A preprint version of: IASME Transactions 2 (2005), 1190-1197 (published by WSEAS)

Incompressible ionized fluid mixtures: a non-Newtonian approach

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Abstract: The model combining non-Newtonian p-power-law generalization of the Navier-Stokes equation for barycentric velocity with Nernst-Planck equation for concentrations of particular mutually reacting ionic constituents, the heat equation, and also the Poisson equation for self-induced quasistatic electric field is presented. Existence of weak solutions for certain specific values of $p \geq 9/4$ and, in a special isothermal case, also uniqueness are proved.

Key Words: non-Newtonian fluids, mixtures, Eckart-Prigogine description, existence, uniqueness.

1 Introduction

Chemically reacting mixtures represent a framework for modelling of various complicated processes in biology and chemistry. My research in this area has been initiated by J. Nečas who, during many years before he passed away, spoke about "living fluids", although he never elaborated any concept of such fluids. To compromise thermodynamic amenability and mathematical rigor, the model proposed in [20, 21] uses incompressible Newtonian framework with the barycentric impulse balance. This "barycentric" approach is called the Eckart-Prigogine's [7, 17] concept; in the compressible case, see also [1, 4, 5, 9]. The incompressibility refers here both to each particular constituent and, through volume-additivity hypothesis as in e.g. [13, 19], also to the overall mixture. To cover biological applications on a cellular or subcellular level where intensity of electric field on cell membranes is very high, the self-induced electrostatic field must be considered; recall that the intra-cellular electric potential ranges usually over 60-100 mV while the thickness of cell membranes is of the order of 10 nm, which results to intensity of electric field of the order of 10 MV/m.

In comparison with [20, 21] or [22, Sect. 12.6], we consider here a non-Newtonian concept and use deep regularity results of Málek, Nečas, and Růžička [12] for such fluids with a shear-thickening p-power-law viscosity. Being an extended version of [23], this paper proves existence of a weak solution for the full system if $2.25 \leq p \leq 2.3027$ and uniqueness for the isothermal case, which extends the results from [23] where only a weak solution in the case of one specified value of p has been considered.[1] Anyhow, this paper confirms that [23] is correct at least in the sense that a specific p, for which weak solutions exist, does exist. Due to an extremely late distribution of specific strict requirements from WSEAS concerning the extended version of [23], the great part of this paper could arise during a couple of weeks only (occupied, in addition, primarily by making already scheduled 400-page proofs of [22]) and therefore the author apologizes for incidental imperfections.

2 The model

We consider a mixture of L mutually reacting chemical ionic constituents. Our model consists in a system

[1] To be more specific, [23] considers $p = 5/2$ but the arguments supporting just this value of p does not seem fully justified in [23] because the last space in (28) below is only $L^{4/3}(I;L^4(\Omega))$ for $p = 5/2$ but not $L^{4/3}(I;L^5(\Omega))$ as incorrectly claimed in [23].

of $n{+}L{+}2$ differential equations combining the *non-Newtonian* modification of the *Navier-Stokes equation* (balancing the barycentric momentum ρv), the *Nernst-Planck equation* modified for moving media (balancing the mass of particular constituents), the *heat equation* (balancing the internal energy $c_\mathrm{v}\theta$), and the quasistatic *Poisson equation* for the electrostatic field (balancing the electric induction $\varepsilon\nabla\phi$):

$$\rho\frac{\partial v}{\partial t}+\rho(v{\cdot}\nabla)v-\mathrm{div}\,\tau(\mathrm{D}v)+\nabla\pi=-q\nabla\phi\,,\qquad \mathrm{div}(v)=0\,,\tag{1a}$$

$$\frac{\partial c_\ell}{\partial t}-\mathrm{div}\big(d\nabla c_\ell+mc_\ell(e_\ell{-}q)\nabla\phi-c_\ell v\big)=r_\ell(c_1,...,c_L,\theta)\,,\qquad \ell=1,...,L\,,\tag{1b}$$

$$c_\mathrm{v}\frac{\partial\theta}{\partial t}-\mathrm{div}\big(\kappa\nabla\theta-c_\mathrm{v}v\theta\big)=\tau(\mathrm{D}v){:}\mathrm{D}v+d\nabla q{\cdot}\nabla\phi+\sum_{\ell=1}^{L}mc_\ell e_\ell^2|\nabla\phi|^2-mq^2|\nabla\phi|^2-\sum_{\ell=1}^{L}h_\ell(\theta)r_\ell(c,\theta),\tag{1c}$$

$$\mathrm{div}(\varepsilon\nabla\phi)+q=0,\qquad q=\sum_{\ell=1}^{L}e_\ell c_\ell\,.\tag{1d}$$

The variables v, π, c_ℓ, θ, ϕ and q have the following meaning:
v barycenter velocity,
π pressure,
c_ℓ concentration of ℓ-constituent,
ϕ electrostatic potential,
θ temperature,
q the total electric charge,
where the concentrations c_ℓ are to satisfy

$$\sum_{\ell=1}^{L}c_\ell=1,\qquad c_\ell\geq 0.\tag{2}$$

In (1c) and later on, c abbreviates $(c_1,...,c_L)$. The meaning of the data is:
$\tau=\tau(\mathrm{D}v)$ stress tensor, $\mathrm{D}v=\frac12(\nabla v)^\top+\frac12\nabla v$,
$\rho>0$ mass density,
e_ℓ valence (=charge) of ℓ-constituent,
$\varepsilon>0$ permitivity,
$r_\ell(c_1,...,c_L,\theta)$ ℓ-constituent production rate,
$h_\ell=h_\ell(\theta)$ enthalpy of the ℓ-constituent,
$\kappa>0$ thermal conductivity,
$c_\mathrm{v}>0$ heat capacity,
$d>0$ a diffusion coefficient, and
$m>0$ a mobility coefficient.

The system (1) is to be completed by the initial conditions

$$v(0,\cdot)=v_0\,,\quad c_\ell(0,\cdot)=c_{\ell 0}\,,\quad \theta(0,\cdot)=\theta_0\tag{3}$$

on the considered fixed bounded Lipschitz domain $\Omega\subset\mathbb{R}^n$, and by the boundary conditions corresponding, e.g., to a closed container, which, in some simplified version, leads to:

$$v=0,\quad c_\ell=c_{\ell\Sigma},\quad \varepsilon\frac{\partial\phi}{\partial\vec n}=\alpha(\phi_\Sigma{-}\phi),\quad \kappa\frac{\partial\theta}{\partial\vec n}=0\tag{4}$$

on $\Sigma:=(0,T)\times\partial\Omega$, where $\vec n$ is the unit outward normal to the boundary $\partial\Omega$ and $c_{\ell\Sigma}$ and ϕ_Σ are prescribed.

3 Physical comments to the model

The body force in (1a) comes from *Lorenz' force* acting on a charge q moving in the electromagnetic field (E,B), i.e. $q(E+v\times B)$ after the simplification that the intensity of electric field is $E=-\nabla\phi$ and the magnetic induction B vanishes.

The phenomenological flux $j_\ell:=-d\nabla c_\ell+mc_\ell(q{-}e_\ell)\nabla\phi$ in (1b) equals to $-m(c_\ell\nabla\mu_\ell-f_\mathrm{R})$ where

$$\mu_\ell=e_\ell\phi+\frac{d}{m}\ln(c_\ell),\tag{5}$$

plays the role of an *electrochemical potential* and where

$$f_\mathrm{R}:=q\nabla\phi\tag{6}$$

is a "*reaction force*" keeping the natural requirement $\sum_{\ell=1}^{L}j_\ell=0$ satisfied, which eventually fixes also the equality constraint in (2).

To show conservation of the *total energy*, let us assume naturally the electric-charge conservation in chemical reactions, i.e.

$$\sum_{\ell=1}^{L}e_\ell r_\ell(c,\theta)=0\tag{7}$$

and put, for simplicity, $\alpha=0$ in the boundary conditions (4), and then calculate the rate of electrostatic energy:

$$\frac{\varepsilon}{2}\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega|\nabla\phi|^2\mathrm{d}x = \int_\Omega \varepsilon\nabla\phi\cdot\nabla\frac{\partial\phi}{\partial t}\mathrm{d}x$$
$$= -\int_\Omega \varepsilon\phi\Delta\frac{\partial\phi}{\partial t}\mathrm{d}x = \int_\Omega \phi\sum_{\ell=1}^L e_\ell\frac{\partial c_\ell}{\partial t}\mathrm{d}x$$
$$= \int_\Omega \phi\sum_{\ell=1}^L e_\ell\big(r_\ell(c,\theta) - \mathrm{div}(j_\ell + c_\ell v)\big)\mathrm{d}x$$
$$= -\int_\Omega \phi\sum_{\ell=1}^L e_\ell \mathrm{div}(j_\ell + c_\ell v)\mathrm{d}x$$
$$= \int_\Omega \nabla\phi\cdot\sum_{\ell=1}^L e_\ell(j_\ell + c_\ell v)\mathrm{d}x - \int_\Gamma \phi\sum_{\ell=1}^L e_\ell j_\ell\cdot\vec{n}\,\mathrm{d}S \quad (8)$$

where (1d) and (1b) have been used together with (7) and twice Green's formula counting also with the boundary conditions (4). Testing (1a) by v, we obtain rate of kinetic energy

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega \rho\frac{|v|^2}{2}\mathrm{d}x = \int_\Omega \sum_{\ell=1}^L c_\ell(f_\ell\cdot v) - \rho\big((v\cdot\nabla)v\big)\cdot v$$
$$-\nu|\nabla v|^2\,\mathrm{d}x = -\int_\Omega \nu|\nabla v|^2 + \sum_{\ell=1}^L c_\ell e_\ell\nabla\phi\cdot v\,\mathrm{d}x. \quad (9)$$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega c_\mathrm{v}\theta\mathrm{d}x = \int_\Omega \nu|\nabla v|^2$$
$$-\sum_{\ell=1}^L\big(e_\ell j_\ell\nabla\phi + h_\ell(\theta)r_\ell(c,\theta)\big)\mathrm{d}x. \quad (10)$$

Altogether, summing (8)–(10) and using also (1b) integrated over Ω and Green's formula, we obtain the following balance:

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega\Big(\rho\frac{|v|^2}{2} + \varepsilon\frac{|\nabla\phi|^2}{2} + c_\mathrm{v}\theta\Big)\mathrm{d}x$$
$$= -\int_\Omega\sum_{\ell=1}^L h_\ell(\theta)r_\ell(c,\theta)\mathrm{d}x - \int_\Gamma\phi\sum_{\ell=1}^L e_\ell j_\ell\cdot\vec{n}\,\mathrm{d}S, \quad (11)$$

where we used the boundary conditions (4). Hence, (11) just says that the total energy rate, i.e. the rate of the sum of kinetic, electrostatic, and internal energy $\frac{1}{2}\rho|v|^2 + \frac{1}{2}\varepsilon|\nabla\phi|^2 + c_\mathrm{v}\theta$ over Ω, is balanced with the enthalpy production rate $\sum_{\ell=1}^L h_\ell r_\ell$ over Ω and the normal flux of electro-energy $\sum_{\ell=1}^L \phi e_\ell j_\ell\cdot\vec{n}$ through the boundary Γ.

The meaning of the five heat-source terms on the right-hand side of (1c) is the following:

- The first term $\tau(\mathrm{D}v):\mathrm{D}v$ represents the heat production rate due to the loss of kinetic energy by viscosity.
- The second term $d\nabla q\cdot\nabla\phi$ is the power (per unit volume) of the electric current arising by the diffusion flux, which can create local cooling effects. A global cooling effect seems possible via interaction with the environment if $\alpha \neq 0$, expectedly related with the so-called *Peltier effect*. If $\alpha = 0$, one can however see that the overall production due to this term over Ω is nonnegative: indeed, by using Green's formula twice, one gets

$$\int_\Omega\nabla q\cdot\nabla\phi\,\mathrm{d}x = -\int_\Omega\varepsilon\nabla(\Delta\phi)\cdot\nabla\phi\mathrm{d}x = \int_\Omega\varepsilon|\Delta\phi|^2\mathrm{d}x$$
$$-\int_\Gamma\varepsilon\Delta\phi\frac{\partial\phi}{\partial\vec{n}}\mathrm{d}S \geq \int_\Gamma q\alpha(\phi_\Gamma - \phi)\mathrm{d}S = 0. \quad (12)$$

- The third term $\sum_{\ell=1}^L mc_\ell e_\ell^2|\nabla\phi|^2$ is the power of *Joule's heat* produced by the electric currents j_ℓ.
- The fourth term $-mq^2|\nabla\phi|^2 = -mf_\mathrm{R}^2$ is the rate of cooling by the force which balances the volume-additivity constraint, and its influence is presumably very small as usually $|q|$ is much smaller than $\max_{\ell=1,\dots,L}|e_\ell|$. Besides, Joule's heat always dominates this cooling effect because

$$\sum_{\ell=1}^L c_\ell e_\ell^2 \geq \Big(\sum_{\ell=1}^L c_\ell e_\ell\Big)^2 \quad (13)$$

  if (2) holds, cf. [20, Remark 2.2].
- The last term $\sum_{\ell=1}^L h_\ell(\theta)r_\ell(c,\theta)$ is the heat produced or consumed by chemical reactions.

It should be emphasized that many simplifications are adopted in the presented model:

- we consider small electrical currents (i.e. magnetic field is neglected),
- we adopt the mentioned volume-additivity and incompressibility assumption,
- we 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)
- in agreement with Onsager's reciprocity principle, we also assume the heat flux independent of the concentration gradients (i.e. Dufour's effect is neglected),
- we assume the temperature-independent diffusion coefficients, mobility coefficients, and mass densities that are the same for each constituents, i.e. d, m, and ρ, respectively.

In 60ties, there appeared a newer and more rational concept by Truesdell [29, 30, 31] balancing impulses $\rho c_\ell v_\ell$ (with v_ℓ denoting the velocity of the ℓ-constituent) of all constituents separately together with interactive forces between them, see also [2, 14, 15, 18, 24, 25, 26, 28]. Then our barycentric velocity v equals to $\sum_{\ell=1}^L c_\ell v_\ell$. Recently, Samohýl [27] derived the model (1) by various simplifications from this rational model of Truesdell. In particular, [27] showed that the reaction force $f_{\rm R}$ from (6) in (1b) can be derived from a so-called Hittorf referential system related to the velocity of a dominant un-charged non-reacting constituent (typically water) after transformation to the barycentric system related to our velocity v under the assumptions (among others) of very diluted solution and negligible diffusion velocities.

4 Existence of weak solutions

We naturally assume the mass conservation in all chemical reactions and nonnegative production rate of ℓth constituent if its concentration vanishes, and the volume-additivity constraint holds for the initial and the boundary conditions, i.e.

$$\sum_{\ell=1}^L r_\ell(c_1,...,c_L,\theta)=0\,, \tag{14a}$$

$$r_\ell(c_1,...,c_{\ell-1},0,c_{\ell+1},...,c_L,\theta)\ge 0\,, \tag{14b}$$

$$\sum_{\ell=1}^L c_{\ell 0}=\sum_{\ell=1}^L c_{\ell\Sigma}=1, \quad c_{\ell 0}\ge 0, \quad c_{\ell\Sigma}\ge 0. \tag{14c}$$

Further, we assume $\tau(D)=\Phi'(|D|^2)$, $\Phi:\mathbb{R}\to\mathbb{R}^+$, and, for some $\varepsilon>0, C\in\mathbb{R}$, it satisfies

$$\Phi(0)=0, \quad \Phi'(0)=0, \tag{15a}$$

$$\Phi''(|D|^2)(B,B)\ge\varepsilon\big(1+|D|^{p-2}\big)|B|^2, \tag{15b}$$

$$\big|\Phi''(|D|^2)\big|\le C\big(1+|D|^{p-2}\big) \tag{15c}$$

for any $D,B\in\mathbb{R}^{n\times n}$ symmetric. The Korn inequality and (15a,b) imply (cf. [12, Lemma 2.1]) that, for any $v\in W_0^{1,2}(\Omega;\mathbb{R}^n)$,

$$\int_\Omega(\tau({\rm D}v_1)-\tau({\rm D}v_2)){:}{\rm D}(v_1-v_2)\,{\rm d}x\ge\zeta\big\|\nabla v^{12}\big\|_2^2 \tag{16}$$

for some $\zeta>0$ depending on ε and on Ω and for $\|\cdot\|_p$ the norm in $L^p(\Omega;\mathbb{R}^{n\times n})$; later, it will also abbreviate the norm in $L^p(\Omega)$ or $L^p(\Omega;\mathbb{R}^n)$.

We will prove the existence of a weak solution by Schauder's fixed point technique like in [20]. We define a retract $K:\mathcal{M}\to\{\xi{\in}\mathcal{M};\ \xi_\ell\ge 0,\ \ell=1,...,L\}$ by

$$K_\ell(\xi):=\frac{\xi_\ell^+}{\sum_{k=1}^L\xi_k^+}, \quad \xi_\ell^+:=\max(\xi_\ell,0), \tag{17}$$

where $\mathcal{M}$ denotes the affine manifold

$$\mathcal{M}:=\Big\{\xi\in\mathbb{R}^L;\ \sum_{\ell=1}^L\xi_\ell=1\Big\}. \tag{18}$$

Let us note that K is continuous and bounded on $\mathcal{M}$. Considering $\gamma=(\gamma_1,...,\gamma_L)=$ "old" concentrations and $\vartheta=$ an "old" temperature field, we define the quadruple (v,c,θ,ϕ) as the weak solution to the *decoupled "retracted" system*:

$$\rho\frac{\partial v}{\partial t}+\rho(v{\cdot}\nabla)v-{\rm div}\,\tau({\rm D}v)$$
$$+\nabla\pi=-q\nabla\phi\,, \qquad {\rm div}(v)=0\,, \tag{19a}$$

$$\frac{\partial c_\ell}{\partial t}-{\rm div}\big(d\nabla c_\ell+mK_\ell(\gamma)(e_\ell{-}q)\nabla\phi-c_\ell v\big)$$
$$=r_\ell(K(\gamma),\vartheta)\,, \qquad \ell=1,...,L\,, \tag{19b}$$

$$c_{\rm v}\frac{\partial\theta}{\partial t}-{\rm div}\big(\kappa\nabla\theta-c_{\rm v}v\theta\big)=\tau({\rm D}v){:}{\rm D}v$$
$$+d\sum_{\ell=1}^L e_\ell\nabla c_\ell{\cdot}\nabla\phi+m\sum_{\ell=1}^L K_\ell(\gamma)e_\ell^2|\nabla\phi|^2$$
$$-mq^2|\nabla\phi|^2-\sum_{\ell=1}^L h_\ell(\vartheta)r_\ell(K(\gamma),\vartheta), \tag{19c}$$

$${\rm div}(\varepsilon\nabla\phi)+q=0, \quad q=\sum_{\ell=1}^L e_\ell K_\ell(\gamma) \tag{19d}$$

with the initial and boundary conditions (3)–(4). Obviously, given (γ,ϑ), we are to solve subsequently the (now decoupled) equations (19d), (19a), (19b), and (19c) to obtain ϕ, v, c, and θ, respectively.

For simplicity we assume

$$r_\ell, h_\ell\ \text{ continuous and bounded}. \tag{20}$$

In some simplified cases, a certain (although only sub-linear) growth of $r_\ell(c,\cdot)$ may be admitted, too; cf. [20]. Let us abbreviate $I:=(0,T)$ and $Q=I\times\Omega$.

Proposition 1 *Let the assumptions (14), (15), (20) hold, let $v_0\in W^{1,p}_{0,{\rm DIV}}(\Omega;\mathbb{R}^n)$, $c_0\in L^2(\Omega;\mathbb{R}^L)$, $\theta_0\in L^2(\Omega)$, let Ω be of class C^3, and α and $\phi_\Sigma(t,\cdot)$ be smooth, $n\le 3$, and*

$$\frac{9}{4}\le p<\frac{1+\sqrt{13}}{2}. \tag{21}$$

Let $(\gamma,\vartheta)\in L^2(Q;\mathbb{R}^L)\times L^2(I;W^{1,2}(\Omega))$ be given such that $\sum_{\ell=1}^L\gamma_\ell=1$ a.e. on Q. Then, for some $C<+\infty$ independent of (γ,ϑ), (19) has a unique weak solution which satisfies

$$\sigma:=\sum_{\ell=1}^L c_\ell=1\quad \textit{a.e. on } Q \tag{22}$$

(although $c_\ell\ge 0$ need not hold!), and also the following a-priori estimates

$$\|v\|_{L^\infty(I;W^{1,p}(\Omega;\mathbb{R}^n))\cap L^{\frac{2}{p-1}}(I;W^{2,\frac{6}{p+1}}(\Omega;\mathbb{R}^n))}\le C, \tag{23a}$$
$$\Big\|\frac{\partial v}{\partial t}\Big\|_{L^2(I;L^2(\Omega;\mathbb{R}^n))}\le C, \tag{23b}$$
$$\|\theta\|_{L^2(I;W^{1,2}(\Omega))\cap L^\infty(I;L^2(\Omega))}\le C, \tag{23c}$$
$$\Big\|\frac{\partial \theta}{\partial t}\Big\|_{L^2(I;W^{1,2}(\Omega)^*)}\le C, \tag{23d}$$
$$\|c\|_{L^2(I;W^{1,2}(\Omega;\mathbb{R}^L))\cap L^\infty(I;L^2(\Omega;\mathbb{R}^L))}\le C, \tag{23e}$$
$$\Big\|\frac{\partial c}{\partial t}\Big\|_{L^2(I;W^{1,2}(\Omega;\mathbb{R}^L)^*)}\le C, \tag{23f}$$
$$\|\phi\|_{L^\infty(I;W^{2,2}(\Omega))}\le C. \tag{23g}$$

Proof. First, we prove (22). By summing (19c) for $\ell=1,...,L$ and by (14a), one gets

$$\begin{aligned}\frac{\partial\sigma}{\partial t}&=\sum_{\ell=1}^L r_\ell\big(K(\gamma),\vartheta\big)+\mathrm{div}\bigg(d\nabla\sigma+v\sigma\\&\quad-\sum_{\ell=1}^L mK_\ell(\gamma)\Big(e_\ell-\sum_{l=1}^L e_lK_l(\gamma)\Big)\nabla\phi\bigg)\\&=d\Delta\sigma-v\cdot\nabla\sigma,\end{aligned} \tag{24}$$

cf. also [20, Formula (3.18)]. Due to (14c), the unique solution to thus obtained equation

$$\frac{\partial\sigma}{\partial t}-d\Delta\sigma+v\cdot\nabla\sigma=0 \tag{25}$$

is $\sigma\equiv 1$.

Further, we realize that the charge $q=e\cdot K(\gamma)$ in (19d) is always bounded and, in particular, it is in $L^\infty(I;L^2(\Omega))$, and (23g) follows by usual $W^{2,2}$-regularity of the Δ-operator with (4). Then also the driving force $q\nabla\phi$ in (19a) is bounded in $L^\infty(I;L^6(\Omega;\mathbb{R}^n))$, hence certainly in $L^2(Q;\mathbb{R}^n)$, and we can use [12] where the estimates (23a,b) have been derived by a very sophisticated usage of a shift technique and a test by a truncated Laplacean under the restriction $p\ge 9/4$, which is just the lower bound in (21).

Testing (19b) by c_ℓ gives (23e) standardly when we realize that the term

$$\mathrm{div}(mK_\ell(\gamma)(e_\ell-q)\nabla\phi)-r_\ell(K(\gamma),\vartheta) \tag{26}$$

is certainly bounded in $L^\infty(I;W^{1,6/5}(\Omega)^*)\subset L^2(I;W^{1,2}(\Omega)^*)$ and when we also use

$$\begin{aligned}\int_\Omega c_\ell v\cdot\nabla c_\ell\,\mathrm{d}x&=\frac12\int_\Omega v\cdot\nabla c_\ell^2\,\mathrm{d}x\\&=-\frac12\int_\Omega(\mathrm{div}\,v)c_\ell^2\,\mathrm{d}x=0.\end{aligned} \tag{27}$$

Then (23f) follows by testing (19b) by arbitrary $z\in L^2(I;W^{1,2}(\Omega))$.

Now, by the Sobolev embedding $W^{1,6/(p+1)}(\Omega)\subset L^{6/(p-1)}(\Omega)$ which holds for $n\le 3$, let us realize that (23a) is the estimate of

$$\nabla v \text{ in } L^\infty(I;L^p(\Omega;\mathbb{R}^n))\cap L^{\frac{2}{p-1}}(I;L^{\frac{6}{p-1}}(\Omega;\mathbb{R}^n)). \tag{28}$$

To work in terms of weak solutions of the heat equation, we need to embed this space into $L^{2p}(I;L^{6p/5+\varepsilon}(\Omega;\mathbb{R}^n))$ with some $\varepsilon>0$. By usual interpolation between the spaces in (28) with a coefficient $\lambda\in[0,1]$, it needs the conditions

$$\frac{\lambda}{\infty}+\frac{(1-\lambda)(p-1)}{2}\le\frac{1}{2p}\,,\quad\text{and} \tag{29a}$$
$$\frac{\lambda}{p}+\frac{(1-\lambda)(p-1)}{6}<\frac{5}{6p}. \tag{29b}$$

The smallest $\lambda\ge 0$ satisfying (29a) is $\lambda=(p^2-p-1)/(p^2-p)$. For this λ, (29b) results to $p^2-p-3<0$ after a simple algebra. This condition just gives the upper bound in (21). Having now $v\in L^{2p}(I;L^{6p/5+\varepsilon}(\Omega;\mathbb{R}^n))$, due to (15a,c), $\tau(\mathrm{D}v){:}\mathrm{D}v$ is then certainly bounded in $L^2(I;L^{6/5}(\Omega))$ which is a subset of the natural "right-hand-side space" $L^2(I;W^{1,2}(\Omega)^*)$ for the heat equation. By (23e,g), we also know that $(e\cdot\nabla c)\cdot\nabla\phi$ is bounded in $L^2(I;L^{3/2}(\Omega))$. The other three terms on the right-hand side of (19c) are even better. Then (23c) follows standardly by testing (19c) by θ, and (23d) then follows by using a test by arbitrary $z\in L^2(I;W^{1,2}(\Omega))$ for (19c).

Eventually, the uniqueness of solutions to (19b,c,d) follows standardly because these equations are decoupled and linear, while uniqueness for (19a) is nontrivial and has been proved in [12] if $p\ge 9/4$. $\square$

Proposition 2 *Let the assumptions of Proposition 1 hold, then the mapping $(\gamma,\vartheta)\mapsto(v,c,\theta,\phi)$ with*

$\sum_{\ell=1}^{L}\gamma_\ell = 1$ *is continuous from the weak topology on* $\mathcal{W}^{L+1}$ *with*

$$\mathcal{W} := L^2(I;W^{1,2}(\Omega)) \cap W^{1,2}(I;W^{1,2}(\Omega)^*) \tag{30}$$

to the weak topology related to the spaces from the estimates (23).*

Proof. Take a sequence $\{(\gamma_k,\vartheta_k)\}_{k\in\mathbb{N}}$ converging weakly to some (γ,ϑ) in $\mathcal{W}^{L+1}$. Take the corresponding $(v_k,c_k,\theta_k,\phi_k)$ and choose a subsequence converging weakly* in the spaces specified in the estimates (23). By Aubin-Lions' compact-embedding theorem [3, 10], cf. also e.g. [22, Lemma 7.7], the estimates (23c,d) imply that

$$\gamma_k \to \gamma \ \text{ in } \ L^2(I;L^{6-\varepsilon}(\Omega;\mathbb{R}^L)) \tag{31}$$

in the norm topology with any $\varepsilon > 0$, which allows us to pass to the limit $K(\gamma_k) \to K(\gamma)$ and also ensures $\phi_k \to \phi$ strongly in $L^{1/\varepsilon}(I;W^{2,2}(\Omega))$. Then we get $|\nabla\phi_k|^2 \to |\nabla\phi|^2$ in $L^{1/(2\varepsilon)}(I;L^3(\Omega))$ to exploit for (19c). Using again Aubin-Lions' theorem shows $\vartheta_k \to \vartheta$ strongly in $L^2(I;L^{6-\varepsilon}(\Omega))$, which allows us to pass to the limit $h_\ell(\vartheta_k) \to h_\ell(\vartheta)$ and $r_\ell(\gamma_k,\vartheta_k) \to r_\ell(\gamma,\vartheta)$. Moreover, again by Aubin-Lions' theorem and by interpolation like in the proof of Proposition 1,

$$\nabla v_k \to \nabla v \ \text{ in } \ L^{2p}(I;L^{6p/5}(\Omega;\mathbb{R}^n)) \tag{32}$$

in the norm topology, hence

$$\tau(\mathrm{D}v_k){:}\mathrm{D}v_k \to \tau(\mathrm{D}v){:}\mathrm{D}v \ \text{ in } \ L^2(I;L^{6/5}(\Omega)), \tag{33}$$

which is essential for the limit passage in (19c) to obtain a conventional weak solution. The limit passage in (19) is then routine. The uniqueness proved in Proposition 1 with help of [12] ensures eventually the convergence of the whole sequence. □

Proposition 3 *Let again the assumptions of Proposition 1 hold, then the mapping* $\mathcal{F} : (\gamma,\vartheta) \mapsto (c,\theta)$, *where* (c,θ) *is uniquely determined by (19), maps the set*

$$\mathcal{C} := \big\{(c,\theta)\in\mathcal{W}^{L+1};\ \|c\|_{\mathcal{W}^L} \le C,\\ \|\theta\|_{\mathcal{W}} \le C,\ c(\cdot,\cdot)\in\mathcal{M} \text{ a.e. on } Q\big\} \tag{34}$$

with C from (23c-f) into itself and has a fixed point $(c,\theta) \in \mathcal{C}$. *Moreover, considering the corresponding* ϕ *and* v, *the quadruple* (v,c,θ,ϕ) *is a weak solution to (1)–(4).*

Proof. The fact that $\mathcal{F} : \mathcal{C} \to \mathcal{C}$ follows from Proposition 1 because C from (23c-f) does not depend on (γ,ϑ) at all, hence even $\mathcal{F} : \mathcal{W}^{L+1} \to \mathcal{C}$. We use $\mathcal{C}$ equipped with the weak topology. The continuity of $\mathcal{F}$ in this topology was proved in Proposition 2. The fixed point then exists by Schauder's theorem (in Tikhonov's modification).

Finally, by testing by c_ℓ^- the resulted equation for c_ℓ, i.e. (19b) with $K(c)$ in place of $K(\gamma)$, we obtain $c_\ell^- = 0$ if (14b,c) is taken into account; the important fact is that $K_\ell(u)\nabla c_\ell^- = 0$ because, for a.a. $(t,x) \in Q$, either $K_\ell(u(t,x)) = 0$ (if $c_\ell(t,x) \le 0$) or $\nabla c_\ell(t,x)^- = 0$ (if $c_\ell(t,x) > 0$). Hence (2) is proved, and $c_\ell = K_\ell(c)$, so that the retract K can eventually be forgotten at this fixed point. □

Let us remark that the bounds in (21) are very tight; note that the length of this interval is only about 0.0528. Therefore, it would be worth trying either to improve regularity results from [12] by using also the fact that the driving force on the right-hand side $q\nabla\phi$ of (1a) is not only in $L^2(Q)$ but even in $L^\infty(I;W^{1,1/\varepsilon}(\Omega;\mathbb{R}^n))$ if a $W^{2,1/\varepsilon}$-regularity for the Δ-operator would be used, $\varepsilon > 0$ arbitrary, or to seek for a more general solution. The former option is certainly extremely difficult, while the latter one seems to be more promising although there are some technical obstacles too. E.g., one can think about a distributional solution $\theta \in L^\infty(I;L^1(\Omega))$ as in [16], which might allow for $p < 3$, but, due to the advection term $\mathrm{div}(v\nabla\theta)$ in (19c), it is not obvious whether such distributional solution θ depends depends continuously on (γ,ϑ) as needed for the fixed-point argument.

5 Uniqueness in the isothermal case

Let us confine ourselves on the case that the temperature variations can be neglected, hence instead of $r_\ell = r_\ell(c,\theta)$ we consider only $r_\ell = r_\ell(c)$; it is certainly well satisfied, e.g., in biological applications on cellular level. Then (1) decouples to (1a,b,d) and (1c). To show uniqueness, it suffices to consider only (1a,b,d) because (1c) will follow.

Proposition 4 *Let (15c) hold,* r_ℓ *be Lipschitz continuous,* Ω *be of the* C^3*-class,* α *and* ϕ_Σ *be smooth,* $n\le 3$, *and* $p\ge 5/2$. *Then there is at most one weak solution to the problem (1a,b,d),(3),(4).*

Proof. For notational simplicity, let $\rho{=}1$. Recall that $q = \sum_{\ell=1}^{L} e_\ell c_\ell =: e{\cdot}u$. Consider the two weak solutions (ϕ^1,c^1,v^1) and (ϕ^2,c^2,v^2) to (1a,b,d), and denote $\phi^{12} := \phi^1{-}\phi^2$, $c^{12} := c^1{-}c^2$, and $v^{12} := v^1{-}v^2$.

Test the difference of (1a) (resp. (1b)) written for two solutions by v^{12} (resp. c_ℓ^{12}), and use (16) to get:

$$\begin{aligned}&\frac{\mathrm{d}}{\mathrm{d}t}\Big(\big\|v^{12}\big\|_2^2+\sum_{\ell=1}^{L}\big\|c_\ell^{12}\big\|_2^2\Big)+\zeta\big\|\nabla v^{12}\big\|_2^2\\&\quad+d\sum_{\ell=1}^{L}\big\|\nabla c_\ell^{12}\big\|_2^2=\int_\Omega\Big(\big((v^2\cdot\nabla)v^2-(v^1\cdot\nabla)v^1\big)v^{12}\\&\quad+\big(q^2\nabla\phi^2-q^1\nabla\phi^1\big)\cdot v^{12}\\&\quad+m\sum_{\ell=1}^{L}\Big(c_\ell^2(e_\ell-q^2)\nabla\phi^2-c_\ell^1(e_\ell-q^1)\nabla\phi^1\Big)\cdot\nabla c_\ell^{12}\\&\quad+\sum_{\ell=1}^{L}\big(c_\ell^1v^1-c_\ell^2v^2\big)\nabla c_\ell^{12}\\&\quad+\big(r(c^1)-r(c^2)\big)\cdot c^{12}\Big)\mathrm{d}x=:I_1+\ldots+I_5\end{aligned}\tag{35}$$

The term I_1 in (35), arising from the convective term, can be handled as in [11, Theorem 4.29] modified with zero-Dirichlet boundary condition provided $p\geq 5/2$, namely

$$\begin{aligned}I_1&=-\int_\Omega(v^{12}\cdot\nabla)v^1\cdot v^{12}\mathrm{d}x\\&\leq\varepsilon\big\|\nabla v^{12}\big\|_2^2+C_\varepsilon\big\|\nabla v^1\big\|_p^{2p/(2p-n)}\big\|\nabla v^{12}\big\|_2^2\end{aligned}$$

for $\varepsilon<\zeta$ and then treated by Gronwall's inequality.

Furthermore, from (1d) we get $\phi^{12}=\Delta^{-1}(e\cdot c^{12})$ where Δ^{-1} denotes the inverse operator to Δ under the homogeneous boundary conditions (4), i.e. $\varepsilon\partial\phi/\partial\vec{n}+\alpha\phi=0$. Estimate the term I_2 in (35), for each $\ell=1,\ldots L$, as

$$\begin{aligned}I_2&:=\int_\Omega\Big(c_\ell^2\nabla\phi^2-c_\ell^1\nabla\phi^1\Big)\cdot v^{12}\,\mathrm{d}x\\&\leq\frac{1}{4\varepsilon}\big\|c_\ell^{12}\big\|_2^2\big\|\nabla\phi^1\big\|_4^2+\varepsilon\big\|v^{12}\big\|_4^2\\&\quad+\big\|c_\ell^2\big\|_\infty^2\big\|\nabla\Delta^{-1}(e\cdot c^{12})\big\|_2^2+\frac{1}{4}\big\|v^{12}\big\|_2^2=:T_1+..T_4.\end{aligned}$$

By (23e), $q\in L^2(I;W^{1,2}(\Omega))$, and then $\nabla\phi^1\in L^2(I;W^{2,2}(\Omega;\mathbb{R}^n))\subset L^2(I;L^4(\Omega;\mathbb{R}^n))$ for $n\leq 3$ (here even $n\leq 8$ is allowed) through standard $W^{3,2}$-regularity results for the linear boundary-value problem (1d)–(4). Then the term T_1 will be handled by Gronwall's inequality. As to $T_2\leq\varepsilon N^2\|\nabla v^{12}\|_2^2$, we will absorb it in the respective term coming from the viscosity term (1a) if $\varepsilon<\zeta/N^2$ where N is the norm of the embedding $W^{1,2}(\Omega)\subset L^4(\Omega)$. As to T_3, we use $\|\nabla\phi^{12}\|_2\leq C\|e\cdot c^{12}\|_2$ with some C depending on Ω and on α, and then will handle it together with T_4 by Gronwall's inequality. Now we estimate the terms $I_{3\ell}$ with $I_3=\sum_{\ell=1}^{L}I_{3\ell}$ in (35) as

$$\begin{aligned}\frac{I_{3\ell}}{m}&:=\int_\Omega\Big(c_\ell^1(e_\ell-q^1)\nabla\phi^1-c_\ell^2(e_\ell-q^2)\nabla\phi^2\Big)\cdot\nabla c_\ell^{12}\mathrm{d}x\\&\leq\frac{3m}{d}\big\|c_\ell^{12}\big\|_2^2\big\|e_\ell-q^1\big\|_\infty^2\big\|\nabla\phi^1\big\|_\infty^2\\&\quad+\frac{3m}{d}\big\|c_\ell^2\big\|_\infty^2\big\|e\cdot c^{12}\big\|_2^2\big\|\nabla\phi^1\big\|_\infty^2\\&\quad+\frac{3m}{d}\big\|c_\ell^2\big\|_\infty^2\big\|e_\ell-q^2\big\|_\infty^2\big\|\nabla\phi^{12}\big\|_2^2\\&\quad+\frac{d}{4m}\big\|\nabla c_\ell^{12}\big\|_2^2=T_1+\ldots+T_4.\end{aligned}\tag{36}$$

Now we employ the regularity of $\Delta^{-1}:L^\infty(\Omega)\to W^{1,\infty}(\Omega)$; this follows by the standard $W^{2,1/\varepsilon}$-regularity theory with $\varepsilon<1/n$, cf. e.g. [8], so that $\nabla\phi^1\in L^\infty(Q;\mathbb{R}^n)$, which is needed for both T_1 and T_2. These terms are then to be treated by Gronwall's inequality. As to T_3, estimate $\|\nabla\phi^{12}\|_2^2\leq C\|e\cdot c^{12}\|_2^2$, which will lead to Gronwall's inequality, while T_4 is to be absorbed in the left-hand side. Further, using also (27) (here with v^1 and c_ℓ^{12} instead of v and c_ℓ, respectively) we estimate $I_{4\ell}$ in the term $I_4=\sum_{\ell=1}^{L}I_{4\ell}$ in (35) as

$$\begin{aligned}I_{4\ell}&:=\int_\Omega\big(c_\ell^1v^1-c_\ell^2v^2\big)\cdot\nabla c_\ell^{12}\mathrm{d}x=\int_\Omega c_\ell^2v^{12}\cdot\nabla c_\ell^{12}\mathrm{d}x\\&\leq\frac{1}{d}\big\|c_\ell^2\big\|_\infty^2\big\|v^{12}\big\|_2^2+\frac{d}{4}\big\|\nabla c_\ell^{12}\big\|_2^2.\end{aligned}\tag{37}$$

Eventually, denoting by L_r the Lipschitz constant of $r:\mathbb{R}^L\to\mathbb{R}^L$, we estimate the term I_5 in as

$$I_5:=\int_\Omega\big(r(c^1)-r(c^2)\big)\cdot c^{12}\mathrm{d}x\leq L_r\big\|c^{12}\big\|_2^2.\tag{38}$$

Then we sum $I_1+\ldots+I_5$ and use the mentioned Gronwall's inequality to obtain both $v^{12}=0$ and $c_\ell^{12}=0$. $\square$

Let us remark that, in fact, more sophisticated technique from [12] for I_1 allows even for $p\geq\frac{9}{4}$, which is consistent with the investigations in Section 4. In the isothermal case, the existence of a weak solution was shown also in [21] or [22, Sect.12.6] in the Navier-Stokes case (i.e. $p=2$ was admitted).

Acknowledgments: This work has been partly supported by the grants 201/03/0934 (GA ČR) and MSM 0021620839 (MŠMT ČR).

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