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Reaction–diffusion systems of Maxwell–Stefan type with reversible mass-action kinetics

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ABSTRACT

The mass-based Maxwell–Stefan approach to one-phase multicomponent reactive mixtures is mathematically analyzed. It is shown that the resulting quasilinear, strongly coupled reaction–diffusion system is locally well-posed in an L_p-setting and generates a local semiflow on its natural state space. Solutions regularize instantly and become strictly positive if their initial components are all nonnegative and nontrivial. For a class of reversible mass-action kinetics, the positive equilibria are identified: these are precisely the constant chemical equilibria of the system, which may form a manifold. Here the total free energy of the system is employed which serves as a Lyapunov function for the system. By the generalized principle of linearized stability, positive equilibria are proved to be normally stable.

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1. Introduction

1.1. Reaction–diffusion systems of Maxwell–Stefan type

The Maxwell–Stefan approach modeling diffusion in multicomponent mixtures is well-known in the engineering literature, cf. [7,12,13,21,25]. In the mathematical community the resulting reaction–diffusion equations seem much less known, but have recently attracted a lot of attention, see [1,3,9]. Therefore, we begin with a review of the basic ideas of this approach.

Let $\Omega \subset \mathbb{R}^n$ be an open bounded domain with boundary $\partial\Omega$ of class $C^{2+\alpha}$ and outer normal field ν. We consider a mixture of $N \geq 2$ species A_k with *molar masses* $M_k > 0$ and *individual mass densities* $\rho_k \geq 0$ filling the container Ω. Mass balance of the single component A_k reads

$$\partial_t \rho_k + \operatorname{div}_x(\rho_k \mathbf{u}_k) = M_k r_k \quad \text{in } \Omega,\ t > 0,$$

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where $\mathbf{u}_k$ denotes the *individual velocity* of species A_k, satisfying $(\mathbf{u}_k|\nu) = 0$ on $\partial\Omega$, and r_k is the rate of production of species A_k due to chemical reactions. Observe that the kinetics r should be *positivity preserving*, i.e., subject to the condition

$$\rho_j \geq 0, \quad \rho_k = 0 \quad \Rightarrow \quad r_k \geq 0,$$

and should satisfy $\sum_k M_k r_k = 0$, which results in *conservation of total mass*. The quantities of interest are the mass densities ρ_k, while the individual velocities $\mathbf{u}_k$ are in general unknown and have to be modeled, as well as the kinetics r_k. To reduce the complexity of these balance laws, we introduce the *total density* $\rho = \sum_k \rho_k$, the *barycentric velocity* $\mathbf{u} = \sum_k \rho_k \mathbf{u}_k/\rho$, the *mass fractions* $y_k = \rho_k/\rho$, and the *concentrations* $c_k = \rho_k/M_k = y_k\rho/M_k$. With these new variables, we obtain the overall mass balance

$$\partial_t \rho + \operatorname{div}_x(\rho\mathbf{u}) = 0 \quad \text{in } \Omega,\ t > 0,$$

and $(\mathbf{u}|\nu) = 0$ on $\partial\Omega$. The individual mass balances now become

$$\rho(\partial_t y_k + \mathbf{u}\cdot\nabla_x y_k) + \operatorname{div}_x J_k = M_k r_k \quad \text{in } \Omega,\ t > 0,$$

where the *diffusive fluxes* J_k are given by

$$J_k = \rho_k(\mathbf{u}_k - \mathbf{u}), \quad k = 1,\dots,N.$$

Note that, by definition, $\sum_k y_k = 1$ and $\sum_k J_k = 0$.

So far everything is physically exact in the framework of continuum mechanics. However, to obtain a closed model one has to prescribe laws for $\mathbf{u}$, r_k, and most importantly for the diffusive fluxes J_k. In this paper, we are interested in the *incompressible*, *isobaric*, *isothermal case*, which means

$$\rho = const, \qquad \mathbf{u} = 0,$$

and no temperature dependence. We note that most of the engineering literature, as well as the papers [1,9], is *molar-based*, i.e., instead of the total mass ρ the *total molar concentration* $c_{\text{tot}} = \sum_k c_k$ is assumed be constant and the *molar averaged velocity* $\mathbf{v} = \frac{1}{c_{\text{tot}}}\sum_k c_k\mathbf{u}_k$ vanishes. However, adding up the individual mass balances, this leads to $\sum_k r_k = 0$, which is only satisfied in special situations. Hence, also having in mind the more general case of nontrivial velocity field and temperature, we prefer the *mass-based ansatz* $\rho = const$.

The above assumptions lead to the problem

$$\rho\partial_t y_k + \operatorname{div}_x J_k = M_k r_k(y) \quad \text{in } \Omega, \qquad (J_k|\nu) = 0 \quad \text{on } \partial\Omega, \tag{1.1}$$

for $k = 1,\dots,N$, completed by initial data $y_k(0) = y_0^k \geq 0$. We again emphasize the constraints

$$\sum_{k=1}^N J_k = 0, \qquad \sum_{k=1}^N y_k = 1. \tag{1.2}$$

Together with $y \geq 0$ this already implies L_∞-bounds for y, a very important property. Therefore, when modeling the diffusive fluxes it is essential that positivity as well as conservation of mass are ensured.

A classical approach to model the diffusive fluxes J_k is now as follows. One of the species, say A_N, acts as a solvent for the mixture, say water, or tuluol, benzol, etc. This means that y_N is close to 1 and the remaining y_k are small, hence the A_k are dilute for $k \neq N$. As A_N will in general not be involved in the reactions, the equation for y_N is ignored and the remaining diffusive fluxes are modeled by *Fick's law*, i.e. $J_k = -d_k\nabla_x y_k$, $k = 1,\dots,N-1$, where $d_k > 0$. This way (1.1) becomes a semilinear reaction–diffusion system with diagonal main part which preserves nonnegativity of $y_1,\dots,y_{N-1}$. However, now (1.2) forces an unrealistic diffusive flux J_N for y_N, such that nonnegativity and *a priori* L_∞-bounds for the mass fractions might get lost. This might be one reason for the notorious problem of global existence in the Fickian approach, see [16,22].

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