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Existence analysis of Maxwell-Stefan systems for multicomponent mixtures

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EXISTENCE ANALYSIS OF MAXWELL-STEFAN SYSTEMS FOR MULTICOMPONENT MIXTURES

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ABSTRACT. Maxwell-Stefan systems describing the dynamics of the molar concentrations of a gas mixture with an arbitrary number of components are analyzed in a bounded domain under isobaric, isothermal conditions. The systems consist of mass balance equations and equations for the chemical potentials, depending on the relative velocities, supplemented with initial and homogeneous Neumann boundary conditions. Global-in-time existence of bounded weak solutions to the quasilinear parabolic system and their exponential decay to the homogeneous steady state are proved. The mathematical difficulties are due to the singular Maxwell-Stefan diffusion matrix, the cross-diffusion coupling, and the lack of standard maximum principles. Key ideas of the proofs are the Perron-Frobenius theory for quasi-positive matrices, entropy-dissipation methods, and a new entropy variable formulation allowing for the proof of nonnegative lower and upper bounds for the concentrations.

1. INTRODUCTION

The Maxwell-Stefan equations describe the diffusive transport of multicomponent mixtures [22, 24]. Applications include various fields like sedimentation, dialysis, electrolysis, ion exchange, ultrafiltration, and respiratory airways [5, 27]. The model bases upon inter-species force balances, relating the velocities of the species of the mixture. It is well-known that the usual Fickian diffusion model, which states that the flux of a chemical substance is proportional to its concentration gradient, is not able to describe, e.g., uphill or osmotic diffusion phenomena in multicomponent mixtures, as demonstrated experimentally by Duncan and Toor [13]. These phenomena can be modeled by using the theory of non-equilibrium thermodynamics, in which the fluxes are assumed to be linear combinations of the thermodynamic forces [11, Chap. 4]. However, this model requires the knowledge of all binary diffusion coefficients, which are not always easy to determine, and the positive semi-definiteness of the diffusion matrix. The advantage of the Maxwell-Stefan approach is that it is capable to describe uphill diffusion effects without assuming particular properties on the diffusivities (besides symmetry).

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Key words and phrases. Maxwell-Stefan systems, cross-diffusion, Perron-Frobenius theory, entropy-dissipation methods, existence of solutions, long-time behavior of solutions.

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We consider an ideal gaseous mixture consisting of $N + 1$ components with molar concentrations $c_i(x, t)$ for $i = 1, \dots, N + 1$ (see Appendix A). Since we concentrate our study on cross-diffusion effects, we suppose isothermal and isobaric conditions. Then the total molar concentration $\sum_{i=1}^{N+1} c_i$ is constant and we set this constant equal to one. More general situations are investigated, e.g., in [15]. The dynamics of the mixture is given by the mass balance equations

$$(1) \quad \partial_t c_i + \operatorname{div} J_i = r_i(c) \quad \text{in } \Omega, \quad t > 0, \quad i = 1, \dots, N + 1,$$

where $J_i = c_i u_i$ denotes the molar flux, u_i the mean velocity, r_i the net production rate of the i -th component, $c = (c_1, \dots, c_{N+1})^\top$, and $\Omega \subset \mathbb{R}^d$ ($d \geq 1$) is a bounded domain. We have assumed above that the averaged mean velocity vanishes, $\sum_{i=1}^{N+1} c_i u_i = 0$. Then the conservation of the total mass implies that the total production rate vanishes, $\sum_{i=1}^{N+1} r_i(c) = 0$. The fluxes are related to the concentration gradients by

$$(2) \quad \nabla c_i = - \sum_{j=1, j \neq i}^{N+1} \frac{c_j J_i - c_i J_j}{D_{ij}}, \quad i = 1, \dots, N + 1,$$

where $D_{ij} > 0$ for $i \neq j$ are some diffusion coefficients. The derivation of these relations is sketched in Appendix A.

The aim of this paper is to prove the global-in-time existence of weak solutions to system (1)-(2) for constant coefficients $D_{ij} > 0$, supplemented with the boundary and initial conditions

$$(3) \quad \nabla c_i \cdot \nu = 0 \quad \text{on } \partial\Omega, \quad t > 0, \quad c_i(\cdot, 0) = c_i^0 \quad \text{in } \Omega, \quad i = 1, \dots, N + 1,$$

where ν is the exterior unit normal vector on $\partial\Omega$. There are several difficulties to overcome in the analysis of the Maxwell-Stefan system.

First, the molar fluxes are not defined *a priori* as a linear combination of the concentration gradients, which makes it necessary to invert the flux-gradient relations (2). As the Maxwell-Stefan equations are linearly dependent, we need to invert the system on a subspace, yielding the diffusion matrix \tilde{A}^{-1} . In the engineering literature, this inversion is often done in an approximate way. For instance, a numerical solution procedure for $N = 3$ was developed in [2] and the special case $D_{ij} = 1/(f_i f_j)$ for some constants $f_i > 0$ was investigated in [3].

Second, equations (1)-(2) are coupled, which translates into the fact that \tilde{A}^{-1} is generally a full matrix with nonlinear solution-dependent coefficients. Thus, standard tools like the maximum principle or regularity theory are not available. In particular, it is not clear how to prove nonnegative lower and upper bounds for the concentrations. Moreover, it is not clear whether \tilde{A}^{-1} is positive semi-definite or not, such that even the proof of local-in-time existence of solutions is nontrivial.

Third, it is not standard to find suitable a priori estimates which allow us to conclude the global-in-time existence of solutions.

In view of these difficulties, it is not surprising that there are only very few analytical results in the mathematical literature for Maxwell-Stefan systems. Under some general

assumptions on the nonlinearities, Giovangigli proved that there exists a unique global solution to the whole-space Maxwell-Stefan system if the initial datum is sufficiently close to the equilibrium state [15, Theorem 9.4.1]. Bothe [4] showed the existence of a unique local solution for general initial data. Boudin et al. [7] considered a ternary system ($N = 2$) and assumed that two diffusivities are equal. In this situation, the Maxwell-Stefan system reduces to a heat equation for the first component and a drift-diffusion-type equation for the second species. Boudin et al. [7] proved the existence of a unique global solution and investigated its long-time decay to the stationary state. Up to now, there does not exist a global existence theory for (1)-(2) for general initial data. We provide such a result in this work.

After inverting the flux-gradient relations (2) on a suitable subspace, the Maxwell-Stefan equations become a parabolic cross-diffusion system. Amann derived in [1] sufficient conditions for the solutions to such systems to exist globally in time. The question if a given local solution exists globally is reduced to the problem of finding a priori estimates in suitable Sobolev spaces. Another approach was developed in [8, 9, 14, 17, 19] for systems arising in granular material modeling, population dynamics, cell biology, and thermodynamics to treat cross-diffusion systems whose diffusion matrix may be neither symmetric nor positive semi-definite. The idea is to exploit the entropy structure of the model by introducing so-called entropy variables. In these variables, the new diffusion matrix becomes positive semi-definite and an entropy-dissipation relation can be derived. However, in all of the mentioned papers (except [9]) systems with two equations only have been considered.

In this paper, we combine and extend the entropy-dissipation technique of [8, 9, 14, 17, 19] as well as ideas of Bothe [4] to overcome the above mathematical difficulties. We are able to prove the global-in-time existence of weak solutions to (1)-(3) for arbitrary diffusion matrices and general initial data. This result is obtained under the following assumptions:

- Domain: $\Omega \subset \mathbb{R}^d$ ($d \leq 3$) is a bounded domain with $\partial\Omega \in C^{1,1}$.
- Initial data: c_1^0, \dots, c_N^0 ($N \geq 2$) are nonnegative measurable functions, $c_{N+1}^0 = 1 - \sum_{i=1}^N c_i^0$, and

$$(4) \quad \sum_{i=1}^N c_i^0 \leq 1.$$

- Diffusion matrix: $(D_{ij}) \in \mathbb{R}^{(N+1) \times (N+1)}$ is a symmetric matrix with elements $D_{ij} > 0$ for $i \neq j$.
- Production rates: The functions $r_i \in C^0([0, 1]^{N+1}; \mathbb{R})$, $i = 1, \dots, N + 1$, satisfy

$$(5) \quad \sum_{i=1}^{N+1} r_i(c) = 0, \quad \sum_{i=1}^{N+1} r_i(c) \log c_i \leq 0 \quad \text{for all } 0 < c_1, \dots, c_{N+1} \leq 1.$$

We stress the fact that, although the diffusion coefficients D_{ij} are constant, the diffusion matrix of the inverted Maxwell-Stefan system depends on the molar concentrations in a nonlinear way (see below) and we need to deal with a fully coupled nonlinear parabolic

system. Our proof also works for diffusion coefficients depending on the concentrations c_i if the coefficients d_{ij} are bounded from above and below.

The regularity on the boundary $\partial\Omega$ is needed for the a priori estimate $\|w\|_{H^2(\Omega)} \leq C\|f\|_{L^2(\Omega)}$ of the elliptic problem $-\Delta w + w = f$ in Ω , $\nabla w \cdot \nu = 0$ on $\partial\Omega$.

The inequality imposed on the production rates is needed to prove that the entropy is nonincreasing in time. It is satisfied if, for instance, $N = 4$ and $r_1 = r_3 = c_2c_4 - c_1c_3$, $r_2 = r_4 = c_1c_3 - c_2c_4$ [10]. For the existence result, the inequality can be weakened by

$$(6) \quad \sum_{i=1}^{N+1} r_i(c) \log c_i \leq C_r \quad \text{for all } 0 < c_1, \dots, c_{N+1} \leq 1,$$

where $C_r > 0$ is some constant independent of c_i (see (27)). This condition is satisfied, for instance, for the tumor-growth model in [19].

Our first main result is the global existence of solutions to (1)-(3).

Theorem 1 (Global existence of solutions). *Let the above assumptions hold. Then there exists a weak solution (c_1, \dots, c_{N+1}) to (1)-(3) satisfying*

$$\begin{aligned} c_i &\in L^2_{\text{loc}}(0, \infty; H^1(\Omega)), \quad \partial_t c_i \in L^2_{\text{loc}}(0, \infty; \mathcal{V}'), \\ 0 \leq c_i &\leq 1, \quad i = 1, \dots, N, \quad c_{N+1} = 1 - \sum_{i=1}^N c_i \geq 0 \quad \text{in } \Omega, \quad t > 0, \end{aligned}$$

where \mathcal{V}' is the dual space of $\mathcal{V} = \{u \in H^2(\Omega) : \nabla u \cdot \nu = 0 \text{ on } \partial\Omega\}$.

To be precise, the existence theorem for (1)-(3) has to be understood as an existence result for a system in N components (see below), which is equivalent to (1)-(3) as long as $c_i > 0$ for all $i = 1, \dots, N$ and $\sum_{i=1}^N c_i < 1$ are satisfied.

We explain the key ideas of the proof. For this, we write (2) more compactly as

$$(7) \quad \nabla c = A(c)J,$$

where $A(c) \in \mathbb{R}^{(N+1) \times (N+1)}$ and $\nabla c = (\partial c_i / \partial x_j)_{ij}$, $J = (J_1, \dots, J_{N+1})^\top \in \mathbb{R}^{(N+1) \times d}$. Using the Perron-Frobenius theory for quasi-positive matrices, Bothe [4] characterized the spectrum of $A(c)$ in case that $c_i > 0$ for $i = 1, \dots, N$ and $\sum_{i=1}^N c_i < 1$. Under these conditions, $A(c)$ can be inverted on its image. Then, denoting its inverse by $\tilde{A}(c)^{-1}$, (1)-(2) can be formulated as

$$(8) \quad \partial_t c - \text{div}(-\tilde{A}(c)^{-1} \nabla c) = r(c) \quad \text{in } \Omega, \quad t > 0,$$

where $r(c) = (r_1(c), \dots, r_{N+1}(c))^\top$.

It turns out that it is more convenient to eliminate the last equation for c_{N+1} , which is determined by $c_{N+1} = 1 - \sum_{i=1}^N c_i$, and to work only with the system in N components. We set $c' = (c_1, \dots, c_N)^\top$, $J' = (J_1, \dots, J_N)^\top$, and $r'(c) = (r_1(c), \dots, r_N(c))^\top$. Using the facts that $c_{N+1} = 1 - \sum_{i=1}^N c_i$ and $\sum_{i=1}^N J_i = -J_{N+1}$, system (7) can be written as $\nabla c' = -A_0(c')J'$. The matrix $A_0(c')$ defined in Section 2 is generally not symmetric and it

is not clear if it is positive definite. If $A_0(c')$ is invertible (and we prove in Section 2 that this is the case), we can write system (1)-(2) as

$$(9) \quad \partial_t c' - \operatorname{div}(A_0(c')^{-1} \nabla c') = r'(c) \quad \text{in } \Omega, \quad t > 0.$$

Still, $A_0(c')^{-1}$ may be not positive (semi-) definite.

Our main idea to handle (9) is to exploit its entropy structure. We associate to this system the entropy density

$$(10) \quad h(c') = \sum_{i=1}^N c_i (\log c_i - 1) + c_{N+1} (\log c_{N+1} - 1), \quad c_1, \dots, c_N \geq 0, \quad \sum_{i=1}^N c_i \leq 1,$$

where $c_{N+1} = 1 - \sum_{i=1}^N c_i$ is interpreted as a function of the other concentrations. Furthermore, we define the entropy variables

$$(11) \quad w_i = \frac{\partial h}{\partial c_i} = \log \frac{c_i}{c_{N+1}}, \quad i = 1, \dots, N,$$

and we denote by $H(c') = \nabla^2 h(c')$ the Hessian of h with respect to c' . Then (9) becomes

$$(12) \quad \partial_t c' - \operatorname{div}(B(w) \nabla w) = r'(c) \quad \text{in } \Omega, \quad t > 0,$$

where $w = (w_1, \dots, w_N)^\top$ and $B(w) = A_0(c)^{-1} H(c)^{-1}$ is symmetric and positive definite (see Lemma 6). The advantage of the formulation in terms of the entropy variables is not only that the diffusion matrix $B(w)$ is positive definite (which allows us to apply the Lax-Milgram lemma to a linearized version of (12)) but it yields also positive lower and upper bounds for the concentrations. Indeed, inverting (11), we find that

$$(13) \quad c_i = \frac{e^{w_i}}{1 + e^{w_1} + \dots + e^{w_N}}, \quad i = 1, \dots, N.$$

Therefore, if the functions w_i are bounded, the concentrations c_i are positive and $\sum_{i=1}^N c_i < 1$ which implies that $c_{N+1} = 1 - \sum_{i=1}^N c_i > 0$. This observation is a key novelty of the paper.

Formulation (8) is needed to derive a priori estimates which are an important ingredient for the global existence proof. Differentiating the entropy $\mathcal{H}[c] = \int_{\Omega} h(c) dx$ (now $h(c)$ is interpreted as a function of all c_1, \dots, c_{N+1}) formally with respect to time, a computation (made rigorous in Lemma 9) shows the entropy-dissipation inequality

$$(14) \quad \frac{d\mathcal{H}}{dt} + K \int_{\Omega} \sum_{i=1}^{N+1} |\nabla \sqrt{c_i}|^2 dx \leq 0,$$

where $K > 0$ is a constant which depends only on (D_{ij}) . This estimate yields H^1 bounds for $\sqrt{c_i}$.

The existence proof is based on the construction of a problem which approximates (12). We replace the time derivative by an implicit Euler discretization with time step $\tau > 0$ and we add the fourth-order operator $\varepsilon(\Delta^2 w + w)$, which guarantees the uniform coercivity of the elliptic system in \mathcal{V} with respect to w . The existence of approximating weak solutions is shown by means of the Leray-Schauder fixed-point theorem. The discrete analogon of the

above entropy-dissipation estimate implies a priori bounds uniform in the approximation parameters τ and ε , which allows us to pass to the limit $(\tau, \varepsilon) \rightarrow 0$. In particular, the entropy inequality provides global solutions.

System (1)-(3) with vanishing production rates, $r = (r_1, \dots, r_{N+1})^\top = 0$, admits the homogeneous steady state $(\bar{c}_1^0, \dots, \bar{c}_{N+1}^0)$, where $\bar{c}_i^0 = \text{meas}(\Omega)^{-1} \int_{\Omega} c_i^0 dx$. We are able to prove that the solution, constructed in Theorem 1, converges exponentially fast to this stationary state. For this, we introduce the relative entropy

$$\mathcal{H}^*[c] = \sum_{i=1}^{N+1} \int_{\Omega} c_i \log \frac{c_i}{\bar{c}_i^0} dx.$$

Theorem 2 (Exponential decay). *Let the assumptions of Theorem 1 hold. We suppose that $r = 0$ and $\min_{i=1, \dots, N+1} \|c_i^0\|_{L^1(\Omega)} > 0$. Let (c_1, \dots, c_{N+1}) be the weak solution constructed in Theorem 1 and define $c^0 = (c_1^0, \dots, c_{N+1}^0)^\top$. Then there exist constants $C > 0$, depending only on Ω , and $\lambda > 0$, depending only on Ω and (D_{ij}) , such that*

$$\|c_i(\cdot, t) - \bar{c}_i^0\|_{L^1(\Omega)} \leq C e^{-\lambda t} \sqrt{\mathcal{H}^*[c^0]}, \quad i = 1, \dots, N+1.$$

The proof of this result is based on the entropy-dissipation inequality (14) and the logarithmic Sobolev inequality [16], which links the entropy dissipation to the relative entropy, as well as on the Csiszár-Kullback inequality [26], which bounds the squared L^1 norm in terms of the relative entropy. The difficulty of the proof is that the approximate solutions do not conserve the L^1 -norm because of the presence of the regularizing ε -terms, and we need to derive appropriate bounds.

The paper is organized as follows. In Section 2, we prove some properties of the diffusion matrices $A(c)$ and $A_0(c)$ and we show how system (1)-(2) of $N+1$ equations can be reduced to a system of N equations. Based on these properties, Theorems 1 and 2 are proved in Sections 3 and 4, respectively. For the convenience of the reader, the derivation of the Maxwell-Stefan relations (2) is sketched in Appendix A and some definitions and results from matrix theory needed in Section 2 are summarized in Appendix B.

2. PROPERTIES OF THE DIFFUSION MATRICES

Let the Maxwell-Stefan diffusion matrix $(D_{ij}) \in \mathbb{R}^{(N+1) \times (N+1)}$ ($N \geq 2$) be symmetric with $D_{ij} > 0$ for $i \neq j$ and $D_{ii} = 0$ for all i and set $d_{ij} = 1/D_{ij}$ for $i \neq j$. Let $c = (c_i) \in \mathbb{R}^{N+1}$ be a strictly positive vector satisfying $\sum_{i=1}^{N+1} c_i = 1$. We refer to Appendix B for the definitions and results from matrix analysis used in this section. According to (2) and (7), the matrix $A = A(c) = (a_{ij}) \in \mathbb{R}^{(N+1) \times (N+1)}$ is given by

$$a_{ij} = d_{ij} c_i \quad \text{for } i, j = 1, \dots, N+1, \quad i \neq j, \quad a_{ii} = - \sum_{j=1, j \neq i}^{N+1} d_{ij} c_j \quad \text{for } i = 1, \dots, N+1.$$

In [15, Section 7.7.1], the matrix with elements $-a_{ij} c_j$ is analyzed and it is shown that it is symmetric, positive semi-definite, irreducible, and a singular M-matrix as well as that a generalized inverse can be defined. Our approach is to apply the Perron-Frobenius theory to A , following [4].

Lemma 3 (Properties of A). *Let $\delta = \min_{i,j=1,\dots,N+1, i \neq j} d_{ij} > 0$ and $\Delta = 2 \sum_{i,j=1, i \neq j}^{N+1} d_{ij}$. Then the spectrum $\sigma(-A)$ of $-A$ satisfies*

$$\sigma(-A) \subset \{0\} \cup [\delta, \Delta].$$

The inclusion $\sigma(-A) \subset \{0\} \cup [\delta, \infty)$ is shown in [4, Section 5]. For the convenience of the reader and since some less known results from matrix analysis are needed, we present a full proof.

Proof. The matrix A is quasi-positive and irreducible. Therefore, by Theorem 13 of Perron-Frobenius (see Appendix B), the spectral bound of A , $s(A) = \max\{\Re(\lambda) : \lambda \in \sigma(A)\}$, is a simple eigenvalue of A associated with a strictly positive eigenvector and $s(A) > \Re(\lambda)$ for all $\lambda \in \sigma(A)$, $\lambda \neq s(A)$. Here, $\Re(z)$ denotes the real part of the complex number z . Thus,

$$\sigma(A) \subset \{s(A)\} \cup \{z \in \mathbb{C} : \Re(z) < s(A)\}.$$

An elementary computation shows that c is a (strictly) positive eigenvector to the eigenvalue $\lambda = 0$ of A . According to the Perron-Frobenius theory, only the eigenvector to $s(A)$ is positive. This implies that $s(A) = 0$ and

$$\sigma(A) \subset \{0\} \cup \{z \in \mathbb{C} : \Re(z) < 0\}.$$

We can describe the spectrum of $\sigma(A)$ in more detail. Let $C^{1/2} = \text{diag}(\sqrt{c_1}, \dots, \sqrt{c_{N+1}})$ be a diagonal matrix in $\mathbb{R}^{(N+1) \times (N+1)}$ with inverse $C^{-1/2}$. Then we can introduce the symmetric matrix $A_S = C^{-1/2} A C^{1/2}$ whose elements are given by

$$a_{ij}^S = \begin{cases} a_{ii} & \text{if } i = 1, \dots, N+1, \\ d_{ij} \sqrt{c_i c_j} & \text{if } i, j = 1, \dots, N+1, i \neq j. \end{cases}$$

The matrix A_S is real and symmetric since $d_{ij} = d_{ji}$ and therefore, it has only real eigenvalues. Since A and A_S are similar, their spectra coincide:

$$\sigma(A_S) = \sigma(A) \subset \{0\} \cup \{z \in \mathbb{R} : z < 0\} = (-\infty, 0].$$

Now, consider the matrix $A_S(\alpha) = A_S - \alpha \sqrt{c} \otimes \sqrt{c}$, where $0 < \alpha < \delta$ and $\sqrt{c} = (\sqrt{c_1}, \dots, \sqrt{c_{N+1}})^\top$. Then $A_S(\alpha)$ is quasi-positive and irreducible (since $\alpha < \delta \leq d_{ij}$). Using $\sum_{i=1}^{N+1} c_i = 1$, a computation shows that $-\alpha$ is an eigenvalue of $A_S(\alpha)$ associated to the strictly positive eigenvector \sqrt{c} . By Theorem 13 of Perron-Frobenius, the spectral bound of $A_S(\alpha)$ equals $-\alpha$ and

$$\sigma(A_S(\alpha)) \subset (-\infty, -\alpha].$$

Since $A_S(\alpha)$ and $\alpha \sqrt{c} \otimes \sqrt{c}$ are symmetric, we can apply Theorem 16 of Weyl:

$$\lambda_i(A_S) = \lambda_i(\alpha \sqrt{c} \otimes \sqrt{c} + A_S(\alpha)) \leq \lambda_i(\alpha \sqrt{c} \otimes \sqrt{c}) + \lambda_{N+1}(A_S(\alpha)),$$

where $i = 1, \dots, N+1$ and the eigenvalues $\lambda_i(\cdot)$ are arranged in increasing order. Because of $\lambda_{N+1}(A_S(\alpha)) = -\alpha$ and $\lambda_i(\alpha \sqrt{c} \otimes \sqrt{c}) = 0$ for $i = 1, \dots, N$, $\lambda_{N+1}(\alpha \sqrt{c} \otimes \sqrt{c}) = \alpha$ (see Proposition 14), we find that $\lambda_i(A_S) \leq -\alpha$ for $i = 1, \dots, N$ and $\lambda_{N+1}(A_S) \leq 0$. Thus, for all $\alpha < \delta$,

$$\sigma(A) = \sigma(A_S) \subset \{0\} \cup (-\infty, -\alpha],$$

implying that $\sigma(-A) \subset \{0\} \cup [\delta, \infty)$.

It remains to prove the upper bound of the spectrum. Denoting by $\|\cdot\|_F$ the Frobenius norm, we find for the spectral radius of $-A$ that

$$\begin{aligned} r(-A) &\leq \| -A \|_F = \left(\sum_{i,j=1}^{N+1} a_{ij}^2 \right)^{1/2} = \left(\sum_{i=1}^{N+1} \left(\sum_{j=1, j \neq i}^{N+1} d_{ij} c_j \right)^2 + \sum_{i,j=1, j \neq i}^{N+1} (d_{ij} c_i)^2 \right)^{1/2} \\ &< 2 \sum_{i,j=1, j \neq i}^{N+1} d_{ij} = \Delta, \end{aligned}$$

since $0 < c_i < 1$, finishing the proof. \square

Lemma 4 (Properties of restrictions of A and A_S). *Let $\tilde{A} = A|_{\text{im}(A)}$ and $\tilde{A}_S = A_S|_{\text{im}(A_S)}$. Then \tilde{A} and \tilde{A}_S are invertible on the images $\text{im}(A)$ and $\text{im}(A_S)$, respectively, and*

$$(15) \quad \sigma(-\tilde{A}), \sigma(-\tilde{A}_S) \subset [\delta, \Delta), \quad \sigma((-\tilde{A}_S)^{-1}) \subset (1/\Delta, 1/\delta).$$

Proof. Direct inspection shows that $\ker(A) = \text{span}\{c\}$, $\text{im}(A) = \{\mathbf{1}\}^\perp$, where $\mathbf{1} = (1, \dots, 1)^\top \in \mathbb{R}^{N+1}$, and $\ker(A_S) = \text{span}\{\sqrt{c}\}$. By the symmetry of A_S , it follows that

$$(16) \quad \mathbb{R}^{N+1} = \ker(A_S)^\perp \oplus \ker(A_S) = \text{im}(A_S^\top) \oplus \ker(A_S) = \text{im}(A_S) \oplus \ker(A_S).$$

Furthermore, using Theorem 12, since $\lambda = 0$ is a semisimple eigenvalue of A ,

$$(17) \quad \mathbb{R}^{N+1} = \text{im}(A) \oplus \ker(A).$$

We observe that both \tilde{A} and \tilde{A}_S are endomorphisms. Clearly, $\sigma(\tilde{A}) \subset \sigma(A)$ and $\sigma(\tilde{A}_S) \subset \sigma(A_S)$. We claim that 0 is not contained in $\sigma(\tilde{A})$ or $\sigma(\tilde{A}_S)$. Indeed, otherwise there exists $x \in \text{im}(A)$ (or $x \in \text{im}(A_S)$), $x \neq 0$, such that $\tilde{A}x = 0$ (or $\tilde{A}_S x = 0$). But this implies that $x \in \ker(A)$ (or $x \in \ker(A_S)$) and because of (17) (or (16)), it follows that $x = 0$, contradiction. Hence, \tilde{A} and \tilde{A}_S are invertible on their respective domain, and (15) follows. \square

The above lemma shows that the flux-gradient relation (7) can be inverted since $\sum_{i=1}^{N+1} J_i = 0$ implies that each column of J is an element of $\{\mathbf{1}\}^\perp = \text{im}(A)$. In fact, we can write (7) as $\nabla c = \tilde{A}J$ and hence, $J = \tilde{A}^{-1}\nabla c$. Therefore, we can formulate (1) and (2) as

$$(18) \quad \partial_t c - \text{div}(-\tilde{A}^{-1}\nabla c) = r(c) \quad \text{in } \Omega, \quad t > 0.$$

The next step is to reduce the Maxwell-Stefan system of $N + 1$ components to a system of N components only. Still, we assume that $c_i > 0$ for all i and $\sum_{i=1}^{N+1} c_i = 1$. We define the matrices

$$X = I_{N+1} - \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ \vdots \\ 1 \\ 0 \end{pmatrix}, \quad X^{-1} = I_{N+1} + \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ \vdots \\ 1 \\ 0 \end{pmatrix} \in \mathbb{R}^{(N+1) \times (N+1)},$$

where X^{-1} is the inverse of X and I_{N+1} is the unit matrix of $\mathbb{R}^{(N+1) \times (N+1)}$. A computation shows that

$$X^{-1}AX = \begin{pmatrix} -A_0 & b \\ 0 & 0 \end{pmatrix},$$

where the $(N \times N)$ -matrix $A_0 = (a_{ij}^0)$ is defined by

$$(19) \quad a_{ij}^0 = \begin{cases} -(d_{ij} - d_{i,N+1})c_i & \text{if } i \neq j, \quad i, j = 1, \dots, N, \\ \sum_{j=1, j \neq i}^N (d_{ij} - d_{i,N+1})c_j + d_{i,N+1} & \text{if } i = j = 1, \dots, N, \end{cases}$$

and the vector $b = (b_i)$ is given by $b_i = d_{i,N+1}c_i$, $i = 1, \dots, N$. In Lemma 5 below we show that A_0 is invertible. Then, writing $c' = (c_1, \dots, c_N)^\top$ and $J' = (J_1, \dots, J_N)^\top$,

$$\begin{pmatrix} \nabla c' \\ 0 \end{pmatrix} = X^{-1}\nabla c = (X^{-1}AX)X^{-1}J = \begin{pmatrix} -A_0 J' \\ 0 \end{pmatrix}.$$

Thus, applying X^{-1} to (18), since $X^{-1}\partial_t c = (\partial_t c', 0)^\top$ and $X^{-1}r(c) = (r'(c), 0)^\top$,

$$(20) \quad \partial_t c' - \operatorname{div}(A_0^{-1}\nabla c') = r' \quad \text{in } \Omega, \quad t > 0.$$

We note that every solution c' to this problem defines a solution to (18) and hence to (1)-(2) by multiplying (20) (augmented via $(c', 0)^\top$) by X and setting $c_{N+1} = 1 - \sum_{i=1}^N c_i$.

Lemma 5 (Properties of A_0). *The matrix $A_0 \in \mathbb{R}^{N \times N}$, defined in (19), is invertible with spectrum*

$$\sigma(A_0) \subset [\delta, \Delta].$$

Furthermore, the elements of its inverse A_0^{-1} are uniformly bounded in $c_1, \dots, c_N \in [0, 1]$.

Proof. Since the blockwise upper triangular matrix $-X^{-1}AX$ is similar to $-A$, their spectra coincide and

$$(21) \quad \sigma(A_0) \cup \{0\} = \sigma(-X^{-1}AX) = \sigma(-A) \subset \{0\} \cup [\delta, \Delta].$$

Observing that 0 is a simple eigenvalue of $-A$, it follows that $\sigma(A_0) \subset [\delta, \Delta]$ and hence, A_0 is invertible.

It remains to show the uniform bound for the elements α_{ij} of A_0^{-1} . By Cramer's rule, $A_0^{-1} = \operatorname{adj}(A_0)/\det A_0$, where $\operatorname{adj}(A_0)$ is the adjugate of A_0 . The definition of A_0 in (19) implies that

$$|a_{ij}^0| \leq \sum_{k=1, k \neq i}^N |d_{ik} - d_{i,N+1}| + |d_{i,N+1}| = K_i \leq K, \quad i, j = 1, \dots, N,$$

where $K = \max_{i=1, \dots, N} K_i$. Therefore, the elements of $\operatorname{adj}(A_0)$ are not larger than $(N-1)!K^{N-1}$. By (21), the eigenvalues of A_0 are bounded from below by δ . Consequently, since the determinant of a matrix equals the product of its eigenvalues, $\det(A_0) \geq \delta^N$. This shows that $|\alpha_{ij}| \leq (N-1)!K^{N-1}\delta^{-N}$ for all i, j . \square

Consider the Hessian $\nabla^2 h$ of the entropy density (10) in the variables c_1, \dots, c_N . Then $H = (h_{ij}) = \nabla^2 h \in \mathbb{R}^{N \times N}$ is given by

$$h_{ij} = \frac{1}{c_{N+1}} + \frac{\delta_{ij}}{c_i}, \quad i, j = 1, \dots, N,$$

where δ_{ij} denotes the Kronecker delta. The matrix H is symmetric and positive definite by Sylvester's criterion, since all principle minors $\det H_k$ of H are positive:

$$\det H_k = (c_1 \cdots c_k c_{N+1})^{-1} \left(\sum_{i=1}^k c_i + c_{N+1} \right) > 0, \quad k = 1, \dots, N.$$

Lemma 6 (Properties of B). *The matrix $B = A_0^{-1} H^{-1}$ is symmetric and positive definite. Furthermore, the elements of B are bounded uniformly in $c_1, \dots, c_{N+1} \in [0, 1]$.*

Proof. Using $d_{ij} = d_{ji}$ and $\sum_{i=1}^{N+1} c_i = 1$, a calculation shows that the elements β_{ij} of $B^{-1} = H A_0$ equal

$$\begin{aligned} \beta_{ii} &= d_{i,N+1} \left(1 - \sum_{k=1, k \neq i}^N c_k \right) \left(\frac{1}{c_i} + \frac{1}{c_{N+1}} \right) + \sum_{k=1, k \neq i}^N \left(\frac{d_{k,N+1}}{c_{N+1}} + \frac{d_{ik}}{c_i} \right) c_k, \\ \beta_{ij} &= \frac{d_{i,N+1}}{c_{N+1}} \left(1 - \sum_{k=1, k \neq i}^N c_k \right) + \frac{d_{j,N+1}}{c_{N+1}} \left(1 - \sum_{k=1, k \neq j}^N c_k \right) + \sum_{k=1, k \neq i, j}^N d_{k,N+1} \frac{c_k}{c_{N+1}} - d_{ij}, \end{aligned}$$

where $i, j = 1, \dots, N$ and $i \neq j$. Hence, B^{-1} is symmetric. We have proved above that H^{-1} is symmetric and positive definite. According to Theorem 15, the number of positive eigenvalues of $A_0 = H^{-1} B^{-1}$ equals that for B^{-1} . However, by (21), A_0 has only positive eigenvalues. Therefore, also B^{-1} has only positive eigenvalues. This shows that B^{-1} and consequently B are symmetric and positive definite.

It remains to show the uniform boundedness of B . The inverse $H^{-1} = (\eta_{ij})$ can be computed explicitly:

$$\eta_{ij} = \begin{cases} (1 - c_i)c_i & \text{if } i = j = 1, \dots, N, \\ -c_i c_j & \text{if } i \neq j, i, j = 1, \dots, N. \end{cases}$$

Denoting the elements of A_0^{-1} by α_{ij} , the elements b_{ij} of B equal

$$\begin{aligned} b_{ii} &= \alpha_{ii}(1 - c_i)c_i - \sum_{k=1, k \neq i}^N \alpha_{ik}c_i c_k, \quad i = 1, \dots, N, \\ b_{ij} &= -\alpha_{ii}c_i c_j + \alpha_{ij}(1 - c_j)c_j - \sum_{k=1, k \neq i, j}^N \alpha_{ik}c_j c_k, \quad i \neq j, i, j = 1, \dots, N. \end{aligned}$$

By Lemma 5, the elements α_{ij} are uniformly bounded. Then, since $c_i \in [0, 1]$, the uniform bound for b_{ij} follows. \square

3. PROOF OF THEOREM 1

The analysis in Section 2 shows that the Maxwell-Stefan system can be reduced to the problem

$$(22) \quad \partial_t c' - \operatorname{div}(B(w)\nabla w) = r'(c) \quad \text{in } \Omega, \quad t > 0,$$

$$(23) \quad \nabla w_i \cdot \nu = 0 \quad \text{on } \partial\Omega, \quad w_i(\cdot, 0) = w_i^0 \quad \text{in } \Omega, \quad i = 1, \dots, N,$$

where $B = B(w)$ is symmetric and positive definite for $c_1, \dots, c_{N+1} > 0$ and $c_i = c_i(w)$ is given by (13). Furthermore, any solution $c' = c'(w)$ to this problem defines formally a solution to the original problem (1)-(3) by setting $c_{N+1} = 1 - \sum_{i=1}^N c_i$. We assume that there exists $0 < \eta < 1$ such that $c_i^0 \geq \eta$ for $i = 1, \dots, N$ and $c_{N+1}^0 = 1 - \sum_{i=1}^N c_i^0 \geq \eta$. Then $w_i^0 = \log(c_i^0/c_{N+1}^0)$ satisfies $w_i^0 \in L^\infty(\Omega)$, $i = 1, \dots, N$.

Step 1: Existence of an approximate system. Let $T > 0$, $m \in \mathbb{N}$ and set $\tau = T/m$, $t_k = \tau k$ for $k = 0, \dots, m$. We prove the existence of weak solutions to the approximate system

$$(24) \quad \begin{aligned} & \frac{1}{\tau} \int_{\Omega} (c'(w^k) - c'(w^{k-1})) \cdot v dx + \int_{\Omega} \nabla v : B(w^k) \nabla w^k dx \\ & + \varepsilon \int_{\Omega} (\Delta w^k \cdot \Delta v + w^k \cdot v) dx = \int_{\Omega} r'(c(w^k)) \cdot v dx, \quad v \in \mathcal{V}^N, \end{aligned}$$

where w^k approximates $w(\cdot, t_k)$ and $\varepsilon > 0$. The notation “:” signifies summation over both matrix indices; in particular,

$$\int_{\Omega} \nabla v : B(w^k) \nabla w^k dx = \sum_{i,j=1}^N \int_{\Omega} b_{ij}(w^k) \nabla v_i \cdot \nabla w_j^k dx,$$

and we recall that $\mathcal{V} = \{u \in H^2(\Omega) : \nabla u \cdot \nu = 0 \text{ on } \partial\Omega\}$. The implicit Euler discretization of the time derivative makes the system elliptic which avoids problems related to the regularity in time. The additional ε -term guarantees the coercivity of the elliptic system.

Lemma 7. *Let the assumptions of Theorem 1 hold and let $w^{k-1} \in L^\infty(\Omega)^N$. Then there exists a weak solution $w^k \in \mathcal{V}^N$ to (24).*

Proof. The idea of the proof is to apply the Leray-Schauder fixed-point theorem. Let $\bar{w} \in L^\infty(\Omega)^N$ and $\sigma \in [0, 1]$. We wish to find $w \in \mathcal{V}^N$ such that

$$(25) \quad a(w, v) = F(v) \quad \text{for all } v \in \mathcal{V}^N,$$

where

$$\begin{aligned} a(w, v) &= \int_{\Omega} \nabla v : B(\bar{w}) \nabla w dx + \varepsilon \int_{\Omega} (\Delta w \cdot \Delta v + w \cdot v) dx, \\ F(v) &= -\frac{\sigma}{\tau} \int_{\Omega} (c'(\bar{w}) - c'(w^{k-1})) \cdot v dx + \sigma \int_{\Omega} r'(c(\bar{w})) \cdot v dx. \end{aligned}$$

Since $B(\bar{w})$ is positive definite, by Lemma 6, the bilinear form a is coercive,

$$a(w, w) = \int_{\Omega} \sum_{i,j=1}^N b_{ij}(\bar{w}) \nabla w_i \cdot \nabla w_j dx + \varepsilon \int_{\Omega} (|\Delta w|^2 + |w|^2) dx \geq C\varepsilon \|w\|_{H^2(\Omega)^N}^2,$$

where $C > 0$ is a constant. The inequality follows from elliptic regularity, using the assumption $\partial\Omega \in C^{1,1}$. By Lemma 6 again, the elements of $B(\bar{w})$ are bounded uniformly in c , and thus, a is continuous in $\mathcal{V}^N \times \mathcal{V}^N$. Using $0 < c_i(\bar{w}), c_i(w^{k-1}) < 1$ and the continuity of r_i , we can show that F is bounded in \mathcal{V}^N . Then the Lax-Milgram lemma provides the existence of a unique solution $w \in \mathcal{V}^N$ to (25). Since the space dimension is assumed to be at most three, the embedding $H^2(\Omega) \hookrightarrow L^\infty(\Omega)$ is continuous (and compact) such that $w \in L^\infty(\Omega)^N$. This shows that the fixed-point operator $S : L^\infty(\Omega)^N \times [0, 1] \rightarrow L^\infty(\Omega)^N$, $S(\bar{w}, \sigma) = w$, is well-defined. By construction, $S(\bar{w}, 0) = 0$ for all $\bar{w} \in L^\infty(\Omega)^N$. Standard arguments show that S is continuous and compact. It remains to prove a uniform bound for all fixed points of $S(\cdot, \sigma)$ in $L^\infty(\Omega)^N$.

Let $w \in L^\infty(\Omega)^N$ be such a fixed point. Then w solves (25) with \bar{w} replaced by w . Taking the test function $v = w \in \mathcal{V}^N$, it follows that

$$\begin{aligned} & \frac{\sigma}{\tau} \int_{\Omega} (c'(w) - c'(w^{k-1})) \cdot w dx + \int_{\Omega} (\nabla w : B(w) \nabla w + \varepsilon (|\Delta w|^2 + |w|^2)) dx \\ (26) \quad & = \sigma \int_{\Omega} r'(c(w)) \cdot w dx. \end{aligned}$$

In order to estimate the first term on the left-hand side, we consider the entropy density h , defined in (10). Its Hessian is positive definite if $c_1, \dots, c_{N+1} > 0$ and hence, h is convex, i.e.

$$h(c) - h(\hat{c}) \leq \nabla h(c) \cdot (c - \hat{c}) \quad \text{for all } c, \hat{c} \in \mathbb{R}^N \text{ with } 0 < c_i, \hat{c}_i, \sum_{j=1}^N c_j, \sum_{j=1}^N \hat{c}_j < 1.$$

Using $w = \nabla h(c')$, we find that

$$\frac{\sigma}{\tau} \int_{\Omega} (c'(w) - c'(w^{k-1})) \cdot w dx \geq \frac{\sigma}{\tau} \int_{\Omega} (h(c'(w)) - h(c'(w^{k-1}))) dx.$$

By Lemma 6, B is positive definite:

$$\int_{\Omega} \nabla w : B(w) \nabla w dx \geq 0.$$

Finally, using the assumptions $\sum_{i=1}^N r_i(c) = -r_{N+1}(c)$ and $\sum_{i=1}^{N+1} r_i(c) \log c_i \leq 0$,

$$\begin{aligned} \int_{\Omega} r'(c(w)) \cdot w dx &= \int_{\Omega} \left(\sum_{i=1}^N r_i(c(w)) (\log c_i(w) - \log c_{N+1}(w)) \right) dx \\ &= \int_{\Omega} \sum_{i=1}^{N+1} r_i(c(w)) \log c_i(w) dx \leq 0. \end{aligned}$$

Therefore, (26) becomes

$$\sigma \int_{\Omega} h(c'(w)) dx + \varepsilon \tau \int_{\Omega} (|\Delta w|^2 + |w|^2) dx \leq \sigma \int_{\Omega} h(c'(w^{k-1})) dx.$$

This yields an H^2 bound uniform in w and σ (but depending on ε and τ). The embedding $H^2(\Omega) \hookrightarrow L^\infty(\Omega)$ implies the desired uniform bound in $L^\infty(\Omega)$, and the Leray-Schauder theorem gives a solution to (24). \square

Note that we obtain the uniform bounds also under the weaker condition (6). In this case, (26) can be estimated as

$$(27) \quad \sigma \int_{\Omega} h(c'(w)) dx + \varepsilon \tau \int_{\Omega} (|\Delta w|^2 + |w|^2) dx \leq \sigma \int_{\Omega} h(c'(w^{k-1})) dx + \sigma C_r \tau \text{meas}(\Omega).$$

Step 2: Entropy dissipation. Since the diffusion matrix $B(w^k)$ defines a self-adjoint endomorphism, the entropy-dissipation estimate

$$\int_{\Omega} \nabla w^k : B(w^k) \nabla w^k dx \geq \int_{\Omega} \lambda |\nabla w^k|^2 dx$$

holds, where λ is the smallest eigenvalue of $B(w^k)$. Unfortunately, λ depends on $c(w^k)$ and we do not have a positive lower bound independent of w^k . However, we are able to prove an entropy-dissipation inequality in the variables $\sqrt{c_i(w^k)}$ with a uniform positive lower bound. In the following, we employ the notation $f(c^k) = (f(c_1^k), \dots, f(c_{N+1}^k))^\top$ for arbitrary functions f .

Lemma 8. *Let $w^k \in \mathcal{V}^N$ be a weak solution to (24). Then*

$$\int_{\Omega} \nabla w^k : B(w^k) \nabla w^k dx \geq \frac{4}{\Delta} \int_{\Omega} |\nabla \sqrt{c^k}|^2 dx,$$

where $c^k = c(w^k) = (c_1(w^k), \dots, c_{N+1}(w^k))^\top$ is defined in (13) and $c_{N+1}(w^k) = 1 - \sum_{i=1}^N c_i(w^k)$.

Proof. First, we claim that

$$\int_{\Omega} \nabla w^k : B(w^k) \nabla w^k dx = \int_{\Omega} \nabla \log c^k : (-\tilde{A})^{-1} \nabla c^k dx,$$

where \tilde{A} is defined in Lemma 4. To prove this identity we set $z' = (z_1, \dots, z_N)^\top = B(w^k) \nabla w^k \in \mathbb{R}^{N \times d}$ and $z_{N+1} = -\sum_{i=1}^N z_i \in \mathbb{R}^d$. Then the definitions of w^k and z_{N+1} yield

$$(28) \quad \begin{aligned} \nabla w^k : B(w^k) \nabla w^k &= \nabla w^k : z' = \sum_{i=1}^N (\nabla \log c_i^k - \nabla \log c_{N+1}^k) \cdot z_i \\ &= \sum_{i=1}^{N+1} \nabla \log c_i^k \cdot z_i = \nabla \log c^k : z, \end{aligned}$$

where $z = (z', z_{N+1})^\top$. Using $\nabla w^k = H\nabla c'(w^k)$ and $B = A_0^{-1}H^{-1}$, where $H = H(c'(w^k))$ is the Hessian of h , it follows that $z' = A_0^{-1}\nabla c'(w^k)$ or, equivalently, $\nabla c'(w^k) = A_0 z'$. A computation shows that for $i = 1, \dots, N$,

$$\nabla c_i^k = (A_0 z')_i = \sum_{j=1, j \neq i}^N (d_{ij} - d_{i, N+1})(z_j c_j^k - z_j c_i^k) + d_{i, N+1} z_i = (-Az)_i = (-\tilde{A}z)_i,$$

since each column of z is an element of $\text{im}(A)$. Because of $\tilde{A}z \in \text{im}(A)$, we have $(-\tilde{A}z)_{N+1} = -\sum_{i=1}^N (-\tilde{A}z)_i = \nabla c_{N+1}^k$. We infer that $\nabla c^k = -\tilde{A}z$ and consequently, $z = (-\tilde{A})^{-1}\nabla c^k$. Inserting this into (28) proves the claim.

We recall from the proof of Lemma 4 that the images of $\tilde{A} = A|_{\text{im}(A)}$ and $\tilde{A}_S = A_S|_{\text{im}(A_S)}$ are given by $\text{im}(A) = \{\mathbf{1}\}^\perp$ and $\text{im}(A_S) = \text{span}\{\sqrt{c^k}\}^\perp = \{C^{-1/2}x : x \in \text{im}(A)\}$, where $C^{\pm 1/2} = \text{diag}((c_1^k)^{\pm 1/2}, \dots, (c_{N+1}^k)^{\pm 1/2}) \in \mathbb{R}^{(N+1) \times (N+1)}$. Then the definition $-A = C^{1/2}(-A_S)C^{-1/2}$ implies that $-\tilde{A} = C^{1/2}(-\tilde{A}_S)C^{-1/2}$ and hence, $(-\tilde{A}_S)^{-1} = C^{-1/2}(-\tilde{A})^{-1}C^{1/2}$. We infer that

$$\begin{aligned} \nabla \log c^k : (-\tilde{A})^{-1}\nabla c^k &= 4(\nabla \sqrt{c^k}) : C^{-1/2}(-\tilde{A})^{-1}C^{1/2}\nabla \sqrt{c^k} \\ &= 4\nabla \sqrt{c^k} : (-\tilde{A}_S)^{-1}\nabla \sqrt{c^k} \geq \frac{4}{\Delta} |\nabla \sqrt{c^k}|^2. \end{aligned}$$

The inequality follows from Lemma 4 since $(-\tilde{A}_S)^{-1}$ is a self-adjoint endomorphism whose smallest eigenvalue is larger than $1/\Delta$. \square

Step 3: A priori estimates. Next, we derive some estimates uniform in τ , ε , and η by means of the entropy-dissipation inequality. The following lemma is a consequence of (26), the proof of Lemma 7, and Lemma 8.

Lemma 9 (Discrete entropy inequality). *Let $w^k \in \mathcal{V}^N$ be a weak solution to (24). Then for $k \geq 1$,*

$$\mathcal{H}[c^k] + \frac{4\tau}{\Delta} \int_{\Omega} |\nabla \sqrt{c^k}|^2 dx + \varepsilon\tau \int_{\Omega} (|\Delta w^k|^2 + |w^k|^2) dx \leq \mathcal{H}[c^{k-1}],$$

where $c^k = c(w^k)$ and $\mathcal{H}[c^k] = \int_{\Omega} h(c^k) dx$. Solving this estimate recursively, it follows that

$$\mathcal{H}[c^k] + \frac{4\tau}{\Delta} \sum_{j=1}^k \int_{\Omega} |\nabla \sqrt{c^j}|^2 dx + \varepsilon\tau \sum_{j=1}^k \int_{\Omega} (|\Delta w^j|^2 + |w^j|^2) dx \leq \mathcal{H}[c^0].$$

Let $w^k \in \mathcal{V}^N$ be a weak solution to (24) and set $c^k = c(w^k)$. We define the piecewise-constant-in-time functions $w^{(\tau)}(x, t) = w^k(x)$ and $c^{(\tau)}(x, t) = (c_1^k, \dots, c_N^k)^\top(x)$ for $x \in \Omega$, $t \in ((k-1)\tau, k\tau]$, $k = 1, \dots, m$, $c^{(\tau)}(\cdot, 0) = (c_1^0, \dots, c_N^0)^\top$, and we introduce the discrete time derivative $D_\tau c^{(\tau)} = (c^{(\tau)} - \sigma_\tau c^{(\tau)})/\tau$ with the shift operator $(\sigma_\tau c^{(\tau)})(x, t) = c^{(\tau)}(x, t - \tau)$ for $x \in \Omega$, $t \in (\tau, T]$, $(\sigma_\tau c^{(\tau)})(x, t) = c^0(x)$ for $x \in \Omega$, $t \in (0, \tau]$. The functions $(c^{(\tau)}, w^{(\tau)})$ solve the following equation in the distributional sense:

$$(29) \quad D_\tau c^{(\tau)} - \text{div}(A_0^{-1}(c^{(\tau)})\nabla c^{(\tau)}) + \varepsilon(\Delta^2 w^{(\tau)} + w^{(\tau)}) = r'(c^{(\tau)}), \quad t > 0.$$

Lemma 9 implies the following a priori estimates.

Lemma 10. *There exists a constant $C > 0$ independent of ε , τ , and η such that*

$$(30) \quad \|\sqrt{c^{(\tau)}}\|_{L^2(0,T;H^1(\Omega))} + \sqrt{\varepsilon}\|w^{(\tau)}\|_{L^2(0,T;H^2(\Omega))} \leq C,$$

$$(31) \quad \|c^{(\tau)}\|_{L^2(0,T;H^1(\Omega))} + \|D_\tau c^{(\tau)}\|_{L^2(0,T;\mathcal{V}')} \leq C.$$

In the following, $C > 0$ denotes a generic constant independent of ε , τ , and η .

Proof. Estimate (30) is an immediate consequence of the entropy inequality of Lemma 9 and the L^∞ -bound for $c^{(\tau)}$. To prove (31), we employ the Hölder inequality:

$$\begin{aligned} \|\nabla c_i^{(\tau)}\|_{L^2(0,T;L^2(\Omega))}^2 &= 4 \int_0^T \|\sqrt{c_i^{(\tau)}} \nabla \sqrt{c_i^{(\tau)}}\|_{L^2(\Omega)}^2 dt \\ &\leq 4 \int_0^T \|\sqrt{c_i^{(\tau)}}\|_{L^\infty(\Omega)}^2 \|\nabla \sqrt{c_i^{(\tau)}}\|_{L^2(\Omega)}^2 dt \\ &\leq 4 \|c_i^{(\tau)}\|_{L^\infty(0,T;L^\infty(\Omega))} \|\nabla \sqrt{c_i^{(\tau)}}\|_{L^2(0,T;L^2(\Omega))}^2 \leq C, \end{aligned}$$

using (30) and the fact that $0 < c_i^{(\tau)} < 1$, $i = 1, \dots, N$. Here and in the following, $C > 0$ denotes a generic constant independent of ε , τ , and η . By (29) and $L^2(\Omega) \hookrightarrow (H^1(\Omega))'$,

$$\begin{aligned} \|D_\tau c^{(\tau)}\|_{L^2(0,T;\mathcal{V}')} &\leq C \|A_0^{-1} \nabla c^{(\tau)}\|_{L^2(0,T;L^2(\Omega))} \\ &\quad + \varepsilon C \|w^{(\tau)}\|_{L^2(0,T;H^2(\Omega))} + C \|r'(c^{(\tau)})\|_{L^2(0,T;L^2(\Omega))} \\ &\leq C \|A_0^{-1}\|_{L^\infty(0,T;L^\infty(\Omega))} \|\nabla c^{(\tau)}\|_{L^2(0,T;L^2(\Omega))} \\ &\quad + \varepsilon C \|w^{(\tau)}\|_{L^2(0,T;H^2(\Omega))} + C \|r'(c^{(\tau)})\|_{L^2(0,T;L^2(\Omega))}. \end{aligned}$$

The proof of Lemma 5 shows that the elements of A_0^{-1} are bounded by a constant which depends only on N and (D_{ij}) . Since $0 < c^{(\tau)} < 1$ and r' is continuous, $(r'(c^{(\tau)}))$ is bounded in $L^2(0,T;L^2(\Omega))$. Therefore, in view of (30) and the bound on $c^{(\tau)}$ in $L^2(0,T;H^1(\Omega))$,

$$\|D_\tau c^{(\tau)}\|_{L^2(0,T;\mathcal{V}')} \leq C,$$

finishing the proof. \square

Step 4: Limits $\varepsilon \rightarrow 0$ and $\tau \rightarrow 0$. We apply the compactness result of [12, Theorem 1] to the family $(c^{(\tau)})$. Since the embedding $H^1(\Omega) \hookrightarrow L^p(\Omega)$ is compact for $1 < p < 6$, (31) implies the existence of a subsequence, which is not relabeled, such that, as $(\varepsilon, \tau) \rightarrow 0$,

$$c^{(\tau)} \rightarrow c' = (c_1, \dots, c_N) \quad \text{strongly in } L^2(0,T;L^p(\Omega)), \quad 1 < p < 6.$$

As a consequence, $c_i \geq 0$, $\sum_{i=1}^N c_i \leq 1$, and $c_{N+1} = 1 - \sum_{i=1}^N c_i \geq 0$. Because of the uniform L^∞ -bounds for $c_i^{(\tau)}$, this convergence holds even in the space $L^q(\Omega \times (0,T))$ for all

$1 \leq q < \infty$. Furthermore, by (30)-(31), up to subsequences,

$$\begin{aligned}\nabla c^{(\tau)} &\rightharpoonup \nabla c' \quad \text{weakly in } L^2(0, T; L^2(\Omega)), \\ D_\tau c^{(\tau)} &\rightharpoonup \partial_t c' \quad \text{weakly in } L^2(0, T; \mathcal{V}'), \\ \varepsilon w^{(\tau)} &\rightarrow 0 \quad \text{strongly in } L^2(0, T; H^2(\Omega)).\end{aligned}$$

Since the elements of A_0^{-1} are bounded and $0 < c^{(\tau)} < 1$,

$$\begin{aligned}A_0(c^{(\tau)})^{-1} &\rightarrow A_0(c')^{-1} \quad \text{strongly in } L^q(0, T; L^q(\Omega)) \text{ for all } 1 \leq q < \infty, \\ r'(c^{(\tau)}) &\rightarrow r'(c) \quad \text{strongly in } L^2(0, T; L^2(\Omega)),\end{aligned}$$

setting $c = (c_1, \dots, c_{N+1})^\top$. The above convergence results are sufficient to pass to the limit $(\varepsilon, \tau) \rightarrow 0$ in the weak formulation of (29), showing that c satisfies

$$\partial_t c' - \operatorname{div}(A_0(c')^{-1} \nabla c') = r'(c) \quad \text{in } L^2(0, T; \mathcal{V}').$$

This proves the existence of a weak solution to (9) and (3) with initial data satisfying $c_i^0 \geq \eta > 0$ and $\sum_{i=1}^N c_i^0 \leq 1 - \eta$. In view of the uniform bounds and the finiteness of the initial entropy, we can perform the limit $\eta \rightarrow 0$ to obtain the existence result for general initial data with $c_i^0 \geq 0$ and $\sum_{i=1}^N c_i^0 \leq 1$. This proves Theorem 1.

4. PROOF OF THEOREM 2

First, we prove that, if the production rates vanish, the L^1 norms of the semi-discrete molar concentrations are bounded. We assume that there exists $0 < \eta < 1$ such that $c_i^0 \geq \eta$ for $i = 1, \dots, N + 1$.

Lemma 11 (Bounded L^1 norms). *Let $r = 0$. Then there exists a constant $\gamma_0 > 0$, only depending on c^0 , such that for all $0 < \gamma \leq \min\{1, \gamma_0\}$ and sufficiently small $\varepsilon > 0$, depending on γ , the semi-discrete concentrations $c^k = c(w^k)$, where $w^k \in \mathcal{V}^N$ solves (24), satisfy*

$$(32) \quad (1 - \gamma) \|c_i^0\|_{L^1(\Omega)} \leq \|c_i^k\|_{L^1(\Omega)} \leq (1 + \gamma) \|c_i^0\|_{L^1(\Omega)}, \quad i = 1, \dots, N, \quad k \in \mathbb{N},$$

$$(33) \quad \|c_{N+1}^0\|_{L^1(\Omega)} - \gamma \sum_{i=1}^N \|c_i^0\|_{L^1(\Omega)} \leq \|c_{N+1}^k\|_{L^1(\Omega)} \leq \|c_{N+1}^0\|_{L^1(\Omega)} + \gamma \sum_{i=1}^N \|c_i^0\|_{L^1(\Omega)}.$$

Furthermore, $\|c_{N+1}^k\|_{L^1(\Omega)} \geq \frac{1}{2} \|c_{N+1}^0\|_{L^1(\Omega)} > 0$.

Proof. We recall that $\tau = T/m$ for $T > 0$ and $m \in \mathbb{N}$. Let $k \in \{1, \dots, m\}$. Using the test function $v = e_i$ in (24), where e_i is the i -th unit vector of \mathbb{R}^N , we find that

$$\int_{\Omega} c_i^k dx = \int_{\Omega} c_i^{k-1} dx - \varepsilon \tau \int_{\Omega} w_i^k dx, \quad i = 1, \dots, N,$$

where we abbreviated $c_i^k = c_i(w^k)$. Solving these recursive equations, we obtain

$$(34) \quad \int_{\Omega} c_i^k dx = \int_{\Omega} c_i^0 dx - \varepsilon \tau \sum_{j=1}^k \int_{\Omega} w_i^j dx.$$

Because of the ε -terms, we do not have discrete mass conservation but we will derive uniform L^1 -bounds. The entropy inequality in Lemma 9 shows that

$$(35) \quad \begin{aligned} \mathcal{H}[c^k] + \varepsilon\tau \int_{\Omega} ((\Delta w_i^k)^2 + (w_i^k)^2) dx &\leq \mathcal{H}[c^k] + \varepsilon\tau \int_{\Omega} (|\Delta w^k|^2 + |w^k|^2) dx \\ &\leq \mathcal{H}[c^{k-1}], \quad k \geq 1. \end{aligned}$$

Solving this inequality recursively, we infer from $\mathcal{H}[c^k] \geq -\text{meas}(\Omega)(N+1)$ that

$$\varepsilon\tau \sum_{j=1}^k \|w_i^j\|_{L^2(\Omega)}^2 \leq \mathcal{H}[c^0] - \mathcal{H}[c^k] \leq \mathcal{H}[c^0] + \text{meas}(\Omega)(N+1).$$

Consequently, using $k\tau \leq T$,

$$\begin{aligned} \varepsilon\tau \sum_{j=1}^k \int_{\Omega} |w_i^j| dx &\leq \varepsilon\tau C \sum_{j=1}^k \|w_i^j\|_{L^2(\Omega)} \leq \varepsilon\tau C \sqrt{k} \left(\sum_{j=1}^k \|w_i^j\|_{L^2(\Omega)}^2 \right)^{1/2} \\ &\leq C \sqrt{\varepsilon\tau k (\mathcal{H}[c^0] + \text{meas}(\Omega)(N+1))} \\ &\leq C \sqrt{\varepsilon T (\mathcal{H}[c^0] + \text{meas}(\Omega)(N+1))}. \end{aligned}$$

Let $\gamma > 0$ and $0 < \varepsilon < 1$ satisfy

$$(36) \quad 0 < \gamma \leq \min \left\{ 1, \gamma_0 = \left(2 \sum_{i=1}^N \|c_i^0\|_{L^1(\Omega)} \right)^{-1} \|c_{N+1}^0\|_{L^1(\Omega)} \right\},$$

$$(37) \quad 0 < \sqrt{\varepsilon} \leq \frac{\gamma \min_{\ell=1, \dots, N} \|c_{\ell}^0\|_{L^1(\Omega)}}{C \sqrt{T (\mathcal{H}[c^0] + \text{meas}(\Omega)(N+1))}}.$$

Then, in view of (34),

$$(1 - \gamma) \|c_i^0\|_{L^1(\Omega)} \leq \|c_i^k\|_{L^1(\Omega)} = \|c_i^0\|_{L^1(\Omega)} - \varepsilon\tau \sum_{j=1}^k \int_{\Omega} w_i^j dx \leq (1 + \gamma) \|c_i^0\|_{L^1(\Omega)}.$$

These relations hold for all $i = 1, \dots, N$. For $i = N+1$, we estimate (using (32))

$$\begin{aligned} \int_{\Omega} c_{N+1}^k dx &= \int_{\Omega} \left(1 - \sum_{i=1}^N c_i^k \right) dx \geq \int_{\Omega} \left(1 - (1 + \gamma) \sum_{i=1}^N c_i^0 \right) dx \\ &= \int_{\Omega} c_{N+1}^0 dx - \gamma \sum_{i=1}^N \int_{\Omega} c_i^0 dx \geq \frac{1}{2} \|c_{N+1}^0\|_{L^1(\Omega)} > 0, \end{aligned}$$

by definition of γ_0 . A similar computation yields

$$\int_{\Omega} c_{N+1}^k dx \leq \int_{\Omega} \left(1 - (1 - \gamma) \sum_{i=1}^N c_i^0 \right) dx = \|c_{N+1}^0\|_{L^1(\Omega)} + \gamma \sum_{i=1}^N \|c_i^0\|_{L^1(\Omega)}.$$

This proves the lemma. \square

For the proof of Theorem 2, we introduce the following notations: $c^k = (c_1^k, \dots, c_{N+1}^k)^\top$, $\bar{c}^k = (\bar{c}_1^k, \dots, \bar{c}_{N+1}^k)^\top$, where $\bar{c}_i^k = \text{meas}(\Omega)^{-1} \int_{\Omega} c_i^k dx$ for $i = 1, \dots, N+1$, $k \geq 0$. Furthermore, we set $w^k = (w_1^k, \dots, w_N^k)^\top$, and $\bar{w}^k = (\bar{w}_1^k, \dots, \bar{w}_N^k)^\top$, where $\bar{w}_i^k = \log(\bar{c}_i^k / \bar{c}_{N+1}^k)$ for $i = 1, \dots, N$. We recall the definition of the relative entropy

$$\mathcal{H}^*[c^k] = \sum_{i=1}^{N+1} \int_{\Omega} c_i^k \log \frac{c_i^k}{\bar{c}_i^k} dx.$$

Employing the test function $w^k - \bar{w}^k$ in (24), we obtain

$$\begin{aligned} \frac{1}{\tau} \int_{\Omega} (c'(w^k) - c'(w^{k-1})) \cdot (w^k - \bar{w}^k) dx + \int_{\Omega} \nabla w^k : B(w^k) \nabla w^k dx \\ + \varepsilon \int_{\Omega} (|\Delta w^k|^2 + w^k \cdot (w^k - \bar{w}^k)) dx = 0. \end{aligned}$$

We estimate the integrals term by term.

Using the definition $c_{N+1}^k = 1 - \sum_{i=1}^N c_i^k$, a computation shows that

$$(c'(w^k) - c'(w^{k-1})) \cdot w^k = (c^k - c^{k-1}) \cdot \log c^k.$$

Therefore, we find that

$$\begin{aligned} \int_{\Omega} (c'(w^k) - c'(w^{k-1})) \cdot (w^k - \bar{w}^k) dx &= \int_{\Omega} (c^k - c^{k-1}) \cdot \log \frac{c^k}{\bar{c}^k} dx \\ &= \int_{\Omega} (c^k - c^{k-1}) \cdot \log \frac{c^k}{\bar{c}^0} dx + \int_{\Omega} (c^k - c^{k-1}) \cdot \log \frac{\bar{c}^0}{\bar{c}^k} dx. \end{aligned}$$

The first integral on the right-hand side can be estimated by employing the convexity of $h(c)$ as a function of c_1, \dots, c_{N+1} , which implies that

$$\begin{aligned} h(c(w^k)) - h(c(w^{k+1})) &\leq \nabla h(c(w^k)) \cdot (c(w^k) - c(w^{k-1})) \\ &= \log(c^k) \cdot (c^k - c^{k-1}). \end{aligned}$$

Thus, because of $\sum_{i=1}^{N+1} c_i^k = 1$ and the definition of $\mathcal{H}^*[c^k]$,

$$\int_{\Omega} (c^k - c^{k-1}) \cdot \log \frac{c^k}{\bar{c}^0} dx \geq \mathcal{H}^*[c^k] - \mathcal{H}^*[c^{k-1}].$$

For the second integral, we employ the bounds (32)-(33) as well as $\gamma < 1$ and $\varepsilon > 0$ sufficiently small, which yields

$$\frac{1}{1+\gamma} \leq \frac{\bar{c}_i^0}{\bar{c}_i^k} \leq \frac{1}{1-\gamma}, \quad i = 1, \dots, N, \quad \frac{1}{1+\bar{\gamma}} \leq \frac{\bar{c}_{N+1}^0}{\bar{c}_{N+1}^k} \leq \frac{1}{1-\bar{\gamma}},$$

where $\bar{\gamma} = \gamma(1/\bar{c}_{N+1}^0 - 1) > 0$. Here, we have used again that $\sum_{i=1}^{N+1} \bar{c}_i^0 = 1$. Then, with $C_1 = \text{meas}(\Omega)$,

$$\begin{aligned} \int_{\Omega} (c^k - c^{k-1}) \cdot \log \frac{\bar{c}^0}{c^k} dx &\geq - \int_{\Omega} \sum_{i=1}^N c_i^k \log(1 + \gamma) dx - \int_{\Omega} c_{N+1}^k \log(1 + \bar{\gamma}) dx \\ &\quad + \int_{\Omega} \sum_{i=1}^N c_i^{k-1} \log(1 - \gamma) dx + \int_{\Omega} c_{N+1}^{k-1} \log(1 - \bar{\gamma}) dx \\ &\geq -C_1 \log \frac{(1 + \gamma)(1 + \bar{\gamma})}{(1 - \gamma)(1 - \bar{\gamma})}. \end{aligned}$$

We have already proved that

$$\int_{\Omega} \nabla w^k : B(w^k) \nabla w^k dx \geq \frac{4}{\Delta} \int_{\Omega} |\nabla \sqrt{c^k}|^2 dx.$$

Applying Young's inequality to the ε -term, it follows that

$$\mathcal{H}^*[c^k] - \mathcal{H}^*[c^{k-1}] + \frac{4\tau}{\Delta} \int_{\Omega} |\nabla \sqrt{c^k}|^2 dx \leq \frac{\varepsilon\tau}{2} \int_{\Omega} |\bar{w}^k|^2 dx + C_1 \log \frac{(1 + \gamma)(1 + \bar{\gamma})}{(1 - \gamma)(1 - \bar{\gamma})}.$$

The logarithmic Sobolev inequality [16] as well as the bounds (32)-(33) show that

$$\begin{aligned} \mathcal{H}^*[c^k] &= \sum_{i=1}^{N+1} \int_{\Omega} c_i^k \log \frac{c_i^k}{\bar{c}_i^k} dx + \sum_{i=1}^{N+1} \int_{\Omega} c_i^k \log \frac{\bar{c}_i^k}{c_i^0} dx \\ &\leq C(\Omega) \sum_{i=1}^{N+1} \int_{\Omega} |\nabla \sqrt{c_i^k}|^2 dx + \sum_{i=1}^N \int_{\Omega} c_i^k \log(1 + \gamma) dx + \int_{\Omega} c_{N+1}^k \log(1 + \bar{\gamma}) dx \\ &\leq C(\Omega) \int_{\Omega} |\nabla \sqrt{c^k}|^2 dx + C_1 \log((1 + \gamma)(1 + \bar{\gamma})), \end{aligned}$$

from which we infer that

$$(1 + C_2\tau)\mathcal{H}^*[c^k] \leq \mathcal{H}^*[c^{k-1}] + \frac{\varepsilon\tau}{2} \int_{\Omega} |\bar{w}^k|^2 dx + C_{\gamma},$$

where $C_2 = 4/(C(\Omega)\Delta)$ and, for $\tau \leq 1$,

$$C_{\gamma} = C_1 \log \frac{(1 + \gamma)(1 + \bar{\gamma})}{(1 - \gamma)(1 - \bar{\gamma})} + \frac{4C_1}{C(\Omega)\Delta} \log((1 + \gamma)(1 + \bar{\gamma})).$$

We can estimate \bar{w}^k by using the bounds for \bar{c}^k of Lemma 11:

$$\int_{\Omega} |\bar{w}^k|^2 dx \leq \sum_{i=1}^N \int_{\Omega} (|\log \bar{c}_i^k| + |\log \bar{c}_{N+1}^k|)^2 dx \leq C_3,$$

where $C_3 > 0$ depends on the L^1 -norm of c^0 and γ . Hence

$$\mathcal{H}^*[c^k] \leq (1 + C_2\tau)^{-1} \mathcal{H}^*[c^{k-1}] + \frac{\varepsilon\tau}{2} C_3 (1 + C_2\tau)^{-1} + C_{\gamma} (1 + C_2\tau)^{-1}.$$

Solving these recursive inequalities, we conclude that

$$\mathcal{H}^*[c^k] \leq (1 + C_2\tau)^{-k} \mathcal{H}^*[c^0] + \frac{\varepsilon\tau}{2} C_3 \sum_{j=1}^k (1 + C_2\tau)^{-j} + C_\gamma \sum_{j=1}^k (1 + C_2\tau)^{-j}.$$

The sum contains the first terms of the geometric series:

$$\sum_{j=1}^k (1 + C_2\tau)^{-j} \leq \frac{1}{1 - (1 + C_2\tau)^{-1}} - 1 = \frac{1}{C_2\tau},$$

yielding

$$\mathcal{H}^*[c^{(\tau)}(\cdot, t)] \leq (1 + C_2\tau)^{-t/\tau} \mathcal{H}^*[c^0] + \frac{\varepsilon C_3}{2C_2} + \frac{C_\gamma}{C_2\tau}, \quad t > 0.$$

Now, we choose sequences for ε , τ , and γ such that $\gamma \rightarrow 0$, $C_\gamma/\tau \rightarrow 0$, and (37) is satisfied (then also $\varepsilon \rightarrow 0$). This is possible since $C_\gamma \rightarrow 0$ as $\gamma \rightarrow 0$. Then, because of $c_i^{(\tau)} \rightarrow c_i$ in $L^2(0, T; L^2(\Omega))$ for $i = 1, \dots, N + 1$, the limit $(\varepsilon, \tau, \gamma) \rightarrow 0$ leads to

$$\mathcal{H}^*[c(\cdot, t)] \leq e^{-C_2 t} \mathcal{H}^*[c^0], \quad t \geq 0.$$

Moreover, we can pass to the limit $\eta \rightarrow 0$. Finally, since $\int_\Omega c_i(\cdot, t) dx = \int_\Omega c_i^0 dx$ for $i = 1, \dots, N + 1$ (see Lemma 11), we can apply the Csiszár-Kullback inequality [26] to finish the proof.

APPENDIX A. DERIVATION OF THE MAXWELL-STEFAN RELATIONS

The Maxwell-Stefan relations (2) for an ideal gas mixture of $N+1$ components are derived by assuming that the thermodynamical driving force d_i of the i -th component balances the friction force f_i . We suppose constant temperature and pressure. Our derivation follows [4]. For details on the modeling, we refer to the monographs [15, 27].

The driving force d_i is assumed to be proportional to the gradient of the chemical potential μ_i [27, Section 3.3]:

$$(38) \quad d_i = \frac{c_i}{RT} \nabla \mu_i, \quad i = 1, \dots, N + 1.$$

Here, R is the gas constant, T the (constant) temperature, and $c_i = \rho_i/m_i$ is the molar concentration of the i -th species with the mass density ρ_i and the molar mass m_i of the i -th species. For more general expressions of d_i , we refer to [15, Chapter 7]. The chemical potential under isothermal, isobaric conditions is defined by $\mu_i = \partial G/\partial c_i$, where G is the Gibbs free energy. In an ideal gas, we have $\nabla \mu_i = RT \nabla \log c_i$ implying that $d_i = \nabla c_i$.

The mutual friction force between the i -th and the j -th component is supposed to be proportional to the relative velocity and the amount of molar mass such that

$$(39) \quad f_i = - \sum_{j=1, j \neq i}^{N+1} \frac{c_i c_j (u_i - u_j)}{D_{ij}},$$

where D_{ij} are the binary Maxwell-Stefan diffusivities [21, Formula (16)]. By the Onsager reciprocal relation, the diffusion matrix (D_{ij}) is symmetric [20]. Then, using (38), (39), and the definition $J_k = c_k u_k$, the balance $d_i = f_i$ becomes

$$\nabla c_i = - \sum_{j=1, j \neq i}^{N+1} \frac{c_j J_i - c_i J_j}{D_{ij}}, \quad i = 1, \dots, N+1,$$

which equals (2).

Another derivation of the Maxwell-Stefan equations (1) and (2) starts from the Boltzmann transport equation for an isothermal ideal gas mixture [6]. The main assumptions are that a diffusion scaling is possible and that the scattering rates are independent of the microscopic velocities. Then, in the formal limit of vanishing mean-free paths, (1) and (2) are derived. The diffusivities D_{ij} are determined by

$$D_{ij} = \frac{T(m_i + m_j)}{m_i m_j S_{ij}},$$

where S_{ij} are the averaged scattering rates of the collision operator associated to the components i and j . Since $S_{ij} = S_{ji}$, the diffusion matrix (D_{ij}) is symmetric. We also observe that (D_{ij}) does not depend on the concentrations which is consistent with the assumption made in this paper.

APPENDIX B. MATRIX ANALYSIS

We recall some results on the eigenvalues of special matrices such as symmetric, quasi-positive, or rank-one matrices. Although most of the results in this appendix are valid for matrices with complex elements, we consider the real case only and refer to the literature for the general situation [18, 23, 25].

A vector $x \in \mathbb{R}^n$ ($n \in \mathbb{N}$) is called *positive* if all components are nonnegative and at least one component is positive. It is called *strictly positive* if all components are positive [25]. Let $A = (a_{ij}) \in \mathbb{R}^{n \times n}$ be a square matrix. The unit matrix in $\mathbb{R}^{n \times n}$ is denoted by I_n . Let $\sigma(A)$ denote the spectrum of A . The spectral radius of A is defined by $r(A) = \max\{|\lambda| : \lambda \in \sigma(A)\}$, and the spectral bound of A equals $s(A) = \max\{\Re(\lambda) : \lambda \in \sigma(A)\}$. An eigenvalue of A is called *semisimple* if its algebraic and geometric multiplicities coincide and *simple* if its algebraic multiplicity (and hence also its geometric multiplicity) equals one. The following theorem is proved in [23, Theorem 3.4].

Theorem 12. *Let $A \in \mathbb{R}^{n \times n}$ and let $\lambda \in \sigma(A)$ be a real eigenvalue. Then λ is semisimple if and only if*

$$\mathbb{R}^n = \text{im}(A - \lambda I_n) \oplus \ker(A - \lambda I_n).$$

The matrix A is called *quasi-positive* if $A \neq 0$ and $a_{ij} \geq 0$ for all $i \neq j$ and *irreducible* if for any proper nonempty subset $M \subset \{1, \dots, n\}$ there exist $i \in M$ and $j \notin M$ such that $a_{ji} \neq 0$. If $n = 1$, A is called irreducible if $A \neq 0$. For quasi-positive and irreducible matrices, the following result holds [25, Theorem A.45, Remark A.46].

Theorem 13 (Perron-Frobenius). *Let A be a quasi-positive and irreducible matrix. Then its spectral bound $s(A)$ is a simple eigenvalue of A associated with a strictly positive eigenvector and $s(A) > \Re(\lambda)$ for all $\lambda \in \sigma(A)$, $\lambda \neq s(A)$. All eigenvalues of A different from $s(A)$ have no positive eigenvector.*

The spectrum of rank-one matrices can be determined explicitly [23, Section 3.8, Lemma 2]. Notice that any rank-one matrix $A \in \mathbb{R}^{n \times m}$ can be written in the form $A = x \otimes y$, where $x \in \mathbb{R}^n$, $y \in \mathbb{R}^m$.

Proposition 14 (Spectrum of rank-one matrix). *Let $x, y \in \mathbb{R}^n$. Then $\sigma(x \otimes y) = \{0, \dots, 0, x \cdot y\}$, i.e., $x \cdot y$ is a simple eigenvalue.*

We recall two results on eigenvalues of products and sums of symmetric matrices.

Theorem 15. *Let $A \in \mathbb{R}^{n \times n}$ be symmetric and positive definite and let $B \in \mathbb{R}^{n \times n}$ be symmetric. Then the number of positive eigenvalues of AB equals that for B .*

For a proof, we refer to [23, Prop. 6.1].

Theorem 16 (Weyl). *Let $A, B \in \mathbb{R}^{n \times n}$ be symmetric and let the eigenvalues $\lambda_i(A)$ of A and $\lambda_i(B)$ of B be arranged in increasing order. Then, for $i = 1, \dots, n$,*

$$\lambda_i(A) + \lambda_1(B) \leq \lambda_i(A + B) \leq \lambda_i(A) + \lambda_n(B).$$

A proof is given in [18, Theorem 4.3.1].

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