

Incompressible Fluid Mixtures of Ionized Constituents

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Abstract. A model of a fluid mixture of incompressible chemically reacting charged constituents in Prigogine's description (i.e. balancing the barycentric momentum but not momenta of particular constituents) is presented. Under the volume-additivity hypothesis, incompressibility of all constituents, and some other simplifying assumptions, the model combines the Navier-Stokes equation together with the Nernst-Planck equation with advection for the concentrations of the particular mutually reacting constituents, the heat equation, and finally the Poisson equation for the self-induced quasistatic electric field. The isothermal variant is analyzed by Galerkin's method.

1 Introduction

Various complicated processes in biology on a (sub-)cellular level can use a framework of chemically reacting mixtures of ionic constituents, cf. [6,8]. Although theory of mixtures has undergone an intensive scrutiny during many decades, there is still no description that would be thermodynamically undoubtless, practically implementable as far as data accessibility concerns, and mathematically justified at least as far as mere existence of a weak solution concerns (although the last requirement is often over-ambitious).

Two mainstreams in the theory of mixtures can be distinguished. First, a so-called Truesdell's description balances momenta for each constituent separately. Proposed in Truesdell et al. [22,23], it has been further developed in particular in [2,5,9-11,13,14,17-19,21]. It exhibits great rigor (although its thermodynamics is also not entirely complete) and suppresses phenomenology to minimum but involves, in concrete problems usually unknown, interaction terms between the particular constituents and richer investigations can be done rather in two-component mixtures only, cf. [2,9] and [13, Chapter 7]. The second mainstream, called Prigogine's [12] concept, balances the momentum of barycenter only and postulates phenomenological fluxes of particular constituents. Introducing such a phenomenology allows for a better applicability but exhibits difficulties with a definition of an entropy that would satisfy the Clausius-Duhem inequality. In the compressible case, this barycentric concept has been developed among others in [1,3,4,7].

The model suggested here compromises the thermodynamical rigor with mathematical amenability with the aim to provide as much thermodynamical consistency as possible and simultaneously to allow for rigorous mathematical analysis at least in important special cases and for expectedly easy computational implementation, and also to keep a high complexity of the model which would not restrict desirable biological applications. This led to a choice of *Prigogine's description* in the *incompressible Newtonian framework*. The incompressibility refers here both to each particular constituent and, through volume-additivity hypothesis as in e.g. [9,14], also to the overall mixture. This incompressibility is definitely a simplifying assumption to be subjected to a discussion because it brings "traditional" difficulties in the Clausius-Duhem inequality as well as in the definition of the electrochemical potential but, on the other hand, it just allows for a relatively simple mathematical/numerical treatment. Substantial feature is that the self-induced electrostatic field is

considered and the electro-neutrality hypothesis is not assumed. This hypothesis is indeed not realistic in certain biological applications: the electrostatic potential of each cell is of the order 100 mV while thickness of its membrane is of the order 10 nm, which obviously leads to a tremendous intensity of the electric field (of the order 10 MV/m) on each cell membrane, i.e. e.g. in each ionic channel, although intensities inside fluidic media occurring in biological systems are certainly smaller. However, many simplifications are adopted in the presented model, too. In particular, we consider small electric currents (i.e. magnetic field is neglected), adopt the mentioned volume-additivity assumption, assume the diffusion fluxes independent of other constituent's gradients (cross-effects are neglected) as well as of the temperature gradient (i.e. Soret's effect is neglected) and (in agreement with Onsager's reciprocity principle) also the heat flux independent of the concentration gradients (i.e. Dufour's effect is neglected), and finally the diffusion and mobility coefficients and mass densities that are the same for each constituents. This contribution, beside reviewing (and slightly expanding) the main results from [16], proposes the Galerkin approximation of the isothermal case that is conceptually amenable for computer implementation.

2 Formulation of an Anisothermal Model

Although biological processes on cellular and sub-cellular level can well be considered as isothermal (i.e. temperature is only a constant given parameter), for theoretical reason it is worth formulating the model anisothermally. We consider a mixture of L constituents occupying a bounded fixed domain $\Omega \subset \mathbb{R}^3$ with a boundary $\Gamma := \partial\Omega$. Our model consists of a system of $3 + L + 2$ differential equations combining the Navier-Stokes system (1a), the Nernst-Planck equation generalized for moving media (1b), the Poisson equation (1c), and the heat equation (1d):

$$\rho \frac{\partial v}{\partial t} + \rho(v \cdot \nabla)v - \operatorname{div}(\nu(c, \theta)\nabla v) + \nabla p = -q\nabla\phi, \quad \operatorname{div}(v) = 0, \quad c = (c_1, \dots, c_L), \quad (1a)$$

$$\frac{\partial c_\ell}{\partial t} + \operatorname{div}(j_\ell + c_\ell v) = r_\ell(c, \theta), \quad j_\ell = -d(c, \theta)\nabla c_\ell - m(c, \theta)c_\ell e_\ell \nabla\phi + m(c, \theta)c_\ell f_R, \quad (1b)$$

$$\varepsilon \Delta\phi = -q, \quad q = \sum_{\ell=1}^L e_\ell c_\ell, \quad (1c)$$

$$c_v \frac{\partial \theta}{\partial t} - \operatorname{div}(\kappa \nabla \theta + c_v v \theta) = \nu(c, \theta)|\nabla v|^2 + \sum_{\ell=1}^L (f_\ell \cdot j_\ell - h_\ell(\theta)r_\ell(c, \theta)), \quad f_\ell = -e_\ell \nabla\phi, \quad (1d)$$

where $\ell = 1, \dots, L$ in (1b) and where “ \cdot ” means the scalar product between vectors. The meaning of the variables is:

v barycentric velocity,

p pressure,

c_ℓ concentration of ℓ^{th} -constituent, presumably to satisfy $\sum_{\ell=1}^L c_\ell = 1$, $c_\ell \geq 0$,

ϕ electrostatic potential,

θ temperature,

q the total electric charge.

The data are: $\rho > 0$ mass density both of the mixture and of the constituents, i.e. ρ does not depend on $c = (c_1, \dots, c_L)$, further $\nu(c, \theta) > 0$ denotes the viscosity of the mixture, e_ℓ valence (i.e. electric charge) of ℓ^{th} -constituent, $\varepsilon > 0$ permittivity, $r_\ell(c, \theta)$ production rate of the ℓ^{th} -constituent by chemical reactions, $h_\ell(\theta)$ the enthalpy contained in the ℓ^{th} -constituent,

$f_\ell = -e_\ell \nabla \phi$ body force acting on ℓ^{th} -constituent, j_ℓ phenomenological flux of ℓ^{th} -constituent given in (1b), $d(c, \theta)$, $m(c, \theta) > 0$ diffusion and mobility coefficients, respectively, $c_v > 0$ specific heat (within constant volume), $\kappa > 0$ heat conductivity. A bit speculative force f_R acting equally on each constituent is to hold the *volume-additivity* constraint

$$\sum_{\ell=1}^L c_\ell = 1, \quad (2)$$

assuming naturally that also the initial and boundary conditions (6)–(7) below satisfy it, cf. the assumption (20d). In view of (2) and the constraint $c_\ell \geq 0$, the variables $c = (c_1, \dots, c_L)$ can also be called *volume fractions*; as all constituents are assumed incompressible, c_ℓ 's are simultaneously mass fractions. Summing (1b) for $\ell = 1, \dots, L$ and using (8) below, one gets $\frac{\partial}{\partial t} \sigma + v \cdot \nabla \sigma = -\text{div} \sum_{\ell=1}^L j_\ell$ with $\sigma := \sum_{\ell=1}^L c_\ell$, hence the key to hold σ constant as required in (2) is to ensure that the sum of diffusive fluxes vanishes, i.e.,

$$\sum_{\ell=1}^L j_\ell = 0. \quad (3)$$

Now we can postulate the force f_R as a *reaction force* holding (3), which (assuming (2) for a moment), gives

$$\sum_{\ell=1}^L j_\ell = m(c, \theta) \sum_{\ell=1}^L c_\ell f_R - m(c, \theta) \left(\sum_{\ell=1}^L c_\ell e_\ell \right) \nabla \phi - d(c, \theta) \nabla \left(\sum_{\ell=1}^L c_\ell \right) = m(c, \theta) (f_R - q \nabla \phi), \quad (4)$$

hence, if (3) is to be satisfied, we obtain

$$f_R = q \nabla \phi. \quad (5)$$

Usually, f_R is small because $|q|$ is much smaller in comparison with $\max_{\ell=1, \dots, L} |e_\ell|$. Some other models postulate even the electro-neutrality assumption $q = 0$, which obviously makes this reaction force zero. Let us also remark that, in very diluted water solutions of salts, an alternative option is to consider velocity of water as the referential velocity instead of the barycentric one as used here. This is sometimes called Hittorf's referential system. Then, assuming again that diffusivity and mobility coefficients do not depend on a particular constituent and after suitable simplification relying on small concentrations of non-water constituents, the “reaction force” $f_R = q \nabla \phi$ arises simply by transformation from the Hittorf's system to the barycentric one; see [17,20].

Eventually, the initial conditions are assumed:

$$v(0, \cdot) = v_0, \quad c_\ell(0, \cdot) = c_{0\ell}, \quad \theta(0, \cdot) = \theta_0 \quad \text{on } \Omega. \quad (6)$$

We have still to consider some boundary conditions, e.g. a closed thermally isolated container which in some simplified version leads, for a.a. $t \geq 0$, to:

$$v = 0, \quad c_\ell = c_\ell^\Gamma, \quad \varepsilon \frac{\partial \phi}{\partial n} = \alpha (\phi_\Gamma - \phi), \quad \frac{\partial \theta}{\partial n} = 0 \quad \text{on } \Gamma, \quad (7)$$

where n denotes the unit outward normal to the boundary Γ and the coefficient $\alpha > 0$ can be interpreted as a “surface permittivity” of the boundary and ϕ_Γ is an outer potential. Yet, more sophisticated conditions are definitely to be used for nontrivial biological applications in cell biology.

3 Discussion of the Model and Its Thermodynamics

Derivation of the model is briefly motivated as follows: The *Navier-Stokes equation* (1a) is based on Hamilton's dissipation principle generalized for dissipative systems, cf. [5]; the body force $q\nabla\phi = \sum_{\ell=1}^L f_\ell$ is due to the electrostatic interaction of the charge e_ℓ when assuming that the velocities of particles and the rate of the electric field are small so that the magnetic effects are negligible, as it is certainly the case in usual applications in biology. The equation (1b) balances concentration of the particular constituents as usual in the *Nernst-Planck equation* but here completed *with the advection* term $\text{div}(c_\ell v)$ related with moving medium in Eulerian coordinates, while (1c) is the rest from the full electro-magnetical Maxwell's system which remains if assuming relatively slow movements of electric charges and small electric currents which do not create any fast variation of electric fields and any substantial magnetic field, and eventually (1d) is the usual *heat equation* balancing energy again in a moving medium in Eulerian coordinates, see e.g. [1,7]. The volume-additivity assumption (2) is often accepted in the theory of mixtures, although it should be emphasized that it is only a certain approximation of reality; cf. the discussion in [13, Sect. 2.8].

To show conservation of the total energy, we naturally assume the mass and electric charge conservation in all chemical reactions and nonnegative production of the ℓ^{th} -constituent if its concentration vanishes, i.e.,

$$\sum_{\ell=1}^L r_\ell(c, \theta) = 0, \quad \sum_{\ell=1}^L e_\ell r_\ell(c, \theta) = 0, \quad r_\ell(c_1, \dots, c_{\ell-1}, 0, c_{\ell+1}, \dots, c_L, \theta) \geq 0. \quad (8)$$

Let us first calculate the rate of the electrostatic energy (i.e. its power), using (1c) and (1b) together with the electric-charge-preservation assumption (8) and twice Green's formula counting also with the boundary conditions (7):

$$\begin{aligned} \frac{d}{dt} \left(\int_{\Omega} \frac{\varepsilon}{2} |\nabla\phi|^2 dx + \int_{\Gamma} \frac{\alpha}{2} (\phi - \phi_{\Gamma})^2 dS \right) &= \int_{\Omega} \varepsilon \nabla\phi \cdot \nabla \frac{\partial\phi}{\partial t} dx + \int_{\Gamma} \alpha (\phi - \phi_{\Gamma}) \frac{\partial(\phi - \phi_{\Gamma})}{\partial t} dS \\ &= \int_{\Omega} \varepsilon \nabla\phi \cdot \nabla \frac{\partial\phi}{\partial t} dx - \int_{\Gamma} \varepsilon (\phi - \phi_{\Gamma}) \frac{\partial}{\partial t} \left(\frac{\partial\phi}{\partial n} \right) dS \\ &= - \int_{\Omega} \varepsilon \phi \Delta \frac{\partial\phi}{\partial t} dx + \int_{\Gamma} \varepsilon \phi_{\Gamma} \frac{\partial}{\partial t} \left(\frac{\partial\phi}{\partial n} \right) dS \\ &= \int_{\Omega} \phi \sum_{\ell=1}^L e_\ell \frac{\partial c_\ell}{\partial t} dx + \int_{\Gamma} \varepsilon \phi_{\Gamma} \frac{\partial}{\partial t} \left(\frac{\partial\phi}{\partial n} \right) dS \\ &= \int_{\Omega} \phi \sum_{\ell=1}^L e_\ell \left(r_\ell(c, \theta) - \text{div}(j_\ell + c_\ell v) \right) dx + \int_{\Gamma} \varepsilon \phi_{\Gamma} \frac{\partial}{\partial t} \left(\frac{\partial\phi}{\partial n} \right) dS \\ &= - \int_{\Omega} \phi \sum_{\ell=1}^L e_\ell \text{div}(j_\ell + c_\ell v) dx + \int_{\Gamma} \varepsilon \phi_{\Gamma} \frac{\partial}{\partial t} \left(\frac{\partial\phi}{\partial n} \right) dS \\ &= \int_{\Omega} \nabla\phi \cdot \sum_{\ell=1}^L e_\ell (j_\ell + c_\ell v) dx + \int_{\Gamma} \left(\varepsilon \phi_{\Gamma} \frac{\partial}{\partial t} \left(\frac{\partial\phi}{\partial n} \right) - \phi \sum_{\ell=1}^L e_\ell j_\ell \cdot n \right) dS. \quad (9) \end{aligned}$$

Testing (1a) by v , we obtain the rate of the kinetic energy

$$\begin{aligned} \frac{d}{dt} \int_{\Omega} \varrho \frac{|v|^2}{2} dx &= \int_{\Omega} \sum_{\ell=1}^L c_{\ell} (f_{\ell} \cdot v) - \varrho ((v \cdot \nabla)v) \cdot v - \nu(c, \theta) |\nabla v|^2 dx \\ &= - \int_{\Omega} \nu(c, \theta) |\nabla v|^2 + \sum_{\ell=1}^L c_{\ell} e_{\ell} \nabla \phi \cdot v dx. \end{aligned} \quad (10)$$

The rate of the thermal part of the internal energy can be obtained simply by integration of (1d) over Ω and using Green's theorem with the considered boundary conditions $\partial\theta/\partial n = 0$:

$$\frac{d}{dt} \int_{\Omega} c_v \theta dx = \int_{\Omega} \nu(c, \theta) |\nabla v|^2 - \sum_{\ell=1}^L \left(e_{\ell} j_{\ell} \cdot \nabla \phi + h_{\ell}(\theta) r_{\ell}(c, \theta) \right) dx. \quad (11)$$

Altogether, summing (9)–(11) and using also (1b) integrated over Ω and Green's formula, we obtain the following balance:

$$\begin{aligned} \frac{d}{dt} \left(\int_{\Omega} \left(\frac{\varrho}{2} |v|^2 + \frac{\varepsilon}{2} |\nabla \phi|^2 + c_v \theta \right) dx + \int_{\Gamma} \frac{\alpha}{2} (\phi - \phi_{\Gamma})^2 dS \right) \\ = - \int_{\Omega} \sum_{\ell=1}^L h_{\ell}(\theta) r_{\ell}(c, \theta) dx + \int_{\Gamma} \left(\varepsilon \phi_{\Gamma} \frac{\partial}{\partial t} \left(\frac{\partial \phi}{\partial n} \right) - \phi \sum_{\ell=1}^L e_{\ell} j_{\ell} \cdot n \right) dS \end{aligned} \quad (12)$$

where we used the boundary conditions (7). Hence, (12) just says that the total energy rate, i.e. the rate of the sum of the kinetic, the electrostatic, and the internal energies $\frac{1}{2}\varrho|v|^2 + \frac{1}{2}\varepsilon|\nabla\phi|^2 + c_v\theta$ over Ω and the electrostatic energy $\frac{1}{2}\alpha(\phi - \phi_{\Gamma})^2$ deposited on Γ is balanced with the enthalpy production rate $\sum_{\ell=1}^L h_{\ell}r_{\ell}$ over Ω and the flux of an electro-energy through the boundary Γ (i.e. power of the outer voltage ϕ_{Γ}).

Another interesting observation is how the *heat sources* in (1d) look like. When substituting f_{ℓ} and j_{ℓ} from (1a)–(1b), the right-hand side of (1d) equals

$$\begin{aligned} f(v, c, \phi, \theta) &:= \nu(c, \theta) |\nabla v|^2 + d(c, \theta) \nabla q \cdot \nabla \phi \\ &+ \sum_{\ell=1}^L m(c, \theta) c_{\ell} e_{\ell}^2 |\nabla \phi|^2 - m(c, \theta) q^2 |\nabla \phi|^2 - \sum_{\ell=1}^L h_{\ell}(\theta) r_{\ell}(c, \theta). \end{aligned} \quad (13)$$

The first term in (13) represents the heat production due to a loss of kinetic energy by viscosity. The second one is the power (per unit volume) of the electric current arising by the diffusion flux, which can create local cooling effects as well as a global cooling effect seems possible via interaction with the environment if $\alpha \neq 0$, expectedly related with the so-called *Peltier effect*. In some special occasions, namely d constant and $\alpha = 0$, one can even see an interesting phenomenon, namely that the overall production due to this term over Ω is nonnegative: indeed, by using Green's formula twice, we get

$$\begin{aligned} \int_{\Omega} d \nabla q \cdot \nabla \phi dx &= \varepsilon \int_{\Omega} -d \nabla(\Delta \phi) \cdot \nabla \phi dx \\ &= \varepsilon \int_{\Omega} d |\Delta \phi|^2 dx - \varepsilon \int_{\Gamma} d \Delta \phi \frac{\partial \phi}{\partial n} dS \geq \int_{\Gamma} dq \alpha (\phi_{\Gamma} - \phi) dS = 0. \end{aligned} \quad (14)$$

The third term in (13) is the power of *Joule's heat* produced by the electric currents j_{ℓ} . The fourth term is the rate of cooling by the force which balances the volume-additivity

constraint, and its influence is presumably very small as usually $|q| \ll \max_{\ell=1,\dots,L} |e_\ell|$. Besides, Joule's heat always dominates this cooling effect because $\sum_{\ell=1}^L c_\ell e_\ell^2 \geq (\sum_{\ell=1}^L c_\ell e_\ell)^2$ if $\sum_{\ell=1}^L c_\ell = 1$ and all c_ℓ 's are non-negative, cf. [16, Remark 2.2]. The last term in (13) is the heat produced or consumed by chemical reactions.

The specific *entropy* s is then defined by the Gibbs' relation $s := -\partial\psi/\partial\theta$ and, when we define standardly the specific Helmholtz' *free energy* $\psi(v, \phi, c, \theta) = \frac{1}{2}\varepsilon|\nabla\phi|^2 - c_v\theta\ln(\theta)$, we come to $s = c_v(1 + \ln(\theta))$. The *internal energy* is then $e := \psi + \theta s = c_v\theta + \frac{1}{2}\varepsilon|\nabla\phi|^2$. The requirement of preservation of total energy (i.e. the sum of the kinetic and the internal ones) leads to the energy balance

$$\theta \left[\frac{\partial}{\partial t} + v \cdot \nabla \right] (s) + \operatorname{div} j = f \quad (15)$$

where the heat flux j is subjected to Fourier's law $j = -\kappa\nabla\theta$ and $f = f(v, c, \phi, \theta)$ is the dissipation rate identified in (13); note that (15) is just (1d). Formally, the non-negativity of θ can be ensured by a physically (not mathematically!) acceptable requirement $\lim_{\theta \rightarrow 0^+} d(c, \theta) = 0$ and $\lim_{\theta \rightarrow 0^+} r_\ell(c, \theta) = 0$. Another physically natural assumption is $\sum_{\ell=1}^L h_\ell(\theta) r_\ell(c, \theta)/\theta \geq 0$, i.e. the chemical-reaction rates do not to consume entropy. Then, if even $\theta > 0$, one could claim the *Clausius-Duhem inequality*

$$\frac{d}{dt} \int_{\Omega} s \, dx = \int_{\Omega} \left(\frac{f(v, c, \phi, \theta)}{\theta} + \operatorname{div} \left(\frac{\kappa\nabla\theta}{\theta} \right) + \kappa \frac{|\nabla\theta|^2}{\theta^2} \right) dx \geq 0 \quad (16)$$

if one would prove still non-negativity of the ‘‘Peltier-effect’’ term $\int_{\Omega} \nabla q \cdot \nabla\phi/\theta \, dx$; let us note that $\int_{\Omega} \operatorname{div}(\kappa\nabla\theta/\theta) \, dx = -\int_{\Gamma} \kappa\theta^{-1}\partial\theta/\partial n \, dS = 0$ due to the isolation on the boundary (7). The mentioned non-negativity of the Peltier-like term is, however, not obvious. On the other hand, as the electro-neutrality deviation (i.e. the overall charge q) is usually small, the violation of the entropy balance is presumably also small, if any at all, and may be related with the idealization of the incompressibility of all constituents and volume-additivity of the mixture; note that this term is just to hold the volume-additivity (4). In addition, in isolated and spatially isothermal systems (which is well satisfied in living biological systems on cellular level), the Clausius-Duhem inequality is satisfied due to the calculations (14).

4 Analysis of the Isothermal Case by Galerkin's Method

The mere existence of a weak solution of the full model (1a)–(1d) with (5) and with the initial/boundary conditions (6)–(7), likely needed regularity of Navier-Stokes system in the 3-dimensional case, seems to be difficult. A special ‘‘laminar’’ case (i.e. with the convective term $\varrho(v \cdot \nabla v)v$ in (1a) neglected) has been treated in [16] for ν , d and m constant and Ω smooth. The generalization for d and m continuously dependent on (c, θ) as considered here would be a relatively simple modification, contrary to ν whose constancy makes possible to employ regularity results for the 3D Stokes problem, as used in [16].

Here we focus on another special case, namely the ‘‘isothermal’’ one, i.e. θ constant and fixed, and (1d) neglected. It should be emphasized that in biological application on a (sub)cellular level, the simplifying assumption of a constant temperature is very well acceptable. This has been treated in [16] for ν , d and m constant by the Schauder fixed-point theorem. Here we outline this isothermal case allowing, in addition, for ν , d and m continuously dependent on the volume fractions $c = (c_1, \dots, c_L)$ by using the Galerkin method, which constructively suggests numerical implementation at least on a conceptual

level, i.e. neglected numerical integration that would be desirable to implement the scheme (18a)–(18c) below.

Let, for simplicity, Ω be polyhedral and discretized by a nested sequence of simplectic triangulations \mathcal{T}_h , $h > 0$ being a mesh parameter, and let $V_h := \{v \in W^{1,2}(\Omega); \forall S \in \mathcal{T}_h : v|_S \text{ affine}\}$. Let us agree to extend, if need be, the nonlinearities ν , d , m , and r_ℓ on the whole affine manifold $\mathcal{M} := \{\xi \in \mathbb{R}^L; \sum_{\ell=1}^L \xi_\ell = 1\}$, although eventually only their values for non-negative arguments will matter. We define a retract $K : \mathcal{M} \rightarrow \{\xi \in \mathcal{M} : \xi_\ell \geq 0, \ell = 1, \dots, L\}$ by

$$K_\ell(\xi) := \xi_\ell^+ / \left(\sum_{l=1}^L \xi_l^+ \right), \quad \xi_\ell^+ := \max(\xi_\ell, 0). \quad (17)$$

Note that K is continuous and bounded. We consider a fixed finite time horizon $T > 0$, and define the Galerkin approximate solution (v_h, ϕ_h, c_h) such that $[(v_h, \phi_h, c_h)](t, \cdot) \in V_h^3 \times V_h \times V_h^L$ for a.a. $t \in [0, T]$, $v_h(0, \cdot) = v_0$, $c_h(0, \cdot) = c_0$, $\operatorname{div} v_h = 0$, $c_h|_\Gamma(t, \cdot) = c_\ell^T$, and the following identities hold for a.a. $t \in [0, T]$:

$$\forall z \in V_h : \quad \int_\Omega \varepsilon \nabla \phi_h \cdot \nabla z - q_h z \, dx = \int_\Gamma \alpha(\phi_\Gamma - \phi_h) z \, dS, \quad q_h = \sum_{\ell=1}^L e_\ell K_\ell(c_h), \quad (18a)$$

$$\forall z \in V_h^3, \operatorname{div} z = 0 : \quad \int_\Omega \varrho \left(\frac{\partial v_h}{\partial t} + (v_h \cdot \nabla) v_h \right) \cdot z + \nu(c_h) \nabla v_h : \nabla z - q_h \nabla \phi_h \cdot z \, dx = 0, \quad (18b)$$

$$\forall z \in V_h, z|_\Gamma = 0 : \quad \int_\Omega \frac{\partial c_{h\ell}}{\partial t} z + (d(c_h) \nabla c_{h\ell} - c_{h\ell} v_h) \cdot \nabla z \, dx = \int_\Omega r_\ell(c_h) z - m(c_h) K_\ell(c_h) (e_\ell - q_h) \nabla \phi_h \cdot \nabla z \, dx, \quad (18c)$$

with $\ell = 1, \dots, L$ in (18c). For further analysis, we define seminorms on the linear spaces $L^{4/3}([0, T]; W_{0,\operatorname{DIV}}^{1,2}(\Omega; \mathbb{R}^3)^*)$ and $L^{4/3}([0, T]; W^{1,2}(\Omega)^*)$ respectively by:

$$|\xi|_{\operatorname{DIV},h} = \sup_{\substack{z(t,\cdot) \in V_h^3 \text{ for a.a. } t \in [0,T] \\ \|z\|_{L^4([0,T]; W_{0,\operatorname{DIV}}^{1,2}(\Omega; \mathbb{R}^3))} \leq 1}} \int_0^T \langle \xi(t, \cdot), z(t, \cdot) \rangle dt, \quad (19a)$$

$$|\xi|_h = \sup_{\substack{z(t,\cdot) \in V_h \text{ for a.a. } t \in [0,T] \\ \|z\|_{L^4([0,T]; W^{1,2}(\Omega))} \leq 1}} \int_0^T \langle \xi(t, \cdot), z(t, \cdot) \rangle dt. \quad (19b)$$

Let us assume

$$\nu, d, m, r_\ell : \mathcal{M} \rightarrow \mathbb{R} \text{ continuous, bounded, nonnegative,} \quad (20a)$$

$$\nu_m := \inf_{c \in \mathcal{M}} \nu(c) > 0, \quad d_m := \inf_{c \in \mathcal{M}} d(c) > 0, \quad (20b)$$

$$\exists h_0 > 0 : \quad v_0 \in V_{h_0}^3, \quad c_0 \in V_{h_0}^L, \quad c^T(t, \cdot) \in V_{h_0}^L|_\Gamma \text{ for a.a. } t \in [0, T], \quad (20c)$$

$$\sum_{\ell=1}^L c_{0\ell} = 1, \quad c_{0\ell} \geq 0, \quad \sum_{\ell=1}^L c_\ell^T = 1, \quad c_\ell^T \geq 0. \quad (20d)$$

Lemma 1. *Let (8), and (20a)–(20d) hold. The equations (18a)–(18c) have a solution (v_h, ϕ_h, c_h) which satisfies the following a-priori bounds:*

$$\|\phi_h\|_{L^\infty([0,T];W^{1,2}(\Omega))} \leq C, \quad (21a)$$

$$\|v_h\|_{L^2([0,T];W^{1,2}(\Omega;\mathbb{R}^3)) \cap L^\infty([0,T];L^2(\Omega;\mathbb{R}^3))} \leq C, \quad \left| \frac{\partial v_h}{\partial t} \right|_{\text{DIV}, h_0} \leq C, \quad (21b)$$

$$\|c_{h\ell}\|_{L^2([0,T];W^{1,2}(\Omega)) \cap L^\infty([0,T];L^2(\Omega))} \leq C, \quad \left| \frac{\partial c_{h\ell}}{\partial t} \right|_{h_0} \leq C, \quad (21c)$$

with the constant C independent of h and h_0 provided $h \leq h_0$. Besides, c_h satisfies the volume-additivity constraint $\sum_{\ell=1}^L c_{h\ell} = 1$ (but not necessarily $c_{h\ell} \geq 0$).

Sketch of the proof. Existence of the Galerkin's solution is due to standard arguments from ODEs (after elimination of the linear algebraic system arising from (18a) with a regular matrix) with subsequent prolongation due to the L^∞ -estimates derived below.

The important fact is that the constraint $\sum_{\ell=1}^L c_{h\ell} = 1$ is satisfied. To show it, let us abbreviate $\sigma_h(t, \cdot) := \sum_{\ell=1}^L c_{h\ell}(t, \cdot) \in V_h$. By summing (18c) for $\ell = 1, \dots, L$, one gets

$$\begin{aligned} \int_{\Omega} \frac{\partial \sigma_h}{\partial t} z \, dx &= \int_{\Omega} \left(\sum_{\ell=1}^L r_{\ell}(c_h) \right) z - \left(\sum_{\ell=1}^L m(c_h) K_{\ell}(c_h) \left(e_{\ell} - \sum_{l=1}^L e_l K_l(c_h) \right) \right) \nabla \phi_h \\ &\quad + d(c_h) \nabla \sigma_h - v_h \sigma_h \cdot \nabla z \, dx = - \int_{\Omega} d(c_h) \nabla \sigma_h \cdot \nabla z + (v_h \cdot \nabla \sigma_h) z \, dx \end{aligned} \quad (22)$$

for all $z \in V_h$, where (8) has been used.

Thus (22) results in the corresponding Galerkin approximation of the linear equation $\frac{\partial}{\partial t} \sigma_h + v_h \cdot \nabla \sigma_h - \text{div}(d(c_h) \nabla \sigma_h) = 0$. We assumed $\sigma_h|_{t=0} = \sum_{\ell=1}^L c_{0\ell} = 1$ and $\sigma_h|_{\Sigma} = \sum_{\ell=1}^L c_{\ell}^{\Gamma} = 1$ on Σ , cf. (6) and (7) with (20d), so that the unique solution to this equation is $\sigma_h(t, \cdot) \equiv 1$ for any $t > 0$.

As to (21a), it just suffices to test (18a) by ϕ_h itself and to realize that, since we proved $\sum_{\ell=1}^L c_h(t, \cdot) = 1$, it holds $|q_h(t, \cdot)| \leq \max_{\ell=1, \dots, L} |e_{\ell}|$ because then $0 \leq K_{\ell}(\cdot) \leq 1$. The estimate (21b) can be obtained by testing (18b) by v_h itself and using that $\int_{\Omega} (v_h \cdot \nabla) v_h \cdot v_h \, dx = 0$. The second part of (21b) can be obtained by testing (18b) by a suitable z as follows:

$$\begin{aligned} \varrho \left| \frac{\partial v_h}{\partial t} \right|_{\text{DIV}, h_0} &:= \sup_{\substack{z(t, \cdot) \in V_{h_0}^3 \text{ for a.a. } t \in [0, T] \\ \|z\|_{L^4([0, T]; W_{0, \text{DIV}}^{1, 2}(\Omega; \mathbb{R}^3))} \leq 1}} \int_Q \nu(c_h) \nabla v_h \cdot \nabla z + \varrho (v_h \cdot \nabla) v_h \cdot z - q_h \nabla \phi_h \cdot z \, dx dt \\ &\leq \|\nabla v_h\|_{L^2(Q; \mathbb{R}^{3 \times 3})} \left(T^{1/4} \nu_M + \varrho N^{3/2} \|v_h\|_{L^2([0, T]; W^{1, 2}(\Omega; \mathbb{R}^3))}^{1/2} \right) \times \\ &\quad \times \|v_h\|_{L^\infty([0, T]; L^2(\Omega; \mathbb{R}^3))}^{1/2} + 2N \max_{\ell=1, \dots, L} |e_{\ell}| \|\nabla \phi_h\|_{L^{4/3}([0, T]; L^{6/5}(\Omega))} \end{aligned} \quad (23)$$

where $\nu_M := \sup_{c \in \mathcal{M}} \nu(c)$ and $Q := (0, T) \times \Omega$, and where the convective term has been interpolated as

$$\begin{aligned} \int_Q (v_h \cdot \nabla) v_h \cdot z \, dx dt &\leq \|v_h\|_{L^4([0, T]; L^3(\Omega; \mathbb{R}^3))} \|\nabla v_h\|_{L^2(Q; \mathbb{R}^{3 \times 3})} \|z\|_{L^4([0, T]; L^6(\Omega; \mathbb{R}^3))} \\ &\leq \|v_h\|_{L^2([0, T]; L^6(\Omega; \mathbb{R}^3))}^{1/2} \|v_h\|_{L^\infty([0, T]; L^2(\Omega; \mathbb{R}^3))}^{1/2} \|\nabla v_h\|_{L^2(Q; \mathbb{R}^{3 \times 3})} \|z\|_{L^4([0, T]; L^6(\Omega; \mathbb{R}^3))} \end{aligned}$$

and where N denotes the norm of the embedding $W^{1,2}(\Omega) \subset L^6(\Omega)$. Using the already obtained estimate (21a) and the first part of (21b), the second part of (21b) follows.

Now we test (18c) by $c_{h\ell}$ and use Green's formula for both the left-hand and the right-hand sides and the identities

$$\int_{\Omega} \operatorname{div}(c_{h\ell} v_h) c_{h\ell} dx = - \int_{\Omega} c_{h\ell} v_h \cdot \nabla c_{h\ell} dx = - \int_{\Omega} v_h \cdot \frac{\nabla |c_{h\ell}|^2}{2} dx = \int_{\Omega} \operatorname{div}(v_h) \frac{|c_{h\ell}|^2}{2} dx = 0 \quad (24)$$

and, when employing the boundary conditions (7), also

$$\begin{aligned} \int_{\Omega} -\operatorname{div}(m(c_h) K_{\ell}(c_h) (e_{h\ell} - q_h) \nabla \phi_h) c_{h\ell} dx &= \int_{\Omega} (m(c_h) K_{\ell}(c_h) (e_{\ell} - q_h) \nabla \phi_h) \cdot \nabla c_{h\ell} dx \\ &+ \int_{\Gamma} m(c_h) K_{\ell}(c_h) (e_{\ell} - q_h) \alpha(\phi_h - \phi_{\Gamma}) c_{\ell}^{\Gamma} dS. \end{aligned} \quad (25)$$

By this way, denoting $m_M := \sup_{c \in \mathcal{M}} m(c)$ and $r_{\ell, M} := \sup_{c \in \mathcal{M}} r_{\ell}(c)$, we obtain the estimate

$$\begin{aligned} \frac{d}{dt} \|c_{h\ell}\|_{L^2(\Omega)}^2 + d_m \|\nabla c_{h\ell}\|_{L^2(\Omega; \mathbb{R}^3)}^2 &\leq \int_{\Omega} r_{\ell}(c_h) c_{h\ell} - (m(c_h) K_{\ell}(c_h) (e_{\ell} - q_h) \nabla \phi_h) \cdot \nabla c_{h\ell} dx \\ &- \int_{\Gamma} m(c_h) K_{\ell}(c_h) (e_{\ell} - q_h) \alpha(\phi_h - \phi_{\Gamma}) c_{h\ell} dS \\ &\leq |\Omega| r_{\ell, M} + \|c_{\ell}\|_{L^2(\Omega)}^2 + 2 \frac{m_M}{d_m} \max_{l=1, \dots, L} e_l^2 \|\nabla \phi_h\|_{L^2(\Omega; \mathbb{R}^3)}^2 + \frac{d_m}{2} \|\nabla c_{\ell}\|_{L^2(\Omega; \mathbb{R}^3)}^2 \\ &+ 2m_M \alpha \max_{l=1, \dots, L} |e_l| \left(N_1 \|\phi_h(t, \cdot)\|_{W^{1,2}(\Omega)} + N_2 \|\phi_{\Gamma}\|_{W^{1/2,2}(\Gamma)} \right) \end{aligned} \quad (26)$$

where N_1 and N_2 denote the norms of the trace operator $\phi \mapsto \phi|_{\Gamma} : W^{1,2}(\Omega) \rightarrow L^1(\Gamma)$ and the embedding $W^{1/2,2}(\Gamma) \subset L^1(\Gamma)$, respectively. Note that we used a trivial estimate $\|e_{\ell} - q\|_{L^{\infty}(\Omega)} \leq 2 \max_{l=1, \dots, L} |e_l|$. Altogether, the first estimate (21c) follows by Gronwall's inequality. The second estimate in (21c) can be obtained by testing (18c) by a suitable $z \in L^2([0, T]; W^{1,2}(\Omega))$ as follows:

$$\begin{aligned} \left| \frac{\partial c_{h\ell}}{\partial t} \right|_{h_0} &:= \sup_{\substack{z(t, \cdot) \in V_{h_0} \\ \|z\|_{L^4([0, T]; W^{1,2}(\Omega))} \leq 1}} \left(\int_{\Omega} d(c_h) \nabla c_{h\ell} \cdot \nabla z - c_{h\ell} v_h \cdot \nabla z - r_{\ell}(c_h) z \right. \\ &\left. + m(c_h) K_{\ell}(c_h) (e_{\ell} - q_h) \nabla \phi_h \cdot \nabla z dx dt + \int_{\Sigma} m(c_h) \alpha K_{\ell}(c_h) (e_{\ell} - q_h) (\phi_h - \phi_{\Gamma}) z dS dt \right) \\ &\leq C \left(\|\nabla c_{h\ell}\|_{L^2(Q; \mathbb{R}^3)} + \|c_{h\ell}\|_{L^2([0, T]; L^6(\Omega))} \|v_h\|_{L^2([0, T]; L^6(\Omega; \mathbb{R}^3))}^{1/2} \|v_h\|_{L^{\infty}([0, T]; L^2(\Omega; \mathbb{R}^3))}^{1/2} \right. \\ &\quad \left. + \|\nabla \phi_h\|_{L^2(Q; \mathbb{R}^3)} + \|\phi_h - \phi_{\Gamma}\|_{L^2([0, T]; W^{1/2}(\Gamma))} \right) \end{aligned} \quad (27)$$

where $C = C(\Omega, \sup d(\mathcal{M}), m_M, \alpha, \max_{\ell} |e_{\ell}|, T)$ is a constant. Then we use (21b) and the already proved part of (21c). \square

Note that we did not claim that $c_{h\ell} \geq 0$, which indeed is not obvious because the usual test by the negative part $c_{h\ell}^-$ is not legal for (18c) as $c_{h\ell}^-(t, \cdot) \notin V_h$ in general. This is also why we involved the retract K in (18a) and in (18c).

Proposition 1. *Let (8) and (20a)–(20d) hold. Then one can select a subsequence of $\{(v_h, c_h, \phi_h)\}_{h>0}$ converging in the weak* topologies indicated by the a-priori estimates (21a)–(21c) to some (v, c, ϕ) , and each such triple obtained by this way is a (very) weak solution to the isothermal variant of the original system (1a)–(1c) with (5), i.e. considered with θ omitted.*

Sketch of the proof. In view of the a-priori estimates (21a)–(21c), we can select a subsequence converging as claimed. Realizing that our equations are semilinear (i.e. linear in terms of all derivatives) and using the Aubin-Lions compact-embedding lemma (modified for a locally-convex topologies induced by the seminorms (19a)–(19b) as in [15]), one can easily deduce the convergence to a very weak solution to the isothermal variant of the system (1a)–(1c) with (5) and with the retract K occurring at the respective spots, namely:

$$\varrho \frac{\partial v}{\partial t} + \varrho(v \cdot \nabla)v - \operatorname{div}(\nu(c)\nabla v) + \nabla p = -\hat{q}\nabla\phi, \quad \operatorname{div}(v) = 0, \quad (28a)$$

$$\frac{\partial c_\ell}{\partial t} - \operatorname{div}\left(d(c)\nabla c_\ell + m(c)K_\ell(c)(e_\ell - \hat{q})\nabla\phi - c_\ell v\right) = r_\ell(c), \quad \ell = 1, \dots, L, \quad (28b)$$

$$\varepsilon\Delta\phi = -\hat{q}, \quad \hat{q} = \sum_{\ell=1}^L e_\ell K_\ell(c)\nabla\phi, \quad (28c)$$

completed naturally by the respective initial and boundary conditions (6)–(7). The adjective “very weak” refers to the fact that $\frac{\partial}{\partial t}c_\ell$ and $\frac{\partial}{\partial t}v$ is not in any duality with c_ℓ and v , respectively.

The constraint $\sum_{\ell=1}^L c_\ell = 1$ is inherited from (22) for $h \rightarrow 0+$, and now, at this limit point, we have additionally also $c_\ell(t, \cdot) \geq 0$ satisfied for any t . To see this, test (28b) by the negative part c_ℓ^- of c_ℓ . Realizing $K_\ell(c)\nabla c_\ell^- = 0$ because, for a.a. $(t, x) \in Q$, either $K_\ell(c(t, x)) = 0$ (if $c_\ell(t, x) \leq 0$) or $\nabla c_\ell(t, x)^- = 0$ (if $c_\ell(t, x) > 0$), and $r_\ell(\cdot)c_\ell^- \geq 0$ because of (8), we obtain $c_\ell^- = 0$ a.e. on Q .

The non-negativity of c_ℓ together with $\sum_{\ell=1}^L c_\ell = 1$ ensures that $c(t, x) \in \operatorname{Range}(K)$ for a.a. $(t, x) \in Q$ so that $c_\ell = K_\ell(c)$ and thus the triple (ϕ, v, c) is a weak solution to (28a)–(28c) with the retract K omitted, i.e. the isothermal variant of the original system (1a)–(1c) with (5) when θ is omitted. \square

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A corrigendum:

As pointed out by prof. W.H.Alt, if ν is not constant, only a symmetric part of ∇v should occur in (1a). The relevant modification of formulae (10), (11), (13), etc. are obvious. Korn's inequality is then to be exploited for the estimate of v . This corrigendum unfortunately will not occur in the printed version.