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A phase-field model for liquid-gas mixtures: mathematical modelling and Discontinuous Galerkin discretization

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Abstract

In this article we propose a phase-field approach to model a liquid-gas mixture that might also provide a description of the expansion stage of a metal foam inside a hollow mold. We conceive the mixture as a two-phase incompressible-compressible fluid governed by a Navier-Stokes-Cahn-Hilliard system of equations, and we adapt the Lowengrub-Truskinowsky model to take into account the expansion of the gaseous phase. The resulting system of equations is characterized by a velocity field that fails to be divergence-free, by a logarithmic term for the pressure that enters the Gibbs free-energy expression and by the viscosity that degenerates in the gas phase. In the second part of the article we propose an energy-based numerical scheme that, at the discrete level, preserves the mass conservation property and the energy dissipation law of the original system. We use a Discontinuous Galerkin approximation for the spatial approximation and a modified midpoint based scheme for the time approximation.

Keywords: liquid-gas mixtures, metal foams, phase-field, Navier-Stokes-Cahn-Hilliard, energy-based numerical methods, Discontinuous Galerkin, modified midpoint.

1 Introduction.

Two-phase flows have been studied in depth for their broad range of applications. They pose several formidable problems both from the modelling point of view and from the numerical implementation of schemes apt to capture their complex evolution. Two-phase flows can be classified according to the nature of the phases involved, whether they are liquid, solid or gaseous, each class of phases having its own peculiarities. Here we are concerned with liquid-gas mixtures, that have a rich and complex history as attested, for instance, by the variety of treatments for the simplest problem for a gas-liquid mixture: the expansion of an isolated gas bubble within a fluid governed by the Rayleigh-Plesset equation. There are two main difficulties: the former, quite obvious, lies in the extreme variability of constitutive hypotheses that one can adopt for either the gas or the fluid phase: the gas can be ideal, a van der Waals gas, etc.; the fluid can be ideal, newtonian [21], polymeric [6], etc. More intricate points concern the boundary conditions at the interface [25], the finite amount of the fluid phase [6, 31], the shape of the gas bubble [12] and, in any case, the need to take in due account the compressibility of the gas drop. These difficulties are amplified when the evolution of a family of bubbles is considered and several techniques have been put forward to tackle the problem, ranging from kinetic [28] to phase-field models [27]. A particularly interesting gas-fluid mixture is provided by metal foams during the foaming process. Metal foams are special cases of cellular metals with closed cells that attracted the attention of researchers and engineers for their high capability of energy absorption, high stiffness and low weight, that make them suitable for a wide range of applications, in particular in the automotive industry. The complex process of foaming can be divided into three main steps; gas bubbles *nucleate* within a liquid matrix; they *grow* to yield a complex morphology that finally undergoes a *coarsening* when small bubbles coalesce together to form larger ones. At the beginning of the foaming process, the metal is a powder within which a blowing agent, *e.g.* titanium hydride TiH_2, is dispersed. When the compound is suddenly heated, not only the metal powder passes into the liquid state, but the TiH_2 particles release hydrogen that starts forming bubbles which in turn deeply modify the morphology of the matrix. These bubbles can recombine, breakup or even escape from the boundary of the fluid matrix. At a certain moment the process is stopped by a fast cooling that freezes the foam morphology that can be then analyzed. This avenue to arrive at a metal foam is known as *precursor foaming* and it is this method that has been adopted in the experiments that two of us (E.R. and M.V.) followed in collaboration with M.U.S.P. laboratory in Piacenza, Italy (www.musp.it) [23]. As an aside, we note that, depending on whether the precursor is prepared through a metallurgical or a melt route, the foaming process can be referred as the "Powder line" or "Formgrip line": in the experiment described in [23] only the powder line has been considered. The outcome of the foaming process depends upon many factors like the content of the blowing agent, the heating rate, the size of the precursor, etc. The expansion stage of a metal foam within a hollow mold served as a motivation for the subsequent study that, admittedly, is still far from being apt to capture the evolution of this process.

Up to a few years ago, it was generally believed that the large contrasts in the properties pertaining to the gas and to the fluid phase were responsible for the properties of metal foams. However, it was later realized that such contrasts alone were insufficient to justify the stability of a metal foam. Moreover, the presence of an oxide net within the foam, that can be fragmented into small oxide particles during foaming, was proved experimentally. When these particles are trapped between two bubbles, they exert a *disjoining pressure* that enhances separation of gas bubbles, preventing the collapse of the foam [13, 14]. The effects of disjoining pressure on metal-foam stability have been incorporated into a phenomenological model [14] then subsumed within a numerical scheme based upon a lattice Boltzmann model [15]: actually, it was the impossibility of reproducing accurate foam morphologies numerically [16] that led to search a new stabilizing mechanism. This feature, together with the well known versatility of phase-field models to handle with topological changes, induced us to adapt the phase-field model introduced almost two decades ago by Lowengrub and Truskinovsky [17] to a gas-fluid mixture. In particular, we were led into such an attempt by the remark, contained in [17] itself, that in the mushy region modelling the diffuse interface between two phases, the stress tensor acquires an extra-pressure term. This term might be used, this is our point, to mimic the disjoining pressure that appears as an essential ingredient for the stability of a metal foam.

Phase-field models belong to the vast family of diffuse-interface models. They have been used to describe a variety of physical problems in which phase transitions –like condensation, evaporation, crystallization, etc. –play a role. The importance of phase-field techniques has grown considerably as they can be implemented numerically in an effective way. In their simplest version, they are characterized by a scalar parameter, called the *order parameter*, that serves to dinstinguish one phase from the other. There are different choices for the order parameter: for example, the average volume fraction of a phase [26] or the mass concentration of a phase [5, 17–19]. In both cases, the order parameter has a clear physical meaning and its evolution is described by a nonlinear diffusion equation. In Section 2 we propose a thermodynamically consistent phase-field model for the description of a fluid-gas mixture, adopting the mass concentration of the liquid phase as phase-field variable.

The resulting system of equations associated with the phase-field model is an incompressible-compressible version of a Navier-Stokes-Cahn-Hilliard (IC-NSCH) system. Several numerical approximations of the classical Navier-Stokes-Cahn-Hilliard (NSCH) system have been proposed in literature in the case of incompressible two-phase fluids (see, e.g., [7]) and very recently (see [9] and [10]) numerical techniques have been developed for quasi-incompressible fluids, i.e., fluids in which both phases are incompressible, but the mixing is compressible. However, up to our knowledge, the numerical analysis in the incompressible-compressible case is missing. The main difficulties in the numerical approximation of these systems are represented by the presence of the pressure in the chemical potential definition and by the velocity field that is no longer divergence-free. In this paper we build a numerical scheme that, at the discrete level, preserves mass conservation and the energy dissipation law associated to the original system. In particular, mass conservation and energy dissipation properties for the IC-NSCH system are proved in Section 3, while Section 4 describes an energy-based numerical method for the IC-NSCH system using a modified-midpoint time-discretization (inspired by the one adopted in [10] for the Lowengrub-Truskinowsky model), and using Discontinuous Galerkin finite elements for the spatial discretization (similarly to [8] and [9] where a Navier-Stokes-Korteweg system and a quasi-incompressible two phase flow model have been considered).

2 A phase-field model for gas-liquid mixtures.

In this section we propose a thermodynamically consistent phase-field model for the description of a gas-fluid mixture. Inspired by the expansion stage of the foam inside a hollow mould, we shall suppose hereafter that the expansion of the gas phase occurs at a constant temperature, and that the fluid phase is incompressible. We consider the concentration c of the liquid phase as the phase-field function: if we fix a spatial domain Ω and a time interval $[0, T]$,

$$c = c(\mathbf{x}, t) : \Omega \times [0, T] \to [0, 1] \tag{2.1}$$

is such that $c = 1$ if $\mathbf{x}$ belongs to the liquid phase, $c = 0$ if $\mathbf{x}$ belongs to the gas phase, $0 < c < 1$ if $\mathbf{x}$ belongs to a transition layer between liquid and gas. Our model depends on mass, energy, and momentum balance-equations (Navier-Stokes equations) for the two-phase incompressible-compressible system and a nonlinear evolution equation for the phase-field function c (Cahn-Hilliard equation).

2.1 Thermodynamically consistent phase-field models.

As a general framework we shall consider models where the phase-field variable is governed by an equation of the type

$$\rho\dot{c} = -\mathrm{div}\mathbf{j}(\rho, c, \theta, \nabla\rho, \nabla c, \nabla\theta), \tag{2.2}$$

where ρ is the fluid density, θ is the absolute temperature, $\mathbf{j}$ is a suitable current. We will enforce the constraint $\theta = \text{const.}$ later on in our treatment. We have neglected, for simplicity, dependence on higher order gradients in the scalar fields. Together with (2.2), we shall also suppose that the balance equations of mass, momentum and energy

$$\begin{cases} \dot{\rho} = -\rho\,\mathrm{div}\,\mathbf{u}, \\ \rho\dot{\mathbf{u}} = \mathrm{div}\mathbf{T} + \rho\mathbf{b}, \\ \rho\dot{e} = \mathbf{T}\cdot\mathbf{D} - \mathrm{div}\mathbf{q} + \rho r \end{cases} \tag{2.3}$$

hold in the mixture, in which $\mathbf{u}$ is the fluid velocity, $\mathbf{T}$ is the stess tensor, $\mathbf{b}$ represents the body force, e is the internal energy, $\mathbf{D}$ is the symmetric part of the velocity gradient, $\mathbf{q}$ is the energy flux and r represents the energy supply. In addition to these averaged balance equations, we must ensure the validity of the second law of thermodynamics, through the following Clausius-Duhem inequality:

Entropy principle. *Let η be the entropy density. The Clausius-Duhem inequality*

$$\rho\dot{\eta} \geq -\mathrm{div}\left(\frac{\mathbf{q}}{\theta} + \mathbf{k}\right) + \frac{\rho r}{\theta} \tag{2.4}$$

must hold and must be compatible with the balance equations (2.3). The extra-entropy flux $\mathbf{k}$ is another constitutive quantity that accounts for entropy flux due to phase changes.

We find it expedient to introduce the Gibbs free-energy g that is related to the Helmholtz free-energy $\psi := e - \theta\eta$ by the Legendre transformation

$$\psi(p, \theta, c) = g(p, \theta, c) - p\frac{\partial g}{\partial p}. \tag{2.5}$$

By use of (2.3) and (2.5), we can rewrite (2.4) as

$$\rho\left(\dot{g} + \eta\dot{\theta} + \frac{1}{\rho^2}\dot{\rho}p - \frac{1}{\rho}\dot{p}\right) - \mathbf{T}\cdot\mathbf{D} - \theta\,\mathrm{div}\,\mathbf{k} + \frac{1}{\theta}\mathbf{q}\cdot\nabla\theta \leq 0. \tag{2.6}$$

Hereafter, we suppose that g and also $\mathbf{T}$, η, $\mathbf{k}$, $\mathbf{q}$ and $\mathbf{j}$ could depend upon $p, c, \theta, \nabla\theta$, $\mathbf{D}, \nabla c$. The validity of (2.6) imposes restrictions on the constitutive functions $\mathbf{T}$, ψ, η, $\mathbf{k}$, $\mathbf{q}$ and $\mathbf{j}$, as stated by the next theorem (*see* [18] for a proof), where a subscript denotes differentiation with respect to the indicated variable.

Theorem 2.1 *The functions* $\mathbf{T}$, g, η, $\mathbf{k}$, $\mathbf{q}$ *and* $\mathbf{j}$ *are compatible with the second law of thermodynamics in the form (2.6) if*

$$g_\theta + \eta = 0, \quad g_{\mathbf{D}} = 0, \quad g_{\nabla\theta} = 0, \tag{2.7}$$

$$\mathbf{q} = -\kappa(c,p,\theta)\nabla\theta, \tag{2.8}$$

$$\mathrm{div}\mathbf{j} = \hat{f}(c,p,\theta)\left(\frac{1}{\theta}g_c - \frac{1}{\rho}\mathrm{div}\left(\frac{\rho}{\theta}g_{\nabla c}\right)\right), \tag{2.9}$$

$$\mathbf{T} = -p\mathbf{I} - \mathrm{sym}(\rho\nabla c \otimes g_{\nabla c}) + 2\mu\mathbf{D} + \lambda(\mathrm{div}\mathbf{v})\mathbf{I}, \tag{2.10}$$

where the functions κ *and* $\hat{f}$ *are positive;* μ *and* λ *can be, in principle, taken as functions of* p, θ, c, *and they must obey the constraints* $\mu > 0$ *and* $2\mu + 3\lambda > 0$.

Since $\mathbf{L} := \nabla\mathbf{u}$ might have a skew-symmetric part, we have the further restriction

$$\mathrm{skw}(\rho\nabla c \otimes g_{\nabla c}) = 0 \tag{2.11}$$

that, however, is easily accounted for. In fact, since the scalar function g can depend on the vector ∇c only through its scalar invariant $|\nabla c|$, we can set $g_{\nabla c} = g(|\nabla c|)\nabla c$ so that (2.11) is automatically satisfied and (2.10) can be recast as

$$\mathbf{T} = \mathbf{T}_0 + \mathbf{T}_v, \tag{2.12}$$

where

$$\mathbf{T}_0 = -p\mathbf{I} - \nu\rho\nabla c \otimes \nabla c, \quad \mathbf{T}_v = 2\mu\mathbf{D} + \lambda(\mathrm{div}\mathbf{v})\mathbf{I} \tag{2.13}$$

are the non-viscous part and the viscous part of the stress tensor, respectively. Since in our problem the fluid component can be regarded as incompressible, while the gaseous phase is clearly compressible, we shall assume

$$\lambda = \lambda(c) = \lambda_g(1-c)$$

where λ_g is characteristic of the gas dispersed in the mixture. As to the viscosity μ, we take the simplest formula interpolating between the bulk values of the gas and the fluid phase:

$$\mu = \mu(c) := \mu_f c + \mu_g(1-c) \tag{2.14}$$

where μ_g and μ_f pertain to the gas and to the fluid phase, respectively. Following Lowengrub and Truskinovsky [17], we decompose the capillary stress $\mathbf{T}_0$ into a pressure and into a shear component. Actually, we limit our attention to a free-energy ψ such that $\psi_{\nabla c} = \nu\nabla c$, with $\nu > 0$ a constant. Then, we have

$$\mathbf{T}_0 = -(p + \nu\rho|\nabla c|^2)\mathbf{I} + \nu\rho|\nabla c|^2\left(\mathbf{I} - \frac{\nabla c}{|\nabla c|} \otimes \frac{\nabla c}{|\nabla c|}\right). \tag{2.15}$$

Since $\frac{\nabla c}{|\nabla c|} = \mathbf{n}$, the unit normal to the interface, following the analogy with the level-set method described in [17], the last term in (2.15) can be viewed as a regularised extra-surface term, from which the surface tension can be derived (see [17]). It is tempting to interpret the phase-field dependent correction to the pressure $\nu\rho|\nabla c|^2$ as a disjoining pressure, but a more refined microscopic treatment would be needed to corroborate this claim. Nevertheless, at variance with [13], we do not add an extra term to account for disjoining pressure but we are content with the correction just found. The use of Gibbs free-energy is justified by the argument discussed in [17]: usually, Helmholtz free-energy $\psi(\rho, \theta, c, \nabla c)$ allows to obtain pressure through the relation

$$p = \rho^2 \partial_\rho \psi.$$

However, this is possible only if the fluid is compressible and if the equation of state $p = p(\rho, T)$ can be inverted at a given temperature. For an incompressible fluid, however, the density is constant at a given temperature and so $\rho = \rho(\theta)$, from which it is impossible to recover information about pressure. The use of the Gibbs free-energy g makes it possible to overcome this difficulty, as remarked in [17], since from g it is possible to recover ρ through

$$\rho^{-1} = \frac{\partial g}{\partial p}. \tag{2.16}$$

For future reference, we also list here the expressions of the entropy density η and the (generalised) chemical potential μ in terms of g

$$\eta = -\frac{\partial g}{\partial \theta} \qquad \mu = \frac{\partial g}{\partial c}.$$

When g has been assigned, it is possible to turn back to the Helmholtz free-energy ψ, then expressed in terms of p and θ. By virtue of (2.16), requiring $\rho =$ const. is tantamount as having

$$\frac{\partial^2 g}{\partial p^2} = 0. \tag{2.17}$$

In our context, it seems reasonable to set [17]

$$\rho^{-1} = \frac{c}{\rho_1} + nR\theta(1-c)\frac{1}{p}, \tag{2.18}$$

so that, when $c \equiv 1$, $\rho = \rho_1$, the density of the fluid phase, whereas when $c \equiv 0$, ρ obeys the law of ideal gases. By use of (2.16), we obtain

$$g(p, \theta, c, \nabla c) = \frac{c}{\rho_1} p + nR\theta(1-c) \ln \frac{p}{p_0} + g_0(c, \theta) + g_1(c) + g_2(\nabla c),$$

where p_0 is a reference pressure. The mixing energy g_0 is taken as

$$g_0(c, \theta) := (1-c)\left(\left(\frac{7}{2}nR - S_0\right)(\theta - \theta_0) + nR\theta \ln \left(\frac{\theta_0}{\theta}\right)^{\frac{7}{2}}\right)$$

so that, when $c \equiv 0$ the Gibbs free energy reduces to the standard expression for a perfect, diatomic gas ([22], p. 54): here S_0 and θ_0 are constants. As to g_1, we propose the standard double well potential

$$g_1(c) = \beta c^2 (1-c)^2.$$

Since, on passing from the gas phase where $c = 0$ to a level surface for c within the transition layer, the mixing energy changes from 0 to $\beta c^2(1-c)^2$, following [20] we can interpret $\beta c^2(1-c)^2$ as an *osmotic* pressure

$$p_g = \beta c^2 (1-c)^2. \tag{2.19}$$

If we only consider the leading term in (2.19) when $c \ll 1$, we find that

$$c = \sqrt{\frac{p_g}{\beta}} \tag{2.20}$$

at the interface between the gas and the liquid metal. Equation (2.20) shows the same relation between c and p_g as in Sievert's law. Sievert's law can be expressed by the relation

$$c(\theta, p_g) = K_s \sqrt{\frac{p_g}{p_a}} \tag{2.21}$$

where p_a is the atmospheric pressure and K_s is a temperature-dependent parameter that, in the case of hydrogen in liquid aluminium, is given by [27, 29]

$$K_s = 8.9 \cdot 10^{-5} \cdot 10^{-\frac{2760}{T}+2.796}.$$

Comparing (2.20) and (2.21), we find that

$$\beta = \frac{p_a}{K_s^2}$$

and so, also the Sievert's law can be accounted for in this model. The term $g_2(\nabla c)$ is defined by

$$g_2(\nabla c) = \frac{\gamma}{2}|\nabla c|^2.$$

Collecting together all the terms, the Gibbs free-energy is given by

$$\begin{aligned} g(p, \theta, c, \nabla c) \quad &= \quad \frac{c}{\rho_1} p + nR\theta(1-c)\ln\frac{p}{p_0} \\ &\quad + (1-c)\left(\left(\frac{7}{2}nR - S_0\right)(\theta - \theta_0) + nR\theta \ln\left(\frac{\theta_0}{\theta}\right)^{\frac{7}{2}}\right) \\ &\quad + \beta c^2(1-c)^2 + \frac{\gamma}{2}|\nabla c|^2. \end{aligned} \tag{2.22}$$

To summarize, since we limit ourselves to the case where the temperature θ is constant (according to the hypotheses we discussed for the expansion of the foaming process) and choosing $\hat{f} = \theta$ in (2.9), the set of Navier-Stokes-Cahn-Hilliard equations for incompressible-compressible fluids can be written in the form:

$$\rho^{-1} = \frac{c}{\rho_1} + \frac{(1-c)nR\theta}{p}, \tag{2.23}$$

$$\dot{\rho} = -\rho \operatorname{div} \mathbf{u}, \tag{2.24}$$

$$\rho\dot{\mathbf{u}} = \operatorname{div} \mathbf{T} + \rho\mathbf{b}, \tag{2.25}$$

$$\rho\dot{c} = \operatorname{div}\left(\zeta \nabla \left(\rho^{-1}\delta_c g\right)\right), \tag{2.26}$$

where ζ is a positive constant,

$$\mathbf{T} = -p\mathbf{I} - \nu\rho\nabla c \otimes \nabla c + 2\mu c\mathbf{D}, \tag{2.27}$$

$$\delta_c g := \rho g_c - \operatorname{div}\left(\rho g_{\nabla c}\right), \tag{2.28}$$

$$
\begin{aligned}
g(p,c,\nabla c) \quad = \quad & \frac{c}{\rho_1}p + nR\theta(1-c)\ln\frac{p}{p_0} \\
& +(1-c)\left(\left(\frac{7}{2}nR - S_0\right)(\theta-\theta_0) + nR\theta\ln\left(\frac{\theta_0}{\theta}\right)^{\frac{7}{2}}\right) \\
& +\beta c^2(1-c)^2 + \frac{\gamma}{2}|\nabla c|^2. \qquad (2.29)
\end{aligned}
$$

2.2 Geometry and boundary-initial conditions.

For simplicity, we consider a 2D geometry so that, at the initial time, we have a gas-liquid mixture within a rectangular box $\mathcal{B}$ (see Figure 1). The gas is present not only within bubbles but can escape the fluid phase occupying the upper part of the box, too.

We have now to impose a suitable set of boundary conditions on the fields $\mathbf{u}$, p, and c characterising our system. We first consider the rigid portions of the boundary, $\partial\mathcal{B}_l$ and $\partial\mathcal{B}_b$ for the lateral part and the bottom part of the boundary, respectively. For the velocity field we

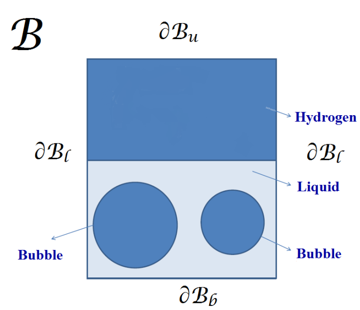

Figure 1: Test case for the metal-foam model.

enforce

$$\mathbf{u} = \mathbf{0} \qquad \text{on } \partial\mathcal{B}_b, \tag{2.30}$$

$$\mathbf{u}\cdot\mathbf{n} = 0 \qquad \text{on } \partial\mathcal{B}_l. \tag{2.31}$$

Moreover we assume

$$\mathbf{Tn}\cdot\boldsymbol{\tau} = 0 \qquad \text{on } \partial\mathcal{B}_l, \tag{2.32}$$

where $\mathbf{Tn}\cdot\boldsymbol{\tau}$ identifies the tangential component of $\mathbf{Tn}$ and we also suppose that

$$\mathbf{Tn} = \mathbf{0} \qquad \text{on } \partial\mathcal{B}_u \tag{2.33}$$

on the upper part of the box.

For the concentration c, we have two types of boundary conditions. First, we suppose that

$$\nabla c\cdot\mathbf{n} = 0 \qquad \text{on } \partial\mathcal{B}. \tag{2.34}$$

Moreover, we recall that the evolution of c is ruled by

$$\rho\dot{c} = -\text{div}\mathbf{j} \tag{2.35}$$

where the current $\mathbf{j}$ is given by

$$\mathbf{j} := \zeta \nabla \left(\frac{1}{\rho} \delta_c g \right).$$

By integrating on $\mathcal{B}$ and using both Reynolds' transport theorem and the divergence theorem, we arrive at

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_{\mathcal{B}} \rho c \mathrm{d}V = \int_{\partial \mathcal{B}} \mathbf{j} \cdot \mathbf{n} \mathrm{d}A :$$

imposing

$$\mathbf{j} \cdot \mathbf{n} = 0 \qquad \text{on } \partial \mathcal{B} \tag{2.36}$$

amounts at saying that there is no flux across the boundaries of the box. As to initial conditions, we have to assign an initial configuration c_0 of the bubbles and we can suppose that the initial velocity is equal to zero.

2.3 Dimensionless equations.

To deal with the evolution equations (2.23), we need to recast them into a dimensionless form. To this aim, we introduce as basic characteristic quantities the length L^*, the velocity V^*, the density ρ^*, the chemical potential μ^*, the temperature θ^* [17], from which we can obtain a characteristic time $t^* = \frac{L^*}{V^*}$ and a characteristic pressure $p^* = \rho^* \mu^*$. If $\mathbb{M} = \frac{\mu^*}{V^*}$ is the Mach number, $\mathbb{C} = \frac{\nu}{\mu^* L^{*2}}$ is the Cahn number (or capillary number), $\mathbb{R}e = \frac{\rho^* V^* L^*}{\mu}$ is the Reynolds number and $\mathbb{P}e = \frac{\rho^* V^* L^*}{\zeta \mu^*}$ is the Péclet number, then the incompressible-compressible version of the Navier-Stokes-Cahn-Hilliard (IC-NSCH) system of equations in dimensionless form is given by

$$\dot{\rho} = -\rho \operatorname{div} \mathbf{u}, \tag{2.37}$$

$$\rho \dot{\mathbf{u}} = \operatorname{div} \mathbf{T}, \tag{2.38}$$

$$\rho \dot{c} = \operatorname{div} \left(\frac{1}{\mathbb{P}e} \nabla \left(\rho^{-1} \delta_c g \right) \right), \tag{2.39}$$

where

$$\rho^{-1} = \frac{c}{\rho_1} + \frac{(1-c) N_1 \theta}{p}, \tag{2.40}$$

$$\mathbf{T} = -\frac{1}{\mathbb{M}} \left(p \mathbf{I} + \mathbb{C} \rho \nabla c \otimes \nabla c \right) + \frac{2}{\mathbb{R}e} c \mathbf{D}, \tag{2.41}$$

$$\delta_c g = \rho g_c - \operatorname{div} \left(\rho g_{\nabla c} \right), \tag{2.42}$$

$$\begin{aligned} g(p, c, \nabla c) = {} & \frac{c}{\rho_1} p + N_1 \theta (1-c) \ln \frac{p}{p_0} \\ & + (1-c) \left(\left(\frac{7}{2} N_1 - \sigma_0 \right) (\theta - 1) + N_1 \theta \ln \left(\frac{\theta_0}{\theta} \right)^{\frac{7}{2}} \right) \\ & + b c^2 (1-c)^2 + \frac{\mathbb{C}}{2} |\nabla c|^2, \end{aligned} \tag{2.43}$$

and $N_1 = \frac{R\theta_0}{M_w \mu^*}$, in which M_w is the molecular weight of the gas, $\sigma_0 = \frac{S_0\theta_0}{\mu^*}$, $b = \frac{\beta}{\mu^*}$, together with the following boundary conditions:

$$\mathbf{u} = \mathbf{0} \qquad \text{on } \partial\mathcal{B}_b, \tag{2.44}$$

$$\mathbf{u} \cdot \mathbf{n} = 0 \qquad \text{on } \partial\mathcal{B}_l, \tag{2.45}$$

$$\mathbf{T}\mathbf{n} \cdot \boldsymbol{\tau} = 0 \qquad \text{on } \partial\mathcal{B}_l, \tag{2.46}$$

$$\mathbf{T}\mathbf{n} = \mathbf{0} \qquad \text{on } \partial\mathcal{B}_u, \tag{2.47}$$

$$\nabla c \cdot \mathbf{n} = 0 \qquad \text{on } \partial\mathcal{B}, \tag{2.48}$$

$$\mathbf{j} \cdot \mathbf{n} = 0 \qquad \text{on } \partial\mathcal{B}. \tag{2.49}$$

3 A continuous mixed formulation of IC-NSCH system of equations.

In this section we prove mass conservation and energy dissipation properties for the incompressible-compressible Navier-Stokes-Cahn-Hilliard (IC-NSCH) system of equations (2.37)-(2.39). To this aim it is instrumental to rewrite (2.37)-(2.39) by resorting to a mixed formulation as follows:

$$\begin{aligned}
0 &= \rho(\partial_t c) + \rho(\mathbf{u} \cdot \nabla)c - \frac{1}{\mathbb{P}e}\Delta\mu, && (3.1)\\
\mathbf{0} &= \sqrt{\rho}\,\partial_t(\sqrt{\rho}\mathbf{u}) + \rho(\mathbf{u} \cdot \nabla)\mathbf{u} + \frac{1}{2}\operatorname{div}(\rho\mathbf{u})\mathbf{u} + \frac{1}{\mathbb{M}}\nabla p \\
&\quad + \frac{\mathbb{C}}{\mathbb{M}}\operatorname{div}(\rho\nabla c \otimes \nabla c) - \frac{2}{\mathbb{R}e}\operatorname{div}(c\mathbf{D}), && (3.2)\\
0 &= \partial_t\rho + \operatorname{div}(\rho\mathbf{u}), && (3.3)\\
0 &= \mu - \mu_0(c) - \frac{p}{\rho_1} + N_1\theta\ln p + \frac{\mathbb{C}}{\rho}\operatorname{div}(\rho\nabla c) + K && (3.4)
\end{aligned}$$

where

$$\begin{aligned}
\rho^{-1} &= \frac{c}{\rho_1} + \frac{(1-c)N_1\theta}{p}, && (3.5)\\
K &= \left(\frac{7}{2}N_1 - \sigma_0\right)(\theta - 1) + N_1\theta\ln\left(\frac{\theta_0}{\theta}\right)^{\frac{7}{2}}, && (3.6)\\
\mu_0(c) &= \frac{dg_1(c)}{dc} = 2bc(1-c)(1-2c), && (3.7)
\end{aligned}$$

in which we have introduced the chemical potential μ as $\rho^{-1}\delta_c g$ (cf. (2.42) and (2.43)) in order to split the fourth-order Cahn-Hilliard equation (2.39) into two second order equations, namely (3.1) and (3.4). Notice that, for ease of notation, we have supposed that the reference pressure p_0 is equal to 1. For the analysis, we will consider the following initial and boundary conditions:

$$\mathbf{u}(x,0) = \mathbf{u}_0(x), \qquad c(x,0) = c_0(x), \qquad \text{for all } x \in \Omega, \tag{3.8}$$

$$\mathbf{u} = \mathbf{0}, \qquad \nabla c \cdot \mathbf{n} = \nabla\mu \cdot \mathbf{n} = 0, \qquad \text{on } \partial\Omega \times (0,T). \tag{3.9}$$

Conditions (3.9) are simplified boundary conditions with respect to the ones introduced in Section 2. However, the analysis can be extended to the original boundary conditions.
Introducing a new variable $\mathbf{q} = \nabla c$ and manipulating the momentum equation (3.2), the system (3.1)-(3.4) can be written as follows:

$$\begin{aligned}
0 &= \rho\,\partial_t c + \rho(\mathbf{u}\cdot\nabla)c - \frac{1}{\mathbb{P}e}\Delta\mu, && (3.10)\\
\mathbf{0} &= \sqrt{\rho}\,\partial_t(\sqrt{\rho}\mathbf{u}) + \rho(\mathbf{u}\cdot\nabla)\mathbf{u} + \frac{1}{2}\operatorname{div}(\rho\mathbf{u})\mathbf{u} + \frac{1}{\mathbb{M}}\nabla p - \frac{1}{\mathbb{M}}\rho\mu\nabla c + \frac{1}{\mathbb{M}}\frac{1}{\rho_1}\rho p\nabla c\\
&\quad - \frac{1}{\mathbb{M}}N_1\theta\rho\ln p\nabla c - \frac{1}{\mathbb{M}}K\rho\nabla c + \frac{\mathbb{C}}{2\mathbb{M}}\rho\nabla(|\mathbf{q}|^2) + \frac{1}{\mathbb{M}}\rho\mu_0(c)\nabla c - \frac{2}{\mathbb{R}e}\operatorname{div}(c\mathbf{D}), && (3.11)\\
0 &= \partial_t\rho + \operatorname{div}(\rho\mathbf{u}), && (3.12)\\
0 &= \rho\mu - \rho\mu_0(c) - \frac{p}{\rho_1}\rho + N_1\theta\rho\ln p + \mathbb{C}\operatorname{div}(\,\rho\,\mathbf{q}\,) + K\rho, && (3.13)\\
\mathbf{0} &= \mathbf{q} - \nabla c. && (3.14)
\end{aligned}$$

with the following initial and boundary conditions:

$$\mathbf{u}(x,0) = \mathbf{u}_0(x), \qquad c(x,0) = c_0(x), \quad \text{for all } x\in\Omega, \tag{3.15}$$

$$\mathbf{u} = \mathbf{0}, \qquad \mathbf{q}\cdot\mathbf{n} = \nabla\mu\cdot\mathbf{n} = 0, \qquad \text{on } \partial\Omega\times(0,T). \tag{3.16}$$

Indeed, using the following identity

$$\operatorname{div}(\rho\,\nabla c\otimes\nabla c) = \operatorname{div}(\rho\,\nabla c)\nabla c + \frac{1}{2}\,\rho\,\nabla(|\nabla c|^2), \tag{3.17}$$

we can rewrite (3.2) as follows:

$$\begin{aligned}
\mathbf{0} &= \sqrt{\rho}\,\partial_t(\sqrt{\rho}\mathbf{u}) + \rho(\mathbf{u}\cdot\nabla)\mathbf{u} + \frac{1}{2}\operatorname{div}(\rho\mathbf{u})\mathbf{u} + \frac{1}{\mathbb{M}}\nabla p\\
&\quad + \frac{\mathbb{C}}{\mathbb{M}}\operatorname{div}(\rho\nabla c)\nabla c + \frac{\mathbb{C}}{2\,\mathbb{M}}\rho\nabla\left(|\nabla c|^2\right) - \frac{2}{\mathbb{R}e}\operatorname{div}(c\mathbf{D}). && (3.18)
\end{aligned}$$

Using, from equation (3.4), the fact that

$$\frac{\mathbb{C}}{\mathbb{M}}\operatorname{div}(\rho\nabla c)\nabla c = \frac{1}{\mathbb{M}}\rho\mu_0(c)\nabla c - \frac{1}{\mathbb{M}}\rho\mu\nabla c + \frac{1}{\mathbb{M}}\frac{1}{\rho_1}\rho p\nabla c - \frac{1}{\mathbb{M}}N_1\theta\rho\ln p\nabla c - \frac{1}{\mathbb{M}}K\rho\nabla c,$$

we can rewrite equation (3.18) as (3.11).

Now, the mass conservation property of the IC-NSCH system (3.10)-(3.14) reads as follows.

Theorem 3.1 (Mass conservation) *If $(c,\mathbf{u},p,\mu,\mathbf{q})$ is a strong solution of the system (3.10)-(3.14) which satisfies the boundary conditions (3.16), then*

$$\frac{d}{dt}\left(\int_\Omega \rho\,dx\right) = 0. \tag{3.19}$$

Proof. Let us consider the local mass conservation equation (3.12) and integrate it over the domain Ω:

$$\int_\Omega (\partial_t \rho + \mathrm{div}(\rho \mathbf{u}))\, dx = 0. \tag{3.20}$$

Due to the boundary conditions (3.16),

$$\int_\Omega \mathrm{div}(\rho \mathbf{u})\, dx = \int_{\partial\Omega} \rho \mathbf{u} \cdot \mathbf{n}\, ds = 0, \tag{3.21}$$

so equation (3.20) can be rewritten as

$$\int_\Omega \partial_t \rho \, dx = 0 \tag{3.22}$$

that yields the global mass conservation relation (3.19). □

We can also derive a continuous energy dissipation law for the IC-NSCH system. The derivation will be consistent with the mixed formulation (3.10)-(3.14) given above. The main technical difficulties are due to the presence of logarithmic pressure terms both in the momentum equation (3.11) and in the chemical potential definition (3.13). Let us preliminary introduce the total energy associated to the system (3.10)-(3.14):

$$E := \int_\Omega \left(\frac{1}{2} \rho\, |\mathbf{u}|^2 + \frac{1}{\mathbb{M}} \rho\, g(p, c, \mathbf{q}) - \frac{1}{\mathbb{M}} p \right) dx, \tag{3.23}$$

where

$$\begin{aligned} g(p, c, \mathbf{q}) &= \frac{c}{\rho_1} p + N_1 \theta (1 - c) \ln p + g_0(c) + g_1(c) + g_2(\mathbf{q}), && (3.24)\\ g_0(c) &= (1 - c) K, && (3.25)\\ g_1(c) &= b c^2 (1 - c)^2, && (3.26)\\ g_2(\mathbf{q}) &= \frac{\mathbb{C}}{2} |\mathbf{q}|^2. && (3.27) \end{aligned}$$

Theorem 3.2 (Energy dissipation) *Let $(c, \mathbf{u}, p, \mu, \mathbf{q})$ be a sufficiently smooth solution of the system (3.10)-(3.14). Then there holds*

$$\begin{aligned} \frac{dE}{dt} &= \frac{d}{dt} \int_\Omega \left(\frac{1}{2} \rho |\mathbf{u}|^2 + \frac{1}{\mathbb{M}} \rho g(p, c, \mathbf{q}) - \frac{1}{\mathbb{M}} p \right) dx \\ &= -\frac{1}{\mathbb{P}e\mathbb{M}} \int_\Omega |\nabla \mu|^2 dx - \frac{2}{\mathbb{R}e} \int_\Omega c\, (\mathbf{D} : \mathbf{D})\, dx. \end{aligned} \tag{3.28}$$

Proof. Let us test equation (3.10) with $\dfrac{\mu}{\mathbb{M}}$ and equation (3.11) with $\mathbf{u}$ and sum them together. If we use the following identity

$$\int_\Omega \left(\rho\, (\mathbf{u} \cdot \nabla)\, \mathbf{u} \cdot \mathbf{u} + \frac{1}{2} \mathrm{div}(\rho \mathbf{u}) \mathbf{u} \cdot \mathbf{u} \right) dx = 0 \tag{3.29}$$

and equation (3.13), integrating by parts the viscous term and the term containing $\Delta\mu$, we obtain:

$$
\begin{aligned}
0 \; = \; \int_\Omega \Big(& \sqrt{\rho}\partial_t(\sqrt{\rho}\mathbf{u})\cdot\mathbf{u} + \frac{1}{\mathbb{M}}\nabla p\cdot\mathbf{u} + \frac{1}{\mathbb{M}}\frac{1}{\rho_1}\rho p\nabla c\cdot\mathbf{u} - \frac{1}{\mathbb{M}}N_1\theta\rho\ln p\nabla c\cdot\mathbf{u} + \frac{1}{\mathbb{M}}\frac{1}{\rho_1}\rho p(\partial_t c) \\
& - \frac{1}{\mathbb{M}}N_1\theta\rho\ln p(\partial_t c) + \frac{1}{\mathbb{M}}\rho\mu_0(c)\nabla c\cdot\mathbf{u} + \frac{1}{\mathbb{M}}\rho\mu_0(c)(\partial_t c) + \frac{\mathbb{C}}{2\,\mathbb{M}}\rho\nabla(|\mathbf{q}|^2)\cdot\mathbf{u} \\
& - \frac{\mathbb{C}}{\mathbb{M}}\operatorname{div}(\rho\mathbf{q})(\partial_t c) - \frac{1}{\mathbb{M}}K\rho\nabla c\cdot\mathbf{u} - \frac{1}{\mathbb{M}}K\rho(\partial_t c) + \frac{1}{\mathbb{P}e\mathbb{M}}|\nabla\mu|^2 + \frac{2}{\mathbb{R}e}c\mathbf{D}:\mathbf{D}\Big)\,dx.
\end{aligned}
\tag{3.30}
$$

We get the following relations:

(I) the first term in (3.30) is

$$\int_\Omega \sqrt{\rho}\,\partial_t(\sqrt{\rho}\mathbf{u})\cdot\mathbf{u}\,dx = \int_\Omega \partial_t\left(\frac{\rho}{2}|\mathbf{u}|^2\right)\,dx, \tag{3.31}$$

(II) integrating by parts, using the boundary conditions (3.16) and the mass conservation equation (3.12), the terms containing $\mu_0(c)$ are equal to

$$\int_\Omega \left(\frac{1}{\mathbb{M}}\rho\mu_0(c)\nabla c\cdot\mathbf{u} + \frac{1}{\mathbb{M}}\rho\mu_0(c)(\partial_t c)\right)\,dx = \int_\Omega \partial_t\left(\frac{1}{\mathbb{M}}\rho g_1(c)\right)\,dx, \tag{3.32}$$

(III) integrating by parts, using the boundary conditions (3.16) and the mass conservation equation (3.12), the terms containing the variable $\mathbf{q}$ are equal to

$$\int_\Omega \left(\frac{\mathbb{C}}{2\,\mathbb{M}}\rho\nabla(|\mathbf{q}|^2)\cdot\mathbf{u} - \frac{\mathbb{C}}{\mathbb{M}}\operatorname{div}(\rho\mathbf{q})(\partial_t c)\right)\,dx = \int_\Omega \partial_t\left(\frac{1}{\mathbb{M}}\rho g_2(\mathbf{q})\right)\,dx, \tag{3.33}$$

(IV) integrating by parts, using the boundary conditions (3.16) and the mass conservation equation (3.12), the terms containing the constant K are equal to

$$\int_\Omega \left(-\frac{1}{\mathbb{M}}K\rho\nabla c\cdot\mathbf{u} - \frac{1}{\mathbb{M}}K\rho(\partial_t c)\right)\,dx = \int_\Omega \partial_t\left(\frac{1}{\mathbb{M}}\rho g_0(c)\right)\,dx. \tag{3.34}$$

Now, let us consider pressure terms:

$$
\begin{aligned}
\int_\Omega \Big(& \frac{1}{\mathbb{M}}\nabla p\cdot\mathbf{u} + \frac{1}{\mathbb{M}}\frac{1}{\rho_1}\rho p\nabla c\cdot\mathbf{u} - \frac{1}{\mathbb{M}}N_1\theta\rho\ln p\nabla c\cdot\mathbf{u} \\
& + \frac{1}{\mathbb{M}}\frac{1}{\rho_1}\rho p(\partial_t c) - \frac{1}{\mathbb{M}}N_1\theta\rho\ln p(\partial_t c)\Big)\,dx.
\end{aligned}
\tag{3.35}
$$

Notice that, integrating by parts, using boundary conditions (3.16) and mass conservation equation (3.12):

(a)

$$\int_\Omega \frac{1}{\mathbb{M}}\frac{1}{\rho_1}\rho p\nabla c\cdot\mathbf{u}\,dx = \int_\Omega \left(\frac{1}{\mathbb{M}}\frac{1}{\rho_1}cp(\partial_t\rho) - \frac{1}{\mathbb{M}}\frac{1}{\rho_1}\rho c\mathbf{u}\cdot\nabla p\right)\,dx, \tag{3.36}$$

(b)

$$\int_\Omega -\frac{1}{\mathbb{M}}N_1\theta\rho\ln p\nabla c\cdot\mathbf{u}\,dx = \int_\Omega\Big(\frac{1}{\mathbb{M}}N_1\theta(1-c)\ln p(\partial_t\rho) - \frac{1}{\mathbb{M}}N_1\theta\rho(1-c)\frac{\nabla p}{p}\cdot\mathbf{u}\Big)\,dx. \tag{3.37}$$

Using (3.36) and (3.37) into (3.35) we obtain:

$$\int_\Omega\Big(\frac{1}{\mathbb{M}}\nabla p\cdot\mathbf{u} - \frac{1}{\mathbb{M}}\frac{1}{\rho_1}\rho c\mathbf{u}\cdot\nabla p - \frac{1}{\mathbb{M}}N_1\theta\rho(1-c)\frac{\nabla p}{p}\cdot\mathbf{u} + \frac{1}{\mathbb{M}}\frac{1}{\rho_1}cp(\partial_t\rho) + \frac{1}{\mathbb{M}}\frac{1}{\rho_1}\rho p(\partial_t c) + \frac{1}{\mathbb{M}}N_1\theta(1-c)\ln p(\partial_t\rho) - \frac{1}{\mathbb{M}}N_1\theta\rho\ln p(\partial_t c)\Big)\,dx. \tag{3.38}$$

If we notice the fact that, remembering the definition of ρ,

$$\int_\Omega\Big(\frac{1}{\mathbb{M}}\nabla p\cdot\mathbf{u} - \frac{1}{\mathbb{M}}\frac{1}{\rho_1}\rho c\mathbf{u}\cdot\nabla p - \frac{1}{\mathbb{M}}N_1\theta\rho(1-c)\frac{\nabla p}{p}\cdot\mathbf{u}\Big)\,dx = 0, \tag{3.39}$$

then (3.38) can be rewritten as

$$\int_\Omega\Big(\frac{1}{\mathbb{M}}\frac{1}{\rho_1}cp(\partial_t\rho) + \frac{1}{\mathbb{M}}\frac{1}{\rho_1}p\rho(\partial_t c) - \frac{1}{\mathbb{M}}N_1\theta\rho(1-c)\frac{\partial_t p}{p} + \frac{1}{\mathbb{M}}N_1\theta\rho(1-c)\frac{\partial_t p}{p} + \frac{1}{\mathbb{M}}N_1\theta(1-c)\ln p(\partial_t\rho) - \frac{1}{\mathbb{M}}N_1\theta\rho\ln p(\partial_t c)\Big)\,dx, \tag{3.40}$$

in which we have added and subtracted the quantity $\frac{1}{\mathbb{M}}N_1\theta\rho(1-c)\frac{\partial_t p}{p}$. Using the fact that p can be written, in terms of ρ and c, as

$$p = \frac{N_1\theta\rho_1\rho(1-c)}{\rho_1-\rho c}, \tag{3.41}$$

we obtain:

$$\int_\Omega\Big(-\frac{1}{\mathbb{M}}N_1\theta\rho(1-c)\frac{\partial_t p}{p}\Big)\,dx = \int_\Omega\Big(-\frac{1}{\mathbb{M}}\partial_t p + \frac{1}{\mathbb{M}}\frac{1}{\rho_1}\rho c(\partial_t p)\Big)\,dx. \tag{3.42}$$

Using (3.42) into (3.40), we get:

$$\begin{aligned}&\int_\Omega\Big(\frac{1}{\mathbb{M}}\frac{1}{\rho_1}cp(\partial_t\rho) + \frac{1}{\mathbb{M}}\frac{1}{\rho_1}\rho p(\partial_t c) + \frac{1}{\mathbb{M}}\frac{1}{\rho_1}\rho c(\partial_t p) + \frac{1}{\mathbb{M}}N_1\theta(1-c)\ln p(\partial_t\rho) \\ &\quad + \frac{1}{\mathbb{M}}N_1\theta\rho\ln p\,\partial_t(1-c) + \frac{1}{\mathbb{M}}N_1\theta\rho(1-c)\frac{\partial_t p}{p} - \frac{1}{\mathbb{M}}\partial_t p\Big)\,dx \\ = &\int_\Omega\frac{1}{\mathbb{M}}\partial_t\Big(\frac{c}{\rho_1}p\rho + N_1\theta\rho(1-c)\ln p - p\Big)\,dx.\end{aligned} \tag{3.43}$$

Using (3.31)-(3.34) and (3.35)-(3.43) into (3.30), we obtain:

$$\int_\Omega\partial_t\Big(\frac{\rho}{2}|\mathbf{u}|^2 + \frac{1}{\mathbb{M}}\rho g(p,c,\mathbf{q}) - \frac{1}{\mathbb{M}}p\Big)\,dx = -\int_\Omega\frac{1}{\mathbb{P}e\mathbb{M}}|\nabla\mu|^2\,dx - \int_\Omega\frac{2}{\mathbb{R}e}c\mathbf{D}:\mathbf{D}\,dx, \tag{3.44}$$

that is equivalent to the thesis (3.28). □

Remark 3.3 *Notice that the phase-field variable c enters the viscous term in the right-hand side of (3.2). Due to the choice of $g_1(c)$ as a double-well potential, it is not guaranteed that the variable c belongs to the interval $[0, 1]$. In order to enforce this constraint, another choice of $g_1(c)$ has to be done, e.g. a logarithmic potential (see [2], [3]). In order to reduce the complexity of the problem, it is well accepted in the literature the use of double-well potentials. The fact that c remains in the interval $[0, 1]$ has influence on the dissipation of the energy (see Theorem 3.2).*

4 Numerical discretisation.

In this section we propose a numerical scheme that, at discrete level, preserves the mass conservation property and the energy dissipation law associated to the original system. Here we use a Discontinuous Galerkin spatial approximation and a modified-midpoint based scheme for the time-approximation. We point out that the main technical difficulties in the design of numerical methods for the IC-NSCH system of equations are due to the velocity field that is not divergence free, to the presence of logarithmic pressure terms in the Gibbs free-energy and to the degenerate viscosity in the gas phase.

Let $\mathscr{T}_h$ be a conforming, shape-regular family of partitions of Ω into disjoint open triangles T such that $\bar{\Omega} = \bigcup_{T\in\mathscr{T}_h} \bar{T}$. Let us denote with h_T the diameter of an element T of $\mathscr{T}_h$ and let h be the maximum element diameter. Let e denote an edge of the triangulation and $\mathcal{E}$ the set of all interior edges of $\mathcal{T}_h$.

Let us recall the definition of some useful broken Sobolev spaces:

$$H^k(\mathscr{T}_h) := \left\{ v \in L^2(\Omega) : v|_T \in H^k(T),\ \forall T \in \mathscr{T}_h \right\}, \tag{4.1}$$

$$H(\mathrm{div}; \mathscr{T}_h) := \left\{ \mathbf{w} \in (L^2(\Omega))^2 : \mathrm{div}(\mathbf{w}|_T) \in L^2(T),\ \forall T \in \mathscr{T}_h \right\}, \tag{4.2}$$

$$H^1_0(\mathscr{T}_h) := \left\{ v \in H^1(\mathscr{T}_h) : \gamma_0 v = 0 \right\}, \tag{4.3}$$

$$H^1_{\mathbf{n}}(\mathscr{T}_h) := \left\{ \mathbf{w} \in (H^1(\mathscr{T}_h))^2 : \gamma^* \mathbf{w} = 0 \right\}. \tag{4.4}$$

If v is a scalar function in $H^1(\mathscr{T}_h)$, we can define the piecewise gradient $\nabla_h v$ to be the function whose restriction to every element $T \in \mathscr{T}_h$ is equal to ∇v. In the same way, we can define the piecewise divergence $\mathrm{div}_h\, \mathbf{w}$ of a vector function $\mathbf{w} \in H(\mathrm{div}; \mathscr{T}_h)$ as the function whose restriction to every element $T \in \mathscr{T}_h$ is equal to $\mathrm{div}\, \mathbf{w}$. In the rest of the section, for ease of writing, we will suppress the subscript h in the notation of both the piecewise gradient and the piecewise divergence. The traces of functions in $H^1(\mathscr{T}_h)$ belong to the trace space

$$\mathbb{T}(\mathcal{E} \cup \partial\Omega) := \prod_{T\in\mathscr{T}_h} L^2(\partial T). \tag{4.5}$$

Let $\mathbb{P}^p(\mathscr{T}_h)$ denote the space of piecewise polynomials of degree p over $\mathscr{T}_h$. We can define the following finite element spaces:

$$\mathbb{V} := \mathbb{P}^p(\mathscr{T}_h), \quad \mathbb{V}_0 := \mathbb{V} \cap H^1_0(\mathscr{T}_h), \quad \mathbb{V}_{\mathbf{n}} := \mathbb{V}^2 \cap H^1_{\mathbf{n}}(\mathscr{T}_h). \tag{4.6}$$

For simplicity we assume that $\mathbb{V}$ is constant in time.

For $\varphi \in \mathbb{T}(\mathcal{E} \cup \partial\Omega)$, we define the jump $[\![\varphi]\!] \in (L^2(\mathcal{E} \cup \partial\Omega))^2$ and average $\{\!\{\varphi\}\!\} \in L^2(\mathcal{E} \cup \partial\Omega)$ of φ as follows. For every edge $e \in \mathcal{E}$ shared by the (open) triangles T^+ and T^-,

$$[\![\varphi]\!]_e := (\varphi^+|_e)\mathbf{n}^+ + (\varphi^-|_e)\mathbf{n}^-, \qquad \{\!\{\varphi\}\!\}_e := \frac{1}{2}(\varphi^+|_e + \varphi^-|_e), \tag{4.7}$$

where, for $i = +, -$, $v^i = v|_{\bar{T}^i}$ and $\mathbf{n}^i$ is the unit normal vector on e pointing outward of T^i. If $e \in \partial\Omega$, then

$$[\![\varphi]\!]_e := \varphi\mathbf{n}, \qquad \{\!\{\varphi\}\!\}_e := \varphi, \tag{4.8}$$

where $\mathbf{n}$ is the outward unit normal.
In the same way, we can define the jumps $[\![\boldsymbol{\varphi}]\!] \in L^2(\mathcal{E} \cup \partial\Omega)$, $[\![\boldsymbol{\varphi}]\!]_\otimes \in (L^2(\mathcal{E} \cup \partial\Omega))^{2\times 2}$ and average $\{\!\{\boldsymbol{\varphi}\}\!\} \in (L^2(\mathcal{E} \cup \partial\Omega))^2$ of the vector function $\boldsymbol{\varphi} \in (\mathbb{T}(\mathcal{E} \cup \partial\Omega))^2$ as follows. For every $e \in \mathcal{E}$ shared by the (open) triangles T^+ and T^-,

$$[\![\boldsymbol{\varphi}]\!]_e := (\boldsymbol{\varphi}^+|_e) \cdot \mathbf{n}^+ + (\boldsymbol{\varphi}^-|_e) \cdot \mathbf{n}^-, \tag{4.9}$$

$$[\![\boldsymbol{\varphi}]\!]_{e\otimes} := (\boldsymbol{\varphi}^+|_e) \otimes \mathbf{n}^+ + (\boldsymbol{\varphi}^-|_e) \otimes \mathbf{n}^-, \tag{4.10}$$

$$\{\!\{\boldsymbol{\varphi}\}\!\}_e := \frac{1}{2}(\boldsymbol{\varphi}^+|_e + \boldsymbol{\varphi}^-|_e). \tag{4.11}$$

If $e \in \partial\Omega$, then

$$[\![\boldsymbol{\varphi}]\!]_e := \boldsymbol{\varphi} \cdot \mathbf{n}, \quad [\![\boldsymbol{\varphi}]\!]_{e\otimes} := \boldsymbol{\varphi} \otimes \mathbf{n}, \quad \{\!\{\boldsymbol{\varphi}\}\!\}_e := \boldsymbol{\varphi}. \tag{4.12}$$

In the next sections we will suppress the subscript e in the notations of jumps and averages.

4.1 Spatial DG discretisation.

In this section we propose a Discontinuous Galerkin spatial approximation of the IC-NSCH system of equations (3.10)-(3.14), inspired by the one proposed in [9] for a quasi-incompressible system. This DG discrete formulation will be consistent with the mass conservation and energy dissipation properties of the original system.

We first give the elementwise variational formulation of the problem (3.10)-(3.14) in mixed form. We have to find

$$\begin{aligned}(c, \mathbf{u}, p, \mu, \mathbf{q}) \quad \in \quad & L^2(0,T; H^1(\mathscr{T}_h)) \times L^2(0,T; (H^1_0(\mathscr{T}_h))^2) \times L^2(0,T; H^1(\mathscr{T}_h)) \times \\ & L^2(0,T; H^1(\mathscr{T}_h)) \times L^2(0,T; H^1_{\mathbf{n}}(\mathscr{T}_h))\end{aligned}$$

such that

$$0 = \sum_{T\in\mathscr{T}_h}\int_T \left(\rho\,(\partial_t c)\,X + \rho(\mathbf{u}\cdot\nabla)cX\right)\,dx - \frac{1}{\mathbb{P}e}\mathcal{A}(\mu,X) + \int_{\mathcal{E}} F_1(c,\mathbf{u},p,\mu,\mathbf{q},X)\,ds, \tag{4.13}$$

$$\begin{aligned}0 \;=\; & \sum_{T\in\mathscr{T}_h}\int_T \Big(\sqrt{\rho}\,\partial_t\,(\sqrt{\rho}\mathbf{u})\cdot\boldsymbol{\xi} + \rho(\mathbf{u}\cdot\nabla)\mathbf{u}\cdot\boldsymbol{\xi} + \frac{1}{2}\operatorname{div}(\rho\mathbf{u})\mathbf{u}\cdot\boldsymbol{\xi} + \frac{1}{\mathbb{M}}\nabla p\cdot\boldsymbol{\xi}\\ & -\frac{1}{\mathbb{M}}\rho\mu\,\nabla c\cdot\boldsymbol{\xi} + \frac{1}{\mathbb{M}}\frac{1}{\rho_1}\rho p\nabla c\cdot\boldsymbol{\xi} - \frac{1}{\mathbb{M}}N_1\theta\rho\ln p\nabla c\cdot\boldsymbol{\xi} - \frac{1}{\mathbb{M}}K\rho\nabla c\cdot\boldsymbol{\xi}\\ & + \frac{\mathbb{C}}{2\mathbb{M}}\rho\nabla(|\mathbf{q}|^2)\cdot\boldsymbol{\xi} + \frac{1}{\mathbb{M}}\rho\mu_0(c)\nabla c\cdot\boldsymbol{\xi}\Big)\,dx - \frac{2}{\mathbb{R}e}\mathcal{B}(c,\mathbf{u},\boldsymbol{\xi})\\ & + \int_{\mathcal{E}} F_2(c,\mathbf{u},p,\mu,\mathbf{q},\boldsymbol{\xi})\,ds,\end{aligned} \tag{4.14}$$

$$0 = \sum_{T\in\mathscr{T}_h}\int_T \left((\partial_t\rho)\,Z + \operatorname{div}(\rho\mathbf{u})Z\right)\,dx + \int_{\mathcal{E}} F_3(c,\mathbf{u},p,\mu,\mathbf{q},Z)\,ds, \tag{4.15}$$

$$\begin{aligned}0 \;=\; & \sum_{T\in\mathscr{T}_h}\int_T \Big(\rho\mu\psi - \rho\mu_0(c)\psi - \frac{p}{\rho_1}\rho\psi + N_1\theta\rho\ln p\psi + \mathbb{C}\operatorname{div}(\,\rho\,\mathbf{q}\,)\psi + K\rho\psi\Big)\,dx\\ & + \int_{\mathcal{E}} F_4(c,\mathbf{u},p,\mu,\mathbf{q},\psi)\,ds,\end{aligned} \tag{4.16}$$

$$0 = \sum_{T\in\mathscr{T}_h}\int_T \left(\mathbf{q}\cdot\mathbf{T} - \nabla c\cdot\mathbf{T}\right)\,dx + \int_{\mathcal{E}} F_5(c,\mathbf{u},p,\mu,\mathbf{q},\mathbf{T})\,ds, \tag{4.17}$$

$$\forall\,(X,\boldsymbol{\xi},Z,\psi,\mathbf{T})\in H^1(\mathscr{T}_h)\times(H^1_0(\mathscr{T}_h))^2\times H^1(\mathscr{T}_h)\times H^1(\mathscr{T}_h)\times H^1_{\mathbf{n}}(\mathscr{T}_h),$$

in which

$$\begin{aligned}\mathcal{A}(\mu,X) \;:=\; & -\sum_{T\in\mathscr{T}_h}\int_T \nabla\mu\cdot\nabla X\,dx + \int_{\mathcal{E}} \{\!\!\{\nabla X\}\!\!\}\cdot[\![\mu]\!]\,ds\\ & + \int_{\mathcal{E}} [\![X]\!]\cdot\{\!\!\{\nabla\mu\}\!\!\}\,ds - \int_{\mathcal{E}}\frac{\sigma}{h}\,[\![\mu]\!]\cdot[\![X]\!]\,ds,\end{aligned} \tag{4.18}$$

$$\begin{aligned}\mathcal{B}(c,\mathbf{u},\boldsymbol{\xi}) \;:=\; & -\sum_{T\in\mathscr{T}_h}\int_T \left(c\,\epsilon(\mathbf{u}):\epsilon(\boldsymbol{\xi})\right)\,dx + \int_{\mathcal{E}\cup\partial\Omega}\left(\{\!\!\{c\,\epsilon(\boldsymbol{\xi})\}\!\!\}:[\![\mathbf{u}]\!]_{\otimes}\right)\,ds\\ & + \int_{\mathcal{E}\cup\partial\Omega}\left(\{\!\!\{c\,\epsilon(\mathbf{u})\}\!\!\}:[\![\boldsymbol{\xi}]\!]_{\otimes}\right)\,ds - \int_{\mathcal{E}\cup\partial\Omega}\frac{\gamma}{h}\left([\![\mathbf{u}]\!]_{\otimes}:[\![\boldsymbol{\xi}]\!]_{\otimes}\right)\,ds\end{aligned} \tag{4.19}$$

are the symmetric interior penalty discretisation of the laplacian of the chemical potential μ (see [1], [24]) and the DG formulation of the viscous terms (see [11] and [32]), where σ and γ are sufficiently large parameters and $\epsilon(\mathbf{u}) := 1/2(\nabla\mathbf{u} + (\nabla\mathbf{u})^T)$.

The elementwise numerical fluxes F_i, for $i = 1,...,5$, will be chosen later (see (4.52)-(4.56)) according to the properties that our discrete formulation will have to obey. We suppose that the numerical fluxes only depend on the traces of their arguments and are linear in the test functions.

Now, let us give a spatially discrete DG mixed formulation of (4.13)-(4.17): find

$$(c_h, \mathbf{u}_h, p_h, \mu_h, \mathbf{q}_h) \in L^2(0,T;\mathbb{V}) \times L^2(0,T;\mathbb{V}_0^2) \times L^2(0,T;\mathbb{V}) \times L^2(0,T;\mathbb{V}) \times L^2(0,T;\mathbb{V}_{\mathbf{n}})$$

such that

$$\begin{aligned}
0 &= \sum_{T\in\mathscr{T}_h}\int_T \left(\rho_h\left(\partial_t c_h\right)X + \rho_h(\mathbf{u}_h\cdot\nabla)c_h X\right)\,dx - \frac{1}{\mathbb{P}e}\mathcal{A}(\mu_h, X) \\
&\quad + \int_{\mathcal{E}} F_1(c_h, \mathbf{u}_h, p_h, \mu_h, \mathbf{q}_h, X)\,ds, && (4.20)\\
0 &= \sum_{T\in\mathscr{T}_h}\int_T \Big(\sqrt{\rho_h}\,\partial_t\left(\sqrt{\rho_h}\mathbf{u}_h\right)\cdot\boldsymbol{\xi} + \rho_h(\mathbf{u}_h\cdot\nabla)\mathbf{u}_h\cdot\boldsymbol{\xi} + \frac{1}{2}\operatorname{div}(\rho_h\mathbf{u}_h)\mathbf{u}_h\cdot\boldsymbol{\xi} \\
&\quad + \frac{1}{\mathbb{M}}\nabla p_h\cdot\boldsymbol{\xi} - \frac{1}{\mathbb{M}}\rho_h\mu_h\nabla c_h\cdot\boldsymbol{\xi} + \frac{1}{\mathbb{M}}\frac{1}{\rho_1}\rho_h p_h\nabla c_h\cdot\boldsymbol{\xi} - \frac{1}{\mathbb{M}}N_1\theta\rho_h\ln p_h\nabla c_h\cdot\boldsymbol{\xi} \\
&\quad - \frac{1}{\mathbb{M}}K\rho_h\nabla c_h\cdot\boldsymbol{\xi} + \frac{\mathbb{C}}{2\mathbb{M}}\rho_h\nabla(|\mathbf{q}_h|^2)\cdot\boldsymbol{\xi} + \frac{1}{\mathbb{M}}\rho_h\mu_0(c_h)\nabla c_h\cdot\boldsymbol{\xi}\Big)\,dx \\
&\quad - \frac{2}{\mathbb{R}e}\mathcal{B}(c_h, \mathbf{u}_h, \boldsymbol{\xi}) + \int_{\mathcal{E}} F_2(c_h, \mathbf{u}_h, p_h, \mu_h, \mathbf{q}_h, \boldsymbol{\xi})\,ds, && (4.21)\\
0 &= \sum_{T\in\mathscr{T}_h}\int_T \left((\partial_t\rho_h)\,Z + \operatorname{div}(\rho_h\mathbf{u}_h)Z\right)\,dx + \int_{\mathcal{E}} F_3(c_h, \mathbf{u}_h, p_h, \mu_h, \mathbf{q}_h, Z)\,ds, && (4.22)\\
0 &= \sum_{T\in\mathscr{T}_h}\int_T \Big(\rho_h\mu_h\psi - \rho_h\mu_0(c_h)\psi - \frac{p_h}{\rho_1}\rho_h\psi + N_1\theta\rho_h\ln p_h\psi \\
&\quad + \mathbb{C}\operatorname{div}(\rho_h\,\mathbf{q}_h)\psi + K\rho_h\psi\Big)\,dx + \int_{\mathcal{E}} F_4(c_h, \mathbf{u}_h, p_h, \mu_h, \mathbf{q}_h, \psi)\,ds, && (4.23)\\
0 &= \sum_{T\in\mathscr{T}_h}\int_T \left(\mathbf{q}_h\cdot\mathbf{T} - \nabla c_h\cdot\mathbf{T}\right)\,dx + \int_{\mathcal{E}} F_5(c_h, \mathbf{u}_h, p_h, \mu_h, \mathbf{q}_h, \mathbf{T})\,ds, && (4.24)
\end{aligned}$$

$$\forall\,(X, \boldsymbol{\xi}, Z, \psi, \mathbf{T}) \in \mathbb{V}\times\mathbb{V}_0^2\times\mathbb{V}\times\mathbb{V}\times\mathbb{V}_{\mathbf{n}}.$$

In the DG formulation (4.20)-(4.24) we have used, for simplicity, $\rho_h := \rho(c_h, p_h)$. Now we recall a proposition that will be useful to prove the discrete mass conservation property and the discrete version of the energy law for the spatially discrete DG formulation (4.20)-(4.24) (see [1], [8] for the proof).

Proposition 4.1 *If $\mathbf{w}\in H(\operatorname{div};\mathscr{T}_h)$ and $v\in H^1(\mathscr{T}_h)$, then*

$$\sum_{T\in\mathscr{T}_h}\int_T \operatorname{div}(\mathbf{w})v\,dx = \sum_{T\in\mathscr{T}_h}\left(-\int_T \mathbf{w}\cdot\nabla v\,dx + \int_{\partial T} v\mathbf{w}\cdot\mathbf{n}_T\,ds\right). \tag{4.25}$$

In particular, $\mathbf{w}\in(\mathbb{T}(\mathcal{E}\cup\partial\Omega))^2$, $v\in\mathbb{T}(\mathcal{E}\cup\partial\Omega)$ and

$$\sum_{T\in\mathscr{T}_h}\int_{\partial T} v\mathbf{w}\cdot\mathbf{n}\,ds = \int_{\mathcal{E}} [\![\mathbf{w}]\!]\,\{\!\{v\}\!\}\,ds + \int_{\mathcal{E}\cup\partial\Omega} [\![v]\!]\cdot\{\!\{\mathbf{w}\}\!\}\,ds = \int_{\mathcal{E}\cup\partial\Omega} [\![v\mathbf{w}]\!]\,ds. \tag{4.26}$$

In the sequel, the elementwise numerical fluxes F_i, for $i = 1, ..., 5$, will be chosen by imposing:

- spatially discrete mass conservation,
- spatially discrete energy dissipation law,
- consistency of the discrete DG formulation (4.20)-(4.24), i.e.

$$F_i(c, \mathbf{u}, p, \mu, \mathbf{q}, \cdot) = 0 \tag{4.27}$$

  for $i = 1, \ldots, 5$ and for all smooth functions $c, \mathbf{u}, p, \mu, \mathbf{q}$.

In particular, the conditions to be imposed on the numerical fluxes $F_i, i = 1, ..., 5$, in order to ensure that a mass conservation relation holds for the spatial discretisation (4.20)-(4.24) will be defined by the following result.

Theorem 4.2 (Spatially discrete conservation of mass) *If $(c_h, \mathbf{u}_h, p_h, \mu_h, \mathbf{q}_h)$ is a solution of the spatially discrete system (4.20)-(4.24) then*

$$\frac{d}{dt}\left(\sum_{T\in\mathscr{T}_h}\int_T \rho_h\, dx\right) = 0 \tag{4.28}$$

if and only if

$$\int_{\mathcal{E}} F_3(c_h, \mathbf{u}_h, p_h, \mu_h, \mathbf{q}_h, 1)\, ds = -\int_{\mathcal{E}} [\![\rho_h \mathbf{u}_h]\!]\, ds. \tag{4.29}$$

Proof. Let $Z = 1$ be the scalar function equal to 1 everywhere on the spatial domain Ω. Using $Z = 1$ in (4.22), we obtain

$$0 = \sum_{T\in\mathscr{T}_h}\int_T \left(\partial_t \rho_h + \operatorname{div}(\rho_h \mathbf{u}_h)\right)\, dx + \int_{\mathcal{E}} F_3(c_h, \mathbf{u}_h, \bar{p}_h, \mu_h, \mathbf{q}_h, 1)\, ds. \tag{4.30}$$

Integration by parts of the second term leads to

$$0 = \sum_{T\in\mathscr{T}_h}\int_T \partial_t \rho_h\, dx + \int_{\mathcal{E}} [\![\rho_h \mathbf{u}_h]\!]\, ds + \int_{\mathcal{E}} F_3(c_h, \mathbf{u}_h, \bar{p}_h, \mu_h, \mathbf{q}_h, 1)\, ds \tag{4.31}$$

which implies the thesis. □

Now, if we define the spatially discrete total energy associated to the system (4.20)-(4.24) as

$$E_h := \sum_{T\in\mathscr{T}_h}\int_T \left(\frac{\rho_h}{2}|\mathbf{u}_h|^2 + \frac{1}{\mathbb{M}}\rho_h g(p_h, c_h, \mathbf{q}_h) - \frac{1}{\mathbb{M}}p_h\right)\, dx, \tag{4.32}$$

that is the spatially discrete version of the continuous total energy (3.23), we can set conditions on the numerical fluxes F_i, $i = 1, \ldots, 5$, under which the spatially discrete system (4.20)-(4.24) preserves a spatially discrete version of the energy dissipation law (3.28). The proof of the following theorem shares the same structure of the continuous case and has been inspired by the proof given in [9] for a volume-fraction based quasi-incompressible phase-field model. For simplicity of notation, we set

$$F_i(\cdot) := F_i(c_h, \mathbf{u}_h, p_h, \mu_h, \mathbf{q}_h, \cdot), \text{ for all } i = 1, \ldots, 5.$$

Theorem 4.3 (Spatially discrete energy dissipation law) *If $(c_h, \mathbf{u}_h, p_h, \mu_h, \mathbf{q}_h)$ is a solution of the spatially discrete system (4.20)-(4.24) then*

$$\begin{aligned} \frac{dE_h}{dt} &= \frac{d}{dt}\left(\sum_{T\in\mathscr{T}_h}\int_T\left(\frac{\rho_h}{2}|\mathbf{u}_h|^2+\frac{1}{\mathbb{M}}\rho_h g(p_h,c_h,\mathbf{q}_h)-\frac{1}{\mathbb{M}}p_h\right)dx\right)\\ &= \frac{1}{\mathbb{P}e\mathbb{M}}\mathcal{A}(\mu_h,\mu_h)+\frac{2}{\mathbb{R}e}\mathcal{B}(c_h,\mathbf{u}_h,\mathbf{u}_h) \end{aligned} \tag{4.33}$$

if and only if the following conditions on the numerical fluxes F_i, for $i = 1, \ldots, 5$, are satisfied:
a.

$$\begin{aligned} 0 \;=\; &\int_{\mathcal{E}}\left(F_1\left(\frac{\mu_h}{\mathbb{M}}\right)+F_2(\mathbf{u}_h)+F_3\left(\frac{1}{\mathbb{M}}g_1(c_h)+\frac{\mathbb{C}}{2\,\mathbb{M}}|\mathbf{q}_h|^2+\frac{1}{\mathbb{M}}K(1-c_h)\right.\right.\\ &\left.+\frac{1}{\mathbb{M}}\frac{1}{\rho_1}c_hp_h+\frac{1}{\mathbb{M}}N_1\theta(1-c_h)\ln p_h\right)+\frac{1}{2}[\![\rho_h(\mathbf{u}_h\cdot\mathbf{u}_h)\mathbf{u}_h]\!]+\frac{1}{\mathbb{M}}[\![\rho_h g_1(c_h)\mathbf{u}_h]\!]\\ &+\frac{\mathbb{C}}{2\,\mathbb{M}}[\![\rho_h|\mathbf{q}_h|^2\mathbf{u}_h]\!]+\frac{1}{\mathbb{M}}[\![K\rho_h(1-c_h)\mathbf{u}_h]\!]\\ &\left.+\frac{1}{\mathbb{M}}\frac{1}{\rho_1}[\![\rho_h p_h c_h\mathbf{u}_h]\!]+\frac{N_1\theta}{\mathbb{M}}[\![\rho_h(1-c_h)\ln p_h\mathbf{u}_h]\!]\right)ds, \end{aligned} \tag{4.34}$$

b.

$$0 = \int_{\mathcal{E}}\left(\partial_t F_5\left(\frac{\mathbb{C}}{\mathbb{M}}\rho_h\mathbf{q}_h\right)-\frac{\mathbb{C}}{\mathbb{M}}[\![\rho_h\mathbf{q}_h(\partial_t c_h)]\!]-F_4\left(\frac{1}{\mathbb{M}}\partial_t c_h\right)\right)ds. \tag{4.35}$$

Remark 4.4 *Notice that $\mathcal{A}$ and $\mathcal{B}$, by definition, are negative definite. Hence, it holds*

$$\frac{dE_h}{dt} < 0.$$

Proof. Let us test equation (4.20) with $\frac{\mu_h}{\mathbb{M}}$ and equation (4.21) with $\mathbf{u}_h$ and sum them together. If we use the fact that

$$\begin{aligned} &\sum_{T\in\mathscr{T}_h}\int_T\left(\rho_h(\mathbf{u}_h\cdot\nabla)\mathbf{u}_h\cdot\mathbf{u}_h+\frac{1}{2}\operatorname{div}(\rho_h\mathbf{u}_h)\mathbf{u}_h\cdot\mathbf{u}_h\right)dx = \\ = \quad &\int_{\mathcal{E}}\frac{1}{2}[\![\rho_h(\mathbf{u}_h\cdot\mathbf{u}_h)\mathbf{u}_h]\!]\,ds, \end{aligned}$$

and equation (4.23), we obtain:

$$
\begin{aligned}
0 \;=\; & \sum_{T\in\mathscr{T}_h}\int_T \Bigg(\sqrt{\rho_h}\,\partial_t\left(\sqrt{\rho_h}\mathbf{u}_h\right)\cdot\mathbf{u}_h + \frac{1}{\mathbb{M}}\nabla p_h\cdot\mathbf{u}_h + \frac{1}{\mathbb{M}}\frac{1}{\rho_1}\rho_h p_h\nabla c_h\cdot\mathbf{u}_h \\
& \quad - \frac{1}{\mathbb{M}}N_1\theta\rho_h\ln p_h\nabla c_h\cdot\mathbf{u}_h + \frac{1}{\mathbb{M}}\frac{1}{\rho_1}\rho_h p_h(\partial_t c_h) - \frac{1}{\mathbb{M}}N_1\theta\rho_h\ln p_h(\partial_t c_h) \\
& \quad + \frac{1}{\mathbb{M}}\rho_h\mu_0(c_h)\nabla c_h\cdot\mathbf{u}_h + \frac{1}{\mathbb{M}}\rho_h\mu_0(c_h)(\partial_t c_h) + \frac{\mathbb{C}}{2\,\mathbb{M}}\rho_h\nabla(|\mathbf{q}_h|^2)\cdot\mathbf{u}_h \\
& \quad - \frac{\mathbb{C}}{\mathbb{M}}\,\mathrm{div}(\rho_h\mathbf{q}_h)(\partial_t c_h) - \frac{1}{\mathbb{M}}K\rho_h\nabla c_h\cdot\mathbf{u}_h - \frac{1}{\mathbb{M}}K\rho_h(\partial_t c_h)\Bigg)\,dx \\
& + \int_{\mathcal{E}}\left(F_1\left(\frac{\mu_h}{\mathbb{M}}\right) + F_2(\mathbf{u}_h) + F_4\left(\frac{1}{\mathbb{M}}\partial_t c_h\right) + \frac{1}{2}\left[\!\left[\rho_h(\mathbf{u}_h\cdot\mathbf{u}_h)\mathbf{u}_h\right]\!\right]\right)ds \\
& - \frac{1}{\mathbb{P}e\mathbb{M}}\mathcal{A}(\mu_h,\mu_h) - \frac{2}{\mathbb{R}e}\mathcal{B}(c_h,\mathbf{u}_h,\mathbf{u}_h).
\end{aligned}
\tag{4.36}
$$

We get the following relations:

(I) the first term in (4.36) is

$$
\sum_{T\in\mathscr{T}_h}\int_T\sqrt{\rho_h}\,\partial_t(\sqrt{\rho_h}\mathbf{u}_h)\cdot\mathbf{u}_h\,dx = \sum_{T\in\mathscr{T}_h}\int_T\partial_t\left(\frac{\rho_h}{2}|\mathbf{u}_h|^2\right)dx, \tag{4.37}
$$

(II) integrating by parts and using mass conservation equation (4.22), the terms containing $\mu_0(c_h)$ are equal to

$$
\begin{aligned}
& \sum_{T\in\mathscr{T}_h}\int_T\left(\frac{1}{\mathbb{M}}\rho_h\mu_0(c_h)\nabla c_h\cdot\mathbf{u}_h + \frac{1}{\mathbb{M}}\rho_h\mu_0(c_h)(\partial_t c_h)\right)dx \\
= \; & \sum_{T\in\mathscr{T}_h}\int_T\partial_t\left(\frac{1}{\mathbb{M}}\rho_h g_1(c_h)\right)dx + \int_{\mathcal{E}}\left(F_3\left(\frac{1}{\mathbb{M}}g_1(c_h)\right) + \frac{1}{\mathbb{M}}\left[\!\left[\rho_h g_1(c_h)\mathbf{u}_h\right]\!\right]\right)ds,
\end{aligned}
\tag{4.38}
$$

(III) integrating by parts and using the mass conservation equation (4.22), the terms containing the variable $\mathbf{q}_h$ are equal to

$$
\begin{aligned}
& \sum_{T\in\mathscr{T}_h}\int_T\left(\frac{\mathbb{C}}{2\,\mathbb{M}}\rho_h\nabla(|\mathbf{q}_h|^2)\cdot\mathbf{u}_h - \frac{\mathbb{C}}{\mathbb{M}}\,\mathrm{div}(\rho_h\mathbf{q}_h)(\partial_t c_h)\right)dx \\
= \; & \sum_{T\in\mathscr{T}_h}\int_T\partial_t\left(\frac{1}{\mathbb{M}}\rho_h g_2(\mathbf{q}_h)\right)dx + \int_{\mathcal{E}}\left(F_3\left(\frac{\mathbb{C}}{2\,\mathbb{M}}|\mathbf{q}_h|^2\right) + \partial_t F_5\left(\frac{\mathbb{C}}{\mathbb{M}}\,\rho_h\mathbf{q}_h\right)\right)ds \\
& + \int_{\mathcal{E}}\left(\frac{\mathbb{C}}{2\,\mathbb{M}}\left[\!\left[\rho_h|\mathbf{q}_h|^2\mathbf{u}_h\right]\!\right] - \frac{\mathbb{C}}{\mathbb{M}}\left[\!\left[\rho_h\mathbf{q}_h(\partial_t c_h)\right]\!\right]\right)ds,
\end{aligned}
\tag{4.39}
$$

(IV) integrating by parts and using the mass conservation equation (4.22), the terms containing the constant K are equal to

$$\begin{aligned}
&\sum_{T\in\mathscr{T}_h}\int_T\left(-\frac{1}{\mathbb{M}}K\rho_h\nabla c_h\cdot\mathbf{u}_h-\frac{1}{\mathbb{M}}K\rho_h(\partial_t c_h)\right)\,dx\\
=\ &\sum_{T\in\mathscr{T}_h}\int_T\partial_t\left(\frac{1}{\mathbb{M}}\rho_h g_0(c_h)\right)\,dx\\
&+\int_{\mathcal{E}}\left(F_3\left(\frac{1}{\mathbb{M}}K(1-c_h)\right)+\frac{1}{\mathbb{M}}[\![K\rho_h(1-c_h)\mathbf{u}_h]\!]\right)\,ds. \qquad (4.40)
\end{aligned}$$

Now, as in the continuous case, let us consider the pressure terms:

$$\begin{aligned}
&\sum_{T\in\mathscr{T}_h}\int_T\left(\frac{1}{\mathbb{M}}\nabla p_h\cdot\mathbf{u}_h+\frac{1}{\mathbb{M}}\frac{1}{\rho_1}\rho_h p_h\nabla c_h\cdot\mathbf{u}_h-\frac{1}{\mathbb{M}}N_1\theta\rho_h\ln p_h\nabla c_h\cdot\mathbf{u}_h\right.\\
&\qquad\left.+\frac{1}{\mathbb{M}}\frac{1}{\rho_1}\rho_h p_h(\partial_t c_h)-\frac{1}{\mathbb{M}}N_1\theta\rho_h\ln p_h(\partial_t c_h)\right)\,dx. \qquad (4.41)
\end{aligned}$$

Notice that, integrating by parts and using mass conservation equation (4.22):

(a)

$$\begin{aligned}
&\sum_{T\in\mathscr{T}_h}\int_T\left(\frac{1}{\mathbb{M}}\frac{1}{\rho_1}\rho_h p_h\nabla c_h\cdot\mathbf{u}_h\right)\,dx\\
=\ &\sum_{T\in\mathscr{T}_h}\int_T\left(\frac{1}{\mathbb{M}}\frac{1}{\rho_1}c_h p_h(\partial_t\rho_h)-\frac{1}{\mathbb{M}}\frac{1}{\rho_1}\rho_h c_h\mathbf{u}_h\cdot\nabla p_h\right)\,dx\\
&+\int_{\mathcal{E}}\left(F_3\left(\frac{1}{\mathbb{M}}\frac{1}{\rho_1}c_h p_h\right)+\frac{1}{\mathbb{M}}\frac{1}{\rho_1}[\![\rho_h p_h c_h\mathbf{u}_h]\!]\right)\,ds, \qquad (4.42)
\end{aligned}$$

(b)

$$\begin{aligned}
&\sum_{T\in\mathscr{T}_h}\int_T\left(-\frac{1}{\mathbb{M}}N_1\theta\rho_h\ln p_h\nabla c_h\cdot\mathbf{u}_h\right)\,dx\\
=\ &\sum_{T\in\mathscr{T}_h}\int_T\left(\frac{1}{\mathbb{M}}N_1\theta(1-c_h)\ln p_h(\partial_t\rho_h)-\frac{1}{\mathbb{M}}N_1\theta\rho_h(1-c_h)\frac{\nabla p_h}{p_h}\cdot\mathbf{u}_h\right)\,dx\\
&+\int_{\mathcal{E}}\left(F_3\left(\frac{1}{\mathbb{M}}N_1\theta\ln p_h(1-c_h)\right)+\frac{1}{\mathbb{M}}[\![N_1\theta\rho_h(1-c_h)\ln p_h\mathbf{u}_h]\!]\right)\,ds. \\
&\qquad (4.43)
\end{aligned}$$

Using (4.42) and (4.43) into (4.41) we obtain:

$$\begin{aligned}
&\sum_{T\in\mathscr{T}_h}\int_T\Bigg(\frac{1}{\mathbb{M}}\nabla p_h\cdot\mathbf{u}_h-\frac{1}{\mathbb{M}}\frac{1}{\rho_1}\rho_h c_h\mathbf{u}_h\cdot\nabla p_h-\frac{1}{\mathbb{M}}N_1\theta\rho_h(1-c_h)\frac{\nabla p_h}{p_h}\cdot\mathbf{u}_h\\
&+\frac{1}{\mathbb{M}}\frac{1}{\rho_1}c_h p_h(\partial_t\rho_h)+\frac{1}{\mathbb{M}}\frac{1}{\rho_1}\rho_h p_h(\partial_t c_h)+\frac{1}{\mathbb{M}}N_1\theta(1-c_h)\ln p_h(\partial_t\rho_h)\\
&-\frac{1}{\mathbb{M}}N_1\theta\rho_h\ln p_h(\partial_t c_h)\Bigg)\,dx+\int_{\mathcal{E}}F_3\left(\frac{1}{\mathbb{M}}\frac{1}{\rho_1}c_h p_h+\frac{1}{\mathbb{M}}N_1\theta(1-c_h)\ln p_h\right)\,ds\\
&+\int_{\mathcal{E}}\left(\frac{1}{\mathbb{M}}\frac{1}{\rho_1}[\![\rho_h p_h c_h\mathbf{u}_h]\!]+\frac{1}{\mathbb{M}}[\![N_1\theta\rho_h(1-c_h)\ln p_h\mathbf{u}_h]\!]\right)\,ds. \qquad (4.44)
\end{aligned}$$

If we notice the fact that, remembering the definition of ρ_h,

$$\sum_{T\in\mathscr{T}_h}\int_T\left(\frac{1}{\mathbb{M}}\nabla p_h\cdot\mathbf{u}_h-\frac{1}{\mathbb{M}}\frac{1}{\rho_1}\rho_h c_h\mathbf{u}_h\cdot\nabla p_h-\frac{1}{\mathbb{M}}N_1\theta\rho_h(1-c_h)\frac{\nabla p_h}{p_h}\cdot\mathbf{u}_h\right)dx=0, \qquad (4.45)$$

then we can rewrite (4.44) as

$$\begin{aligned}
&\sum_{T\in\mathscr{T}_h}\int_T\Bigg(\frac{1}{\mathbb{M}}\frac{1}{\rho_1}c_h p_h(\partial_t\rho_h)+\frac{1}{\mathbb{M}}\frac{1}{\rho_1}p_h\rho_h(\partial_t c_h)-\frac{1}{\mathbb{M}}N_1\theta\rho_h(1-c_h)\frac{\partial_t p_h}{p_h}\\
&+\frac{1}{\mathbb{M}}N_1\theta\rho_h(1-c_h)\frac{\partial_t p_h}{p_h}+\frac{1}{\mathbb{M}}N_1\theta(1-c_h)\ln p_h(\partial_t\rho_h)-\frac{1}{\mathbb{M}}N_1\theta\rho_h\ln p_h(\partial_t c_h)\Bigg)dx\\
&+\int_{\mathcal{E}}F_3\left(\frac{1}{\mathbb{M}}\frac{1}{\rho_1}c_h p_h+\frac{1}{\mathbb{M}}N_1\theta(1-c_h)\ln p_h\right)\,ds\\
&+\int_{\mathcal{E}}\left(\frac{1}{\mathbb{M}}\frac{1}{\rho_1}[\![\rho_h p_h c_h\mathbf{u}_h]\!]+\frac{1}{\mathbb{M}}[\![N_1\theta\rho_h(1-c_h)\ln p_h\mathbf{u}_h]\!]\right)\,ds \qquad (4.46)
\end{aligned}$$

in which we have added and subtracted the quantity $\frac{1}{\mathbb{M}}N_1\theta\rho_h(1-c_h)\frac{\partial_t p_h}{p_h}$. Using the fact that p_h can be written, in terms of ρ_h and c_h, as

$$p_h=\frac{N_1\theta\rho_1\rho_h(1-c_h)}{\rho_1-\rho_h c_h}, \qquad (4.47)$$

we obtain:

$$\begin{aligned}
&\sum_{T\in\mathscr{T}_h}\int_T\left(-\frac{1}{\mathbb{M}}N_1\theta\rho_h(1-c_h)\frac{\partial_t p_h}{p_h}\right)\,dx=\\
=\ &\sum_{T\in\mathscr{T}_h}\int_T\left(-\frac{1}{\mathbb{M}}\partial_t p_h+\frac{1}{\mathbb{M}}\frac{1}{\rho_1}\rho_h c_h(\partial_t p_h)\right)\,dx. \qquad (4.48)
\end{aligned}$$

Using (4.48) into (4.46), we get:

$$\begin{aligned}
&\sum_{T\in\mathscr{T}_h}\int_T \frac{1}{\mathbb{M}}\partial_t\left(\frac{c_h}{\rho_1}p_h\rho_h+N_1\theta\rho_h(1-c_h)\ln p_h-p_h\right)dx\\
&+\int_{\mathcal{E}}F_3\left(\frac{1}{\mathbb{M}}\frac{1}{\rho_1}c_hp_h+\frac{1}{\mathbb{M}}N_1\theta(1-c_h)\ln p_h\right)ds\\
&+\int_{\mathcal{E}}\left(\frac{1}{\mathbb{M}}\frac{1}{\rho_1}[\![\rho_hp_hc_h\mathbf{u}_h]\!]+\frac{1}{\mathbb{M}}[\![N_1\theta\rho_h(1-c_h)\ln p_h\mathbf{u}_h]\!]\right)ds. \qquad (4.49)
\end{aligned}$$

Then, using (4.37)-(4.40) and (4.41)-(4.49) into (4.36), we obtain:

$$\begin{aligned}
0 \;=\; &\sum_{T\in\mathscr{T}_h}\int_T\partial_t\left(\frac{\rho_h}{2}|\mathbf{u}_h|^2+\frac{1}{\mathbb{M}}\rho_hg(p_h,c_h,\mathbf{q}_h)-\frac{1}{\mathbb{M}}p_h\right)dx\\
&+\int_{\mathcal{E}}\left(F_1\left(\frac{\mu_h}{\mathbb{M}}\right)+F_2\left(\mathbf{u}_h\right)+F_3\left(\frac{1}{\mathbb{M}}g_1(c_h)+\frac{\mathbb{C}}{2\,\mathbb{M}}|\mathbf{q}_h|^2+\frac{1}{\mathbb{M}}K(1-c_h)\right.\right.\\
&\left.+\frac{1}{\mathbb{M}}\frac{1}{\rho_1}c_hp_h+\frac{1}{\mathbb{M}}N_1\theta(1-c_h)\ln p_h\right)-F_4\left(\frac{1}{\mathbb{M}}\partial_tc_h\right)+\partial_tF_5\left(\frac{\mathbb{C}}{\mathbb{M}}\,\rho_h\mathbf{q}_h\right)\\
&+\frac{1}{2}[\![\rho_h(\mathbf{u}_h\cdot\mathbf{u}_h)\mathbf{u}_h]\!]+\frac{1}{\mathbb{M}}[\![\rho_hg_1(c_h)\mathbf{u}_h]\!]\\
&+\frac{\mathbb{C}}{2\,\mathbb{M}}[\![\rho_h|\mathbf{q}_h|^2\mathbf{u}_h]\!]-\frac{\mathbb{C}}{\mathbb{M}}[\![\rho_h\mathbf{q}_h(\partial_tc_h)]\!]\\
&\left.+\frac{1}{\mathbb{M}}[\![K\rho_h(1-c_h)\mathbf{u}_h]\!]+\frac{1}{\mathbb{M}}\frac{1}{\rho_1}[\![\rho_hp_hc_h\mathbf{u}_h]\!]+\frac{N_1\theta}{\mathbb{M}}[\![\rho_h(1-c_h)\ln p_h\mathbf{u}_h]\!]\right)ds\\
&-\frac{1}{\mathbb{P}e\mathbb{M}}\mathcal{A}(\mu_h,\mu_h)-\frac{2}{\mathbb{R}e}\mathcal{B}(c_h,\mathbf{u}_h,\mathbf{u}_h). \qquad (4.50)
\end{aligned}$$

So, the scheme (4.20)-(4.24) preserves the energy law at the spatially discrete level iff

$$\begin{aligned}
0 \;=\; &\int_{\mathcal{E}}\left(F_1\left(\frac{\mu_h}{\mathbb{M}}\right)+F_2\left(\mathbf{u}_h\right)+F_3\left(\frac{1}{\mathbb{M}}g_1(c_h)+\frac{\mathbb{C}}{2\,\mathbb{M}}|\mathbf{q}_h|^2+\frac{1}{\mathbb{M}}K(1-c_h)\right.\right.\\
&\left.+\frac{1}{\mathbb{M}}\frac{1}{\rho_1}c_hp_h+\frac{1}{\mathbb{M}}N_1\theta(1-c_h)\ln p_h\right)+\frac{1}{2}[\![\rho_h(\mathbf{u}_h\cdot\mathbf{u}_h)\mathbf{u}_h]\!]+\frac{1}{\mathbb{M}}[\![\rho_hg_1(c_h)\mathbf{u}_h]\!]\\
&+\frac{\mathbb{C}}{2\,\mathbb{M}}[\![\rho_h|\mathbf{q}_h|^2\mathbf{u}_h]\!]+\frac{1}{\mathbb{M}}[\![K\rho_h(1-c_h)\mathbf{u}_h]\!]\\
&\left.+\frac{1}{\mathbb{M}}\frac{1}{\rho_1}[\![\rho_hp_hc_h\mathbf{u}_h]\!]+\frac{N_1\theta}{\mathbb{M}}[\![\rho_h(1-c_h)\ln p_h\mathbf{u}_h]\!]\right)ds\\
&+\int_{\mathcal{E}}\left(\partial_tF_5\left(\frac{\mathbb{C}}{\mathbb{M}}\,\rho_h\mathbf{q}_h\right)-\frac{\mathbb{C}}{\mathbb{M}}[\![\rho_h\mathbf{q}_h(\partial_tc_h)]\!]-F_4\left(\frac{1}{\mathbb{M}}\partial_tc_h\right)\right)ds. \qquad (4.51)
\end{aligned}$$

It is clear from (4.20)-(4.24) that ∂_tc_h does not depend from the other variables; so conditions (a) and (b) of the thesis are satisfied. □

Summarising, from the spatially discrete mass conservation theorem (Theorem 4.2) and the spatially discrete energy dissipation law theorem (Theorem 4.3), it follows that a possible choice for the numerical fluxes is:

$$
\begin{aligned}
F_1(X) &= 0, && (4.52)\\
F_2(\boldsymbol{\xi}) &= -\frac{1}{2}\,[\![\rho_h\mathbf{u}_h]\!]\,\{\!\{\mathbf{u}_h\cdot\boldsymbol{\xi}\}\!\} - \left(\{\!\{\boldsymbol{\xi}\}\!\}\otimes\{\!\{\rho_h\mathbf{u}_h\}\!\}\right) : [\![\mathbf{u}_h]\!]_{\otimes} - \frac{1}{\mathbb{M}}\,[\![g_1(c_h)]\!]\cdot\{\!\{\rho_h\boldsymbol{\xi}\}\!\}\\
&\quad -\frac{\mathbb{C}}{2\,\mathbb{M}}\,[\![|\mathbf{q}_h|^2]\!]\cdot\{\!\{\rho_h\boldsymbol{\xi}\}\!\} - \frac{1}{\mathbb{M}}\,[\![K(1-c_h)]\!]\cdot\{\!\{\rho_h\boldsymbol{\xi}\}\!\} - \frac{1}{\mathbb{M}}\frac{1}{\rho_1}\,[\![c_hp_h]\!]\cdot\{\!\{\rho_h\boldsymbol{\xi}\}\!\}\\
&\quad -\frac{N_1\theta}{\mathbb{M}}\,[\![(1-c_h)\ln p_h]\!]\cdot\{\!\{\rho_h\boldsymbol{\xi}\}\!\}, && (4.53)\\
F_3(Z) &= -\,[\![\rho_h\mathbf{u}_h]\!]\,\{\!\{Z\}\!\}, && (4.54)\\
F_4(\psi) &= -\mathbb{C}\,[\![\rho_h\mathbf{q}_h]\!]\,\{\!\{\psi\}\!\}, && (4.55)\\
F_5(\mathbf{T}) &= [\![c_h]\!]\cdot\{\!\{\mathbf{T}\}\!\}. && (4.56)
\end{aligned}
$$

4.2 Time-discretisation.

In this section we propose a semi-discretisation in time of the continuous system (3.10)-(3.14) based on a modified midpoint type scheme (see also [4], [30]) used in [10].

Let us subdivide the time interval $[0,T]$ into N equally spaced subintervals whose end-points are $t_0 = 0 < t_1 < \ldots < t_N = T$ and denote with Δt the timestep size, such that $t^{n+1} = t^n + \Delta t$ for all $n = 0,1,...,N-1$; let $h^n(\cdot)$ denote $h(\cdot,t^n)$ for a generic time-dependent function h. The temporally discrete scheme for (3.10)-(3.14) is written as follows. Given initial conditions $(c^0,\mathbf{u}^0,p^0,\mu^0,\mathbf{q}^0)$, for all $n = 0,1,...,N-1$, find $(c^{n+1},\mathbf{u}^{n+1},p^{n+1},\mu^{n+1},\mathbf{q}^{n+1}) \in H^1(\Omega)\times(H^2(\Omega)\cap H^1_0(\Omega))^2 \times H^1(\Omega)\times H^2(\Omega)\times H^1_{\mathbf{n}}(\Omega)$ such that

$$
\begin{aligned}
0 &= \rho^{n+\frac12}\,c_{\bar t}^{n+1} + \rho^{n+\frac12}(\sqrt{\rho}\mathbf{u})^{n+1}\cdot\nabla c^{n+\frac12} - \frac{1}{\mathbb{P}e}\Delta\mu^{n+\frac12}, && (4.57)\\
\mathbf{0} &= \sqrt{\rho}^{\,n+\frac12}\,(\sqrt{\rho}\mathbf{u})_{\bar t}^{n+1} + \rho^{n+\frac12}\left((\sqrt{\rho}\mathbf{u})^{n+1}\cdot\nabla\right)(\sqrt{\rho}\mathbf{u})^{n+1}\\
&\quad +\frac12\,\mathrm{div}(\rho^{n+\frac12}(\sqrt{\rho}\mathbf{u})^{n+1})(\sqrt{\rho}\mathbf{u})^{n+1} + \frac{1}{\mathbb{M}}\nabla p^{n+\frac12}\\
&\quad -\frac{1}{\mathbb{M}}\rho^{n+\frac12}\mu^{n+\frac12}\,\nabla c^{n+\frac12} + \frac{1}{\mathbb{M}}\frac{1}{\rho_1}\rho^{n+\frac12,*}p^{n+\frac12}\nabla c^{n+\frac12}\\
&\quad -\frac{1}{\mathbb{M}}N_1\theta\rho^{n+\frac12,*}\,(\ln p)^{n+\frac12}\,\nabla c^{n+\frac12}\\
&\quad -\frac{1}{\mathbb{M}}K\rho^{n+\frac12,*}\nabla c^{n+\frac12} + \frac{\mathbb{C}}{4\mathbb{M}}\rho^{n+\frac12,*}\nabla\left(\mathbf{q}^{n+1}\cdot\mathbf{q}^{n+1} + \mathbf{q}^n\cdot\mathbf{q}^n\right)\\
&\quad +\frac{1}{2\,\mathbb{M}}\rho^{n+\frac12,*}\nabla\left(g_1(c^{n+1}) + g_1(c^n)\right) - \frac{2}{\mathbb{R}e}\,\mathrm{div}\left(c^{n+\frac12}\mathbf{D}^{n+1}\right), && (4.58)\\
0 &= \rho_{\bar t}^{n+1} + \mathrm{div}\left(\rho^{n+\frac12,*}(\sqrt{\rho}\mathbf{u})^{n+1}\right), && (4.59)\\
0 &= \rho^{n+\frac12}\mu^{n+\frac12} - \rho^{n+\frac12}\frac{g_1(c^{n+1}) - g_1(c^n)}{c^{n+1}-c^n} - \frac{p^{n+\frac12}}{\rho_1}\rho^{n+\frac12} + N_1\theta\rho^{n+\frac12}\,(\ln p)^{n+\frac12}\\
&\quad +\mathbb{C}\,\mathrm{div}\left(\,\rho^{n+\frac12}\,\mathbf{q}^{n+\frac12}\,\right) + K\rho^{n+\frac12}, && (4.60)\\
\mathbf{0} &= \mathbf{q}^{n+\frac12} - \nabla c^{n+\frac12}. && (4.61)
\end{aligned}
$$

Here we have used the following notation:

$$c_{\bar{t}}^{n+1} := \frac{c^{n+1} - c^n}{\Delta t}, \qquad \rho_{\bar{t}}^{n+1} := \frac{\rho^{n+1} - \rho^n}{\Delta t},$$
$$(\sqrt{\rho}\mathbf{u})_{\bar{t}}^{n+1} := \frac{\sqrt{\rho^{n+1}}\mathbf{u}^{n+1} - \sqrt{\rho^n}\mathbf{u}^n}{\Delta t}, \qquad (\sqrt{\rho}\mathbf{u})^{n+1} := \frac{\sqrt{\rho^{n+1}}\mathbf{u}^{n+1} + \sqrt{\rho^n}\mathbf{u}^n}{\sqrt{\rho^{n+1}} + \sqrt{\rho^n}}.$$

We have used, for simplicity,

$$h^{n+\frac{1}{2}} := \frac{h^n + h^{n+1}}{2}$$

for a generic function h. In the time-scheme, the modified midpoint approximation $G(c^{n+1}, c^n)$ of the potential term has been used:

$$\begin{aligned} G(c^{n+1}, c^n) &:= \frac{g_1\left(c^{n+1}\right) - g_1\left(c^n\right)}{c^{n+1} - c^n} & (4.62)\\ &= \frac{1}{4}\left(c^{n+1}\left(c^{n+1} - 1\right) + c^n\left(c^n - 1\right)\right)\left(c^{n+1} + c^n - 1\right). & (4.63) \end{aligned}$$

The density and the logarithmic terms are approximated as follows:

$$\rho^{n+\frac{1}{2}} := \frac{\rho^{n+1} + \rho^n}{2}, \qquad \rho^{n+\frac{1}{2},*} := \rho(c^{n+\frac{1}{2}}, p^{n+\frac{1}{2}}), \tag{4.64}$$

$$(\ln p)^{n+\frac{1}{2}} := \ln p^{n+\frac{1}{2}}, \tag{4.65}$$

$$(\ln p)^{n+1} := \ln p^{n+\frac{1}{2}} + \frac{p^{n+1} - p^n}{2p^{n+1}}, \qquad (\ln p)^n := \ln p^{n+\frac{1}{2}} - \frac{p^{n+1} - p^n}{2p^n}. \tag{4.66}$$

In addition, we set

$$\mathbf{D}^{n+1} := \frac{\nabla(\sqrt{\rho}\mathbf{u})^{n+1} + (\nabla(\sqrt{\rho}\mathbf{u})^{n+1})^T}{2}. \tag{4.67}$$

Remark 4.5 *The choice of the time-approximation related to* $(\ln p)^{n+1}$ *can be justified in the following way. Let us consider the quantity*

$$\ln\frac{p^{n+\frac{1}{2}}}{p^{n+1}} = \ln p^{n+\frac{1}{2}} - \ln p^{n+1}. \tag{4.68}$$

From the Taylor expansion of the left-hand side of (4.68), we obtain

$$\frac{p^n - p^{n+1}}{2p^{n+1}}. \tag{4.69}$$

In a similar way it is possible to justify the choice of the time-approximation related to $(\ln p)^n$.

Now, we will prove that the temporally discrete scheme (4.57)-(4.61) satisfies the mass conservation property as stated by the following result.

Theorem 4.6 (Temporally discrete conservation of mass) *The temporally discrete scheme (4.57)-(4.61) is mass-conservative, i.e.*

$$\int_\Omega \rho^{n+1}\,dx = \int_\Omega \rho^n\,dx, \qquad \textit{for all } n = 0, 1, ..., N-1. \tag{4.70}$$

Proof. Let us integrate equation (4.59) over the spatial domain Ω:

$$\int_\Omega \left(\rho_{\bar{t}}^{n+1} + \operatorname{div}\left(\rho^{n+\frac{1}{2}}(\sqrt{\rho}\mathbf{u})^{n+1}\right)\right) dx = 0. \tag{4.71}$$

Using the fact that

$$\int_\Omega \operatorname{div}\left(\rho^{n+\frac{1}{2}}(\sqrt{\rho}\mathbf{u})^{n+1}\right) dx = \int_{\partial\Omega} \rho^{n+\frac{1}{2}}(\sqrt{\rho}\mathbf{u})^{n+1}\cdot\mathbf{n}\, ds = 0, \tag{4.72}$$

equation (4.71) can be rewritten as

$$\int_\Omega \frac{\rho(c^{n+1}) - \rho(c^n)}{\Delta t}\, dx = 0, \tag{4.73}$$

which implies the thesis. □

If we define

$$E^n := \int_\Omega \left(\frac{1}{2}\rho^n \left|\mathbf{u}^n\right|^2 + \frac{1}{\mathbb{M}}\rho^n g(p^n, c^n, \mathbf{q}^n) - \frac{1}{\mathbb{M}}p^n\right) dx \tag{4.74}$$

as the temporally discrete version of the total energy (3.23), for $n = 0, 1, ..., N$, we can also prove that our scheme (4.57)-(4.61) preserves a temporally discrete formulation of the continuous energy dissipation law (3.28).

Theorem 4.7 (Temporally discrete energy dissipation law) *If* $(c^{n+1}, \mathbf{u}^{n+1}, p^{n+1}, \mu^{n+1}, \mathbf{q}^{n+1})$ *is a solution of the temporally discrete system (4.57)-(4.61). Then*

$$E_{\bar{t}}^{n+1} = -\frac{1}{\mathbb{P}e\mathbb{M}}\int_\Omega \left(\nabla\mu^{n+\frac{1}{2}}\right)^2 dx - \frac{2}{\mathbb{R}e}\int_\Omega c^{n+\frac{1}{2}}\left(\mathbf{D}^{n+1} : \mathbf{D}^{n+1}\right) dx, \tag{4.75}$$

for all $n = 0, 1, ..., N-1$, *where*

$$E_{\bar{t}}^{n+1} := \frac{E^{n+1} - E^n}{\Delta t}.$$

Proof. Let us test equation (4.57) with $\dfrac{\mu^{n+\frac{1}{2}}}{\mathbb{M}}$ and equation (4.58) with $(\sqrt{\rho}\mathbf{u})^{n+1}$ and sum them together. If we use the following identity

$$\begin{aligned}\int_\Omega \Big(&\rho^{n+\frac{1}{2}}\left(\left((\sqrt{\rho}\mathbf{u})^{n+1}\cdot\nabla\right)(\sqrt{\rho}\mathbf{u})^{n+1}\cdot(\sqrt{\rho}\mathbf{u})^{n+1}\right.\\ &+ \frac{1}{2}\operatorname{div}(\rho^{n+\frac{1}{2}}(\sqrt{\rho}\mathbf{u})^{n+1})(\sqrt{\rho}\mathbf{u})^{n+1}\cdot(\sqrt{\rho}\mathbf{u})^{n+1}\Big)\, dx = 0,\end{aligned} \tag{4.76}$$

equation (4.60) and integrate by parts the viscous term and term containing $\Delta\mu^{n+\frac{1}{2}}$, we obtain:

$$
\begin{aligned}
0 \;=\; & \int_\Omega \Bigg(\sqrt{\rho}^{\,n+\frac{1}{2}} \, (\sqrt{\rho}\mathbf{u})_{\bar{t}}^{n+1} \cdot (\sqrt{\rho}\mathbf{u})^{n+1} + \frac{1}{\mathbb{M}} \nabla p^{n+\frac{1}{2}} \cdot (\sqrt{\rho}\mathbf{u})^{n+1} \\
& + \frac{1}{\mathbb{M}} \frac{1}{\rho_1} \rho^{\,n+\frac{1}{2},*} p^{n+\frac{1}{2}} \nabla c^{n+\frac{1}{2}} \cdot (\sqrt{\rho}\mathbf{u})^{n+1} \\
& - \frac{1}{\mathbb{M}} N_1 \theta \rho^{\,n+\frac{1}{2},*} (\ln p)^{n+\frac{1}{2}} \nabla c^{n+\frac{1}{2}} \cdot (\sqrt{\rho}\mathbf{u})^{n+1} \\
& + \frac{1}{\mathbb{M}} \frac{1}{\rho_1} \rho^{n+\frac{1}{2}} p^{n+\frac{1}{2}} \frac{c^{n+1} - c^n}{\Delta t} - \frac{1}{\mathbb{M}} N_1 \theta \rho^{n+\frac{1}{2}} (\ln p)^{n+\frac{1}{2}} \frac{c^{n+1} - c^n}{\Delta t} \\
& + \frac{1}{\mathbb{M}} \rho^{\,n+\frac{1}{2},*} \frac{\nabla (g_1(c^{n+1}) + g_1(c^n))}{2} \cdot (\sqrt{\rho}\mathbf{u})^{n+1} \\
& + \frac{1}{\mathbb{M}} \rho^{n+\frac{1}{2}} \frac{g_1(c^{n+1}) - g_1(c^n)}{c^{n+1} - c^n} \frac{c^{n+1} - c^n}{\Delta t} \\
& + \frac{\mathbb{C}}{4\mathbb{M}} \rho^{\,n+\frac{1}{2},*} \nabla (\mathbf{q}^{n+1} \cdot \mathbf{q}^{n+1} + \mathbf{q}^n \cdot \mathbf{q}^n) \cdot (\sqrt{\rho}\mathbf{u})^{n+1} \\
& - \frac{\mathbb{C}}{\mathbb{M}} \operatorname{div}(\rho^{n+\frac{1}{2}} \mathbf{q}^{n+\frac{1}{2}}) \frac{c^{n+1} - c^n}{\Delta t} \\
& - \frac{1}{\mathbb{M}} K \rho^{\,n+\frac{1}{2},*} \nabla c^{n+\frac{1}{2}} \cdot (\sqrt{\rho}\mathbf{u})^{n+1} - \frac{1}{\mathbb{M}} K \rho^{n+\frac{1}{2}} \frac{c^{n+1} - c^n}{\Delta t} \\
& + \frac{1}{\mathbb{P}e\mathbb{M}} |\nabla \mu^{n+\frac{1}{2}}|^2 + \frac{2}{\mathbb{R}e} c^{n+\frac{1}{2}} (\mathbf{D}^{n+1} : \mathbf{D}^{n+1}) \Bigg) \, dx. \qquad (4.77)
\end{aligned}
$$

We get the following relations:

(I) the first term in (4.77) is

$$
\int_\Omega \sqrt{\rho}^{\,n+\frac{1}{2}} \, (\sqrt{\rho}\mathbf{u})_{\bar{t}}^{n+1} \cdot (\sqrt{\rho}\mathbf{u})^{n+1} \, dx = \int_\Omega \frac{1}{2\Delta t} \left(\rho^{n+1} (\mathbf{u}^{n+1})^2 - \rho^n (\mathbf{u}^n)^2 \right) dx, \qquad (4.78)
$$

(II) integrating by parts, and using the mass conservation equation (4.59), the terms containing g_1 are equal to

$$
\begin{aligned}
& \int_\Omega \Bigg(\frac{1}{2\mathbb{M}} \rho^{\,n+\frac{1}{2},*} \nabla (g_1(c^{n+1}) + g_1(c^n)) \cdot (\sqrt{\rho}\mathbf{u})^{n+1} \\
& \qquad + \frac{1}{\mathbb{M}\Delta t} \rho^{n+\frac{1}{2}} (g_1(c^{n+1}) - g_1(c^n)) \Bigg) \, dx \\
= \; & \int_\Omega \frac{1}{\mathbb{M}\Delta t} \left(\rho^{n+1} g_1(c^{n+1}) - \rho^n g_1(c^n) \right) dx, \qquad (4.79)
\end{aligned}
$$

(III) integrating by parts and using mass conservation equation (4.59), the terms containing the variable $\mathbf{q}$ are equal to

$$
\begin{aligned}
& \int_\Omega \Bigg(\frac{\mathbb{C}}{4\mathbb{M}} \rho^{\,n+\frac{1}{2},*} \nabla (\mathbf{q}^{n+1} \cdot \mathbf{q}^{n+1} + \mathbf{q}^n \cdot \mathbf{q}^n) \cdot (\sqrt{\rho}\mathbf{u})^{n+1} \\
& \qquad - \frac{\mathbb{C}}{\mathbb{M}} \operatorname{div}(\rho^{n+\frac{1}{2}} \mathbf{q}^{n+\frac{1}{2}}) \frac{c^{n+1} - c^n}{\Delta t} \Bigg) \, dx \\
= \; & \int_\Omega \frac{1}{\mathbb{M}\Delta t} \left(\rho^{n+1} g_2(\mathbf{q}^{n+1}) - \rho^n g_2(\mathbf{q}^n) \right) dx, \qquad (4.80)
\end{aligned}
$$

(IV) integrating by parts and using mass conservation equation (4.59), the terms containing the constant K are equal to

$$\begin{aligned}&\int_\Omega \left(-\frac{1}{\mathbb{M}} K\rho^{\,n+\frac12,*}\nabla c^{n+\frac12}\cdot(\sqrt{\rho}\mathbf{u})^{n+1} - \frac{1}{\mathbb{M}} K\rho^{n+\frac12}\frac{c^{n+1}-c^n}{\Delta t}\right)dx\\ = &\int_\Omega \frac{1}{\mathbb{M}\Delta t}\left(\rho^{n+1}g_0(c^{n+1}) - \rho^n g_0(c^n)\right)dx.\end{aligned} \tag{4.81}$$

Now, let us consider the pressure terms:

$$\begin{aligned}\int_\Omega \Bigg(&\frac{1}{\mathbb{M}}\nabla p^{n+\frac12}\cdot(\sqrt{\rho}\mathbf{u})^{n+1} + \frac{1}{\mathbb{M}}\frac{1}{\rho_1}\rho^{\,n+\frac12,*}p^{n+\frac12}\nabla c^{n+\frac12}\cdot(\sqrt{\rho}\mathbf{u})^{n+1}\\ &-\frac{1}{\mathbb{M}}N_1\theta\rho^{\,n+\frac12,*}(\ln p)^{n+\frac12}\nabla c^{n+\frac12}\cdot(\sqrt{\rho}\mathbf{u})^{n+1}\\ &+\frac{1}{\mathbb{M}}\frac{1}{\rho_1}\rho^{n+\frac12}p^{n+\frac12}\frac{c^{n+1}-c^n}{\Delta t} - \frac{1}{\mathbb{M}}N_1\theta\rho^{n+\frac12}(\ln p)^{n+\frac12}\frac{c^{n+1}-c^n}{\Delta t}\Bigg)dx.\end{aligned} \tag{4.82}$$

Notice that, integrating by parts and using mass conservation equation (4.59):

(a)

$$\begin{aligned}&\int_\Omega\left(\frac{1}{\mathbb{M}}\frac{1}{\rho_1}\rho^{\,n+\frac12,*}p^{n+\frac12}\nabla c^{n+\frac12}\cdot(\sqrt{\rho}\mathbf{u})^{n+1}\right)dx\\ = &\int_\Omega\left(\frac{1}{\mathbb{M}}\frac{1}{\rho_1}c^{n+\frac12}p^{n+\frac12}\frac{\rho^{n+1}-\rho^n}{\Delta t} - \frac{1}{\mathbb{M}}\frac{1}{\rho_1}\rho^{\,n+\frac12,*}c^{n+\frac12}(\sqrt{\rho}\mathbf{u})^{n+1}\cdot\nabla p^{n+\frac12}\right)dx,\end{aligned} \tag{4.83}$$

(b)

$$\begin{aligned}&\int_\Omega\left(-\frac{1}{\mathbb{M}}N_1\theta\rho^{\,n+\frac12,*}(\ln p)^{n+\frac12}\nabla c^{n+\frac12}\cdot(\sqrt{\rho}\mathbf{u})^{n+1}\right)dx\\ = &\int_\Omega\Bigg(\frac{1}{\mathbb{M}}N_1\theta(1-c^{n+\frac12})(\ln p)^{n+\frac12}\frac{\rho^{n+1}-\rho^n}{\Delta t}\\ &\quad -\frac{1}{\mathbb{M}}N_1\theta\rho^{\,n+\frac12,*}(1-c^{n+\frac12})\frac{\nabla p^{n+\frac12}}{p^{n+\frac12}}\cdot(\sqrt{\rho}\mathbf{u})^{n+1}\Bigg)dx.\end{aligned} \tag{4.84}$$

Using (4.83) and (4.84) into (4.82) we obtain:

$$\begin{aligned}\int_\Omega\Bigg(&\frac{1}{\mathbb{M}}\nabla p^{n+\frac12}\cdot(\sqrt{\rho}\mathbf{u})^{n+1} - \frac{1}{\mathbb{M}}\frac{1}{\rho_1}\rho^{\,n+\frac12,*}c^{n+\frac12}(\sqrt{\rho}\mathbf{u})^{n+1}\cdot\nabla p^{n+\frac12}\\ &-\frac{1}{\mathbb{M}}N_1\theta\rho^{\,n+\frac12,*}(1-c^{n+\frac12})\frac{\nabla p^{n+\frac12}}{p^{n+\frac12}}\cdot(\sqrt{\rho}\mathbf{u})^{n+1}\\ &+\frac{1}{\mathbb{M}}\frac{1}{\rho_1}c^{n+\frac12}p^{n+\frac12}\frac{\rho^{n+1}-\rho^n}{\Delta t} + \frac{1}{\mathbb{M}}\frac{1}{\rho_1}\rho^{n+\frac12}p^{n+\frac12}\frac{c^{n+1}-c^n}{\Delta t}\\ &+\frac{1}{\mathbb{M}}N_1\theta(1-c^{n+\frac12})(\ln p)^{n+\frac12}\frac{\rho^{n+1}-\rho^n}{\Delta t} - \frac{1}{\mathbb{M}}N_1\theta\rho^{n+\frac12}(\ln p)^{n+\frac12}\frac{c^{n+1}-c^n}{\Delta t}\Bigg)dx.\end{aligned} \tag{4.85}$$

If we notice the fact that, remembering the definition of $\rho^{\,n+\frac{1}{2},*}$,

$$
\begin{aligned}
0 \;=\; & \int_\Omega \left(\frac{1}{\mathbb{M}} \nabla p^{n+\frac{1}{2}} \cdot (\sqrt{\rho}\mathbf{u})^{n+1} - \frac{1}{\mathbb{M}} \frac{1}{\rho_1} \rho^{\,n+\frac{1}{2},*} c^{n+\frac{1}{2}} (\sqrt{\rho}\mathbf{u})^{n+1} \cdot \nabla p^{n+\frac{1}{2}} \right. \\
& \left. - \frac{1}{\mathbb{M}} N_1 \theta \rho^{\,n+\frac{1}{2},*} (1 - c^{n+\frac{1}{2}}) \frac{\nabla p^{n+\frac{1}{2}}}{p^{n+\frac{1}{2}}} \cdot (\sqrt{\rho}\mathbf{u})^{n+1} \right) dx, \qquad (4.86)
\end{aligned}
$$

then (4.85) can be rewritten as

$$
\begin{aligned}
& \int_\Omega \left(\frac{1}{\mathbb{M}} \frac{1}{\rho_1} c^{n+\frac{1}{2}} p^{n+\frac{1}{2}} \frac{\rho^{n+1} - \rho^n}{\Delta t} + \frac{1}{\mathbb{M}} \frac{1}{\rho_1} p^{n+\frac{1}{2}} \rho^{n+\frac{1}{2}} \frac{c^{n+1} - c^n}{\Delta t} \right. \\
& - \frac{N_1\theta}{\mathbb{M}} \frac{p^{n+1} - p^n}{\Delta t} \frac{1}{2} \left(\frac{\rho^{n+1}}{p^{n+1}} (1 - c^{n+1}) + \frac{\rho^n}{p^n} (1 - c^n) \right) \\
& + \frac{N_1\theta}{\mathbb{M}} \frac{p^{n+1} - p^n}{\Delta t} \frac{1}{2} \left(\frac{\rho^{n+1}}{p^{n+1}} (1 - c^{n+1}) + \frac{\rho^n}{p^n} (1 - c^n) \right) \\
& \left. + \frac{N_1\theta}{\mathbb{M}} (1 - c^{n+\frac{1}{2}}) (\ln p)^{n+\frac{1}{2}} \frac{\rho^{n+1} - \rho^n}{\Delta t} - \frac{N_1\theta}{\mathbb{M}} \rho^{n+\frac{1}{2}} (\ln p)^{n+\frac{1}{2}} \frac{c^{n+1} - c^n}{\Delta t} \right) dx, \qquad (4.87)
\end{aligned}
$$

in which we have added and subtracted the quantity

$$
\frac{N_1\theta}{\mathbb{M}} \frac{p^{n+1} - p^n}{\Delta t} \frac{1}{2} \left(\frac{\rho^{n+1}}{p^{n+1}} (1 - c^{n+1}) + \frac{\rho^n}{p^n} (1 - c^n) \right).
$$

Using the fact that

$$
p^{n+1} = \frac{N_1 \theta \rho_1 \rho^{n+1} (1 - c^{n+1})}{\rho_1 - \rho^{n+1} c^{n+1}}, \qquad p^n = \frac{N_1 \theta \rho_1 \rho^n (1 - c^n)}{\rho_1 - \rho^n c^n}, \qquad (4.88)
$$

we obtain:

$$
\begin{aligned}
& \int_\Omega \left(- \frac{N_1\theta}{\mathbb{M}} \frac{p^{n+1} - p^n}{\Delta t} \frac{1}{2} \left(\frac{\rho^{n+1}}{p^{n+1}} (1 - c^{n+1}) + \frac{\rho^n}{p^n} (1 - c^n) \right) \right) dx \\
= \; & \int_\Omega \left(- \frac{1}{\mathbb{M}} \frac{p^{n+1} - p^n}{\Delta t} + \frac{1}{\mathbb{M}} \frac{1}{2\rho_1} (\rho^{n+1} c^{n+1} + \rho^n c^n) \frac{p^{n+1} - p^n}{\Delta t} \right) dx. \qquad (4.89)
\end{aligned}
$$

Using (4.89) into (4.87), we get

$$\int_\Omega \left(\frac{1}{\mathbb{M}} \frac{1}{\rho_1} c^{n+\frac{1}{2}} p^{n+\frac{1}{2}} \frac{\rho^{n+1}-\rho^n}{\Delta t} + \frac{1}{\mathbb{M}} \frac{1}{\rho_1} p^{n+\frac{1}{2}} \rho^{n+\frac{1}{2}} \frac{c^{n+1}-c^n}{\Delta t} \right.$$
$$+ \frac{1}{\mathbb{M}} \frac{1}{2\rho_1} (\rho^{n+1} c^{n+1} + \rho^n c^n) \frac{p^{n+1}-p^n}{\Delta t}$$
$$+ \frac{N_1\theta}{\mathbb{M}} (1 - c^{n+\frac{1}{2}}) (\ln p)^{n+\frac{1}{2}} \frac{\rho^{n+1}-\rho^n}{\Delta t}$$
$$+ \frac{N_1\theta}{\mathbb{M}} \rho^{n+\frac{1}{2}} (\ln p)^{n+\frac{1}{2}} \frac{c^n - c^{n+1}}{\Delta t}$$
$$+ \frac{N_1\theta}{\mathbb{M}} \frac{p^{n+1}-p^n}{\Delta t} \frac{1}{2} \left(\frac{\rho^{n+1}}{p^{n+1}} (1-c^{n+1}) + \frac{\rho^n}{p^n} (1-c^n) \right)$$
$$\left. - \frac{1}{\mathbb{M}} \frac{p^{n+1}-p^n}{\Delta t} \right) dx. \tag{4.90}$$

If we notice that

$$\int_\Omega \left(\frac{1}{\mathbb{M}} \frac{1}{\rho_1} c^{n+\frac{1}{2}} p^{n+\frac{1}{2}} \frac{\rho^{n+1}-\rho^n}{\Delta t} + \frac{1}{\mathbb{M}} \frac{1}{\rho_1} p^{n+\frac{1}{2}} \rho^{n+\frac{1}{2}} \frac{c^{n+1}-c^n}{\Delta t} \right.$$
$$\left. + \frac{1}{\mathbb{M}} \frac{1}{2\rho_1} (\rho^{n+1} c^{n+1} + \rho^n c^n) \frac{p^{n+1}-p^n}{\Delta t} \right) dx$$
$$= \int_\Omega \frac{1}{\mathbb{M}\Delta t} \frac{1}{\rho_1} (p^{n+1} c^{n+1} \rho^{n+1} - p^n c^n \rho^n) \, dx, \tag{4.91}$$

and

$$\int_\Omega \left(\frac{N_1\theta}{\mathbb{M}} (1 - c^{n+\frac{1}{2}}) (\ln p)^{n+\frac{1}{2}} \frac{\rho^{n+1}-\rho^n}{\Delta t} + \frac{N_1\theta}{\mathbb{M}} \rho^{n+\frac{1}{2}} (\ln p)^{n+\frac{1}{2}} \frac{c^n - c^{n+1}}{\Delta t} \right.$$
$$\left. + \frac{N_1\theta}{\mathbb{M}} \frac{p^{n+1}-p^n}{\Delta t} \frac{1}{2} \left(\frac{\rho^{n+1}}{p^{n+1}} (1-c^{n+1}) + \frac{\rho^n}{p^n} (1-c^n) \right) \right) dx$$
$$= \int_\Omega \frac{1}{\mathbb{M}\Delta t} N_1 \theta ((\ln p)^{n+1} \rho^{n+1} (1-c^{n+1}) - (\ln p)^n \rho^n (1-c^n)) \, dx, \tag{4.92}$$

we can rewrite (4.90) as

$$\int_\Omega \left(\frac{1}{\mathbb{M}\Delta t} \frac{1}{\rho_1} (p^{n+1} c^{n+1} \rho^{n+1} - p^n c^n \rho^n) - \frac{1}{\mathbb{M}\Delta t} (p^{n+1} - p^n) \right.$$
$$\left. + \frac{1}{\mathbb{M}\Delta t} N_1 \theta ((\ln p)^{n+1} \rho^{n+1} (1-c^{n+1}) - (\ln p)^n \rho^n (1-c^n)) \right) dx. \tag{4.93}$$

Using (4.78)-(4.81) and (4.82)-(4.93) into (4.77), we obtain

$$\int_\Omega \left(\frac{1}{\Delta t} \left(\frac{\rho^{n+1}}{2} (\mathbf{u}^{n+1})^2 - \frac{\rho^n}{2} (\mathbf{u}^n)^2 \right) \right.$$
$$\left. + \frac{1}{\Delta t} \left(\frac{1}{\mathbb{M}} \rho^{n+1} g(p^{n+1}, c^{n+1}, \mathbf{q}^{n+1}) - \frac{1}{\mathbb{M}} \rho^n g(p^n, c^n, \mathbf{q}^n) \right) - \frac{1}{\mathbb{M}} \frac{p^{n+1}-p^n}{\Delta t} \right) dx$$
$$= -\frac{1}{\mathbb{P}e\mathbb{M}} \int_\Omega |\nabla \mu^{n+\frac{1}{2}}|^2 \, dx - \frac{2}{\mathbb{R}e} \int_\Omega c^{n+\frac{1}{2}} \left(\mathbf{D}^{n+1} : \mathbf{D}^{n+1} \right) dx, \tag{4.94}$$

that is equivalent to the thesis (4.75). □

4.3 Fully discrete energy consistent DG numerical method.

In this section we propose a fully discretisation of (3.10)-(3.14) based on the results of the previous sections for the semi-discretisations in space and time.

The fully discrete mixed formulation of (3.10)-(3.14) can be written as follows: given initial conditions $(c_h^0, \mathbf{u}_h^0, p_h^0, \mu_h^0, \mathbf{q}_h^0)$, for all $n = 0, 1, ..., N-1$, find

$$(c_h^{n+1}, \mathbf{u}_h^{n+1}, p_h^{n+1}, \mu_h^{n+1}, \mathbf{q}_h^{n+1}) \in \mathbb{V} \times \mathbb{V}_0^2 \times \mathbb{V} \times \mathbb{V} \times \mathbb{V}_{\mathbf{n}}$$

such that

$$\begin{aligned}
0 &= \sum_{T\in\mathscr{T}_h} \int_T \left(\rho_h^{n+\frac{1}{2}} \, (c_h)_{\bar{t}}^{n+1} X + \rho_h^{n+\frac{1}{2}} ((\sqrt{\rho_h}\mathbf{u}_h)^{n+1}) \cdot \nabla c_h^{n+\frac{1}{2}} X \right) dx \\
&\quad - \frac{1}{\mathbb{P}e} \mathcal{A}(\mu_h^{n+\frac{1}{2}}, X) + \int_{\mathcal{E}} F_1(X)\, ds, \qquad (4.95)
\end{aligned}$$

$$\begin{aligned}
0 &= \sum_{T\in\mathscr{T}_h} \int_T \Big(\sqrt{\rho_h}^{\,n+\frac{1}{2}} \, (\sqrt{\rho_h}\mathbf{u}_h)_{\bar{t}}^{n+1} \cdot \boldsymbol{\xi} \\
&\quad + \rho_h^{n+\frac{1}{2}} \left((\sqrt{\rho_h}\mathbf{u}_h)^{n+1} \cdot \nabla \right) (\sqrt{\rho_h}\mathbf{u}_h)^{n+1} \cdot \boldsymbol{\xi} \\
&\quad + \frac{1}{2} \operatorname{div}(\rho_h^{n+\frac{1}{2}} (\sqrt{\rho_h}\mathbf{u}_h)^{n+1}) (\sqrt{\rho_h}\mathbf{u}_h)^{n+1} \cdot \boldsymbol{\xi} + \frac{1}{\mathbb{M}} \nabla p_h^{n+\frac{1}{2}} \cdot \boldsymbol{\xi} \\
&\quad - \frac{1}{\mathbb{M}} \rho_h^{n+\frac{1}{2}} \mu_h^{n+\frac{1}{2}} \nabla c_h^{n+\frac{1}{2}} \cdot \boldsymbol{\xi} + \frac{1}{\mathbb{M}} \frac{1}{\rho_1} \rho_h^{n+\frac{1}{2},*} p_h^{n+\frac{1}{2}} \nabla c_h^{n+\frac{1}{2}} \cdot \boldsymbol{\xi} \\
&\quad - \frac{1}{\mathbb{M}} N_1 \theta \rho_h^{n+\frac{1}{2},*} (\ln p_h)^{n+\frac{1}{2}} \nabla c_h^{n+\frac{1}{2}} \cdot \boldsymbol{\xi} - \frac{1}{\mathbb{M}} K \rho_h^{n+\frac{1}{2},*} \nabla c_h^{n+\frac{1}{2}} \cdot \boldsymbol{\xi} \\
&\quad + \frac{\mathbb{C}}{4\mathbb{M}} \rho_h^{n+\frac{1}{2},*} \nabla \left(\mathbf{q}_h^{n+1} \cdot \mathbf{q}_h^{n+1} + \mathbf{q}_h^{n} \cdot \mathbf{q}_h^{n} \right) \cdot \boldsymbol{\xi} \\
&\quad + \frac{1}{2\,\mathbb{M}} \rho_h^{n+\frac{1}{2},*} \nabla \left(g_1(c_h^{n+1}) + g_1(c_h^{n}) \right) \cdot \boldsymbol{\xi} \Big) \, dx \\
&\quad - \frac{2}{\mathbb{R}e} \mathcal{B}(c_h^{n+\frac{1}{2}}, (\sqrt{\rho_h}\mathbf{u}_h)^{n+1}, \boldsymbol{\xi}) + \int_{\mathcal{E}} F_2(\boldsymbol{\xi})\, ds, \qquad (4.96)
\end{aligned}$$

$$0 = \sum_{T\in\mathscr{T}_h} \int_T \left((\rho_h)_{\bar{t}}^{n+1} Z + \operatorname{div}\left(\rho_h^{n+\frac{1}{2},*} (\sqrt{\rho_h}\mathbf{u}_h)^{n+1} \right) Z \right) dx + \int_{\mathcal{E}} F_3(Z)\, ds, \qquad (4.97)$$

$$
\begin{aligned}
0 \;=\;& \sum_{T\in\mathscr{T}_h}\int_T \Bigg(\rho_h^{n+\frac{1}{2}}\mu_h^{n+\frac{1}{2}}\psi - \rho_h^{n+\frac{1}{2}}\frac{g_1(c_h^{n+1})-g_1(c_h^n)}{c_h^{n+1}-c_h^n}\psi - \frac{p_h^{n+\frac{1}{2}}}{\rho_1}\rho_h^{n+\frac{1}{2}}\psi \\
&\qquad + N_1\theta\rho_h^{n+\frac{1}{2}}\left(\ln p_h\right)^{n+\frac{1}{2}}\psi + \mathbb{C}\,\mathrm{div}\left(\rho_h^{n+\frac{1}{2}}\,\mathbf{q}_h^{n+\frac{1}{2}}\right)\psi + K\rho_h^{n+\frac{1}{2}}\psi\Bigg)\,dx \\
&+\int_{\mathcal{E}} F_4(\psi)\,ds, && (4.98)\\
0 \;=\;& \sum_{T\in\mathscr{T}_h}\int_T\left(\mathbf{q}_h^{n+\frac{1}{2}}\cdot\mathbf{T}-\nabla c_h^{n+\frac{1}{2}}\cdot\mathbf{T}\right)dx+\int_{\mathcal{E}}F_5(\mathbf{T})\,ds, && (4.99)
\end{aligned}
$$

$$
\forall\,(X,\boldsymbol{\xi},Z,\psi,\mathbf{T})\in\mathbb{V}\times\mathbb{V}_0^2\times\mathbb{V}\times\mathbb{V}\times\mathbb{V}_{\mathbf{n}},
$$

and

$$
\begin{aligned}
F_1(X) \;=\;& 0, && (4.100)\\
F_2(\boldsymbol{\xi}) \;=\;& -\frac{1}{2}\left[\!\left[\rho_h^{n+\frac{1}{2}}(\sqrt{\rho_h}\mathbf{u}_h)^{n+1}\right]\!\right]\left\{\!\!\left\{(\sqrt{\rho_h}\mathbf{u}_h)^{n+1}\cdot\boldsymbol{\xi}\right\}\!\!\right\}\\
&-\left(\{\!\{\boldsymbol{\xi}\}\!\}\otimes\left\{\!\!\left\{\rho_h^{n+\frac{1}{2}}(\sqrt{\rho_h}\mathbf{u}_h)^{n+1}\right\}\!\!\right\}\right):\left[\!\left[(\sqrt{\rho_h}\mathbf{u}_h)^{n+1}\right]\!\right]_{\otimes}\\
&-\frac{1}{2\mathbb{M}}\left[\!\left[g_1(c_h^{n+1})+g_1(c_h^n)\right]\!\right]\cdot\left\{\!\!\left\{\rho_h^{n+\frac{1}{2},*}\boldsymbol{\xi}\right\}\!\!\right\}\\
&-\frac{\mathbb{C}}{4\mathbb{M}}\left[\!\left[\mathbf{q}_h^{n+1}\cdot\mathbf{q}_h^{n+1}+\mathbf{q}_h^{n}\cdot\mathbf{q}_h^{n}\right]\!\right]\cdot\left\{\!\!\left\{\rho_h^{n+\frac{1}{2},*}\boldsymbol{\xi}\right\}\!\!\right\}\\
&-\frac{1}{\mathbb{M}}\left[\!\left[K(1-c_h^{n+\frac{1}{2}})\right]\!\right]\cdot\left\{\!\!\left\{\rho_h^{n+\frac{1}{2},*}\boldsymbol{\xi}\right\}\!\!\right\}-\frac{1}{\mathbb{M}}\frac{1}{\rho_1}\left[\!\left[c_h^{n+\frac{1}{2}}p_h^{n+\frac{1}{2}}\right]\!\right]\cdot\left\{\!\!\left\{\rho_h^{n+\frac{1}{2},*}\boldsymbol{\xi}\right\}\!\!\right\}\\
&-\frac{N_1\theta}{\mathbb{M}}\left[\!\left[(1-c_h^{n+\frac{1}{2}})(\ln p_h)^{n+\frac{1}{2}}\right]\!\right]\cdot\left\{\!\!\left\{\rho_h^{n+\frac{1}{2},*}\boldsymbol{\xi}\right\}\!\!\right\}, && (4.101)\\
F_3(Z) \;=\;& -\left[\!\!\left[\rho_h^{n+\frac{1}{2},*}(\sqrt{\rho_h}\mathbf{u}_h)^{n+1}\right]\!\!\right]\{\!\{Z\}\!\}, && (4.102)\\
F_4(\psi) \;=\;& -\mathbb{C}\left[\!\left[\rho_h^{n+\frac{1}{2}}\mathbf{q}_h^{n+\frac{1}{2}}\right]\!\right]\{\!\{\psi\}\!\}, && (4.103)\\
F_5(\mathbf{T}) \;=\;& \left[\!\!\left[c_h^{n+\frac{1}{2}}\right]\!\!\right]\cdot\{\!\{\mathbf{T}\}\!\}. && (4.104)
\end{aligned}
$$

Now, we can state mass conservation property and energy dissipation law for the fully discrete scheme for MF system. The proofs of these results follow from the combination of the corresponding propositions in the spatial (Theorems 4.2, 4.3) and time (Theorems 4.6, 4.7) approximation.

Theorem 4.8 (Fully discrete conservation of mass) *The fully discrete scheme (4.95)-(4.99) is mass-conservative, i.e.*

$$
\sum_{T\in\mathscr{T}_h}\int_T\rho_h^{n+1}\,dx=\sum_{T\in\mathscr{T}_h}\int_T\rho_h^{n}\,dx,\qquad \textit{for all } n=0,1,...,N-1. \tag{4.105}
$$

Proof. The proof follows from the results proposed by Theorems 4.2 and 4.6 which provide a spatial and a time-semidiscrete mass conservation result, respectively. □

Theorem 4.9 (Fully discrete energy dissipation law) *Let*

$$E_h^n := \sum_{T\in\mathscr{T}_h} \int_T \left(\frac{\rho_h^n}{2}|\mathbf{u}_h^n|^2 + \frac{1}{\mathbb{M}}\rho_h^n g(p_h^n, c_h^n, \mathbf{q}_h^n) - \frac{1}{\mathbb{M}} p_h^n \right) dx \tag{4.106}$$

be the fully discrete version of the total energy (3.23), for $n = 0, 1, ..., N$*. If* $(c_h^{n+1},\ \mathbf{u}_h^{n+1},\ p_h^{n+1}, \mu_h^{n+1}, \mathbf{q}_h^{n+1})$ *is a solution of the fully discrete system (4.95)-(4.99), then*

$$(E_h)_{\bar{t}}^{n+1} \quad = \quad \frac{1}{\mathbb{P}e\mathbb{M}}\mathcal{A}(\mu_h^{n+\frac{1}{2}}, \mu_h^{n+\frac{1}{2}}) + \frac{2}{\mathbb{R}e}\mathcal{B}(c_h^{n+\frac{1}{2}}, (\sqrt{\rho_h}\mathbf{u}_h)^{n+1}, (\sqrt{\rho_h}\mathbf{u}_h)^{n+1}), \tag{4.107}$$

for all $n = 0, 1, ..., N-1$*, where*

$$(E_h)_{\bar{t}}^{n+1} := \frac{E_h^{n+1} - E_h^n}{\Delta t}$$

and $\mathcal{A}, \mathcal{B}$ *are negative definite, by definition.*

Proof. The proof consists in the application of the results proposed by Theorems 4.3 and 4.7 which provide a spatial and a time-semidiscrete energy dissipation law, respectively. □

5 Conclusions and Perspectives.

In this paper we proposed a thermodynamically consistent phase-field model for a liquid-gas mixture that might also provide a description of the expansion stage of a metal foam inside a hollow mold within the so-called "Powder Line". The mixture was studied as a two-phase incompressible-compressible fluid governed by a Navier-Stokes-Cahn-Hilliard system of equations (IC-NSCH). In particular, to take into account the expansion of the gaseous phase, we adapted the so-called Lowengrub-Truskinowsky model. Moreover, we introduced a Discontinuous Galerkin based numerical approximation of the resulting system of equations. We proved that our numerical scheme, at the discrete level, preserves the mass conservation property and the energy dissipation law characterizing the original system. A numerical assessment of the presented method will be the object of a future pubblication.

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