{grad}\, \mathcal{S})^T \mathrm{grad}\, w - w \, \mathrm{grad}(\mathrm{div}\, \mathcal{S})$$
$$+ \iota \, \mathrm{div}\, \mathcal{S}(\mathrm{grad}\, w) + \iota \mathcal{S}(\mathrm{grad}\, \mathrm{grad}\, w) \tag{52}$$

with

$$\mathcal{S} = \gamma_1(|\mathrm{grad}\, w| - 1)\mathbf{n} - \gamma_2|\mathrm{grad}\, w|^{-1}(\mathbf{I} - \mathbf{n} \otimes \mathbf{n})\mathrm{grad}(\mathrm{div}\, \mathbf{n}) \tag{53}$$

and $\mathbf{I}$ is the second-order unit tensor.

(2) *Polyelectrolyte polymers and polymer stars.* In the case of polyelectrolyte polymers suffering possible polarization, we may imagine to assign at each point $\mathbf{x} \in \mathcal{B}$ not only the dyadic tensor $\mathcal{R}$, mentioned at the beginning of section 3, but also a polarization vector $\mathbf{p}$. By indicating with Vec the translation space over $\mathcal{E}$, and with B_p a ball of Vec centred at zero and with radius equal to p, the maximum amplitude of the polarization, we have $\mathcal{M} = \mathrm{Hom}(\mathrm{Vec}, \mathrm{Vec}) \times B_p$ and we may construct the relevant hydrodynamic theory, once an explicit expression for ϕ has been selected (see examples in [17]), adding, in the presence of external electric fields, the electromagnetic energy. When we consider also polymer stars, the picture becomes more articulated and we may imagine having $\mathcal{M} = \mathrm{Hom}(\mathrm{Vec}, \mathrm{Vec}) \times B_p \times [0, b]$. In this case, at each $\mathbf{x} \in \mathcal{B}$, an arbitrary element of the interval $[0, b]$ of the real line describes the *radius of gyration* of the polymeric molecules.

(3) *Superfluid helium* ^4He. The work of Rasetti and Regge [24] allows us to manage suitable Poisson brackets to describe 'directly' the dynamics of vortices in superfluid helium (see also the developments in [25]). However, following the suggestions of [4] (p 7), we may choose to adopt the general point of view used here and to select $\mathcal{M} = S^1 \subset \mathbb{C}$, using in this way a potential ϕ with a Ginzburg–Landau structure with complex entries. The application of proposition 2 and subsequent corollaries follows.

4. Concluding remarks

In the case of Korteweg's fluid, diffuse interfaces modelled by the specific volume may generate an energetic wall against the thermodynamic formation of vorticity. However, there are conditions for which such an excess of energy may favour vorticity even for an isentropic flow.

Analogous phenomena occur in the case of general complex fluids. Note that, excluding possible inertial terms associated with χ, the gradient of ν and the derivative of ϕ with respect to grad ν are prominent ingredients in the vorticity equation (31). This circumstance suggests that inhomogeneous spatial distributions of substructures (preferably with high gradients) in steady-state flows may generate energetic barriers to vorticity or may favour it. Basically, the energy involved is that associated with weakly non-local interactions between neighbouring material elements.

For non-stationary incompressible two-dimensional flows the vorticity is in general not conserved even in the perfect case due to *a mechanism of transfer of energy between the coarse-grained level and the substructural one*, ruled by the tensor $\mathbf{T}^E$. In fact, if we calculate the curl of (40a) taking into account (41), we get

$$\frac{d\boldsymbol{\omega}}{dt} = (\boldsymbol{\omega} \cdot \text{grad})\mathbf{v} + \text{grad}\, \iota \times \text{div}\, \mathbf{T} - \iota\, \text{curl}(\text{div}\, \mathbf{T}^E). \tag{54}$$

When the fluid is incompressible, the addendum grad $\iota \times$ div $\mathbf{T}$ vanishes, and in a two-dimensional flow we have also $(\boldsymbol{\omega} \cdot \text{grad})\mathbf{v} = 0$, but the vorticity is still altered by the term $-\iota\, \text{curl}(\text{div}\, \mathbf{T}^E)$, which is different from zero except when (i) there exists a scalar field $\mathcal{B} \ni \mathbf{x} \longmapsto \pi(\mathbf{x})$ such that grad $\pi = $ div $\mathbf{T}^E$, or (ii) there exists a second-order tensor-valued field $\mathcal{B} \ni \mathbf{x} \longmapsto \mathbf{A}(\mathbf{x}) \in \text{Hom}(\text{Vec}, \text{Vec})$ such that $\text{curl}(\mathbf{T}^E)^T = (\text{curl}\,\mathbf{A})^T$. So that, in time-dependent states, even in a two-dimensional flow of an *incompressible* perfect complex fluid the vorticity can be altered with consequent generation of topological transitions.

Experiments confirming the theoretical predictions of the present paper in some special case could be useful towards the understanding of complex fluids.

Acknowledgments

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