Equilibration for chemically reacting flows with Maxwell-Stefan diffusion

Esther Daus(1), **Ansgar Jüngel**(2), **and Bao Quoc Tang**(3)

(1) D-fine Austria GmbH,
Seilerstätte 13, 1010 Vienna, Austria
(2) Technical University Vienna
Wiedner Hauptstrasse 8-10, 1040 Vienna, Austria
(3) University of Graz
Heinrichstrasse 36, 8010 Graz, Austria

e-mail: `quoc.tang@uni-graz.at`

The large-time asymptotics of weak solutions to Maxwell–Stefan diffusion systems for chemically reacting fluids with different molar masses and reversible reactions are investigated. More precisely, we consider the following reactions of N chemical species

$$\alpha_1^a A_1 + \cdots + \alpha_n^a A_n \underset{k_f^a}{\overset{k_b^a}{\rightleftharpoons}} \beta_1^a A_1 + \cdots + \beta_n^a A_n, \quad a = 1, \ldots, N$$

which results in the evolution system with Maxwell-Stefan diffusion

$$\partial_t \rho_i + \nabla \cdot \boldsymbol{j}_i = r_i(\boldsymbol{x}), \quad \nabla x_i = -\sum_{j=1}^{n} \frac{\rho_j \boldsymbol{j}_i - \rho_i \boldsymbol{j}_j}{c^2 M_i M_j D_{ij}}, \ i = 1, \ldots, n, \tag{1}$$

where ρ_i is partial mass density, M_i is the molar mass, $c_i = \rho_i / M_i$ is the partial concentration, $c = \sum_{i=1}^n c_i$ is the total concentration, and $x_i = c_i / c$ is the molar fraction, and

$$r_i(\boldsymbol{x}) = M_i \sum_{a=1}^{N} (\beta_i^a - \alpha_i^a) \left(k_f^a \boldsymbol{x}^{\boldsymbol{\alpha}^a} - k_b^a \boldsymbol{x}^{\boldsymbol{\beta}^a} \right), \quad \boldsymbol{x}^{\boldsymbol{\alpha}^a} = \prod_{i=1}^{n} x_i^{\alpha_i^a}.$$

The diffusion matrix of the system is generally neither symmetric nor positive definite, but the equations admit a formal gradient-flow structure which provides entropy (free energy) estimates. The main result is the exponential decay to the unique equilibrium with a rate that is constructive up to a finite-dimensional inequality.

Theorem 1 ([1]). *Assume detailed balance condition. Then there exists a non-negative global weak solution to* (1)*. Moreover, if there are no boundary equilibria, then the solution converges exponentially to equilibrium with constructive rates, i.e.*

$$\sum_{i=1}^{n} \|x_i(t) - x_{i,\infty}\|_{L^p(\Omega)} \le C_p e^{-\lambda_p t} \quad \forall t > 0, \forall p \ge 1.$$

The key elements of the proof are the existence of a unique detailed-balance equilibrium and the derivation of an inequality relating the entropy and the entropy production. The main difficulty comes from the fact that the reactions are represented by molar fractions while the conservation laws hold for the concentrations. The idea is to enlarge the space of n partial concentrations by adding the total concentration, viewed as an independent variable, thus working with $n+1$ variables. Further results concern the existence of global bounded weak solutions to the parabolic system and an extension of the results to complex-balance systems.

References

[1] Esther S. Daus, Ansgar Jüngel, and Bao Quoc Tang. "Exponential time decay of solutions to reaction-cross-diffusion systems of Maxwell–Stefan type." *Archive for rational mechanics and analysis* **235.2** (2020): 1059–1104.