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On port-Hamiltonian formulations of 3-dimensional compressible Newtonian fluids

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In this manuscript a general formulation of 3-dimensional compressible fluids based on the port-Hamiltonian framework is presented, both for isentropic and non-isentropic assumptions, describing the energy flux between the mechanical, chemical and thermal domains, with an explicit characterization of the first and the second law of Thermodynamics. For isentropic fluids, the conversion of kinetic energy into heat by viscous friction is considered as energy dissipation associated with the rotation and compression of the fluid. A dissipative port-Hamiltonian formulation is derived for this class of fluids, including vorticity boundary conditions in the port variables. For non-isentropic fluids we consider a fluid mixture with multiple chemical reactions. To describe the energy fluxes we propose a pseudo port-Hamiltonian formulation, which includes the rate of irreversible entropy creation by heat flux, chemical reaction, diffusion of matter and viscous friction.

NOTATION

Symbol	Description
Ω	Spatial domain, $\Omega \subset \mathbb{R}^n$
$\partial\Omega$	Boundary surface enclosing Ω
$H(\Omega)$	Sobolev space of differentiable functions on Ω
ζ_i	Spatial variable of the i-th axis
ζ	Set of spatial variables, $\zeta \in \Omega$
t	Time variable
∂_t	Partial time derivative, $\partial_t = \frac{\partial}{\partial t}$
D_t	Material derivative, $D_t = \partial_t + \mathbf{v} \cdot \mathbf{grad}$
div	Divergence of a vector field
grad	Gradient of a scalar
curl	Curl or rotational of a vector field
Div	Divergence of a tensor
Grad	Gradient of a vector field
$^\top$	Transpose of a vector or matrix
$\boldsymbol{u}_1 \cdot \boldsymbol{u}_2$	Dot product between 2 vectors $\boldsymbol{u}_1 \cdot \boldsymbol{u}_2 = \boldsymbol{u}_1^\top \boldsymbol{u}_2$
$\boldsymbol{u}_1 \times \boldsymbol{u}_2$	Cross product between two vectors
$\boldsymbol{u}_1 \otimes \boldsymbol{u}_2$	External product, $\boldsymbol{u}_1 \otimes \boldsymbol{u}_2 = \boldsymbol{u}_1 \boldsymbol{u}_2^\top$
$\boldsymbol{\sigma}_1 : \boldsymbol{\sigma}_2$	Scalar product between 2 tensors $\boldsymbol{\sigma}_1 : \boldsymbol{\sigma}_2 = tr\left(\boldsymbol{\sigma}_1^\top \boldsymbol{\sigma}_2\right)$
$\boldsymbol{u} \cdot \boldsymbol{\sigma}$	Left dot product between a vector and a tensor, $\boldsymbol{u} \cdot \boldsymbol{\sigma} = \boldsymbol{\sigma}^\top \boldsymbol{u}$
$\boldsymbol{\sigma} \cdot \boldsymbol{u}$	Right dot product between a tensor and a vector, $\boldsymbol{\sigma} \cdot \boldsymbol{u} = \boldsymbol{\sigma} \boldsymbol{u}$
ρ	Fluid density
$\mathbf{v}$	Velocity field
p	Static pressure
$\boldsymbol{\tau}$	Viscous stress tensor
u	Specific internal energy
$\hbar$	Specific enthalpy
s	Specific entropy
T	Temperature
c_i	Concentration of species i
$\boldsymbol{c}$	Set of species
$\boldsymbol{\kappa}$	Thermal conduction tensor
$\mathbf{j}_i$	Diffusive flux of species i
$\boldsymbol{\Upsilon}$	Set of diffusive fluxes
r_i	Chemical reaction rate of species i
$\boldsymbol{r}$	Set of reaction rates
η_i	Chemical potential of species i
$\boldsymbol{\eta}$	Set of chemical potentials
μ	Shear viscosity
κ	Dilatational viscosity
$\mathbf{I}$	Identity matrix of proper dimension
$\mathbf{0}$	Zero matrix of proper dimension
$\mathbf{n}$	Outward unitary vector normal to $\partial\Omega$

I. INTRODUCTION

This work presents a pseudo port-Hamiltonian description of the dynamics of non-isentropic reactive and compressible fluids, using the total energy as generating function, and a skew-symmetric structure that describes the energy flux between the mechanical, chemical and thermal domains, with an explicit characterization of the first and second laws of Thermodynamics.

The use of an appropriate model is fundamental in optimization and control design methods. In particular, passivity-based control strategies, such as Energy-Shaping, Damping-Injection and Interconnection and Damping Assignment-Passivity Based Control (IDA-PBC)[1,2], require an accurate description of the energetic behavior of the system, taking into account the energy fluxes between the different components of the system. These models are obtained using the port-Hamiltonian framework (PHS). This framework has been initially introduced in Refs. 3 and 4 for finite-dimensional systems and extended in Refs. 5–7 for infinite-dimensional systems defined on 1-dimensional (1D) domains. In this framework, the system dynamics are described in terms of driving forces expressed through variational derivatives of a non-negative function that characterizes the total energy stored in the system. Similarly, the boundary port variables are power-conjugated, describing the power supplied through the boundary surface. Additionally, the use of structure-preserving spatial discretization methods, as the ones proposed in Refs. 8–11, allows to preserve the properties of the PHS formulation during the computational analysis of distributed-parameter system. This approach has been used in a variety of applications, such as in the description of the thermo-magneto-hydrodynamics of plasma in Tokamak reactors[12], the modeling and control of nanotweezers for classes of DNA-manipulators[13], the characterization of sound propagation in musical instruments[14,15], among others.

In recent years, the role of the energy flux has become relevant in the analysis and study of various phenomena in fluid dynamics. For example, in the interaction of decaying turbulences with thermal non-equilibrium[16], the analysis of the nonlinear saturation of thermal instabilities[17], and the study of turbulences energy cascade in stochastic fluid systems[18]. On the other hand, some methods used in computational fluid dynamics (CFD) require correction formulas for the computation of the energy flux in the numerical sequence as for instance in the ALEDGKS method[19], or present undesired non-physical oscillations[20]. A formulation which explicitly takes into account the energy flux associated with physical phenomena of the system, as the port-Hamiltonian framework, may help in the analysis and study of this kind of problems.

Different energy-based approaches have been presented in literature to describe Newtonian fluids. However, these approaches are constrained due to the considered assumptions that are made. For ideal isentropic fluids, Ref. 5 proposes a PHS formulation for n-dimensional inviscid fluids. Refs. 21 and 22 present 1D PHS formulations of compressible fluids where the vorticity effects are neglected as a consequence of the 1D assumption. A 3-dimensional (3D) PHS model for irrotational fluids is proposed in Ref. 23, considering only a viscous dissipation due to the fluid dilatation. Ref. 24 proposes general dissipative and pseudo PHS formulations for non-reactive compressible fluids, considering isentropic and non-isentropic assumptions, respectively. Refs. 25 and 26 present geometric PHS formulations, in a space of advected quantities, for compressible and incompressible fluids. Regarding reactive fluids, Ref. 27 proposes a pseudo PHS formulation to describe a 1D reactive mixture fluid of l species, including the thermal domain.

Another way to describe the dynamics and thermodynamics properties of complex fluids is the GENERIC approach[28–30], where the system dynamics are described through Poisson and dissipative brackets defined with respect to the total energy and the entropy, respectively[31,32]. An alternative approach for systems defined on 1D domains is the irreversible port-Hamiltonian systems (IPHS) formulation[33]. IPHS describe the dynamics using a formally skew-symmetric operator which depend on energy and co-energy variables. In IPHS the thermodynamic driving forces are described through locally defined pseudo brackets with respect to the total energy and entropy.

In this work, we extend the PHS formulations proposed in Refs. 24 and 27 to the modeling of 3D isentropic and non-isentropic compressible fluids. Under the isentropic assumption, we present a dissipative PHS formulation where the conversion of kinetic energy into heat by viscous friction is described through dissipative terms associated with the vorticity and compressibility of the flow. The boundary port variables of the proposed formulation include vorticity boundary conditions, neglected in Ref. 24. This formulation is useful for applications where the temperature variation of the fluid can be neglected. For example in the study and analysis of the phonation aerodynamics[34,35]. On the other hand, in applications where the temperature variation is relevant, the second law of Thermodynamics has to be taken into account in the fluid model, otherwise the fluid dynamic can exhibit an inaccurate behavior. For example, a fluid model that is constructed taking into account only the first law of Thermodynamics (total energy conservation), could transfer all of its internal energy into kinetic energy. The result is a very fast, but very cold flow. As commented in Ref. 36, such flow configuration has never been observed in nature. In the case of reactive mixing fluid applications, as hydrogen-oxygen mixture combustion chamber-superheater[37], computational methods, such as the lattice Boltzmann method, take special care dealing with the description of the energy and species mass fractions[38]. For the non-isentropic case, we consider a fluid mixture with multiple simultaneous reactions. Defining the operators, and corresponding formal adjoints, that characterizes each physical phenomenon, a pseudo PHS formulation is proposed to describe the dynamics and thermodynamic behavior of the fluid. This formulation includes boundary conditions associated with the diffusion flux of matter, extending the PHS formulations for non-isentropic fluids proposed in Refs. 24 and 27. This result can be interpreted as a first step towards a 3D IPHS formulation of complex fluids and may have application in areas such as the study and analysis of combustion systems[39–42].

The manuscript is organized as follows: Section II presents a brief background on port-Hamiltonian systems, and the entropy creation in fluids. In Section III we derive a dissipative port-Hamiltonian formulation for 3D compressible fluids under an isentropic assumption. In Section IV we develop a pseudo PHS formulation for reactive fluids in a 3D domain, defining the operators and formal adjoints associated with each of the involved physical phenomenon and the corresponding entropy creation. Conclusions are drawn in Section V. The proof of the theorems and the main identities used in this paper are given in an appendix section.

II. PORT-HAMILTONIAN SYSTEMS

Infinite dimensional PHS are dynamic systems described by PDEs of the form $\partial_t \mathbf{x} = \mathscr{J}\mathbf{e}$ where $\mathscr{J}$ is a formally skew symmetric differential operators and $\mathbf{e}$ is the vector of driving forces related to the energy through the variational derivative of the total energy function with respect to the state $\mathbf{x}$.

In Ref. 6 a parametrization of the boundary flow and effort variables is given in order to define a Dirac structure for linear systems defined on a 1D domain $\{\zeta \in [a,b] \subset \mathbb{R}\}$. In Ref. 5 a free coordinate PHS formulation based on differential geometry is given to describe distributed parameter systems on n-dimensional spatial domains.

Let Ω be a 3D spatial domain with spatial variable ζ and boundary $\partial\Omega$. We denote by $H(\Omega)$ the Sobolev space of weakly differentiable functions and by $\mathcal{X} \subset H(\Omega)$, $\mathscr{E} \subset H(\Omega)$ and $\mathscr{F} \subset H(\Omega)$ the spaces of state variables, efforts and flows on Ω, respectively. The total energy stored in the system with state variables $\mathbf{x}(\zeta,t) \in \mathcal{X}$ is given by the following functional:

$$\mathscr{H} = \int_{\Omega} \mathcal{H}(\mathbf{x})\,\mathrm{d}\Omega \tag{1}$$

where $\mathcal{H} : \mathcal{X} \to L^2(\Omega,\mathbb{R})$ denotes the energy density, such that the co-energy variables $\mathbf{e}$, also called efforts, are given by the variational derivatives $\mathbf{e} = \delta_{\mathbf{x}}\mathscr{H}$. PHS formulation of systems on a 3D space can be defined as follows.

Definition 1. *A distributed-parameter PHS defined on a 3D spatial domain Ω, boundary $\partial\Omega$, state space $\mathcal{X}$, and with Hamiltonian $\mathscr{H}$ is given by*

$$\partial_t \mathbf{x} = \mathscr{J}\,\mathbf{e} \tag{2}$$

$$\begin{bmatrix}\mathbf{f}_\partial \\ \mathbf{e}_\partial\end{bmatrix} = R_{\mathbf{n}}\mathbf{e}|_{\partial\Omega} \tag{3}$$

where $\partial_t\mathbf{x} \in \mathscr{F}$, $\mathscr{J}$ is a skew-symmetric differential operator, $\mathbf{f}_\partial$ and $\mathbf{e}_\partial$ are the boundary flow and effort port variables, $R_{\mathbf{n}}$ is an operator that describes the normal and tangential projections on $\partial\Omega$, induced by $\mathscr{J}$, of the co-energy variables $\mathbf{e}$, such that,

$$\dot{\mathscr{H}} = \int_{\partial\Omega} \mathbf{f}_\partial \cdot \mathbf{e}_\partial\,\mathrm{d}\gamma \tag{4}$$

where $\int_{\partial\Omega} \mathbf{f}_\partial \cdot \mathbf{e}_\partial\,\mathrm{d}\gamma$ describes the power supplied to the system through the boundaries.

When the system is isolated, i.e., considering boundary conditions equal to 0, from (4) total energy $\mathscr{H}$ stored in the system is constant along the trajectories of $\mathbf{x}$. This implies that Definition 1 is valid for conservative systems. In Ref. 7 an extension for dissipative systems defined on a 1D domains is presented, and Ref. 43 shows a coordinate-free formulation using differential geometry. For this class of systems, the effects of the dissipative phenomena on the systems dynamics are described through an additional term $-\mathscr{G}^*S\mathscr{G}\mathbf{e}$, i.e., $\partial_t\mathbf{x} = \mathscr{J}\,\mathbf{e} - \mathscr{G}S\mathscr{G}^*\mathbf{e}$, where $\mathscr{G}$ is a differential operator, $\mathscr{G}^*$ is the corresponding formal adjoint, and $S \geq 0$ is a non-negative matrix of appropriate dimensions. Defining $\mathbf{f}_d = -\mathscr{G}^*\mathbf{e}$ and $\mathbf{e}_s = S\mathbf{f}_d$ as the dissipative flow and effort variables, we then have the following definition.

Definition 2. *A distributed-parameter dissipative PHS defined on a 3D spatial domain Ω, boundary $\partial\Omega$, state space $\mathcal{X}$, and with Hamiltonian $\mathscr{H}$ is given by*

$$\begin{bmatrix}\partial_t\mathbf{x} \\ \mathbf{f}_d\end{bmatrix} = \underbrace{\begin{bmatrix}\mathscr{J} & \mathscr{G} \\ -\mathscr{G}^* & 0\end{bmatrix}}_{\tilde{\mathscr{J}}} \begin{bmatrix}\mathbf{e} \\ \mathbf{e}_d\end{bmatrix} \tag{5}$$

$$\begin{bmatrix}\mathbf{f}_\partial \\ \mathbf{e}_\partial\end{bmatrix} = \tilde{R}_{\mathbf{n}} \begin{bmatrix}\mathbf{e}|_{\partial\Omega} \\ \mathbf{e}_d|_{\partial\Omega}\end{bmatrix} \tag{6}$$

where $\partial_t\mathbf{x} \in \mathscr{F}$, $\tilde{\mathscr{J}}$ is an extended formal skew-symmetric differential operator, $\mathbf{f}_\partial$ and $\mathbf{e}_\partial$ are the boundary flow and effort port variables, $\tilde{R}_{\mathbf{n}}$ is an operator that describes the normal and tangential projections on $\partial\Omega$, induced by $\tilde{\mathscr{J}}$, of the co-energy variables $\mathbf{e}$ and dissipative effort $\mathbf{e}_d$, such that,

$$\dot{\mathscr{H}} = \int_{\partial\Omega} \mathbf{f}_\partial \cdot \mathbf{e}_\partial\,\mathrm{d}\gamma - \int_{\Omega} \mathbf{f}_{\mathrm{d}} \cdot \mathbf{e}_{\mathrm{d}}\,\mathrm{d}\Omega \leq \int_{\partial\Omega} \mathbf{f}_\partial \cdot \mathbf{e}_\partial\,\mathrm{d}\gamma \tag{7}$$

where $\int_{\partial\Omega} \mathbf{f}_\partial \cdot \mathbf{e}_\partial\,\mathrm{d}\gamma$ describes the power supplied to the system through the boundaries and $\int_{\Omega} \mathbf{f}_d \cdot \mathbf{e}_d\,\mathrm{d}\Omega \geq 0$ the power dissipated into heat by the internal phenomena.

Note that Definitions 1 and 2 are also valid for distributed port-Hamiltonian systems on 2D spatial domains. For more background on distributed-parameter port-Hamiltonian systems, we refer the reader to Refs. 5–7, and 43. In the next Section we present a dissipative port-Hamiltonian formulation for isentropic compressible fluids.

III. ISENTROPIC FLUIDS

In this section we consider the dynamics of a non-reactive compressible fluid under an isentropic assumption. Denoting by $\rho = \rho(\zeta,t)$ and $\mathbf{v} = \mathbf{v}(\zeta,t)$ the fluid density and the velocity field, respectively, with $\zeta \in \Omega$ as the vector of spatial variables, the governing equations for this kind of fluids are given by the mass balance

$$\partial_t\rho = -\operatorname{div}\rho\mathbf{v}, \quad \forall\zeta \in \Omega \tag{8}$$

and the equation of motion

$$\rho\,\partial_t\mathbf{v} = -(\rho\mathbf{v}\cdot\mathbf{grad}\,)\,\mathbf{v} - \mathbf{grad}\,p - \mathbf{Div}\,\boldsymbol{\tau}, \quad \forall\zeta \in \Omega \tag{9}$$

where $p = p(\zeta,t)$ is the fluid pressure and $\boldsymbol{\tau}$ is the viscous stress tensor. For Newtonian fluids, $\boldsymbol{\tau}$ satisfies the Newton's law of viscosity, i.e., shear stress is proportional to the velocity gradient[44], as shown in Section 3.1.

Given the isentropic assumption, the Gibbs equation that describes the changes of the specific internal energy in a non-reactive compressible fluid reduces to

$$\mathrm{d}u = -p\,\mathrm{d}\frac{1}{\rho} \tag{10}$$

where u denotes the specific (per unit mass) internal energy. Replacing d by the material derivative D_t on both sides of (10) and using (8), the specific internal energy rate of change is given by

$$\partial_t u + \mathbf{v}\cdot\mathbf{grad}\,u = -\frac{p}{\rho}\operatorname{div}\mathbf{v} \tag{11}$$

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This implies that the effects of the thermal domain on the dynamics of the internal energy are neglected. Then, the total energy of system (8)-(9) is defined as:

$$\mathscr{H} = \int_\Omega \left(\frac{1}{2} \rho \mathbf{v} \cdot \mathbf{v} + \rho u(\rho) \right) \mathrm{d}\Omega \tag{12}$$

with the following co-energy variables:

$$\mathbf{e} = \begin{bmatrix} \delta_\rho \mathscr{H} \\ \delta_\mathbf{v} \mathscr{H} \end{bmatrix} = \begin{bmatrix} \frac{1}{2} \mathbf{v} \cdot \mathbf{v} + \hbar \\ \rho \mathbf{v} \end{bmatrix}, \quad \forall \zeta \in \Omega \tag{13}$$

where $\hbar = \hbar(\zeta, t)$ is the specific enthalpy defined as $\hbar = u + p/\rho$ and $p = \rho^2 \partial_\rho u$.

Note that, as a consequence of (10), the relation $\frac{1}{\rho} \mathbf{grad}\ p = \mathbf{grad}\ \hbar$ is obtained. Similarly, using (A1), we have that

$$(\mathbf{v} \cdot \mathbf{grad}\ ) \mathbf{v} = \mathbf{grad}\ \left(\frac{1}{2} \mathbf{v} \cdot \mathbf{v} \right) + G_\omega \cdot \mathbf{v}$$

where G_ω is the gyroscope tensor defined as follows[45,46].

Definition 3. *The gyroscope* $G_\omega \in L^2\left(\Omega, \mathbb{R}^{3\times3}\right)$ *is the skew-symmetric second order tensor that satisfies the identity* $\boldsymbol{\omega} \times \mathbf{v} = G_\omega \cdot \mathbf{v}$*, where* $\boldsymbol{\omega} = \mathbf{curl}\ \mathbf{v}$ *denotes the vorticity vector. According to Ref. 47,* G_ω *is given by*

$$G_\omega = 2\Xi \tag{14}$$

where $\Xi = \frac{1}{2} \left[\mathbf{Grad}\ \mathbf{v} - [\mathbf{Grad}\ \mathbf{v}]^\top \right]$ *is the skew-symmetric part of the velocity gradient.*

Then, the momentum equation (9) can be rewritten as

$$\partial_t \mathbf{v} = -\mathbf{grad}\ \left(\frac{1}{2} \mathbf{v} \cdot \mathbf{v} + \hbar \right) - G_\omega \cdot \mathbf{v} - \frac{1}{\rho} \mathbf{Div}\ \boldsymbol{\tau} \tag{15}$$

Remark 1. *The cross product and the* **curl** *operator are defined on 3D spatial domains, i.e., the vorticity vector* $\boldsymbol{\omega} = \mathbf{curl}\ \mathbf{v}$ *and the term* $\boldsymbol{\omega} \times \mathbf{v}$ *are valid only on 3D spaces. For the 2D space* Ω_{2D}*, two definitions which allow to extend the curl operator are found in the literature*[48,49]*. The scalar curl operator,* $\mathbf{curl}_{2D} : \mathbb{R}^2 \to \mathbb{R}$ *defined as* $\mathbf{curl}_{2D} \boldsymbol{u} := \partial_{\zeta_1} u_2 - \partial_{\zeta_2} u_1$ *for a given vector* $\boldsymbol{u} = [u_1\ u_2]^\top \in L^2(\Omega_{2D}, \mathbb{R}^2)$*. The vector curl operator* $\mathbf{curl}^*_{2D} : \mathbb{R} \to \mathbb{R}^2$ *defined as* $\mathbf{curl}^*_{2D} u := [\partial_{\zeta_2} u\ \ -\partial_{\zeta_1} u]^\top$ *for a given scalar u. Note that* $\mathbf{curl}^*_{2D}$ *is the formal adjoint of* $\mathbf{curl}_{2D}$[50]*. Then, the vorticity in a 2D space* Ω_{2D} *is a scalar defined as* $\omega = \mathbf{curl}_{2D} \mathbf{v}$*. The rotational effects on the momentum equation, given by the term* $\boldsymbol{\omega} \times \mathbf{v}$ *for 3D spaces, are expressed as* $\omega W \cdot \mathbf{v}$ *for 2D spaces, where* $W = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}$ *is a rotation matrix. Moreover, note that* $\omega W = \left[\mathbf{Grad}\ \mathbf{v} - [\mathbf{Grad}\ \mathbf{v}]^\top \right]$*. This implies that the definition of* G_ω *in* (14) *can be also used, i.e.,* $\omega W \cdot \mathbf{v} = G_\omega \cdot \mathbf{v}$*. As a consequence, the expression* (15) *for the momentum equation based on the Gyroscope* G_ω*, is also valid for fluids in 2D spaces under these considerations.*

A. Viscous friction and kinetic energy dissipation

The term $\frac{1}{\rho} \mathbf{Div}\ \boldsymbol{\tau}$ in (15) describes the conversion of kinetic energy into heat by viscous friction. The viscous stress tensor $\boldsymbol{\tau}$ of Newtonian fluids[44] is given by

$$\boldsymbol{\tau} = -\mu \left[\mathbf{Grad}\ \mathbf{v} + [\mathbf{Grad}\ \mathbf{v}]^\top \right] + \left(\frac{2}{3} \mu - \kappa \right) (\mathrm{div}\ \mathbf{v})\, \mathbf{I} \tag{16}$$

where $\mathbf{I}$ is the identity matrix, μ is the shear viscosity of the fluid (or simply viscosity) and κ is the dilatational viscosity, also referred to as the bulk viscosity. Assuming that the viscosities μ and κ are constant, the term $\frac{1}{\rho} \mathbf{Div}\ \boldsymbol{\tau}$ can be expressed as a dissipative element[7], as shown in the following lemma.

Lemma 1. *Consider a viscous Newtonian fluid. Define the operators* $\mathscr{G}_r(\star) = \mathbf{curl}\ \left(\frac{1}{\rho} \star \right)$ *and* $\mathscr{G}_c(\star) = \mathrm{div}\ \left(\frac{1}{\rho} \star \right)$*, and the corresponding formal adjoints* $\mathscr{G}^*_r(\star) = \frac{1}{\rho} \mathbf{curl}\ (\star)$ *and* $\mathscr{G}^*_c(\star) = -\frac{1}{\rho} \mathbf{grad}\ (\star)$*. The rate of change of the velocity associated with the viscous tensor,* $\frac{1}{\rho} \mathbf{Div}\ \boldsymbol{\tau}$*, can be expressed as a dissipative port-Hamiltonian term associated with the velocity effort* $\delta_\mathbf{v} \mathscr{H} = \rho \mathbf{v}$*, namely,*

$$\frac{1}{\rho} \mathbf{Div}\ \boldsymbol{\tau} = \mathscr{G}^*_{\boldsymbol{\tau}} S_{\boldsymbol{\tau}} \mathscr{G}_{\boldsymbol{\tau}} \rho \mathbf{v} \tag{17}$$

where $\mathscr{G}^*_{\boldsymbol{\tau}} = \left[\mathscr{G}^*_r\ \ \mathscr{G}^*_c \right]$*,* $S_{\boldsymbol{\tau}} = \begin{bmatrix} \mu \mathbf{I} & 0 \\ 0 & \hat{\mu} \end{bmatrix} \geq 0$ *and* $\mathscr{G}_{\boldsymbol{\tau}} = \begin{bmatrix} \mathscr{G}_r \\ \mathscr{G}_c \end{bmatrix}$*, with* $\hat{\mu} = \frac{4}{3} \mu + \kappa$*.*

Proof. See Appendix B 1. □

As shown in Appendix B1, the dissipative term in (17) can be expressed as $\frac{1}{\rho} \mathbf{Div}\ \boldsymbol{\tau} = \mathscr{G}^*_r \mu \mathscr{G}_r [\rho \mathbf{v}] + \mathscr{G}^*_c \hat{\mu} \mathscr{G}_c [\rho \mathbf{v}]$, i.e., the dissipation of kinetic energy into heat due to the molecular friction is given by two physical phenomena: the flow rotation and the dilatation-compression of the fluid. As a consequence, if the fluid is incompressible and the flow is irrotational, then the system (8)-(9) is conservative.

Remark 2. *Similarly to the Gyroscope, the dissipative formulation in* (17) *for the divergence of the viscous tensor can be extended for fluids in 2D spaces. In this case, operators* $\mathscr{G}_r$ *and* $\mathscr{G}^*_r$ *are defined as* $\mathscr{G}_r(\star) = \mathbf{curl}_{2D} \left(\frac{1}{\rho} \star \right)$ *and* $\mathscr{G}^*_r(\star) = \frac{1}{\rho} \mathbf{curl}^*_{2D}(\star)$*, respectively.*

B. Dissipative PHS formulation

Using Lemma 1, governing equations of an isentropic and non-reactive compressible fluid can be expressed as a dissipative port-Hamiltonian system, as shown in the following theorem.

Theorem 1. *Consider an isentropic Newtonian fluid with state variables given by* $\mathbf{x} = [\rho\ \mathbf{v}^\top]^\top$*. The fluid dynamics can* *be expressed by the following dissipative port-Hamiltonian system:*

$$\begin{bmatrix}\partial_t \mathbf{x}\\ \mathbf{f}_d\end{bmatrix} = \begin{bmatrix}\mathscr{J} & -\mathscr{G}^*\\ \mathscr{G} & \mathbf{0}\end{bmatrix}\begin{bmatrix}\mathbf{e}\\ \mathbf{e}_d\end{bmatrix}, \quad \zeta \in \Omega \tag{18}$$

where $\mathbf{f}_d$ *and* $\mathbf{e}_d = S_{\boldsymbol{\tau}}\mathbf{f}_d$ *are the dissipative flows and efforts, respectively, and operators* $\mathscr{J}$, $\mathscr{G}^*$ *and* $\mathscr{G}$ *are given by*

$$\mathscr{J} = \begin{bmatrix}0 & -\mathrm{div}\\ -\mathbf{grad} & -\frac{1}{\rho}G_{\boldsymbol{\omega}}\cdot\end{bmatrix}, \ \mathscr{G}^* = \begin{bmatrix}\mathbf{0}\\ \mathscr{G}^*_{\boldsymbol{\tau}}\end{bmatrix}, \ \textit{and}\ \mathscr{G} = \begin{bmatrix}\mathbf{0} & \mathscr{G}_{\boldsymbol{\tau}}\end{bmatrix} \tag{19}$$

The energy balance reads

$$\dot{\mathscr{H}} \leq \langle \mathbf{f}_\partial, \mathbf{e}_\partial \rangle_{\partial\Omega} \tag{20}$$

where

$$\mathbf{f}_\partial = \begin{bmatrix}-\left(\mathbf{n}\cdot \frac{\delta_{\mathbf{v}}\mathscr{H}}{\rho}\right)\\ \frac{\delta_{\mathbf{v}}\mathscr{H}}{\rho}|_{\partial\Omega}\end{bmatrix} \ \textit{and}\ \mathbf{e}_\partial = \begin{bmatrix}\left(\rho\,\delta_\rho\mathscr{H} + e_c\right)|_{\partial\Omega}\\ -\mathbf{n}\times\mathbf{e}_r|_{\partial\Omega}\end{bmatrix} \tag{21}$$

are the boundary port variables, with $\mathbf{e}_r$ *and* e_c *the efforts associated with the power dissipation by the flow rotation and fluid compression phenomena, respectively.*

Proof. Considering Lemma 1 and fluid efforts (13), system (8)-(15) can be rewritten as:

$$\partial_t \begin{bmatrix}\rho\\ \mathbf{v}\end{bmatrix} = \begin{bmatrix}-\mathrm{div}\ \delta_{\mathbf{v}}\mathscr{H}\\ -\mathbf{grad}\ \delta_\rho\mathscr{H} - \frac{1}{\rho}G_{\boldsymbol{\omega}}\cdot\delta_{\mathbf{v}}\mathscr{H} - \mathscr{G}^*_{\boldsymbol{\tau}}S_{\boldsymbol{\tau}}\mathscr{G}_{\boldsymbol{\tau}}\delta_{\mathbf{v}}\mathscr{H}\end{bmatrix}$$

We denote by $\mathbf{f}_r = \mathscr{G}_r(\delta_{\mathbf{v}}\mathscr{H})$ and $\mathbf{e}_r = \mu\mathbf{f}_r$, the dissipative flow and effort associated with the flow rotation, respectively, and by $f_c = \mathscr{G}_c(\delta_{\mathbf{v}}\mathscr{H})$ and $e_c = \hat{\mu} f_c$ the dissipative flow and effort associated with the fluid compressibility, with $\mathscr{G}_r$ and $\mathscr{G}_c$ defined as in Lemma 1. Then, governing equations can be expressed as

$$\begin{bmatrix}\partial_t\rho\\ \partial_t\mathbf{v}\\ \mathbf{f}_r\\ f_c\end{bmatrix} = \begin{bmatrix}0 & -\mathrm{div} & 0 & 0\\ -\mathbf{grad} & \frac{1}{\rho}G_{\boldsymbol{\omega}}\cdot & -\mathscr{G}^*_r & -\mathscr{G}^*_c\\ 0 & \mathscr{G}_r & 0 & 0\\ 0 & \mathscr{G}_c & 0 & 0\end{bmatrix}\begin{bmatrix}\delta_\rho\mathscr{H}\\ \delta_{\mathbf{v}}\mathscr{H}\\ \mathbf{e}_r\\ e_c\end{bmatrix} \tag{22}$$

Considering the state vector $\mathbf{x} = [\rho\ \mathbf{v}^\top]^\top$, the dissipative flow and effort can be expressed as $\mathbf{f}_d = \begin{bmatrix}\mathbf{f}_r\\ f_c\end{bmatrix} = \begin{bmatrix}\mathbf{0} & \mathscr{G}_{\boldsymbol{\tau}}\end{bmatrix}\mathbf{e}$ and $\mathbf{e}_d = \begin{bmatrix}\mathbf{e}_r\\ e_c\end{bmatrix} = \begin{bmatrix}\mu\mathbf{I} & \mathbf{0}\\ \mathbf{0} & \hat{\mu}\end{bmatrix}\mathbf{f}_d$, respectively. Then, defining the operators $\mathscr{J}$, $\mathscr{G}^*$ and $\mathscr{G}$ as in (19), the dissipative port-Hamiltonian formulation (18) is obtained.

On the other hand, the time derivative of the total energy is given by:

$$\begin{aligned}\dot{\mathscr{H}} &= \int_\Omega \mathbf{e}\cdot\partial_t\mathbf{x}\,\mathrm{d}\Omega\\ &= \int_\Omega \mathbf{e}\cdot\mathscr{J}\,\mathbf{e}\,\mathrm{d}\Omega - \int_\Omega \delta_{\mathbf{v}}\mathscr{H}\cdot\mathscr{G}^*_{\mathrm{r}}\mathbf{e}_{\mathrm{r}}\,\mathrm{d}\Omega - \int_\Omega \delta_{\mathbf{v}}\mathscr{H}\cdot\mathscr{G}^*_{\mathrm{c}}\mathrm{e}_{\mathrm{c}}\,\mathrm{d}\Omega\end{aligned}$$

with $\mathscr{J}$ defined in (19). Due to the skew-symmetry of $G_{\boldsymbol{\omega}}$, we have that

$$\begin{aligned}\int_\Omega \mathbf{e}\cdot\mathscr{J}\,\mathbf{e}\,\mathrm{d}\Omega &= -\left\langle \delta_\rho\mathscr{H}, \mathrm{div}\ \delta_{\mathbf{v}}\mathscr{H}\right\rangle_{L^2} - \left\langle \delta_{\mathbf{v}}\mathscr{H}, \mathbf{grad}\ \delta_\rho\mathscr{H}\right\rangle_{L^2}\\ &= -\int_\Omega \mathrm{div}\ \left(\delta_\rho\mathscr{H}\,\delta_{\mathbf{v}}\mathscr{H}\right)\,\mathrm{d}\Omega\end{aligned}$$

Using the Gauss-Ostrogradsky divergence theorem, considering the definition of $\mathscr{G}_r$ and $\mathscr{G}_c$ in Lemma 1, and applying Theorems 3 and 4, $\dot{\mathscr{H}}$ can be rewritten as

$$\dot{\mathscr{H}} = -\int_{\partial\Omega}\left(\delta_\rho\mathscr{H}\,(\delta_{\mathbf{v}}\mathscr{H}\cdot\mathbf{n}) + e_c\left(\frac{\delta_{\mathbf{v}}\mathscr{H}}{\rho}\cdot\mathbf{n}\right) + \left[\mathbf{e}_r\times\frac{\delta_{\mathbf{v}}\mathscr{H}}{\rho}\right]\cdot\mathbf{n}\right)\mathrm{d}\gamma - \int_\Omega \left(\mathrm{e}_{\mathrm{c}}\,(\mathscr{G}_{\mathrm{c}}(\delta_{\mathbf{v}}\mathscr{H})) + \mathbf{e}_{\mathrm{r}}\cdot[\mathscr{G}_{\mathrm{r}}(\delta_{\mathbf{v}}\mathscr{H})]\right)\mathrm{d}\Omega$$

Using the definition of the dissipation efforts and the cross product identity $[\boldsymbol{u}_1\times\boldsymbol{u}_2]\cdot\mathbf{n} = \boldsymbol{u}_2\cdot[\mathbf{n}\times\boldsymbol{u}_1]$, $\dot{\mathscr{H}}$ writes

$$\begin{aligned}\dot{\mathscr{H}} = &-\langle \mathbf{f}_r, \mu\mathbf{f}_r\rangle_{L^2} - \langle f_c, \hat{\mu} f_c\rangle_{L^2} - \int_{\partial\Omega}\frac{\delta_{\mathbf{v}}\mathscr{H}}{\rho}\cdot[\mathbf{n}\times\mathbf{e}_r]\,\mathrm{d}\gamma\\ &-\int_{\partial\Omega}\left(\rho\,\delta_\rho\mathscr{H} + e_c\right)\left(\frac{\delta_{\mathbf{v}}\mathscr{H}}{\rho}\cdot\mathbf{n}\right)\mathrm{d}\gamma\end{aligned}$$

On the other hand, using

$$\begin{bmatrix}\mathbf{f}_\partial\\ \mathbf{e}_\partial\end{bmatrix} = \tilde{R}_{\mathbf{n}}\begin{bmatrix}\delta_\rho\mathscr{H}|_{\partial\Omega}\\ \delta_{\mathbf{v}}\mathscr{H}|_{\partial\Omega}\\ \mathbf{e}_r|_{\partial\Omega}\\ e_c|_{\partial\Omega}\end{bmatrix} \tag{23}$$

with

$$\tilde{R}_{\mathbf{n}} = \begin{bmatrix}0 & -\frac{1}{\rho}\mathbf{n}\cdot & 0 & 0\\ 0 & \frac{1}{\rho} & 0 & 0\\ \rho & 0 & 0 & 1\\ 0 & 0 & -\mathbf{n}\times & 0\end{bmatrix}$$

we obtain the boundary flows and efforts in (21). Then, the rate of change of the fluid total energy can be written as

$$\dot{\mathscr{H}} = -\langle \mathbf{f}_d, S_{\boldsymbol{\tau}}\mathbf{f}_d\rangle_\Omega + \langle \mathbf{f}_\partial, \mathbf{e}_\partial\rangle_{\partial\Omega} \tag{24}$$

where $\langle \mathbf{f}_d, S_{\boldsymbol{\tau}}\mathbf{f}_d\rangle_\Omega = \int_\Omega \mathbf{f}_d\cdot[S_{\boldsymbol{\tau}}\mathbf{f}_d]\,\mathrm{d}\Omega$ and $\langle \mathbf{f}_\partial, \mathbf{e}_\partial\rangle_{\partial\Omega} = \int_{\partial\Omega}\mathbf{f}_\partial\cdot\mathbf{e}_\partial\,\mathrm{d}\gamma$. Finally, given that $\mu \geq 0$ and $\hat{\mu} \geq 0$ we have that $\langle \mathbf{f}_d, S_{\boldsymbol{\tau}}\mathbf{f}_d\rangle_\Omega \geq 0$, as stated in (20). □

Note that the boundary effort $-\mathbf{n}\times\mathbf{e}_r|_{\partial\Omega} = \mu\boldsymbol{\omega}\times\mathbf{n}|_{\partial\Omega}$ is equivalent to the vorticity boundary condition[51] $\boldsymbol{\omega}\times\mathbf{n}|_{\partial\Omega}$,

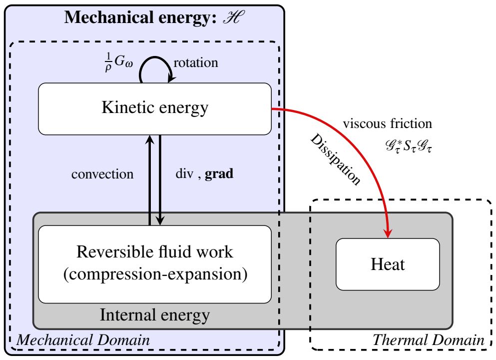

FIG. 1. Energy flux of the PHS formulation of isentropic compressible fluids, described in Theorem 1. Black arrows: reversible energy exchange. Red arrow: irreversible energy transformation.

using only the tangential part of the classical kinematic condition[52] $\omega|_{\partial\Omega}$. Similarly, equation (23) denotes the boundary port variables for the extended skew-symmetric operator in (22), and it is equivalent to the boundary port variables definition for 1D dissipative systems[7]. Additionally, from an energetic point of view, the rate of irreversible work dissipated into heat by viscous friction in the fluid is described through the term $\langle \mathbf{f}_d, S_\tau \mathbf{f}_d \rangle_\Omega \geq 0$ in (24).

Figure 1 shows an illustration of the energy flux described by the system (18) where the reversible energy flux of the fluid are described by operator $\mathscr{J}$. Operators div and **grad** are associated with the conversion between the reversible work of the internal energy and the kinetic energy due to the fluid convection. The energy exchange between the components of the velocity field, due to the fluid rotation, is described through the Gyroscope tensor. Note that in the PHS formulation described in Theorem 1 the functional $\mathscr{H}$ contains only the mechanical energy of the fluid. As a consequence, the irreversible conversion of kinetic energy into heat by viscous friction, described by operator $\mathscr{G}$ and $\mathscr{G}^*$ (red arrow of Figure 1), is considered as a mechanical energy dissipation.

An application example of this kind of fluid model, where the fluid viscosity is pertinent but the thermal domain is neglected, is the study and analysis of the human voice production. The viscosity have a relevant role in the performance and prediction capacity of finite elements models of the phonation aerodynamics[34]. Moreover, the energy exchange between the vocal folds and the intraglottal airflow have a great impact in the study the vocal folds vibration[35]. In this sense, a model focused on the energy flux of the fluid, as the one proposed in Theorem 1, may be useful for this class of applications.

In the following remarks we show that the fluid model proposed in (18) allows to cope with different models of isentropic fluids described in the literature under different assumptions.

Remark 3. *Consider that the isentropic fluid has an irrotational flow. This implies that operators $\mathscr{G}_r$ and $\mathscr{G}_r^*$, and gyroscope tensor G_ω vanish. Then, the port-Hamiltonian formulation in Theorem 1, can be written as*

$$\begin{bmatrix} \partial_t \rho \\ \partial_t \mathbf{v} \\ f_c \end{bmatrix} = \begin{bmatrix} 0 & -\mathrm{div} & 0 \\ -\mathbf{grad} & 0 & -\mathscr{G}_c^* \\ 0 & \mathscr{G}_c & 0 \end{bmatrix} \begin{bmatrix} \delta_\rho \mathscr{H} \\ \delta_{\mathbf{v}} \mathscr{H} \\ e_c \end{bmatrix} \tag{25}$$

satisfying the balance equation $\dot{\mathscr{H}} \leq \langle \mathbf{f}_\partial, \mathbf{e}_\partial \rangle_{\partial\Omega}$, with boundary ports $\mathbf{f}_\partial, \mathbf{e}_\partial$ given by $\mathbf{f}_\partial = -(\mathbf{n} \cdot \delta_{\mathbf{v}} \mathscr{H})|_{\partial\Omega}$ and $\mathbf{e}_\partial = \left(\delta_\rho \mathscr{H} + \frac{e_c}{\rho}\right)|_{\partial\Omega}$, leading to the fluid model proposed in Ref. 23.

Remark 4. *Consider the fluid as isentropic and inviscid. This implies that the operators associated with the viscous tensor vanish. Then, the port-Hamiltonian formulation in Theorem 1, reduces to*

$$\begin{bmatrix} \partial_t \rho \\ \partial_t \mathbf{v} \end{bmatrix} = \begin{bmatrix} 0 & -\mathrm{div} \\ -\mathbf{grad} & -\frac{G_\omega}{\rho} \end{bmatrix} \begin{bmatrix} \delta_\rho \mathscr{H} \\ \delta_{\mathbf{v}} \mathscr{H} \end{bmatrix} \tag{26}$$

satisfying the balance $\dot{\mathscr{H}} = \langle \mathbf{f}_\partial, \mathbf{e}_\partial \rangle_{\partial\Omega}$, with boundary ports given by $\mathbf{f}_\partial = -(\mathbf{n} \cdot \delta_{\mathbf{v}} \mathscr{H})|_{\partial\Omega}$ and $\mathbf{e}_\partial = \delta_\rho \mathscr{H}|_{\partial\Omega}$. This formulation is equivalent to the one given in Ref. 5.

Remark 5. *Note that, as shown in Remarks 1 and 2, the terms associated with the* **curl** *operator in* (22)*, G_ω, $\mathscr{G}_r$ and $\mathscr{G}_r^*$, can be extended to 2D spaces. The dissipative port-Hamiltonian formulation in Theorem 1 is then also valid for 2D isentropic compressible fluids. To simplify the derivation of the boundary fluid and efforts, in Ref. 24 we considered the following equivalent definitions of the 2D curl operator,* $\mathbf{curl}_{2D}(\star) = -\mathrm{div}\ [W\star]$ *and* $\mathbf{curl}^*_{2D}(\star) = W^\top \mathbf{grad}\ (\star)$*, where W is the rotation matrix defined in Remark 1.*

IV. NON ISENTROPIC REACTIVE FLUIDS

In this section a port-Hamiltonian formulation for reactive and non-isentropic compressible reactive fluids is proposed. Due to the non-isentropic assumption, we first analyze the irreversible phenomena in the fluids and the associated entropy production.

A. Irreversible phenomena and entropy production in compressible fluids

Fluid dynamics may involve several irreversible processes, such as diffusion, thermal conduction and viscosity, that are sources of mechanical/chemical energy dissipation into heat[53]. The entropy creation related to these irreversible phenomena is described below leading to an appropriate characterization of the second law of Thermodynamics for non-isentropic compressible fluids.

1. Viscosity and molecular momentum flux

The molecular momentum flux is the transport mechanism associated with the motion, interaction and collisions of fluid molecules[44]. This mechanism is described by the viscous stress tensor $\boldsymbol{\tau}$ in (16). As described in Ref. 44, p. 87 the irreversible production of heat per unit of volume due to viscous friction of fluids is given by $-\boldsymbol{\tau} : [\mathbf{Grad}\,\mathbf{v}]$, i.e., considering a local version of the second law of Thermodynamics[54] we have

$$-\frac{1}{\rho T}\boldsymbol{\tau} : [\mathbf{Grad}\,\mathbf{v}] \geq 0 \tag{27}$$

that describes the specific entropy production rate due to the conversion of kinetic energy into heat by viscous friction.

2. Heat and diffusion fluxes

The heat flux $\mathbf{q}$ describes the energy transport due to thermal conduction. According to Ref. 55, the density of entropy production by heat flux is given by

$$\mathbf{q}\cdot\left[\mathbf{grad}\,\frac{1}{T}\right] = -\frac{\mathbf{q}}{T^2}\cdot[\mathbf{grad}\,T] \geq 0 \tag{28}$$

where T is the absolute temperature of the fluid.

On the other hand, in multi-species fluids, the diffusion flux $\mathbf{j}$ describes the mass transport due to the equalization of concentrations by molecular transfer of species, from one part of the fluid to another[53]. The entropy production density associated with diffusion of l species is given by[55]

$$-\sum_{i=1}^{l}\mathbf{j}_i\cdot\mathbf{grad}\,\frac{\eta_i}{T} = -\boldsymbol{\Upsilon} : \mathbf{Grad}\,\frac{\boldsymbol{\eta}}{T} \geq 0 \tag{29}$$

where η_i is the chemical potential of the i-th species, $\boldsymbol{\Upsilon} = [\mathbf{j}_1,\ldots,\mathbf{j}_l]^\top$ and $\boldsymbol{\eta} = [\eta_1,\ldots,\eta_l]^\top$.

The heat and diffusion fluxes are given by the presence of concentration and temperature gradients. It is commonly assumed that $\mathbf{q}$ depends only on the temperature gradient, and $\mathbf{j}$ only on the concentration gradient. However, in general, these fluxes depend on both gradients; see Refs. 44, 53, and 55 for more details. This implies that the heat flux $\mathbf{q}$ is related to the diffusion flux $\mathbf{j}$, i.e.,

$$\mathbf{q} = -\boldsymbol{\kappa}\cdot\mathbf{grad}\,T + \sum_{i=1}^{l}\eta_i\mathbf{j}_i + q^{(D)} \tag{30}$$

where the first term describes the heat conduction, containing the thermal conductivity, the second term describes the heat diffusion due to the mass flux of the fluid species, and finally $q^{(D)}$ is the Dufour term[44], containing the thermal diffusion coefficients and mass fluxes. This Dufour term is usually neglected. In this work, for simplicity, we consider the heat flux definition (30) without this Dufour term. Then, considering a fluid without mass diffusion, $\mathbf{j}_i = 0$ for all i, we obtain that the heat flux is only given by the heat conduction term, i.e., $\mathbf{q} = -\boldsymbol{\kappa}\cdot\mathbf{grad}\,T$, where $\boldsymbol{\kappa} = \boldsymbol{\kappa}^\top \geq 0$ is a symmetric second order tensor called the thermal conductivity tensor.

Regarding the diffusion flux, the computation of convective transfer phenomena in multi-species systems is generally complicated[56], and simplifications are required to make this problem tractable. Under proper assumptions on the diffusion coefficients, the diffusion equation for multi-species fluids is equivalent to the diffusion equation of binary systems. Then, the most simple formula for the diffusive mass flux is given by[44,55]

$$\mathbf{j}_i = -\mathcal{D}_i\mathbf{grad}\,c_i\,, \tag{31}$$

which is derived from the Fick's law, where $\mathcal{D}_i$ is the diffusion coefficient of species i. An alternative formulation can be found in Ref. 55. Fick's formulation was obtained through empirical studies, and the parameter $\mathcal{D}_i$ can be obtained experimentally.

3. Chemical Reactions

We consider now a general chemical reaction of the form:

$$\xi : \quad a_1C_1 + \cdots + a_kC_k \rightleftharpoons a_{k+1}C_{k+1} + \cdots + a_lC_l \tag{32}$$

where a_i are the stoichiometric reaction coefficients, $C_i, i \in [1,\ldots k]$ are the reactant species, and $C_i, i \in [k+1,\ldots l]$ are the product species. Due to the reaction stoichiometry, the changes in the mole amounts, N_i with $i \in [1,\ldots,l]$, of species satisfy

$$-\frac{dN_1}{a_1} = \cdots = -\frac{dN_k}{a_k} = \frac{dN_{k+1}}{a_{k+1}} = \cdots = \frac{dN_l}{a_l} = d\xi$$

where $d\xi$ denotes the change of reaction ξ. The affinity A of this reaction is defined as

$$A = \sum_{i=1}^{k}a_i\eta_i - \sum_{i=k+1}^{l}a_i\eta_i\,. \tag{33}$$

The entropy production by the chemical reaction is given by $\frac{A}{T}\dot{\xi} \geq 0$ where $\dot{\xi}$ is the reaction velocity[55]. Defining $\upsilon := \dot{\xi}/V$, the reaction velocity per unit volume, we obtain that $A\upsilon/T \geq 0$ is the density of entropy production by reaction ξ. In the case of M simultaneous reactions, we have that the production rate of species i is defined as $r_i = \sum_{m=1}^{M} \pm a_{mi}\upsilon_m$, where the positive sign is used when the species C_i is a reactant of reaction ξ_m and the negative sign when it is a product. Then, the density of entropy production per unit volume is given by

$$\sum_{i=1}^{m}\frac{A_i}{T}\upsilon_i = \sum_{i=1}^{l}\frac{\eta_i}{T}r_i = \frac{\boldsymbol{\eta}}{T}\cdot\boldsymbol{r} \geq 0 \tag{34}$$

where $\boldsymbol{r} = [r_1,\ldots,r_l]^\top$ denotes the set of species reaction rates.

B. Balance equations

Assuming a fluid with l species, additionally to equations (8) and (15), we consider the following constitutive equation to describe the dynamics of species i, $\rho D_t c_i := \rho\,(\partial_t + \mathbf{v}\cdot\mathbf{grad}\,)c_i = -\mathrm{div}\,\mathbf{j}_i - r_i$, i.e.:

$$\partial_t c_i = -\,\mathbf{v}\cdot\mathbf{grad}\,c_i - \frac{1}{\rho}\mathrm{div}\,\mathbf{j}_i - \frac{1}{\rho}r_i \tag{35}$$

where c_i denotes the concentration (mol/kg) of the i-th component, $\mathbf{j}_i$ and r_i are the corresponding diffusive flux and production rate due to the chemical reactions, as shown in Sections IV A 2 and IV A 3, respectively. Then, the dynamics of the l species can be expressed as

$$\partial_t \boldsymbol{c} = -\mathbf{v}\cdot[\mathbf{Grad}\,\boldsymbol{c}] - \frac{1}{\rho}\mathbf{Div}\,\boldsymbol{\Upsilon} - \frac{1}{\rho}\boldsymbol{r} \tag{36}$$

where $\mathbf{c} = [c_1,\dots,c_l]^\top$, $\boldsymbol{\eta} = [\eta_1,\dots,\eta_l]^\top$ and $\boldsymbol{r} = [r_1,\dots,r_l]^\top$ are the vectors of size l, that group the concentration, chemical potential and reaction rate of the fluid species, respectively, and $\boldsymbol{\Upsilon} = [\mathbf{j}_1,\dots,\mathbf{j}_l]^\top$ is a the second order tensor of size $l\times n$ associated with the diffusion flux of species.

Given the non-isentropic assumption, we consider the effect of the thermal domain in the internal energy dynamics. In the non-isentropic case the constitutive equation for the specific internal energy is given by[44]

$$\partial_t u = -\mathbf{v}\cdot\mathbf{grad}\,u - \frac{p}{\rho}\mathrm{div}\,\mathbf{v} - \frac{1}{\rho}\boldsymbol{\tau} : \mathbf{Grad}\,\mathbf{v} - \frac{1}{\rho}\mathrm{div}\,\mathbf{q} \tag{37}$$

where $\mathbf{q}$ is heat flux, described in Section IV A 2, and $-\frac{1}{\rho}\boldsymbol{\tau} : \mathbf{Grad}\,\mathbf{v}$ describes the irreversible rate of internal energy production per unit mass by viscous dissipation.

On the other hand, considering the thermal domain and the chemical species, Gibbs equation can be written as

$$\mathrm{d}u = -p\mathrm{d}\frac{1}{\rho} + T\mathrm{d}s + \sum_{i=1}^{l}\eta_i\mathrm{d}c_i = -p\mathrm{d}\frac{1}{\rho} + T\mathrm{d}s + \boldsymbol{\eta}\cdot\mathrm{d}\boldsymbol{c} \tag{38}$$

where s denotes the specific entropy of the fluid. Considering the local thermodynamic equilibrium assumption $D_t u = \frac{p}{\rho^2}D_t\rho + TD_t s + \sum_{i=1}^{l}\eta_i D_t c_i$, then the following constitutive equation for the specific entropy is obtained:

$$\begin{aligned}\partial_t s = &-\mathbf{v}\cdot\mathbf{grad}\,s - \frac{1}{\rho T}\boldsymbol{\tau} : \mathbf{Grad}\,\mathbf{v} - \frac{1}{\rho T}\mathrm{div}\,\mathbf{q}\\ &+ \frac{1}{\rho T}\boldsymbol{\eta}\cdot[\boldsymbol{r} + \mathbf{Div}\,\boldsymbol{\Upsilon}]\end{aligned} \tag{39}$$

Similarly, assuming that ρ, s and c_i are independent variables, such that $p = \rho^2\partial_\rho u$, from Gibbs equation (38) we obtain the relation $\frac{1}{\rho}\mathbf{grad}\,p = \mathbf{grad}\,\hbar - T\mathbf{grad}\,s - \boldsymbol{\eta}\cdot[\mathbf{Grad}\,\boldsymbol{c}]$ and considering $\frac{1}{\rho T}\boldsymbol{\eta}\cdot\mathbf{Div}\ \boldsymbol{\Upsilon} = \frac{1}{\rho T}\mathrm{div}\ (\boldsymbol{\eta}\cdot\boldsymbol{\Upsilon}) - \frac{1}{\rho T}\boldsymbol{\Upsilon} : \mathbf{Grad}\,\boldsymbol{\eta}$, the governing equation of fluid dynamics can be expressed as:

$$\partial_t\rho = -\,\mathrm{div}\,\rho\mathbf{v} \tag{40a}$$

$$\begin{aligned}\partial_t\mathbf{v} = &-\mathbf{grad}\,\left(\frac{1}{2}\mathbf{v}\cdot\mathbf{v} + \hbar\right) - G_\omega\cdot\mathbf{v} + T\mathbf{grad}\,s\\ &+ [\mathbf{Grad}\,\boldsymbol{c}]\cdot\boldsymbol{\eta} - \frac{1}{\rho}\mathbf{Div}\,\boldsymbol{\tau}\end{aligned} \tag{40b}$$

$$\partial_t\boldsymbol{c} = -\,\mathbf{v}\cdot[\mathbf{Grad}\,\boldsymbol{c}] - \frac{1}{\rho}\mathbf{Div}\,\boldsymbol{\Upsilon} - \frac{1}{\rho}\boldsymbol{r} \tag{40c}$$

$$\begin{aligned}\partial_t s = &-\mathbf{v}\cdot\mathbf{grad}\,s - \frac{1}{\rho T}\boldsymbol{\tau} : [\mathbf{Grad}\,\mathbf{v}] - \frac{1}{\rho T}\boldsymbol{\Upsilon} : [\mathbf{Grad}\,\boldsymbol{\eta}]\\ &+ \boldsymbol{\eta}\cdot\frac{\boldsymbol{r}}{\rho T} - \frac{1}{\rho T}\mathrm{div}\,\mathbf{q}^{(h)}\end{aligned} \tag{40d}$$

where $\mathbf{q}^{(h)} := \mathbf{q} - \sum_{i=1}^{l}\eta_i\mathbf{j}_i = \mathbf{q} - \boldsymbol{\eta}\cdot\boldsymbol{\Upsilon}$ is the heat flux modified by the diffusional enthalpy flux[44].

C. Pseudo port-Hamiltonian formulation

In Section III, due to the isentropic assumption, the thermal domain was neglected, i.e., heat effects were not accounted for in the internal energy description. As a consequence, the conversion of kinetic energy into heat by viscous friction was characterized as a dissipation of energy, and a dissipative port-Hamiltonian formulation was obtained. For non-isentropic reactive fluids, the thermal and chemical domains are described through the dynamics of the specific entropy s and the concentrations of fluid species $\boldsymbol{c}$, respectively. The aim of this section is to obtain a formulation of the form

$$\partial_t\mathbf{x} = \mathscr{J}(\mathbf{x},\mathbf{e})\,\mathbf{e}$$

where $\mathscr{J}(\mathbf{x},\mathbf{e})$ is a formally skew-symmetric operator that describes the energy fluxes between the mechanical, chemical and thermal domains of the fluid dynamics, including the irreversible processes, and satisfying the first and the second law of Thermodynamics.

The chemical and thermal energies are now considered as a part of the total energy, as shown in (38). This implies that u is a function of the specific entropy and the species concentrations. Then, the total energy stored in system (40) with domain Ω is given by:

$$\bar{\mathscr{H}} = \int_\Omega\left(\frac{1}{2}\rho\mathbf{v}\cdot\mathbf{v} + \rho u(\rho,s,\boldsymbol{c})\right)\mathrm{d}\Omega \tag{41}$$

leading to the following co-energy variables

$$\mathbf{e} = \begin{bmatrix}\delta_\rho\bar{\mathscr{H}}\\ \delta_{\mathbf{v}}\bar{\mathscr{H}}\\ \delta_{\boldsymbol{c}}\bar{\mathscr{H}}\\ \delta_s\bar{\mathscr{H}}\end{bmatrix} = \begin{bmatrix}\frac{1}{2}\mathbf{v}\cdot\mathbf{v} + u + \rho\,\partial_\rho u\\ \rho\mathbf{v}\\ \rho\boldsymbol{\eta}\\ \rho T\end{bmatrix} \tag{42}$$

To obtain the port-Hamiltonian formulation for these reactive fluids, we first identify the operators that describe the energy fluxes in(40), as shown in the following lemmas.

Lemma 2. *Let* $\mathscr{A}_{\mathbf{c}} : L^2(\Omega,\mathbb{R}^n) \rightarrow L^2(\Omega,\mathbb{R}^l)$, $\mathscr{A}_s : L^2(\Omega,\mathbb{R}^n) \rightarrow L^2(\Omega,\mathbb{R})$ *and* $\mathscr{R} : L^2(\Omega,\mathbb{R}) \rightarrow L^2(\Omega,\mathbb{R}^l)$ *be the unbounded differential operators defined by* $\mathscr{A}_{\mathbf{c}}(\star) = (\star)\cdot\left[\frac{\mathbf{Grad}\ \boldsymbol{c}}{\rho}\right]$, $\mathscr{A}_s(\star) = (\star)\cdot\left[\frac{\mathbf{grad}\ s}{\rho}\right]$ *and* $\mathscr{R}(\star) = -\frac{1}{\rho^2 T}\boldsymbol{r}(\star)$ *, respectively. Then,* $\mathscr{A}_{\mathbf{c}}^*(\star) = \frac{\mathbf{Grad}\ \mathbf{c}}{\rho}\cdot(\star)$, $\mathscr{A}_s^*(\star) = \frac{\mathbf{grad}\ s}{\rho}(\star)$ *and* $\mathscr{R}^*(\star) = -(\star)\cdot\frac{\boldsymbol{r}}{\rho^2 T}$ *are the formal adjoint operators of* $\mathscr{A}_{\mathbf{c}}$, $\mathscr{A}_s$ *and* $\mathscr{R}$, *respectively.*

Proof. See Appendix B 2. □

Lemma 3. *Let* $\mathscr{D}_{\boldsymbol{\tau}} : L^2(\Omega,\mathbb{R}) \rightarrow L^2(\Omega,\mathbb{R}^n)$, $\mathscr{D}_{\boldsymbol{\Upsilon}} : L^2(\Omega,\mathbb{R}) \rightarrow L^2(\Omega,\mathbb{R})$ *and* $\mathscr{D}_{\mathbf{q}} : L^2(\Omega,\mathbb{R}) \rightarrow L^2(\Omega,\mathbb{R})$ *be the unbounded differential operators defined as* $\mathscr{D}_{\boldsymbol{\tau}}(\star) = -\frac{1}{\rho}\mathbf{Div}\ \left[\frac{\boldsymbol{\tau}}{\rho T}(\star)\right]$, $\mathscr{D}_{\boldsymbol{\Upsilon}}(\star) = -\frac{1}{\rho}\mathbf{Div}\ \left[\frac{\boldsymbol{\Upsilon}}{\rho T}(\star)\right]$ *and* $\mathscr{D}_{\mathbf{q}}(\star) = -\frac{1}{\rho}\mathrm{div}\ \left[\frac{\mathbf{q}^{(h)}}{\rho T^2}(\star)\right]$ *, respectively. Then,* $\mathscr{D}_{\boldsymbol{\tau}}^*(\star) = \frac{\boldsymbol{\tau}}{\rho T} : \mathbf{Grad}\ \frac{(\star)}{\rho}$, $\mathscr{D}_{\boldsymbol{\Upsilon}}^*(\star) = \frac{\boldsymbol{\Upsilon}}{\rho T} : \mathbf{Grad}\ \frac{(\star)}{\rho}$ *and* $\mathscr{D}_{\mathbf{q}}^*(\star) = \frac{\mathbf{q}^{(h)}}{\rho T^2}\cdot\mathbf{grad}\ \frac{(\star)}{\rho}$ *are the formal adjoint operators of* $\mathscr{D}_{\boldsymbol{\tau}}$, $\mathscr{D}_{\boldsymbol{\Upsilon}}$ *and* $\mathscr{D}_{\mathbf{q}}$, *respectively, satisfying the following relations:*

$$\begin{aligned}
&\left\langle \delta_{\mathbf{v}}\bar{\mathscr{H}}, \mathscr{D}_{\tau}(\delta_s\bar{\mathscr{H}})\right\rangle_{L^2} - \left\langle \mathscr{D}_{\boldsymbol{\tau}}^*(\delta_{\mathbf{v}}\bar{\mathscr{H}}), \delta_s\bar{\mathscr{H}}\right\rangle_{L^2} \\
&\qquad = -\int_{\partial\Omega}\frac{\delta_{\mathbf{v}}\bar{\mathscr{H}}}{\rho}\cdot[\boldsymbol{\tau}\cdot\mathbf{n}]\,\mathrm{d}\gamma \qquad (43)\\
&\left\langle \delta_{\mathbf{c}}\bar{\mathscr{H}}, \mathscr{D}_{\boldsymbol{\Upsilon}}(\delta_s\bar{\mathscr{H}})\right\rangle_{L^2} - \left\langle \mathscr{D}_{\boldsymbol{\Upsilon}}^*(\delta_{\mathbf{c}}\bar{\mathscr{H}}), \delta_s\bar{\mathscr{H}}\right\rangle_{L^2} \\
&\qquad = -\int_{\partial\Omega}\frac{\delta_{\mathbf{c}}\bar{\mathscr{H}}}{\rho}\cdot[\boldsymbol{\Upsilon}\cdot\mathbf{n}]\,\mathrm{d}\gamma \qquad (44)\\
&\left\langle \delta_s\bar{\mathscr{H}}, \mathscr{D}_{\mathbf{q}}(\delta_s\bar{\mathscr{H}})\right\rangle_{L^2} - \left\langle \delta_s\bar{\mathscr{H}}, \mathscr{D}_{\mathbf{q}}^*(\delta_s\bar{\mathscr{H}})\right\rangle_{L^2} \\
&\qquad = -\int_{\partial\Omega}\frac{\delta_s\bar{\mathscr{H}}}{\rho}\left[\frac{\mathbf{q}^{(h)}}{T}\cdot\mathbf{n}\right]\mathrm{d}\gamma \qquad (45)
\end{aligned}$$

Proof. See Appendix B 3. □

Note that $\mathscr{A}_s(\delta_{\mathbf{v}}\bar{\mathscr{H}}) = \delta_{\mathbf{v}}\bar{\mathscr{H}}\cdot\frac{\mathbf{grad}\ s}{\rho} = \mathbf{v}\cdot\mathbf{grad}\ s$ and $\mathscr{A}_s(\delta_{\mathbf{v}}\bar{\mathscr{H}}) = \delta_{\mathbf{v}}\bar{\mathscr{H}}\cdot\frac{\mathbf{Grad}\ \boldsymbol{c}}{\rho} = \mathbf{v}\cdot\mathbf{Grad}\ \boldsymbol{c}$ describe the advection terms of the specific entropy and the species concentration dynamics. Similarly, $\mathscr{R}(\delta_s\bar{\mathscr{H}}) = -\frac{\boldsymbol{r}}{\rho^2 T}\delta_s\bar{\mathscr{H}} = -\frac{\boldsymbol{r}}{\rho}$ describes the variation rate of the species concentrations due to chemical reactions, and $-\mathscr{R}(\delta_{\mathbf{c}}\bar{\mathscr{H}}) = \frac{\boldsymbol{r}}{\rho}\cdot\boldsymbol{\eta}$ the corresponding rate of specific entropy production. Then, $\mathscr{D}_{\boldsymbol{\tau}}(\delta_s\bar{\mathscr{H}}) = -\frac{1}{\rho}\mathbf{Div}\ \boldsymbol{\tau}$ and $\mathscr{D}_{\boldsymbol{\Upsilon}}(\delta_s\bar{\mathscr{H}}) = -\frac{1}{\rho}\mathbf{Div}\ \boldsymbol{\Upsilon}$ describe the viscous friction of fluid velocity dynamics and the diffusion phenomena of the species concentration, with $-\mathscr{D}_{\boldsymbol{\tau}}^*(\delta_{\mathbf{v}}\bar{\mathscr{H}}) = -\frac{\boldsymbol{\tau}}{\rho T} : \mathbf{Grad}\ \mathbf{v}$ and $-\mathscr{D}_{\boldsymbol{\Upsilon}}^*(\delta_{\mathbf{v}}\bar{\mathscr{H}}) = -\frac{\boldsymbol{\Upsilon}}{\rho T} : \mathbf{Grad}\ \mathbf{v}$ as the corresponding rate of irreversible entropy production. Finally, $\mathscr{D}_{\mathbf{q}}(\delta_s\bar{\mathscr{H}}) = -\frac{1}{\rho}\mathrm{div}\ \frac{\mathbf{q}^{(h)}}{T}$ and $-\mathscr{D}_{\mathbf{q}}^*(\delta_s\bar{\mathscr{H}}) = -\frac{\mathbf{q}^{(h)}}{\rho T^2}\cdot\mathbf{grad}\ T$ characterize the entropy diffusion and creation by heat flux.

Theorem 2. *Consider a reactive and compressible Newtonian fluid whose total energy* $\bar{\mathscr{H}}$ *on domain* Ω *is defined by* (41), *with state variables* $\mathbf{x} = [\rho\ \mathbf{v}^\top\mathbf{c}^\top\ s]^\top$ *and takes into account the non-negative conditions* (27), (28), (29) *and* (34). *The fluid dynamics can be expressed by the following pseudo port-Hamiltonian system:*

$$\partial_t\mathbf{x} = \mathscr{J}(\mathbf{x},\mathbf{e})\,\mathbf{e}, \qquad (46)$$

where $\mathscr{J}(\mathbf{x},\mathbf{e})$ *is a state and co-energy dependent skew-symmetric operator given by*

$$\mathscr{J}(\mathbf{x},\mathbf{e}) = \begin{bmatrix} 0 & -\mathrm{div} & \mathbf{0} & \mathbf{0} \\ -\mathbf{grad} & -\frac{1}{\rho}G_{\boldsymbol{\omega}}\cdot & \mathscr{A}_{\boldsymbol{c}}^* & \mathscr{A}_s^* + \mathscr{D}_{\boldsymbol{\tau}} \\ \mathbf{0} & -\mathscr{A}_{\boldsymbol{c}} & \mathbf{0} & \mathscr{R} + \mathscr{D}_{\boldsymbol{\Upsilon}} \\ \mathbf{0} & -\mathscr{A}_s - \mathscr{D}_{\boldsymbol{\tau}}^* & -\mathscr{R}^* - \mathscr{D}_{\boldsymbol{\Upsilon}}^* & \mathscr{D}_{\mathbf{q}} - \mathscr{D}_{\mathbf{q}}^* \end{bmatrix} \qquad (47)$$

The energy and entropy balances

$$\dot{\bar{\mathscr{H}}} = \langle\mathbf{f}_\partial,\mathbf{e}_\partial\rangle_{\partial\Omega} \qquad (48)$$

$$\dot{\mathscr{S}} = \int_\Omega \sigma_s\,\mathrm{d}\Omega + \left\langle\mathbf{f}_\partial,\mathbf{e}_\partial^{\mathrm{s}}\right\rangle_{\partial\Omega} \qquad (49)$$

satisfy the first and second law ($\sigma_s \geq 0$) *of Thermodynamics, respectively, and*

$$\mathbf{f}_\partial = \begin{bmatrix} -v_{\mathbf{n}} \\ -v_{\mathbf{t}} \\ -\ \boldsymbol{\Upsilon}|_{\partial\Omega}\cdot\mathbf{n} \\ -\left(\left.\frac{\mathbf{q}^{(h)}}{T}\right|_{\partial\Omega}\cdot\mathbf{n}\right) \end{bmatrix} \quad \textit{and} \quad \mathbf{e}_\partial = \begin{bmatrix} \rho\,\delta_\rho\bar{\mathscr{H}}\big|_{\partial\Omega} + \tau_{\mathbf{n}} \\ \tau_{\mathbf{t}} \\ \left.\frac{\delta_{\mathbf{c}}\bar{\mathscr{H}}}{\rho}\right|_{\partial\Omega} \\ \left.\frac{\delta_s\bar{\mathscr{H}}}{\rho}\right|_{\partial\Omega} \end{bmatrix} \qquad (50)$$

are the boundary port variables, $v_{\mathbf{n}}|_{\partial\Omega} = \mathbf{v}|_{\partial\Omega}\cdot\mathbf{n}$ *and* $v_{\mathbf{t}} = \mathbf{v}|_{\partial\Omega}\cdot\mathbf{t}$ *are the magnitude of the normal and orthogonal projections of the fluid velocity on* $\partial\Omega$. $\tau_{\mathbf{n}}$ *and* $\tau_{\mathbf{t}}$ *are the projections of the viscous tensor and* $\frac{\mathbf{q}^{(h)}}{T}$ *the entropy flux.* $\mathbf{n}$ *is the unitary outward vector normal to* $\partial\Omega$, *and* $\mathbf{t}$ *the tangential unitary vector orthogonal to* $\mathbf{n}$ *such that* $(\mathbf{v}\cdot\mathbf{t})\mathbf{t} = -\mathbf{n}\times[\mathbf{n}\times\mathbf{v}]$. *The term* $\left\langle\mathbf{f}_\partial,\mathbf{e}_\partial^s\right\rangle_{\partial\Omega}$ *describes the entropy exchange with the environment through* $\partial\Omega$, *with* $\mathbf{e}_\partial^s = [\rho s|_{\partial\Omega}\quad 0\quad \mathbf{0}\quad 1]^\top$, *and* $\sigma_s = -\frac{\boldsymbol{\tau}}{T} : \mathbf{Grad}\ \mathbf{v} + \frac{\boldsymbol{r}}{\rho T}\cdot\boldsymbol{\eta} - \frac{\boldsymbol{\Upsilon}}{T} : \mathbf{Grad}\ \boldsymbol{\eta} - \frac{\mathbf{q}^{(h)}}{T^2}\cdot\mathbf{grad}\ T \geq 0$ *characterizes the density of the internal entropy production of the fluid.*

Proof. Considering that $\frac{1}{\rho T}\mathrm{div}\ \mathbf{q}^{(h)} = \frac{\mathbf{q}^{(h)}}{\rho T^2}\cdot\mathbf{grad}\ T + \frac{1}{\rho}\mathrm{div}\ \frac{\mathbf{q}^{(h)}}{T}$ and using the co-energy variables defined in (42), the govern-

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ing equations can be rewritten as:

$$
\begin{aligned}
\partial_t \rho &= -\operatorname{div}\, \delta_{\mathbf{v}}\bar{\mathscr{H}} \\
\partial_t \mathbf{v} &= -\,\mathbf{grad}\ \delta_\rho \bar{\mathscr{H}} - \frac{1}{\rho} G_{\omega} \cdot \delta_{\mathbf{v}}\bar{\mathscr{H}} + \frac{\mathbf{grad}\ s}{\rho}\delta_s \bar{\mathscr{H}} \\
&\quad + \frac{[\mathbf{Grad}\ \boldsymbol{c}]}{\rho}\cdot \delta_{\boldsymbol{c}}\bar{\mathscr{H}} - \frac{1}{\rho}\mathbf{Div}\left[\frac{\boldsymbol{\tau}}{\rho T}\delta_s\bar{\mathscr{H}}\right] \\
\partial_t \boldsymbol{c} &= -\,\delta_{\mathbf{v}}\bar{\mathscr{H}} \cdot \frac{[\mathbf{Grad}\ \boldsymbol{c}]}{\rho} - \frac{1}{\rho}\mathbf{Div}\left[\frac{\boldsymbol{\Upsilon}}{\rho T}\delta_s\bar{\mathscr{H}}\right] - \frac{1}{\rho^2 T}\boldsymbol{r}\,\delta_s\bar{\mathscr{H}} \\
\partial_t s &= -\,\delta_{\mathbf{v}}\bar{\mathscr{H}} \cdot \frac{\mathbf{grad}\ s}{\rho} - \frac{1}{\rho T}\boldsymbol{\tau} : \left[\mathbf{Grad}\ \frac{\delta_{\mathbf{v}}\bar{\mathscr{H}}}{\rho}\right] \\
&\quad - \frac{1}{\rho T}\boldsymbol{\Upsilon} : \left[\mathbf{Grad}\ \frac{\delta_{\boldsymbol{c}}\bar{\mathscr{H}}}{\rho}\right] + \frac{\boldsymbol{r}}{\rho^2 T}\cdot \delta_{\boldsymbol{c}}\bar{\mathscr{H}} \\
&\quad - \frac{\mathbf{q}^{(h)}}{\rho T^2}\mathbf{grad}\ \frac{\delta_s\bar{\mathscr{H}}}{\rho} - \frac{1}{\rho}\operatorname{div}\left[\frac{\mathbf{q}^{(h)}}{\rho T^2}\delta_s\bar{\mathscr{H}}\right]
\end{aligned}
$$

Then, defining the state variables as $\mathbf{x} = \begin{bmatrix}\rho & \mathbf{v}^\top & \boldsymbol{c}^\top & s\end{bmatrix}^\top$, computing the co-energy variables by (42), and using the operators $\mathscr{A}_{\boldsymbol{c}}$, $\mathscr{A}_s$, $\mathscr{R}$, $\mathscr{D}_{\boldsymbol{\tau}}$, $\mathscr{D}_{\boldsymbol{\Upsilon}}$, $\mathscr{D}_{\mathbf{q}}$ and the corresponding formal adjoints defined in Lemmas 2 and 3, we obtain the port-Hamiltonian formulation (46), with the skew-symmetric operator $\mathscr{J}(\mathbf{x},\mathbf{e})$ defined in (47).

On the other hand, the rate of change of the total energy is given by:

$$
\begin{aligned}
\dot{\bar{\mathscr{H}}} &= \int_\Omega \delta_{\mathbf{x}}\bar{\mathscr{H}} \cdot \partial_t \mathbf{x}\, \mathrm{d}\Omega = \int_\Omega \mathbf{e}\cdot [\mathscr{J}(\mathbf{x},\mathbf{e})\,\mathbf{e}]\, \mathrm{d}\Omega \\
&= -\left\langle \delta_\rho\bar{\mathscr{H}}, \operatorname{div}\, \delta_{\mathbf{v}}\bar{\mathscr{H}}\right\rangle_{L^2} - \left\langle \mathbf{grad}\ \delta_\rho\bar{\mathscr{H}}, \delta_{\mathbf{v}}\bar{\mathscr{H}}\right\rangle_{L^2} \\
&\quad + \left\langle \delta_{\mathbf{v}}\bar{\mathscr{H}}, \mathscr{D}_{\boldsymbol{\tau}}(\delta_s\bar{\mathscr{H}})\right\rangle_{L^2} - \left\langle \mathscr{D}^*_{\boldsymbol{\tau}}(\delta_{\mathbf{v}}\bar{\mathscr{H}}), \delta_s\bar{\mathscr{H}}\right\rangle_{L^2} \\
&\quad + \left\langle \delta_{\boldsymbol{c}}\bar{\mathscr{H}}, \mathscr{D}_{\boldsymbol{\Upsilon}}(\delta_s\bar{\mathscr{H}})\right\rangle_{L^2} - \left\langle \mathscr{D}^*_{\boldsymbol{\Upsilon}}(\delta_{\boldsymbol{c}}\bar{\mathscr{H}}), \delta_s\bar{\mathscr{H}}\right\rangle_{L^2} \\
&\quad + \left\langle \delta_s\bar{\mathscr{H}}, \mathscr{D}_{\mathbf{q}}(\delta_s\bar{\mathscr{H}})\right\rangle_{L^2} - \left\langle \delta_s\bar{\mathscr{H}}, \mathscr{D}^*_{\mathbf{q}}(\delta_s\bar{\mathscr{H}})\right\rangle_{L^2}
\end{aligned}
$$

Using identity (A3), the Gauss-Ostrogradsky divergence theorem and the relations given in Lemma 3, we obtain

$$
\begin{aligned}
\dot{\bar{\mathscr{H}}} &= -\int_{\partial\Omega}\left(\delta_\rho\bar{\mathscr{H}}\left(\delta_{\mathbf{v}}\bar{\mathscr{H}}\cdot\mathbf{n}\right) + \frac{\delta_{\mathbf{v}}\bar{\mathscr{H}}}{\rho}\cdot[\boldsymbol{\tau}\cdot\mathbf{n}]\right)\mathrm{d}\gamma \\
&\quad - \int_{\partial\Omega}\left(\frac{\delta_{\boldsymbol{c}}\bar{\mathscr{H}}}{\rho}\cdot[\boldsymbol{\Upsilon}\cdot\mathbf{n}] + \frac{\delta_s\bar{\mathscr{H}}}{\rho}\left(\frac{\mathbf{q}^{(h)}}{T}\cdot\mathbf{n}\right)\right)\mathrm{d}\gamma
\end{aligned}
$$

Consider now the tangential plane Γ to the boundary surface $\partial\Omega$, and the unitary vector $\mathbf{t}\in\Gamma$ orthogonal to $\mathbf{n}$, i.e., $\mathbf{n}\cdot\mathbf{t} = 0$, such that $(\mathbf{v}\cdot\mathbf{t})\mathbf{t} = -\mathbf{n}\times[\mathbf{n}\times\mathbf{v}]$, $\forall\zeta\in\partial\Omega$, describes the orthogonal projection of the fluid velocity with respect to the boundary surface. Then, given that $\frac{\delta_{\mathbf{v}}\bar{\mathscr{H}}}{\rho}\cdot[\boldsymbol{\tau}\cdot\mathbf{n}] = \boldsymbol{\tau} : \left[\frac{\delta_{\mathbf{v}}\bar{\mathscr{H}}}{\rho}\mathbf{n}^\top\right]$ and $\frac{\delta_{\mathbf{v}}\bar{\mathscr{H}}}{\rho} = \left(\frac{\delta_{\mathbf{v}}\bar{\mathscr{H}}}{\rho}\cdot\mathbf{n}\right)\mathbf{n} + \left(\frac{\delta_{\mathbf{v}}\bar{\mathscr{H}}}{\rho}\cdot\mathbf{t}\right)\mathbf{t}$, $\forall\zeta\in\partial\Omega$, the boundary conditions associated with the viscous tensor can be rewritten as:

$$
\frac{\delta_{\mathbf{v}}\bar{\mathscr{H}}}{\rho}\cdot[\boldsymbol{\tau}\cdot\mathbf{n}] = v_{\mathbf{n}}\tau_{\mathbf{n}} + v_{\mathbf{t}}\tau_{\mathbf{t}}, \quad \forall\zeta\in\partial\Omega
$$

where $v_{\mathbf{n}} = \frac{\delta_{\mathbf{v}}\bar{\mathscr{H}}}{\rho}|_{\partial\Omega}\cdot\mathbf{n} = \mathbf{v}|_{\partial\Omega}\cdot\mathbf{n}$ and $v_{\mathbf{t}} = \frac{\delta_{\mathbf{v}}\bar{\mathscr{H}}}{\rho}|_{\partial\Omega}\cdot\mathbf{t} = \mathbf{v}|_{\partial\Omega}\cdot\mathbf{t}$ are the magnitude normal and orthogonal projections of the fluid velocity at $\partial\Omega$, and $\tau_{\mathbf{n}} = \tau : [\mathbf{n}\otimes\mathbf{n}]$ and $\tau_{\mathbf{t}} = \tau : [\mathbf{t}\otimes\mathbf{n}]$ the corresponding projections of the viscous tensor. This implies that $\dot{\bar{\mathscr{H}}}$ can be expressed as:

$$
\begin{aligned}
\dot{\bar{\mathscr{H}}} &= -\int_{\partial\Omega}\left(\left(\rho\,\delta_\rho\bar{\mathscr{H}} + \tau_{\mathbf{n}}\right)v_{\mathbf{n}} + \tau_{\boldsymbol{s}}v_{\boldsymbol{s}}\right)\mathrm{d}\gamma \\
&\quad - \int_{\partial\Omega}\left(\frac{\delta_{\boldsymbol{c}}\bar{\mathscr{H}}}{\rho}\cdot[\boldsymbol{\Upsilon}\cdot\mathbf{n}] + \frac{\delta_s\bar{\mathscr{H}}}{\rho}\left(\frac{\mathbf{q}^{(h)}}{T}\cdot\mathbf{n}\right)\right)\mathrm{d}\gamma \\
&= \int_{\partial\Omega}\mathbf{e}_\partial\cdot\mathbf{f}_\partial\,\mathrm{d}\gamma = \langle\mathbf{e}_\partial,\mathbf{f}_\partial\rangle_{\partial\Omega}
\end{aligned}
$$

where $\mathbf{f}_\partial$ and $\mathbf{e}_\partial$ are the boundary port variables defined in (50).

Regarding the total entropy $\mathscr{S} = \int_\Omega \rho s\,\mathrm{d}\Omega$, with $\delta_{\mathbf{x}}\mathscr{S} = \begin{bmatrix} s & \mathbf{0} & \mathbf{0} & \rho\end{bmatrix}^\top$, we have that its rate of change is given by:

$$
\begin{aligned}
\dot{\mathscr{S}} &= \int_\Omega \delta_{\mathbf{x}}\mathscr{S}\cdot[\mathscr{J}(\mathbf{x})\mathbf{e}]\,\mathrm{d}\Omega \\
&= -\int_\Omega\left(s\operatorname{div}\,\delta_{\mathbf{v}}\bar{\mathscr{H}} + \rho\mathscr{A}_s(\delta_{\mathbf{v}}\bar{\mathscr{H}}) - \rho\mathscr{D}_{\mathbf{q}}(\delta_s\bar{\mathscr{H}})\right)\mathrm{d}\Omega \\
&\quad + \int_\Omega \sigma_s\,\mathrm{d}\Omega \\
&= -\int_\Omega\left(s\operatorname{div}\,\delta_{\mathbf{v}}\bar{\mathscr{H}} + \delta_{\mathbf{v}}\bar{\mathscr{H}}\cdot\mathbf{grad}\ s + \operatorname{div}\frac{\mathbf{q}^{(h)}}{T}\right)\mathrm{d}\Omega \\
&\quad + \int_\Omega \sigma_s\,\mathrm{d}\Omega
\end{aligned}
$$

where $\sigma_s = -\rho\left(\mathscr{D}^*_{\boldsymbol{\tau}}(\delta_{\mathbf{v}}\bar{\mathscr{H}}) + \mathscr{R}^*(\delta_{\boldsymbol{c}}\bar{\mathscr{H}}) + \mathscr{D}^*_{\boldsymbol{\Upsilon}}(\delta_{\boldsymbol{c}}\bar{\mathscr{H}}) + \mathscr{D}^*_{\mathbf{q}}(\delta_s\bar{\mathscr{H}})\right)$ denotes the density of internal entropy production of the reactive fluid dynamics. Using identity (A3) and the Gauss-Ostrogradsky divergence theorem, we obtain

$$
\begin{aligned}
\dot{\mathscr{S}} &= \int_\Omega \sigma_s\,\mathrm{d}\Omega + \int_{\partial\Omega}\left(\mathrm{s}\,\delta_{\mathbf{v}}\bar{\mathscr{H}} + \frac{\mathbf{q}^{(\mathrm{h})}}{\mathrm{T}}\right)\cdot\mathbf{n}\,\mathrm{d}\gamma \\
&= \int_\Omega \sigma_s\,\mathrm{d}\Omega + \langle\mathbf{f}_\partial,\mathbf{e}^{\mathrm{s}}_\partial\rangle_{\partial\Omega}
\end{aligned}
$$

where $\mathbf{e}^s_\partial = [\rho s|_{\partial\Omega} \quad 0 \quad \mathbf{0} \quad 1]^\top$. Considering the non-negative conditions (27), (28), (29) and (34) we have that

$$
\begin{aligned}
\sigma_s &= -\rho\left(\mathscr{D}^*_{\boldsymbol{\tau}}(\delta_{\mathbf{v}}\bar{\mathscr{H}}) + \mathscr{R}^*(\delta_{\boldsymbol{c}}\bar{\mathscr{H}}) + \mathscr{D}^*_{\boldsymbol{\Upsilon}}(\delta_{\boldsymbol{c}}\bar{\mathscr{H}}) + \mathscr{D}^*_{\mathbf{q}}(\delta_s\bar{\mathscr{H}})\right) \\
&= -\frac{\boldsymbol{\tau}}{T} : \mathbf{Grad}\ \mathbf{v} + \frac{\boldsymbol{r}}{\rho T}\cdot\boldsymbol{\eta} - \frac{\boldsymbol{\Upsilon}}{T} : \mathbf{Grad}\ \boldsymbol{\eta} - \frac{\mathbf{q}^{(h)}}{T^2}\cdot\mathbf{grad}\ T \\
&= -\frac{\boldsymbol{\tau}}{T} : \mathbf{Grad}\ \mathbf{v} + \sum_{i=1}^{l}\frac{r_i\eta_i}{\rho T} - \sum_{i=1}^{l}\mathbf{j}_i\cdot\mathbf{grad}\ \frac{\eta_i}{T} - \frac{\mathbf{q}}{T^2}\cdot\mathbf{grad}\ T \\
&\geq 0
\end{aligned}
$$

If the system is isolated, the boundary conditions (50) are equal to 0, and $\dot{\bar{\mathscr{H}}} = 0$, i.e., system (46) is conservative. Similarly, the rate of change of the entropy is given by $\dot{\mathscr{S}} = \int_\Omega \sigma_s\,\mathrm{d}\Omega \geq 0$, i.e., the port-Hamiltonian formulation (46) satisfies the first and second laws of Thermodynamics. $\square$

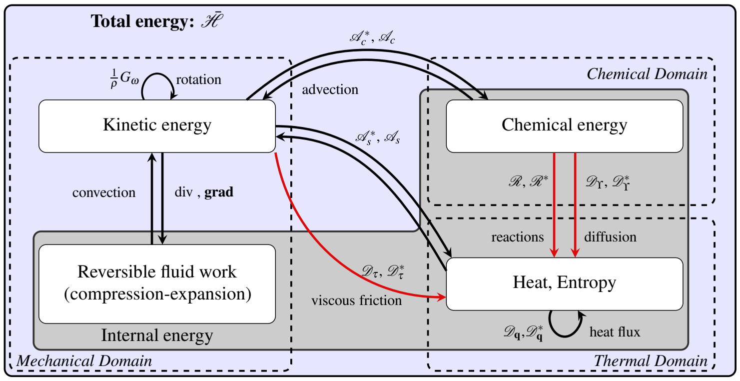

FIG. 2. Energy flux of the PHS formulation of non-isentropic fluids proposed in Theorem 2. Black arrows: reversible energy exchange. Red arrows: irreversible energy transformation.

The PHS formulation described in Theorem 2 can be used in applications where the chemical and thermal domains are relevant for the fluid dynamics, and not only the mechanical domain as in the isentropic case. As for example, in the study and analysis of combustion systems[39–42].

Figure 2 shows the energy flux of the PHS formulation proposed in Theorem 2 due to the physical phenomena of the fluids dynamics. Note that, unlike the isentropic case, the thermal and chemical domains are included in the model of reactive nonisentropic compressible fluids. Additionally to the reversible energy exchange due to the fluid convection and rotation present in the isentropic model, non-isentropic fluids present chemical-mechanical and thermal-mechanical reversible energy transformations. These transformations are associated with the advection terms, described by operators $\mathscr{A}_s$ and $\mathscr{A}_{\mathbf{c}}$, in the entropy and chemical species dynamic equations, respectively, and the corresponding adjoints in the momentum equation. Similarly, the chemical-thermal energy transformation associated with the irreversible entropy creation due to chemical reactions and diffusion are described by operators $\mathscr{R}$, $\mathscr{D}_{\boldsymbol{\Upsilon}}$ and the corresponding adjoints. Finally, entropy production and diffusion by heat flux are described by operators $\mathscr{D}_{\mathbf{q}}^*$ and $\mathscr{D}_{\mathbf{q}}$, respectively.

Remark 6. *Note that different definitions of* $\mathbf{f}_\partial$ *and* $\mathbf{e}_\partial$ *can be proposed such that* $\dot{\bar{\mathscr{H}}} = -\int_{\partial\Omega}\left(\left(\rho\,\delta_\rho\bar{\mathscr{H}} + \tau_{\mathbf{n}}\right)v_{\mathbf{n}} + \tau_t v_t + \frac{\delta_{\mathbf{c}}\bar{\mathscr{H}}}{\rho}\cdot[\boldsymbol{\Upsilon}\cdot\mathbf{n}]\right)\mathrm{d}\gamma - \int_{\partial\Omega}\frac{\delta_s\bar{\mathscr{H}}}{\rho}\left(\frac{\mathbf{q}^{(\mathrm{h})}}{\mathrm{T}}\cdot\mathbf{n}\right)\mathrm{d}\gamma = \langle\mathbf{e}_\partial,\mathbf{f}_\partial\rangle_{\partial\Omega}$. *We selected the realization described in* (50)*, such that* $\mathbf{f}_\partial$ *contains the fluxes of matter and heat between the system* (46) *and its environment, simplifying the analysis of the energy and entropy when the system is isolated.*

Remark 7. *The skew-symmetric operator* $\mathscr{J}(\mathbf{x},\mathbf{e})$ *in* (46) *explicitly depends on the co-energy variable* $\delta_s\bar{\mathscr{H}} = \rho T$*, as shown in* $\mathscr{D}_{\boldsymbol{\tau}}$*,* $\mathscr{D}_{\boldsymbol{\Upsilon}}$*,* $\mathscr{D}_{\mathbf{q}}$*,* $\mathscr{R}$ *and the corresponding formal adjoint operators in Lemma 3. This implies that* $\mathscr{J}(\mathbf{x},\mathbf{e})$ *does not satisfy the Jacobi identity and, as a consequence, the model* (46) *is not a port-Hamiltonian system.*

Similarly to the isentropic case, rotational effects in the momentum equation are characterized using the Gyroscope $G_{\boldsymbol{\omega}}$. As a consequence, from Remark 1, the structure of the pseudo-PHS formulation in Theorem 2, is conserved for the description of 2D reactive non-isentropic compressible fluids.

V. CONCLUSION

In this paper, PHS formulations for isentropic and non-isentropic compressible fluids have been proposed. For isentropic fluids, differential operators and corresponding formal adjoints have been presented to describe the dissipation of kinetic energy into heat viscous friction associated with the vorticity and compressibility of the fluid, separately, leading to a dissipative PHS formulation. Additionally, the boundary port variables include some vorticity boundary conditions, that have not been previously considered in previous works. For the non-isentropic case, a mixture compressible fluid with multiple simultaneous reactions was considered. Operators and corresponding adjoints were defined to characterize the diffusion flux of matter, chemical reactions and the entropy creation associated with these phenomena. The resulting pseudo-PHS is conservative, satisfies the first and second laws of Thermodynamics, and the boundary port variables consider boundary conditions associated with the thermal conduction and diffusive flux of matter of the fluid.

As future work, we consider the development of structure-preserving discretization methods based on finite volumes, finite differences, and/or partitioned finite elements. The aim of these structure-preserving methods is to preserve the properties of the system with respect to the first and second laws of Thermodynamics during numerical implementation of the PHS models in Theorems 1 and 2. In the case of incompressible fluids, a challenge for the discretization methods is the appropriate characterization of the static pressure, such that the structure and properties of the PHS formulation are preserved. On the other hand, we consider the application of passivity-based methods for the control of fluids, and the interconnection of the proposed model with other physical systems, such as in fluid-structure interaction processes. The extension of the PHS formulation to non-Newtonian fluids, such as Maxwell's viscoelastic fluids, is also an interesting topic to consider in the future.

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Appendix A: Useful identities and theorems

Mathematical identities[44] used in this work are listed below:

$$(\boldsymbol{u}\cdot\mathbf{grad}\,)\,\boldsymbol{u} = \mathbf{grad}\left(\frac{1}{2}\boldsymbol{u}\cdot\boldsymbol{u}\right) + [\mathbf{curl}\,\boldsymbol{u}]\times\boldsymbol{u} \tag{A1}$$

$$\boldsymbol{\sigma} : [\mathbf{Grad}\,\boldsymbol{u}] = \mathrm{div}\,[\boldsymbol{\sigma}\cdot\boldsymbol{u}] - \boldsymbol{u}\cdot\mathbf{Div}\,\boldsymbol{\sigma} \tag{A2}$$

$$\mathrm{div}\,[f\boldsymbol{u}] = [\mathbf{grad}\,f]\cdot\boldsymbol{u} + f\,\mathrm{div}\,\boldsymbol{u} \tag{A3}$$

$$\mathbf{Div}\,(\mathbf{Grad}\,\boldsymbol{u}) = \mathbf{grad}\,(\mathrm{div}\,\boldsymbol{u}) - \mathbf{curl}\,[\mathbf{curl}\,\boldsymbol{u}] \tag{A4}$$

$$\mathbf{Div}\left([\mathbf{Grad}\,\boldsymbol{u}]^{\top}\right) = \mathbf{grad}\,(\mathrm{div}\,\boldsymbol{u}) \tag{A5}$$

$$\mathbf{Div}\,[(\mathrm{div}\,\boldsymbol{u})I] = \mathbf{grad}\,(\mathrm{div}\,\boldsymbol{u}) \tag{A6}$$

$$\mathrm{div}\,[\boldsymbol{u}\times\mathbf{v}] = \mathbf{v}\cdot[\mathbf{curl}\,\boldsymbol{u}] - \boldsymbol{u}\cdot[\mathbf{curl}\,\mathbf{v}] \tag{A7}$$

where f is a scalar, $\boldsymbol{u}$ is a vector of dimension 3 and $\boldsymbol{\sigma}$ is a symmetric second order tensor of dimension 3×3.

In the following theorems some useful operators and their adjoints are given, as well as the associted boundary conditions that are used to obtain the port-Hamintonian formulations of fluids. Firstly, we set the adjoint and boundary conditions associated with a modulated rotational operator.

Theorem 3. *Let $\alpha \in C^1\left(\bar{\Omega},\mathbb{R}\right)$ be a continuously differentiable scalar function, such that $(\alpha\boldsymbol{u}) \in H^{\mathrm{curl}}(\Omega,\mathbb{R}^3), \forall\boldsymbol{u} \in H^{\mathrm{curl}}(\Omega,\mathbb{R}^3)$. Denoting by $\mathbf{curl}\ : L^2(\Omega,\mathbb{R}^3) \to L^2(\Omega,\mathbb{R}^3)$ the curl operator, also called rotational, then, $\alpha\,\mathbf{curl}\,(\star)$ is the adjoint of $\mathbf{curl}\,(\alpha\star)$ satisfying the relation*

$$\begin{aligned}\langle\boldsymbol{u}_1,\mathbf{curl}\,(\alpha\boldsymbol{u}_2)\rangle_{L^2} - \langle\alpha\,\mathbf{curl}\,\boldsymbol{u}_1,\boldsymbol{u}_2\rangle_{L^2}\\ = \int_{\partial\Omega}\alpha\,[\boldsymbol{u}_2\times\boldsymbol{u}_1]\cdot\mathbf{n}\,\mathrm{d}\gamma\end{aligned} \tag{A8}$$

for all $(\boldsymbol{u}_1,\boldsymbol{u}_2) \in H^{\mathrm{curl}}(\Omega,\mathbb{R}^3)$, where $\mathbf{n}\in\mathbb{R}^3$ is the outward unitary vector to $\partial\Omega$.

Proof. Using (A7) and the Gauss-Ostrogradsky divergence theorem, the inner product $\langle\boldsymbol{u}_1,\mathbf{curl}\,(\alpha\boldsymbol{u}_2)\rangle_{L^2}$ can be expressed as

$$\begin{aligned}\langle\boldsymbol{u}_1,\mathbf{curl}\,(\alpha\boldsymbol{u}_2)\rangle_{L^2} &= \int_{\Omega}\boldsymbol{u}_1\cdot[\mathbf{curl}\,(\alpha\boldsymbol{u}_2)]\,\mathrm{d}\Omega\\ &= \int_{\Omega}\mathrm{div}\,[(\alpha\boldsymbol{u}_2)\times\boldsymbol{u}_1]\,\mathrm{d}\Omega\\ &\quad+\int_{\Omega}[\alpha\mathbf{curl}\,\boldsymbol{u}_1]\cdot\boldsymbol{u}_2\,\mathrm{d}\Omega\\ &= \langle\alpha\mathbf{curl}\,\boldsymbol{u}_1,\boldsymbol{u}_2\rangle_{L^2}\\ &\quad+\int_{\partial\Omega}[(\alpha\boldsymbol{u}_2)\times\boldsymbol{u}_1]\cdot\mathbf{n}\,\mathrm{d}\gamma\end{aligned}$$

Rewriting the previous equation, we obtain relation (A8). Similarly. As a special case, considering boundary conditions equal to 0, $\langle\boldsymbol{u}_1,\mathbf{curl}\,(\alpha\boldsymbol{u}_2)\rangle_{L^2} = \langle\alpha\,\mathbf{curl}\,\boldsymbol{u}_1,\boldsymbol{u}_2\rangle_{L^2}$, i.e., $\mathbf{curl}\,(\alpha\star)$ is the formal adjoint of $\alpha\,\mathbf{curl}\,(\star)$. ☐

The following theorems define the adjoint and associated boundary conditions for modulated gradient and divergence operators. Note that these theorems are defined on n-dimensional spatial domains, with $n\in\{2,3\}$.

Theorem 4. *Let $\alpha \in C^1\left(\bar{\Omega},\mathbb{R}\right)$ be a continuously differentiable scalar function, such that $(\alpha\boldsymbol{u}) \in H^{\mathrm{div}}(\Omega,\mathbb{R}^n), \forall\boldsymbol{u} \in H^{\mathrm{div}}(\Omega,\mathbb{R}^n)$. Denoting by $\mathrm{div}\ : L^2(\Omega,\mathbb{R}^n) \to L^2(\Omega,\mathbb{R})$ the divergence of a vector of size n, and by $\mathbf{grad}\ : L^2(\Omega,\mathbb{R}) \to L^2(\Omega,\mathbb{R}^n)$ the gradient of a scalar function, then, $\alpha\,\mathbf{grad}\,(\star)$ is the formal adjoint of $\mathrm{div}\,(\alpha\star)$, satisfying the relation*

$$\langle f,\mathrm{div}\,(\alpha\boldsymbol{u})\rangle_{L^2} - \langle\alpha\,\mathbf{grad}\,f,\boldsymbol{u}\rangle_{L^2} = \int_{\partial\Omega}f\,(\alpha\,\boldsymbol{u}\cdot\mathbf{n})\,\mathrm{d}\gamma \tag{A9}$$

for all $\boldsymbol{u}\in H^{\mathrm{div}}(\Omega,\mathbb{R}^n)$ and $f\in H^1(\Omega,\mathbb{R})$ and where $\mathbf{n}\in\mathbb{R}^n$ is the outward unitary vector to $\partial\Omega$.

Proof. The proof follows by using (A3) and Gauss-Ostrogradsky divergence theorem and following a similar procedure as in the proof of Theorem 3. ☐

Theorem 5. *Let $\mathbf{F}\in C^1(\bar{\Omega},\mathbb{R}^n)$ and $\alpha\in C^1(\bar{\Omega},\mathbb{R})$ be continuously differentiable vector and scalar functions, respectively, such that, for any $f\in H^1(\Omega,\mathbb{R})$ we obtain that $(\mathbf{F}f)\in H^1(\Omega,\mathbb{R}^n)$ and $(\alpha f)\in H^1(\Omega,\mathbb{R})$. Define the operator $\mathscr{D}$: $L^2(\Omega,\mathbb{R})\to L^2(\Omega,\mathbb{R})$ as $\mathscr{D}f = \alpha\,\mathrm{div}\,(\mathbf{F}f)$. Then, the formal adjoint $\mathscr{D}^* : L^2(\Omega,\mathbb{R})\to L^2(\Omega,\mathbb{R})$ of $\mathscr{D}$ is given by $\mathscr{D}^*f = -\mathbf{F}\cdot\mathbf{grad}\,(\alpha f)$.*

Proof. Let $f_j, j\in\{1,2\}$ be a continuous differentiable scalar function. Consider $f_j^{\alpha}\in H^1(\Omega,\mathbb{R})$ and $\boldsymbol{f}_j^F\in H^1(\Omega,\mathbb{R}^n)$ as the scalar and vector functions defined as $f_j^{\alpha} = \alpha f_j$ and $\boldsymbol{f}_j^F = \mathbf{F}f_j$, respectively. Using the inner product $\langle f_1, \mathscr{D} f_2\rangle_{L^2}$, we obtain

$$\begin{aligned}\langle f_1, \mathscr{D} f_2\rangle_{L^2} &= \int_\Omega f_1 \alpha \mathrm{div}\ (\mathbf{F} f_2)\,\mathrm{d}\Omega = \int_\Omega \mathrm{f}_1^\alpha \mathrm{div}\ \mathrm{f}_2^\mathrm{F}\,\mathrm{d}\Omega \\ &= -\int_\Omega [\mathbf{grad}\ f_1^\alpha]\cdot \boldsymbol{f}_2^F\,\mathrm{d}\Omega + \int_{\partial\Omega} \mathrm{f}_1^\alpha\left(\mathrm{f}_2^\mathrm{F}\cdot\mathbf{n}\right)\mathrm{d}\gamma \\ &= -\int_\Omega [\mathbf{grad}\ (\alpha f_1)]\cdot F f_2\,\mathrm{d}\Omega + \int_{\partial\Omega} \mathrm{f}_1^\alpha\left(\mathrm{f}_2^\mathrm{F}\cdot\mathbf{n}\right)\mathrm{d}\gamma \\ &= -\int_\Omega (F\cdot\mathbf{grad}\ (\alpha f_1))\, f_2\,\mathrm{d}\Omega \\ &\quad + \int_{\partial\Omega} f_1^\alpha\left(\boldsymbol{f}_2^F\cdot\mathbf{n}\right)\mathrm{d}\gamma \end{aligned} \tag{A10}$$

Then, considering boundary conditions equal to 0, we obtain that $\langle f_1, \mathscr{D} f_2\rangle_{L^2} = \langle -\mathbf{F}\cdot\mathbf{grad}\ (\alpha f_1), f_2\rangle_{L^2}$, i.e., $\mathscr{D}^*(\star) = -\mathbf{F}\cdot\mathbf{grad}\ (\alpha\star)$ is the formal adjoint of $\mathscr{D}$. ☐

Theorem 6. *Let $\bar{\mathscr{D}} : L^2(\Omega,\mathbb{R}) \to L^2(\Omega,\mathbb{R})$ be an unbounded differential operator defined as $\bar{\mathscr{D}} f = \mathbf{F}\cdot\mathbf{grad}\ (\alpha f) + \alpha\,\mathrm{div}\ (\mathbf{F} f)$ where α and $\mathbf{F}$ are continuously differentiable functions, such that, for any $f \in H^1(\Omega,\mathbb{R})$ we obtain that $\boldsymbol{f}^F = \mathbf{F} f \in H^{\mathrm{div}}(\Omega,\mathbb{R}^n)$ and $f^\alpha = \alpha f \in H^1(\Omega,\mathbb{R})$. Then, $\bar{\mathscr{D}}$ is a formally skew-adjoint operator, satisfying*

$$\langle f, \bar{D} f\rangle_{L^2} = \int_{\partial\Omega} f^\alpha\left(\boldsymbol{f}^F\cdot\mathbf{n}\right)\mathrm{d}\gamma \tag{A11}$$

Proof. Let $f_j, j\in\{1,2\}$ be a square integrable scalar function. Consider $f_j^\alpha \in H^1(\Omega,\mathbb{R})$ and $\boldsymbol{f}_j^F \in H^1(\Omega,\mathbb{R}^n)$ as the continuous differentiable scalar and vector functions defined as $f_j^\alpha = \alpha f_j$ and $\boldsymbol{f}_j^F = \mathbf{F} f_j$, respectively. Then, inner product is given by

$$\begin{aligned}\left\langle f_1, \bar{\mathscr{D}} f_2\right\rangle_{L^2} &= \int_\Omega (f_1 \mathbf{F}\cdot\mathbf{grad}\ (\alpha f_2) + f_1\alpha\mathrm{div}\ (\mathbf{F} f_2))\,\mathrm{d}\Omega \\ &= \int_\Omega \left(\boldsymbol{f}_1^F\cdot\mathbf{grad}\ f_2^\alpha + f_1^\alpha \mathrm{div}\ \boldsymbol{f}_2^F\right)\mathrm{d}\Omega\end{aligned}$$

and, using (A10), we have that

$$\begin{aligned}\left\langle f_1, \bar{\mathscr{D}} f_2\right\rangle_{L^2} &= \int_{\partial\Omega}\left(f_1^\alpha\left(\boldsymbol{f}_2^F\cdot\mathbf{n}\right) + f_2^\alpha\left(\boldsymbol{f}_1^F\cdot\mathbf{n}\right)\right)\partial\Omega \\ &\quad - \int_\Omega\left(\boldsymbol{f}_1^F\cdot\mathbf{grad}\ f_2^\alpha + f_1^\alpha\mathrm{div}\ \boldsymbol{f}_2^F\right)\mathrm{d}\Omega \\ &= -\left\langle\bar{\mathscr{D}} f_1, f_2\right\rangle_{L^2} \\ &\quad + \int_{\partial\Omega}\left(f_1^\alpha\left(\boldsymbol{f}_2^F\cdot\mathbf{n}\right) + f_2^\alpha\left(\boldsymbol{f}_1^F\cdot\mathbf{n}\right)\right)\mathrm{d}\gamma\end{aligned}$$

Considering boundary conditions equal to 0, from (A11) we have that $\left\langle f_1, \bar{\mathscr{D}} f_2\right\rangle_{L^2} = \left\langle -\bar{\mathscr{D}} f_1, f_2\right\rangle_{L^2}$. This implies that the formal adjoint of $\bar{\mathscr{D}}$ is given by $\bar{\mathscr{D}}^* = -\bar{\mathscr{D}}$, i.e., $\bar{\mathscr{D}}$ is a formally skew-adjoint operator. Finally, setting $f_1 = f_2 = f$, relation (A11) is obtained. ☐

Regarding the divergence of second order tensors, the corresponding formal adjoint in the space of symmetric tensors is carefully proved in Ref. 57, and extended to non-symmetric square tensors in Ref. 24. In the next result we generalize this approach to second order tensors of size $l\times n$ on an n-dimensional spatial domain Ω, with $n\in\{2,3\}$.

Theorem 7. *Denote by **Div** $: L^2\left(\Omega,\mathbb{R}^{l\times n}\right)\to L^2\left(\Omega,\mathbb{R}^l\right)$ the divergence operator for second order tensors of size $n\times l$ and by **Grad** $: L^2\left(\Omega,\mathbb{R}^l\right)\to L^2\left(\Omega,\mathbb{R}^{l\times n}\right)$ the gradient of a vector field of size l. Then, the formal adjoint of **Div** is $-$**Grad**, satisfying the relation*

$$\langle\boldsymbol{u}, \mathbf{Div}\ \boldsymbol{\sigma}\rangle_{L^2} + \langle\mathbf{Grad}\ \boldsymbol{u}, \boldsymbol{\sigma}\rangle_{L^2} = \int_{\partial\Omega}\boldsymbol{u}\cdot[\mathbf{n}\cdot\boldsymbol{\sigma}]\,\mathrm{d}\gamma \tag{A12}$$

for all $\boldsymbol{u}\in H^1\left(\Omega,\mathbb{R}^l\right)$ and $\boldsymbol{\sigma}\in H^{\mathrm{div}}\left(\Omega,\mathbb{R}^{n\times l}\right)$.

Proof. Consider $\boldsymbol{u} = \begin{bmatrix} u_1\\ \vdots\\ u_l\end{bmatrix}$ and $\boldsymbol{\sigma} = \begin{bmatrix}\sigma_1\\ \vdots\\ \sigma_l\end{bmatrix}$ where $\sigma_i = [\sigma_{i1},\dots,\sigma_{in}], \forall i\in\{1,\dots,l\}$ is the i-th row of tensor $\boldsymbol{\sigma}$. By definition we have that

$$\mathbf{Grad}\ \boldsymbol{u} = \begin{bmatrix}\partial_{\zeta_1}u_1 & \dots & \partial_{\zeta_n}u_1\\ \partial_{\zeta_1}u_2 & \dots & \partial_{\zeta_n}u_2\\ \vdots & \ddots & \vdots\\ \partial_{\zeta_1}u_l & \dots & \partial_{\zeta_n}u_l\end{bmatrix} = \begin{bmatrix}[\mathbf{grad}\ u_1]^\top\\ \vdots\\ [\mathbf{grad}\ u_l]^\top\end{bmatrix} \text{ and}$$

$$\mathbf{Div}\ \boldsymbol{\sigma} = \begin{bmatrix}\partial_{\zeta_1}\sigma_{11}+\dots+\partial_{\zeta_n}\sigma_{1n}\\ \partial_{\zeta_1}\sigma_{21}+\dots+\partial_{\zeta_n}\sigma_{2n}\\ \vdots\\ \partial_{\zeta_1}\sigma_{l1}+\dots+\partial_{\zeta_n}\sigma_{ln}\end{bmatrix} = \begin{bmatrix}\mathrm{div}\ \left(\sigma_1^\top\right)\\ \vdots\\ \mathrm{div}\ \left(\sigma_l^\top\right)\end{bmatrix}$$

Then, the inner product $\langle\boldsymbol{u}, \mathbf{Div}\ \boldsymbol{\sigma}\rangle_{L^2}$ is given by:

$$\begin{aligned}\langle\boldsymbol{u}, \mathbf{Div}\ \boldsymbol{\sigma}\rangle_{L^2} &= \int_\Omega \boldsymbol{u}\cdot[\mathbf{Div}\ \boldsymbol{\sigma}]\,\mathrm{d}\Omega = \int_\Omega\sum_{\mathrm{i}=1}^{1}\mathrm{u_i}\mathrm{div}\ \left(\sigma_\mathrm{i}^\top\right)\mathrm{d}\Omega \\ &\overset{(A3)}{=} -\int_\Omega\sum_{i=1}^{l}[\mathbf{grad}\ u_i]^\top\cdot\sigma_i^\top\,\mathrm{d}\Omega \\ &\quad + \int_\Omega\sum_{i=1}^{l}\mathrm{div}\ \left[\sigma_i^\top u_i\right]\mathrm{d}\Omega \\ &= -\int_\Omega tr\left([\mathbf{Grad}\ \boldsymbol{u}]\,\boldsymbol{\sigma}^\top\right)\mathrm{d}\Omega \\ &\quad + \int_{\partial\Omega}\sum_{i=1}^{l}u_i\sigma_i^\top\cdot\mathbf{n}\,\mathrm{d}\gamma \\ &= -\langle\boldsymbol{\sigma}, \mathbf{Grad}\ \boldsymbol{u}\rangle_{L^2} + \int_{\partial\Omega}\boldsymbol{u}\cdot[\boldsymbol{\sigma}\cdot\mathbf{n}]\,\mathrm{d}\gamma\end{aligned}$$

Regrouping terms, (A12) is obtained. Considering boundary conditions equal to 0 as a special case, we have $\langle\mathbf{Div}\ \boldsymbol{\sigma}, \boldsymbol{u}\rangle_{L^2} = \langle\boldsymbol{\sigma}, -\mathbf{Grad}\ \boldsymbol{u}\rangle_{L^2}$, i.e., $-$**Grad** is the formal adjoint of **Div** . ☐

Theorem 8. *Let $\chi\in C^1\left(\bar{\Omega},\mathbb{R}^{l\times n}\right)$ be a continuous and differentiable second order tensor, and $(\alpha,\beta)\in C^1(\bar{\Omega},\mathbb{R})$ be 2 strictly positive continuous and differentiable scalar functions, such that, $\frac{\chi}{\beta}f\in H^{\mathrm{div}}\left(\Omega,\mathbb{R}^{l\times n}\right),\forall f\in H^1(\Omega,\mathbb{R})$ and $\frac{\boldsymbol{u}}{\alpha}\in H^1\left(\Omega,\mathbb{R}^l\right),\forall\boldsymbol{u}\in H^1\left(\Omega,\mathbb{R}^l\right)$. Then, $\mathscr{D}_\chi^*(\star) = \frac{\chi}{\beta}$:*

$\left[\mathbf{Grad}\,\frac{\star}{\alpha}\right]$ *is the formal adjoint of* $\mathscr{D}_{\chi}(\star) = -\frac{1}{\alpha}\mathbf{Div}\,\left[\frac{\chi}{\beta}\star\right]$, *satisfying the relation*

$$\langle \boldsymbol{u}, \mathscr{D}_{\chi} f\rangle_{L^2} - \langle \mathscr{D}_{\chi}^{*}\boldsymbol{u}, f\rangle_{L^2} = -\int_{\partial\Omega}\left[\frac{f}{\beta}\chi\cdot\mathbf{n}\right]\cdot\frac{\boldsymbol{u}}{\alpha}\,\mathrm{d}\gamma \quad \text{(A13)}$$

Proof. Consider the inner product $\langle \boldsymbol{u}, \mathscr{D}_{\chi} f\rangle_{L^2}$ given by

$$\langle \boldsymbol{u}, \mathscr{D}_{\chi} f\rangle_{L^2} = \int_{\Omega}\boldsymbol{u}\cdot\mathscr{D}_{\chi} f\,\mathrm{d}\Omega = -\int_{\Omega}\frac{\mathrm{u}}{\alpha}\cdot\mathbf{Div}\,\left[\frac{\chi}{\beta}\mathrm{f}\right]\mathrm{d}\Omega$$

Denoting by $\tilde{\boldsymbol{u}} = \boldsymbol{u}/\alpha \in H^1(\Omega, \mathbb{R}^l)$ and $\tilde{\boldsymbol{\sigma}} = \chi f/\beta \in H^{\mathrm{div}}(\Omega, \mathbb{R}^{n\times l})$ and using Theorem 7, we obtain

$$\begin{aligned}\langle \boldsymbol{u}, \mathscr{D}_{\chi} f\rangle_{L^2} =& -\int_{\Omega}\tilde{\boldsymbol{u}}\cdot\mathbf{Div}\,\tilde{\boldsymbol{\sigma}}\,\mathrm{d}\Omega\\ =& \int_{\Omega}\tilde{\boldsymbol{\sigma}} : \mathbf{Grad}\,\tilde{\boldsymbol{u}}\,\mathrm{d}\Omega - \int_{\partial\Omega}\tilde{\mathrm{u}}\cdot[\tilde{\boldsymbol{\sigma}}\cdot\mathbf{n}]\,\mathrm{d}\gamma\\ =& \int_{\Omega} f\frac{\chi}{\beta} : \mathbf{Grad}\,\frac{\boldsymbol{u}}{\alpha}\,\mathrm{d}\Omega - \int_{\partial\Omega}\frac{\mathrm{u}}{\alpha}\cdot\left[\frac{\mathrm{f}}{\beta}\chi\cdot\mathbf{n}\right]\mathrm{d}\gamma\\ =& \langle \mathscr{D}_{\chi}^{*}\boldsymbol{u}, f\rangle_{L^2} - \int_{\partial\Omega}\frac{\boldsymbol{u}}{\alpha}\cdot\left[\frac{f}{\beta}\chi\cdot\mathbf{n}\right]\mathrm{d}\gamma\end{aligned}$$

Regrouping the terms, we obtain (A13). Considering boundary conditions equal to 0, we have that $\langle \boldsymbol{u}, \mathscr{D}_{\chi} f\rangle_{L^2} = \langle \mathscr{D}_{\chi}^{*}\boldsymbol{u}, f\rangle_{L^2}$, i.e., $\mathscr{D}_{\chi}^{*}$ is the formal adjoint of $\mathscr{D}_{\chi}$. □

Appendix B: Proof of Lemmas

1. Proof of Lemma 1

From Theorem 3, considering $\alpha = 1/\rho$, we have that $\mathscr{G}_r^{*}(\star) = \frac{1}{\rho}\mathbf{curl}\,(\star)$ is the formal adjoint of $\mathscr{G}_r(\star) = \mathbf{curl}\left(\frac{1}{\rho}\star\right)$. Similarly, $\mathscr{G}_c^{*}(\star) = -\frac{1}{\rho}\mathbf{grad}\,(\star)$ is the formal adjoint of $\mathscr{G}_c(\star) = \mathrm{div}\left(\frac{1}{\rho}\star\right)$, as shown in Theorem 4. Considering the viscosity tensor (16) and the isotropic assumption, i.e., μ and κ constant, we have that

$$\begin{aligned}\frac{1}{\rho}\mathbf{Div}\,\boldsymbol{\tau} =& \frac{1}{\rho}\mathbf{Div}\,\left[-\mu\left[\mathbf{Grad}\,\mathbf{v} + [\mathbf{Grad}\,\mathbf{v}]^{\top}\right]\right]\\ &+ \frac{1}{\rho}\mathbf{Div}\,\left[\left(\frac{2}{3}\mu - \kappa\right)(\mathrm{div}\,\mathbf{v})\,\mathbf{I}\right]\\ =& -\frac{\mu}{\rho}\mathbf{Div}\,[\mathbf{Grad}\,\mathbf{v}] - \frac{\mu}{\rho}\mathbf{Div}\,\left[[\mathbf{Grad}\,\mathbf{v}]^{\top}\right]\\ &+ \frac{\left(\frac{2}{3}\mu - \kappa\right)}{\rho}\mathbf{Div}\,[(\mathrm{div}\,\mathbf{v})\,\mathbf{I}]\end{aligned}$$

Applying (A4), (A5) and (A6), the terms on the right hand side of previous equation can be rewritten as

$$\begin{aligned}-\frac{\mu}{\rho}\mathbf{Div}\,[\mathbf{Grad}\,\mathbf{v}] =& -\frac{\mu}{\rho}\mathbf{grad}\,(\mathrm{div}\,\mathbf{v}) + \frac{\mu}{\rho}\mathbf{curl}\,[\mathbf{curl}\,\mathbf{v}]\\ =& \mathscr{G}_c^{*}\left(\mu\mathscr{G}_c[\rho\mathbf{v}]\right) + \mathscr{G}_r^{*}\left[\mu\mathscr{G}_r[\rho\mathbf{v}]\right]\\ -\frac{\mu}{\rho}\mathbf{Div}\,[\mathbf{Grad}\,\mathbf{v}]^{\top} =& -\frac{\mu}{\rho}\mathbf{grad}\,(\mathrm{div}\,\mathbf{v})\\ =& \mathscr{G}_c^{*}\left(\mu\mathscr{G}_c[\rho\mathbf{v}]\right)\\ \frac{\left(\frac{2}{3}\mu - \kappa\right)}{\rho}\mathbf{Div}\,[(\mathrm{div}\,\mathbf{v})\,\mathbf{I}] =& \frac{\left(\frac{2}{3}\mu - \kappa\right)}{\rho}\mathbf{grad}\,(\mathrm{div}\,\mathbf{v})\\ =& \mathscr{G}_c^{*}\left(\left(\frac{2}{3}\mu - \kappa\right)\mathscr{G}_c[\rho\mathbf{v}]\right)\end{aligned}$$

Then, the divergence of the fluid viscosity tensor can be expressed as the sum of two dissipative terms, namely:

$$\begin{aligned}\frac{1}{\rho}\mathbf{Div}\,\boldsymbol{\tau} =& \mathscr{G}_r^{*}\mu\mathscr{G}_r\rho\mathbf{v} + \mathscr{G}_c^{*}\hat{\mu}\mathscr{G}_c\rho\mathbf{v}\\ =& \begin{bmatrix}\mathscr{G}_r^{*} & \mathscr{G}_c^{*}\end{bmatrix}\begin{bmatrix}\mu\mathbf{I} & \mathbf{0}\\ \mathbf{0} & \hat{\mu}\end{bmatrix}\begin{bmatrix}\mathscr{G}_r\\ \mathscr{G}_c\end{bmatrix}\rho\mathbf{v}\end{aligned} \quad \text{(B1)}$$

where $\hat{\mu} = \frac{4}{3}\mu + \kappa$, $\mathscr{G}_r^{*}\mu\mathscr{G}_r\rho\mathbf{v}$ is associated with the energy dissipation by the fluid rotation and $\mathscr{G}_c^{*}\hat{\mu}\mathscr{G}_c\rho\mathbf{v}$ with the energy dissipation by fluid compression. Finally, rearranging terms, we obtain (17).

2. Proof of Lemma 2

Consider the weakly differentiable vectors $\boldsymbol{a} \in H^1\left(\Omega, \mathbb{R}^l\right)$ and $\boldsymbol{u} \in H^1\left(\Omega, \mathbb{R}^n\right)$ of size l and n, respectively. Then, the inner product $\langle \boldsymbol{a}, \mathscr{A}_{\boldsymbol{c}}\boldsymbol{u}\rangle_{L^2}$ is given by:

$$\begin{aligned}\langle \boldsymbol{a}, \mathscr{A}_{\boldsymbol{c}}\boldsymbol{u}\rangle_{L^2} =& \int_{\Omega}\boldsymbol{a}\cdot\left[\boldsymbol{u}\cdot\frac{\mathbf{Grad}\,\boldsymbol{c}}{\rho}\right]\mathrm{d}\Omega\\ =& \int_{\Omega}\sum_{j=1}^{l}a_j\left(\boldsymbol{u}\cdot\frac{\mathbf{grad}\,c_j}{\rho}\right)\mathrm{d}\Omega\\ =& \int_{\Omega}\boldsymbol{u}\cdot\left[\sum_{j=1}^{l}a_j\frac{\mathbf{grad}\,c_j}{\rho}\right]\mathrm{d}\Omega\\ =& \int_{\Omega}\boldsymbol{u}\cdot\left[\frac{\mathbf{Grad}\,\boldsymbol{c}}{\rho}\cdot\boldsymbol{a}\right]\mathrm{d}\Omega\\ =& \left\langle\frac{\mathbf{Grad}\,\boldsymbol{c}}{\rho}\cdot\boldsymbol{a}, \boldsymbol{u}\right\rangle_{L^2}\end{aligned}$$

i.e., the formal adjoint of $\mathscr{A}_{\boldsymbol{c}}$ is given by $\mathscr{A}_{\boldsymbol{c}}^{*}(\star) = \left[\frac{\mathbf{Grad}\,\boldsymbol{c}}{\rho}\right]\cdot(\star)$. Following a similar procedure, it is easy to verify that $\mathscr{A}_s^{*}(\star) = \frac{\mathbf{grad}\,s}{\rho}(\star)$ and $\mathscr{R}^{*}(\star) = (\star)\cdot\frac{\boldsymbol{r}}{\rho^2 T}$ are the formal adjoint operators of $\mathscr{A}_s$ and $\mathscr{R}$, respectively.

3. Proof of Lemma 3

The proof that $\mathscr{D}_{\boldsymbol{\tau}}^{*}(\star) = \frac{\boldsymbol{\tau}}{\rho T} : \mathbf{Grad}\,\frac{(\star)}{\rho}$ is the formal adjoint of $\mathscr{D}_{\boldsymbol{\tau}}(\star) = -\frac{1}{\rho}\mathbf{Div}\,\left[\frac{\boldsymbol{\tau}}{\rho T}(\star)\right]$ follows from Theorem 8. Considering $\chi = \boldsymbol{\tau}$, $\alpha = \rho$ and $\beta = \rho T$, we have that

$$\left\langle \delta_{\mathbf{v}}\bar{\mathscr{H}}, \mathscr{D}_{\tau}(\delta_s\bar{\mathscr{H}}) \right\rangle_{L^2} - \left\langle \mathscr{D}^*_{\boldsymbol{\tau}}(\delta_{\mathbf{v}}\bar{\mathscr{H}}), \delta_s\bar{\mathscr{H}} \right\rangle_{L^2} = \int_{\partial\Omega} \frac{\delta_{\mathbf{v}}\bar{\mathscr{H}}}{\rho} \cdot \left[\frac{\boldsymbol{\tau}}{\rho T} \delta_s\bar{\mathscr{H}} \cdot \mathbf{n} \right] \mathrm{d}\gamma$$

Then, since $\boldsymbol{\tau}$ is square and symmetric, and $\delta_s\bar{\mathscr{H}} = \rho T$ we obtain relation (43). The same procedure is used to prove that $\mathscr{D}^*_{\boldsymbol{\Upsilon}}(\star) = \frac{\boldsymbol{\Upsilon}}{\rho T} : \mathbf{Grad}\, \frac{(\star)}{\rho}$ is the formal adjoint of $\mathscr{D}_{\boldsymbol{\Upsilon}}(\star) = -\frac{1}{\rho}\mathbf{Div}\, \left[\frac{\boldsymbol{\Upsilon}}{\rho T}(\star)\right]$ and to obtain (44).

On the other hand, using Theorem 5, considering $\mathbf{F} = \mathbf{q}^{(h)}/\rho T^2$ and $\alpha = 1/\rho$ we can verify that $\mathscr{D}^*_{\mathbf{q}}(\star) = \frac{\mathbf{q}^{(h)}}{\rho T^2} \cdot \mathbf{grad}\, \frac{(\star)}{\rho}$ is the formal adjoint of $\mathscr{D}_{\mathbf{q}}(\star) = -\frac{1}{\rho}\mathrm{div}\, \left[\frac{\mathbf{q}^{(h)}}{\rho T^2}(\star)\right]$. Finally, we note that

$$\left\langle \delta_s\bar{\mathscr{H}}, \mathscr{D}_{\mathbf{q}}(\delta_s\bar{\mathscr{H}}) \right\rangle_{L^2} - \left\langle \delta_s\bar{\mathscr{H}}, \mathscr{D}^*_{\mathbf{q}}(\delta_s\bar{\mathscr{H}}) \right\rangle_{L^2} = \left\langle \delta_s\bar{\mathscr{H}}, \bar{\mathscr{D}}(\delta_s\bar{\mathscr{H}}) \right\rangle_{L^2}$$

where $\bar{\mathscr{D}} = \mathscr{D}_{\mathbf{q}} - \mathscr{D}^*_{\mathbf{q}}$ is a formally skew-symmetric operator. Then, using Theorem 6, relation (45) is obtained.

DATA AVAILABILITY STATEMENT

Data sharing is not applicable to this article as no new data were created or analyzed in this study.

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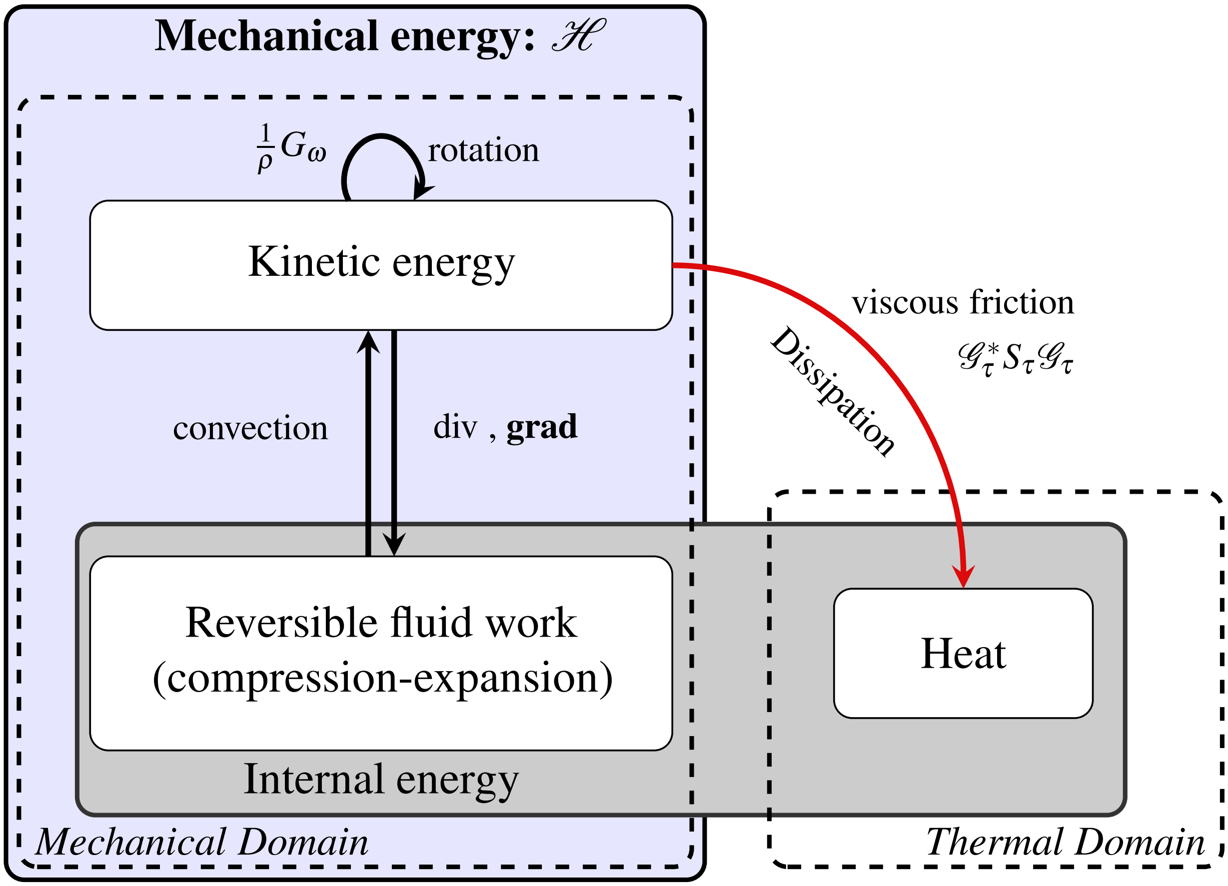
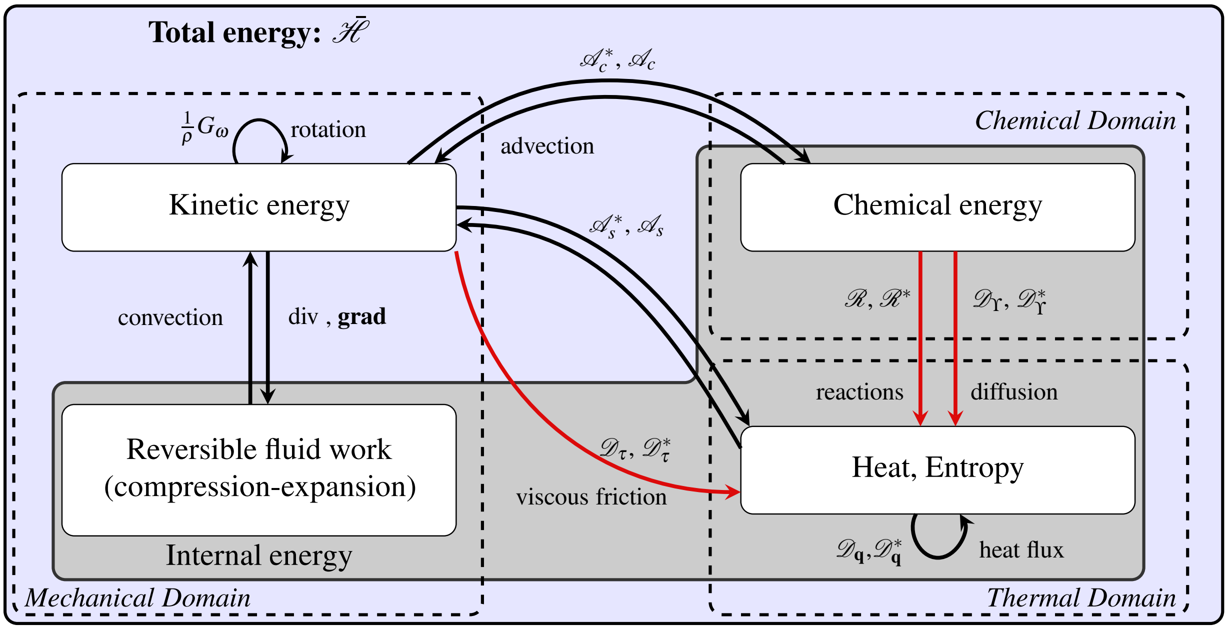

Mechanical energy: $\mathscr{H}$
$\frac{1}{\rho}G_\omega$
rotation
Kinetic energy
viscous friction
$\mathscr{G}_\tau^* S_\tau \mathscr{G}_\tau$
Dissipation
convection
div , grad
Reversible fluid work
(compression-expansion)
Heat
Internal energy
Mechanical Domain
Thermal Domain


Total energy: $\bar{\mathscr{H}}$
$\mathscr{A}_c^*$, $\mathscr{A}_c$
$\frac{1}{\rho}G_\omega$
rotation
advection
Chemical Domain
Kinetic energy
Chemical energy
$\mathscr{A}_s^*$, $\mathscr{A}_s$
convection
div , **grad**
$\mathscr{R}$, $\mathscr{R}^*$
$\mathscr{D}_\Upsilon$, $\mathscr{D}_\Upsilon^*$
reactions
diffusion
$\mathscr{D}_\tau$, $\mathscr{D}_\tau^*$
Reversible fluid work
(compression-expansion)
viscous friction
Heat, Entropy
Internal energy
$\mathscr{D}_{\mathbf{q}}$,$\mathscr{D}_{\mathbf{q}}^*$
heat flux
Mechanical Domain
Thermal Domain