Incompressible ionized fluid mixtures

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A model of a fluid mixture of L incompressible chemically reacting charged constituents in Prigogine's description (i.e. balancing barycentric impulse but not impulses of particular constituents) was presented. Under the volume-additivity hypothesis and some other simplifying assumptions, the model combines the Navier-Stokes equation (1a) for the barycentric velocity v and the pressure p with the Nernst-Planck equation with advection (1b) for the concentrations c_ℓ of the particular mutually reacting constituents, the Poisson equation (1d) for self-induced quasistatic electric field ϕ, and the heat equation (1c) for temperature θ:

$$\varrho\frac{\partial v}{\partial t}+\varrho(v\cdot\nabla)v-\nu\Delta v+\nabla p=\sum_{\ell=1}^{L}c_\ell f_\ell\,,\qquad \operatorname{div}v=0\,, \tag{1a}$$

$$\frac{\partial c_\ell}{\partial t}+\operatorname{div}\big(j_\ell+c_\ell v\big)=r_\ell(c_1,...,c_L,\theta)\,,\qquad \ell=1,...,L\,, \tag{1b}$$

$$\varepsilon\Delta\phi=-q,\qquad q=\sum_{\ell=1}^{L}e_\ell c_\ell\ , \tag{1c}$$

$$c_{\rm v}\frac{\partial\theta}{\partial t}-\operatorname{div}\big(\kappa\nabla\theta+c_{\rm v}v\theta\big)=\nu|\nabla v|^2+\sum_{\ell=1}^{L}\big(f_\ell\cdot j_\ell-h_\ell(\theta)r_\ell(c_1,...,c_L,\theta)\big) \tag{1d}$$

where the Lorenz force and the phenomenological diffusive fluxes are considered as

$$f_\ell=-e_\ell\nabla\phi,\qquad j_\ell=-d\nabla c_\ell-mc_\ell(e_\ell-q)\nabla\phi, \tag{2}$$

and where $\varrho>0$ is the mass density both of the mixture and of the particular constituents, $\nu>0$ is viscosity, e_ℓ valence (i.e. electric charge) of the ℓ-constituent, $\varepsilon>0$ permitivity, $r_\ell(c_1,...,c_L,\theta)$ production rate of the ℓ-constituent by chemical reactions, $h_\ell(\theta)$ the enthalpy contained in the ℓth constituent, $d>0$ a diffusion coefficient, $m>0$ a mobility coefficients, $c_{\rm v}>0$ a specific heat, and $\kappa>0$ a heat conductivity coefficient.

Thermodynamics of this model is based on the energy balance, which sounds essentially as

$$\frac{\rm d}{{\rm d}t}\bigg(\int_\Omega\Big(\underbrace{\frac{\varrho}{2}|v|^2}_{\text{kinetic energy}}+\underbrace{\frac{\varepsilon}{2}|\nabla\phi|^2}_{\text{electrostatic energy}}+\underbrace{c_{\rm v}\theta}_{\text{internal energy}}\Big){\rm d}x\bigg)-\int_\Omega\underbrace{\textstyle\sum_{\ell=1}^{L}h_\ell(\theta)r_\ell(c,\theta)}_{\text{heat production via chemical reactions}}\,{\rm d}x=0 \tag{3}$$

in an isolated system on a fixed domain Ω, i.e. no contribution from (here nonspecified) boundary conditions on $\partial\Omega$ is counted. The heat sources on the right-hand side of (1d), i.e.

$$\nu|\nabla v|^2+d\nabla q\cdot\nabla\phi+\sum_{\ell=1}^{L}mc_\ell e_\ell^2|\nabla\phi|^2-mq^2|\nabla\phi|^2-\sum_{\ell=1}^{L}h_\ell r_\ell, \tag{4}$$

includes respectively the heat production due to viscosity, the power of the electric current arising by due to the diffusion flux which may have a local Peltier-type cooling effects alhough globally it cannot cool because of

$$\int_\Omega d\nabla q\cdot\nabla\phi\,\mathrm{d}x=\varepsilon\int_\Omega -d\nabla(\Delta\phi)\cdot\nabla\phi\,\mathrm{d}x\varepsilon\int_\Omega d|\Delta\phi|^2\,\mathrm{d}x\geq 0, \tag{5}$$

the further term in (4) is Joule's heat produced by the electric currents which always dominates the 4th term (i.e. the rate of cooling by a "reaction force" which balances the volume-additivity constraint $\sum_{\ell=1}^L c_\ell=1$), while the 5th term is the heat produced or consumed by chemical reactions. The entropy balance based on Helmholtz' free energy $\frac{\varepsilon}{2}|\nabla\phi|^2-c_{\rm v}\theta\ln(\theta)$ can formally be established for spatially isothermal processes or electroneutral processes; the violation of Claussius-Duhem inequality for such an entropy may be due to incompressible simplification or due to certain inconsistency of Prigoggine concept with electrostatics.

Existence of a weak solution to an initial-boundary-value problem for (1)–(2) can be shown in two special cases: the Stokes' one (i.e. the convective term $\varrho(v\cdot\nabla)\,v$ in (1a) neglected) or the isothermal one (i.e. the heat equation (1d) neglected). A Kakutani fixed-point argument can be used for both cases [1]. The Galerkin approach has been used for the latter case in [2]. In both cases, fine design of the scheme is necessary, using a certain correcting retract of concentrations from the linear manifold $\sum_{\ell=1}^L c_\ell=1$ to its subset of non-negative c_ℓ's, which eventually may be forgotten in the fixed point or in the limit, respectively. The a-priori L^∞-bound of retracted concentrations facilitates the whole proceedure. In the isothermal case, a (very) weak solution has then the quality: $c_\ell\in L^\infty((0,T)\times\Omega)\cap L^2([0,T];W^{1,2}(\Omega))$ with $\frac{\partial}{\partial t}c_\ell\in L^{4/3}([0,T];W^{1,2}(\Omega)^*)$, and $v\in L^2([0,T];W^{1,2}(\Omega;\mathbb{R}^3))\cap L^\infty([0,T];L^2(\Omega;\mathbb{R}^3))$ with the acceleration $\frac{\partial}{\partial t}v\in L^{4/3}([0,T];W^{1,2}_{0,\mathrm{DIV}}(\Omega;\mathbb{R}^3)^*)$ where the notation $W^{1,2}_{0,\mathrm{DIV}}$ indicates divergence-free functions, and eventually $\phi\in L^\infty([0,T];W^{1,2}(\Omega))$. In case the Stokes the convective term in (1a) is neglected, a regularity for the Poisson and the Stokes equations yields additionally $\phi\in L^\infty([0,T];W^{2,2}(\Omega))$ and $v\in L^6([0,T];W^{2,6}(\Omega;\mathbb{R}^3))$, and then $\theta\in L^2([0,T];W^{1,2}(\Omega))\cap L^\infty([0,T];L^2(\Omega))$ with $\frac{\partial}{\partial t}\theta\in L^2([0,T];W^{1,2}(\Omega)^*)$.

The application of the model is limited to situations where the magnetic field can be neglected and where all constituents are incompressible and have equal mechanical response (i.e. have the same mobility d and diffusivity m as well as the "reaction force" $q\nabla\phi$ in (2) which balances the volume-additivity contraint $\sum_{\ell=1}^L c_\ell=1$ influence them equally). *Acknowledgement*: The work was supported also by the grant 201/03/0934 (GA ČR).

References

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[2] T. Roubíček, *Incompressible Fluid Mixtures of Ionized Constituents*, in Proc. STAMM04, (Eds. K.Hutter, Y.Wang), Shaker Verlag, Aachen, 2005, in print.