Weierstraß-Institut

für Angewandte Analysis und Stochastik

Leibniz-Institut im Forschungsverbund Berlin e. V.

Uniform global bounds for solutions of an implicit Voronoi finite volume method for reaction-diffusion problems

André Fiebach, Annegret Glitzky , Alexander Linke

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Weierstrass Institute
Mohrenstr. 39
10117 Berlin
Germany
email: Andre.Fiebach@wias-berlin.de
        Annegret.Glitzky@wias-berlin.de
        Alexander.Linke@wias-berlin.de

Abstract

We consider discretizations for reaction-diffusion systems with nonlinear diffusion in two space dimensions. The applied model allows to handle heterogeneous materials and uses the chemical potentials of the involved species as primary variables. We propose an implicit Voronoi finite volume discretization on regular Delaunay meshes that allows to prove uniform, mesh-independent global upper and lower L^∞ bounds for the chemical potentials. These bounds provide the main step for a convergence analysis for the full discretized nonlinear evolution problem. The fundamental ideas are energy estimates, a discrete Moser iteration and the use of discrete Gagliardo-Nirenberg inequalities. For the proof of the Gagliardo-Nirenberg inequalities we exploit that the discrete Voronoi finite volume gradient norm in $2d$ coincides with the gradient norm of continuous piecewise linear finite elements.

1 Introduction and model equations

In a bounded domain $\Omega \subset \mathbb{R}^2$ we consider m species X_ν with initial densities U_ν which underly diffusion processes and undergo chemical reactions. The relation between the densities u_ν of the species X_ν and the corresponding chemical potentials v_ν is assumed to be given by Boltzmann statistics, i.e.,

$$u_\nu = \overline{u}_\nu \, e^{v_\nu}, \ \ \nu = 1, \ldots, m. \tag{1}$$

The reference densities $\overline{u}_\nu$ may depend on the spatial position and express the possible heterogeneity of the system under consideration. For the mass fluxes j_ν we make the ansatz

$$j_\nu = -D_\nu(\cdot, e^{v_1}, \ldots, e^{v_m}) u_\nu \nabla v_\nu, = -D_\nu \bar{u}_\nu \, e^{v_\nu} \nabla v_\nu, \ \ \nu = 1, \ldots, m, \tag{2}$$

with diffusion coefficients $D_\nu : \Omega \times \mathbb{R}^m \to \mathbb{R}_+$ which are allowed to depend on the space variable and the state variable. To describe chemical reactions we introduce a finite subset $\mathcal{R} \subset \mathbb{Z}_+^m \times \mathbb{Z}_+^m$. Each pair $(\alpha, \beta) \in \mathcal{R}$ represents the vectors of stoichiometric coefficients of a reversible reaction, written in the form

$$\alpha_1 X_1 + \cdots + \alpha_m X_m \rightleftharpoons \beta_1 X_1 + \cdots + \beta_m X_m.$$
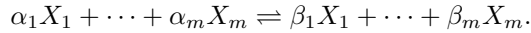
According to the mass action law, the net rate of this pair of reactions is of the form $k_{\alpha\beta}(a^\alpha - a^\beta)$, where $k_{\alpha\beta}$ is a reaction coefficient, $a_\nu := \exp(v_\nu)$ corresponds to the chemical activity of X_ν, and $a^\alpha := \prod_{\nu=1}^m a_\nu^{\alpha_\nu}$. The net production rate of species X_ν corresponding to all accruing reactions is

$$R_\nu := \sum_{(\alpha,\beta) \in \mathcal{R}} k_{\alpha\beta}(a^\alpha - a^\beta)(\beta_\nu - \alpha_\nu). \tag{3}$$

In this notation our reaction-diffusion system consists of m continuity equations with no flux boundary conditions on $\Gamma = \partial\Omega$:

$$\frac{\partial u_\nu}{\partial t} + \nabla \cdot j_\nu = R_\nu \text{ in } \mathbb{R}_+ \times \Omega, \quad \mathbf{n} \cdot j_\nu = 0 \text{ on } \mathbb{R}_+ \times \Gamma,$$
$$u_\nu(0) = U_\nu \text{ in } \Omega, \quad \nu = 1, \ldots, m. \tag{4}$$

The aim of the paper consists in a study of a discretization scheme (Euler backward in time and Voronoi finite volume meshes in space) of Problem (4). It is strongly desired to retain the analytic properties of the continuous problem also in the discretization scheme.

We prove the solvability of the discretized problems and derive global with respect to time a priori estimates for the discretized solutions. Starting from energy estimates we prove as main results of the paper upper bounds and strictly positive lower bounds for the discretized densities. Our special aim is to find uniform bounds (being independent of the underlying mesh) for classes of Voronoi finite volume meshes. The characterization of these classes of meshes is given in (A2). Similar to the continuous setting we use a Moser iteration technique to obtain the uniform upper and lower bounds. This procedure involves the application of a discrete Gagliardo-Nirenberg inequality in the setting of Voronoi finite volume schemes, where the constants are uniform for classes of meshes described by (A2).

In Section 2 we collect the general assumptions concerning the data of the continuous problem and give a summary on results obtained so far for the continuous problem. The main results of the paper concerning the discretization scheme are formulated and proven in Section 3. We start with the description of the discretization, give a local existence result, summarize physically motivated estimates, show uniform global upper bounds of the discretized solution, discuss their asymptotic behavior and derive positive uniform global lower bounds of the densities. These bounds provide the main step for a convergence analysis for the full discretized nonlinear evolution problem in the spirit of [7]. We will present such a convergence analysis in a subsequent paper.

In Appendix A we prove the discrete Gagliardo-Nirenberg inequality in the setting of Voronoi finite volume schemes. Appendix B contains technical lemmas necessary for the treatment of the test functions in the a priori estimates.

2 The continuous problem

2.1 General assumptions on the data

In this section we formulate basic assumptions with respect to the data of the problem, see [13,9].

First we introduce:

Definition 1 (Reaction order, see [9]) A source term of a reaction is of order k, iff there exists a $c > 0$ such that

$$\max_{\nu=1,\ldots,m} \left\{ (\beta_\nu - \alpha_\nu) \left(a^{\boldsymbol{\alpha}} - a^{\boldsymbol{\beta}} \right) \right\} \le c \left(1 + \sum_{\nu=1}^m a_\nu^k \right) \tag{5}$$

$$\forall a \in \mathbb{R}_+^m, \ \forall (\boldsymbol{\alpha}, \boldsymbol{\beta}) \in \mathcal{R}.$$

We will study the problem under the following assumptions:

(A1) $\Omega \subset \mathbb{R}^2$ is a *bounded Lipschitzian domain*, $\Gamma := \partial\Omega$.

Let $m \in \mathbb{N}$ be given and $\mathcal{R}$ a finite subset of $\mathbb{Z}_+^m \times \mathbb{Z}_+^m$. For all $(\boldsymbol{\alpha}, \boldsymbol{\beta}) \in \mathcal{R}$ the reaction rates $k_{(\boldsymbol{\alpha},\boldsymbol{\beta})} : \Omega \times \mathbb{R}^m \to \mathbb{R}_+$ satisfy the *Carathéodory condition* and there exist positive real constants c, C such that $0 < c \le k_{(\boldsymbol{\alpha},\boldsymbol{\beta})}(\boldsymbol{x}, \boldsymbol{y}) \le C < \infty$, f.a.a. $\boldsymbol{x} \in \Omega$, $\forall \boldsymbol{y} \in \mathbb{R}^m$. Source terms of reactions are at most quadratic.

The diffusion coefficients $D_\nu : \Omega \times \mathbb{R}^m \to \mathbb{R}_+$ satisfy the *Carathéodory condition* and $0 < c \le D_\nu(\boldsymbol{x}, \boldsymbol{y}) \le C < \infty$, f.a.a. $\boldsymbol{x} \in \Omega$, $\forall \boldsymbol{y} \in \mathbb{R}^m$ and $\nu = 1, \ldots, m$.

Finally, $\overline{u}_\nu, U_\nu \in L^\infty(\Omega)$ and there exist positive real constants c, C such that $\overline{u}_\nu(\boldsymbol{x}), U_\nu(\boldsymbol{x}) \ge c$ f.a.a. $\boldsymbol{x} \in \Omega$ and $\forall \nu = 1, \ldots, m$.

2.2 Summary of known results for the continuous problem

Let $u := (u_1, \ldots, u_m)$, $v := (v_1, \ldots, v_m)$ denote the vector functions of densities and chemical potentials. In the setting of bounded Lipschitzian domains $\Omega \subset \mathbb{R}^2$, of nonnegative L^∞ coefficients and strictly positive diffusivities, reference densities, and initial densities, a weak formulation

$$\left. \begin{array}{l} u'(t) + Av(t) = 0, \ u(t) = Ev(t) \text{ f.a.a. } t \in \mathbb{R}_+, \ u(0) = U, \\ u \in H^1_{\text{loc}}(\mathbb{R}_+; H^1(\Omega, \mathbb{R}^m)^*), \\ v \in L^2_{\text{loc}}(\mathbb{R}_+; H^1(\Omega, \mathbb{R}^m)) \cap L^\infty_{\text{loc}}(\mathbb{R}_+; L^\infty(\Omega, \mathbb{R}^m)) \end{array} \right\} \tag{P}$$

of (4) is discussed in several papers. The operator A in (P) contains the reaction and diffusion terms of (4) and the operator E incorporates the statistical relation (1). Such problems have been investigated in various papers, see e.g. [20, 13]; the papers [9, 10, 16, 17, 18] treat also electrically charged species, such that the flux terms additionally contain drift contributions and a Poisson equation for the self consistent calculation of the electrostatic potential is added to (4). The papers [9, 10, 14, 16] additionally deal with more general state equations than (1). We shortly summarize results for the continuous reaction-diffusion system (4) obtained in the cited papers.

By means of the stoichiometric subspace $\mathcal{S} := \text{span}\{\boldsymbol{\alpha} - \boldsymbol{\beta} : (\boldsymbol{\alpha}, \boldsymbol{\beta}) \in \mathcal{R}\}$ we define some compatibility class

$$\mathcal{U} := \left\{ u = (u_1, \ldots, u_m) : \left(\int_\Omega u_\nu \, dx \right)_{\nu=1,\ldots,m} \in \mathcal{S} \right\}.$$

If (u, v) is a solution to (P) then $u(t) - U \in \mathcal{U}$ for every $t > 0$. Therefore, if $u^* := \lim_{t \to \infty} u(t)$ exists, then we have necessarily $u^* \in U + \mathcal{U}$. According to [9, 16, 17] there exists a unique stationary solution (u^*, v^*) to (P) additionally fulfilling $u^* \in U + \mathcal{U}$. This (u^*, v^*) is a thermodynamic equilibrium of the system. Along solutions to the instationary problem (P) the free energy

$$F(u) = \int_\Omega \sum_{\nu=1}^m \left\{ u_\nu \left(\ln \frac{u_\nu}{\overline{u}_\nu} - 1 \right) + \overline{u}_\nu \right\} dx$$

decays monotonously and exponentially to its equilibrium value $F(u^*)$,

$$F(u(t)) - F(u^*) \le e^{-\lambda t} (F(U) - F(u^*)) \quad \forall t \ge 0$$

with $\lambda > 0$ depending only on the data, see [16, 18, 14, 17].

If all reactions exhibit source terms of maximal order 2 then all solutions (u, v) to (P) are globally bounded, especially the particle densities are positively bounded away from zero (see e.g. [18]).

Nevertheless, in special cases, using the concrete structure of the underlying reaction system also some systems not fulfilling the general formulated condition of source terms of maximal order 2 can be handled e.g. under the 'intermediate sum condition', where a priori estimates for positive linear combinations of densities are obtained or in the case of cluster reactions of higher order (see [19]) where in the a priori estimates simultaneously different powers of the chemical activities of the different species are used as test functions.

Introducing suitable regularized problems, finding a priori estimates which do not depend on the regularization level, and solving the regularized problems the existence of solutions to (P) is shown in [18,9]. Uniqueness results for (P) can be obtained by standard arguments, if the diffusion coefficients do not depend on the state variables. For cases with diffusion coefficients depending on the state variable we refer to [9].

Let us remark that in three space dimensions there are similar results available, but stronger restrictions on the reactions are needed: reactions of maximal order three can be handled to obtain the exponential decay of the free energy (see [20]). In order to find global upper and lower bounds of the solution and to show solvability of the problem, the order of the source terms in each equation has to be less or equal to $\frac{5}{3}$ (see [9]).

3 Discretized reaction-diffusion systems

3.1 Voronoi finite volume discretization

In the previous part we saw that the solution of reaction diffusion-systems preserve some quantities like mass and positivity. Therefore, the aim is to respect the conservation of this quantities by the approximated solution. The finite volume method has been developed by engineers to study systems of conservation laws.

In the following, we work with Voronoi meshes, which represent one class of admissible finite volume meshes [6]. Our notation is basically taken from [13] and visualized in Figure 1.
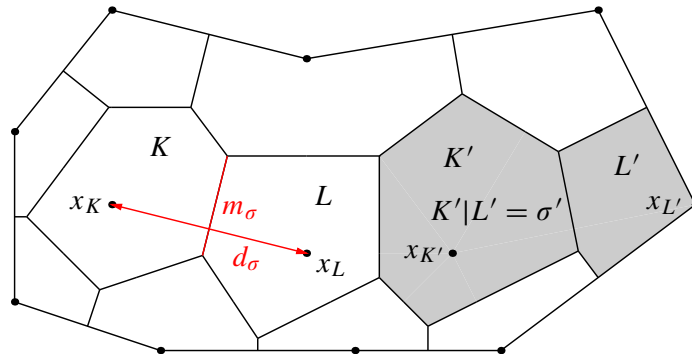
Figure 1: Notation of Voronoi meshes $\mathcal{M} = (\mathcal{P}, \mathcal{V}, \mathcal{E})$.

Let Ω be an open bounded, polyhedral subset of $\mathbb{R}^N$. A Voronoi mesh is defined as triple $\mathcal{M} = (\mathcal{P}, \mathcal{V}, \mathcal{E})$. Here, $\mathcal{P}$ denotes a family of *grid points* in $\bar{\Omega}$, $\mathcal{V}$ denotes a family of *Voronoi control volumes* and $\mathcal{E}$ denotes a family of parts of *hyperplanes* in $\mathbb{R}^{N+1}$. The number of grid points is denoted by $M = \#\mathcal{P}$.

The corresponding control volume K of each grid point $x_K \in \mathcal{P}$ is defined by

$$K = \{x \in \Omega : |x - x_K| < |x - x_L| \qquad \forall x_L \in \mathcal{P}, \, x_L \neq x_K \} .$$

The set of all neighbored control volumes of K are denoted by $\mathcal{N}_{\mathcal{V}}(K)$. The Lebesgue measure of each control volume K is denoted by $|K|$ and the mesh size of $\mathcal{M}$ by

$$\text{size}(\mathcal{M}) = \sup_{K \in \mathcal{V}} \text{diam}(K).$$

For two different $K, L \in \mathcal{V}$ the $(N-1)$ dimensional Lebesgue measure of $\overline{K} \cap \overline{L}$ is either zero or $\overline{K} \cap \overline{L} = \overline{\sigma}$ for one $\sigma \in \mathcal{E}$. Here the symbol $\sigma = K|L$ denotes the $N-1$ dimensional hyperplane between the control volumes K and L and m_{σ} is its Lebesgue measure.

We introduce the subset $\mathcal{E}_{int} \subset \mathcal{E}$ containing all interior hyperplanes and for all $K \in \mathcal{V}$ the subset $\mathcal{E}_K \subset \mathcal{E}$, such that $\partial K = \overline{K} \setminus K = \cup_{L \in \mathcal{N}_{\mathcal{V}}(K)} \overline{L} \cap \overline{K}$.

The Euclidian distance between two neighbored grid points $x_K, x_L \in \mathcal{P}$ over the hyperplane $\sigma = K|L \in \mathcal{E}_{int}$ is denoted by d_{σ}.

Definition 2 (see [13]) Let Ω be an open bounded, polyhedral subset of $\mathbb{R}^N$ and $\mathcal{M} = (\mathcal{P}, \mathcal{V}, \mathcal{E})$ a Voronoi mesh.

– The symbol $X_{\mathcal{V}}(\mathcal{M})$ denotes the set of all piecewise constant functions from Ω to $\mathbb{R}$ which are constant on every Voronoi control volume $K \in \mathcal{V}$. The constant value of $w_h \in X_{\mathcal{V}}(\mathcal{M})$ on the control volume $K \in \mathcal{V}$ is denoted by w_K.
– Let $p \geq 1$. The discrete L^p- norm of $w_h \in X_{\mathcal{V}}(\mathcal{M})$ is defined by

$$\|w_h\|_{L^p, \mathcal{M}, V} = \left(\sum_{K \in \mathcal{V}} |K| |w_K|^p \right)^{1/p}. \tag{3.6}$$

– The discrete H^1 semi-norm of $w_h \in X_{\mathcal{V}}(\mathcal{M})$ is defined by

$$|w_h|^2_{H^1, \mathcal{M}} = \sum_{\sigma = K|L \in \mathcal{E}_{int}} T_{\sigma} |w_K - w_L|^2, \quad T_{\sigma} := \frac{m_{\sigma}}{d_{\sigma}}.$$

Here w_K and w_L are the constant values of w_h in the control volumes K and L. The usual H^1- norm is given by $\|w_h\|^2_{H^1, \mathcal{M}, V} = |w_h|^2_{H^1, \mathcal{M}} + \|w_h\|^2_{L^2, \mathcal{M}, V}$.

We prescribe the approximation of a function $f : \Omega \times \mathbb{R}^m \to \mathbb{R}$ by

$$f_K(\cdot) := \frac{1}{|K|} \int_K f(x, \cdot) \, dx,$$

where $K \in \mathcal{V}$. The corresponding piecewise constant function can be estimated from above and below by the upper and lower bound of the continuous function. For $K \in \mathcal{V}$ we denote by

$$u_{\nu}^{(K)} = \int_K u_{\nu}(x) \, dx = |K| u_{\nu K} = \overline{u}_{\nu K} \, e^{v_{\nu K}} \, |K| \tag{3.7}$$

the mass of the $\nu-$th species in K and by $u_{\nu K}$ the constant density on K. For every species $\nu = 1, \ldots, m$ we introduce the discrete initial values by

$$U_{\nu}^{(K)} := \int_K U_{\nu}(x) \, dx, \quad K \in \mathcal{V}. \tag{3.8}$$

The space-discrete version of the continuous problem (P) is obtained by testing with the characteristic function of K. Using Gauss theorem, we derive the approximated flux term

$$\int_K \nabla \cdot \boldsymbol{j}_{\nu} \, dx = \int_{\partial K} \boldsymbol{j}_{\nu} \cdot \boldsymbol{n}_K d\Gamma \approx \sum_{\sigma = K|L \in \mathcal{E}_K} -T_{\sigma} Y_{\nu}^{\sigma} Z_{\nu}(v_{\nu L}, v_{\nu K})(v_{\nu L} - v_{\nu K}),$$

where $T_{\sigma} = \frac{m_{\sigma}}{d_{\sigma}}$ is the so called transmissibility across the edge $K|L$. Here the term

$$Z^{\sigma}(x, y) = \begin{cases} \frac{e^x - e^y}{x - y}, & \text{for } x \neq y, \\ e^x, & \text{for } x = y, \end{cases}, \qquad x, y \in \mathbb{R}, \tag{3.9}$$

represents some mean value of e^x in the interval $[x, y]$. With this definition of Z^σ it is possible to switch between a gradient in potentials and activities. The symbol Y_ν^σ defines some averaging of $D_\nu \overline{u}_\nu$ over the edge $\sigma = K|L$, which is symmetric in K and L. Possible averagings are

$$Y_\nu^\sigma = \frac{D_{\nu K} \overline{u}_{\nu K} + D_{\nu L} \overline{u}_{\nu L}}{2}, \qquad Y_\nu^\sigma = \frac{D_{\nu K} + D_{\nu L}}{2} \frac{\overline{u}_{\nu K} + \overline{u}_{\nu L}}{2}, \qquad \sigma = K|L.$$

By $D_{\nu K}$ we mean $D_{\nu K} = D_\nu(x_K, e^{v_{1K}}, \ldots, e^{v_{mK}})$. For another averaging which is exact along an aligned edge we refer to [5]. In the sequel all results are independent of the particular chosen Y_ν^σ.

Following [12] we use the notation

$$\begin{aligned}
\boldsymbol{u}_\nu &= (u_\nu^{(K)})_{K \in \mathcal{V}}, & \boldsymbol{u} &= (u_1, \ldots, u_m), & \boldsymbol{u}_K &= (u_{\nu K})_{\nu=1}^m, \\
\boldsymbol{v}_\nu &= (v_{\nu K})_{K \in \mathcal{V}}, & \boldsymbol{v} &= (v_1, \ldots, v_m), & \boldsymbol{v}_K &= (v_{\nu K})_{\nu=1}^m, \\
\boldsymbol{U}_\nu &= (U_\nu^{(K)})_{K \in \mathcal{V}}, & \boldsymbol{U} &= (U_1, \ldots, U_m), & & \\
\boldsymbol{a}_K &= (e^{v_{\nu K}})_{\nu=1}^m, & \boldsymbol{a}_\nu &= (e^{v_{\nu K}})_{K \in \mathcal{V}}, & \nu &= 1, \ldots, m.
\end{aligned}$$

We mention that $u_{\nu,h} \in X_\mathcal{V}(\mathcal{M})$ is equivalent to $(u_{\nu K})_{K \in \mathcal{V}}$. Furthermore, we define the scalar products

$$\langle \boldsymbol{u}_\nu, \boldsymbol{v}_\nu \rangle_{\mathbb{R}^M} = \sum_{K \in \mathcal{V}} |K| u_{\nu K} v_{\nu K}, \qquad \langle \boldsymbol{u}, \boldsymbol{v} \rangle_{\mathbb{R}^{Mm}} = \sum_{\nu=1}^m \langle \boldsymbol{u}_\nu, \boldsymbol{v}_\nu \rangle_{\mathbb{R}^M}.$$

Since our problem is a time evolution problem, we also need the following definition:

Definition 3 (Time discretization, see [13, (A5)]) A time discretization of $\mathbb{R}_+$ is defined as a strictly increasing sequence of real numbers $(t_n)_{n \in \mathbb{N}} \subset \mathbb{R}_+$ with $t_0 = 0$ and $t_n \to +\infty$ for $n \to \infty$. The time step is defined by

$$t_\delta^{(n)} = t_n - t_{n-1} < \infty, \quad \text{for} \quad n \in \mathbb{N}$$

and the largest possible time step by $\overline{t}_\delta = \sup_{n \in \mathbb{N}} t_\delta^{(n)}$.

Now, we introduce the operator $\widehat{E} : \mathbb{R}^{Mm} \to \mathbb{R}_+^{Mm}$ by

$$\widehat{E}\boldsymbol{v} = \left((\overline{u}_{\nu K} \, e^{v_{\nu K}} \, |K|)_{\nu=1,\ldots,m} \right)_{K \in \mathcal{V}}.$$

which maps in every control volume the chemical potential of every species to its mass. Furthermore we define $\widehat{A} : \mathbb{R}^{Mm} \to \mathbb{R}^{Mm}$ by

$$\widehat{A}\boldsymbol{v} = \left(\sum_{L \in \mathcal{N}_\mathcal{V}(K)} -T_{K|L} Y_\nu^{K|L} Z^{K|L} (v_{\nu L} - v_{\nu K}) \right. \tag{3.10}$$
$$\left. - |K| R_\nu(\cdot, e^{\boldsymbol{v}_K}) \right)_{\substack{K \in \mathcal{V}, \\ \nu=1,\ldots,m}}.$$

Using these definitions we can state the discrete problem of (P) by: Find a tuple $(\boldsymbol{u}, \boldsymbol{v})$ such that

$$\left.\begin{aligned}
\frac{\boldsymbol{u}(t_n) - \boldsymbol{u}(t_{n-1})}{t_\delta^{(n)}} + \widehat{A}\boldsymbol{v}(t_n) &= \boldsymbol{0}, \quad \boldsymbol{u}(t_n) = \widehat{E}\boldsymbol{v}(t_n), \quad n \geq 1 \\
\boldsymbol{u}(0) &= \boldsymbol{U}.
\end{aligned}\right\} \tag{P_D}$$

The discrete variational form of $\widehat{A}$ is given by

$$\left\langle \widehat{A}\boldsymbol{w}, \boldsymbol{v} \right\rangle_{\mathbb{R}^{Mm}} = \sum_{\nu=1}^m \sum_{\sigma = K|L \in \mathcal{E}_{int}} T_\sigma Y_\nu^\sigma Z^\sigma (w_{\nu L} - w_{\nu K})(v_{\nu L} - v_{\nu K})$$
$$- \sum_{\nu=1}^m \sum_{K \in \mathcal{V}} |K| R_\nu(x_K, e^{\boldsymbol{w}_K}) v_{\nu K} \quad \forall \boldsymbol{w}, \boldsymbol{v} \in \mathbb{R}^{Mm}.$$

3.2 Local existence result

In analogy to the continuous setting we define the supspaces

$$\widehat{\mathcal{U}} = \left\{ \boldsymbol{u} \in \mathbb{R}^{Mm} : (\langle \boldsymbol{u}_\nu, \mathbf{1} \rangle_{\mathbb{R}^M})_{\nu=1}^m \in \mathcal{S} \right\} \tag{3.11}$$

and

$$\widehat{\mathcal{U}}^\perp = \left\{ \boldsymbol{v} \in \mathbb{R}^{Mm} : \langle \boldsymbol{u}, \boldsymbol{v} \rangle_{\mathbb{R}^{Mm}} = 0 \, \forall \boldsymbol{u} \in \widehat{\mathcal{U}} \right\}. \tag{3.12}$$

Another characterization of $\widehat{\mathcal{U}}^\perp$ is given by

$$\widehat{\mathcal{U}}^\perp = \left\{ \boldsymbol{v} \in \mathbb{R}^{Mm} : v_{\nu K} = \hat{v}_\nu \, \forall K \in \mathcal{V}, \, \nu = 1, \dots, m, \, (\hat{v}_\nu)_{\nu=1}^m \in \mathcal{S}^\perp \right\}.$$

From the definition of $\widehat{A}$ it follows immediately that

$$\left\langle \widehat{A} \boldsymbol{v}, \boldsymbol{v}^\perp \right\rangle = 0 \quad \forall \boldsymbol{v}^\perp \in \widehat{\mathcal{U}}^\perp \text{ and } \forall \boldsymbol{v} \in \mathbb{R}^{Mm}. \tag{3.13}$$

Next we define the operator $\widehat{B} : \mathbb{R}^{Mm} \to \mathbb{R}^{Mm}$, by

$$\widehat{B} \boldsymbol{u} = \left(\sum_{L \in \mathcal{N}_\mathcal{V}(K)} -T_{K|L} Y_\nu^{K|L} \left(\frac{u_{\nu L}}{\overline{u}_{\nu L}} - \frac{u_{\nu K}}{\overline{u}_{\nu K}} \right) - |K| R_\nu \left(\frac{u_{\nu K}}{\overline{u}_{\nu K}} \right) \right)_{K \in \mathcal{V}, \nu = 1, \dots, m},$$

for all $\boldsymbol{u} \in \mathbb{R}^{Mm}$. The solvability of (P_D) can be proved by the investigation of the solvability of the following problem: Find a positive $\boldsymbol{u} \in \mathbb{R}^{Mm}$ such that

$$\left. \begin{array}{l} \frac{\boldsymbol{u}(t_n) - \boldsymbol{u}(t_{n-1})}{t_\delta^{(n)}} + \widehat{B} \boldsymbol{u}(t_n) = \mathbf{0}, \quad n \geq 1, \\ \boldsymbol{u}(t_0) = \boldsymbol{U} \end{array} \right\}. \tag{$P_{\widetilde{D}}$}$$

The relation between $\widehat{A}$ and $\widehat{B}$ is given by $\widehat{B} \boldsymbol{u} = \widehat{A}(\ln(\boldsymbol{u}/\overline{\boldsymbol{u}}))$ for all positive $\boldsymbol{u} \in \mathbb{R}^{Mm}$.

Next, we prove existence under additional assumptions with respect to the reaction terms. We assume that

$$R_\nu(\cdot, (a_1, \dots, a_{\nu-1}, 0, a_{\nu+1}, \dots, a_m)) \geq 0 \quad \forall \nu = 1, \dots, m, \, 0 \leq \boldsymbol{a} \in \mathbb{R}^m \tag{3.14}$$

and

$$\exists \boldsymbol{s}^\perp \in S^\perp : \boldsymbol{s}^\perp > \mathbf{0}. \tag{3.15}$$

Condition (3.14) is known as quasi positivity, see [1,24]. The second condition (3.15) imposes conservation of atom number, see[11, (Th$_2$)]. From the quasi positivity we deduce for one $u_{\nu K} = 0$, $K \in \mathcal{V}$ and $\nu = 1, \dots, m$ that

$$\begin{aligned} (\widehat{B} \boldsymbol{u})_{\nu K} = \sum_{L \in \mathcal{N}_\mathcal{V}(K)} &-T_{K|L} Y_\nu^{K|L} \left(\frac{u_{\nu L}}{\overline{u}_{\nu L}} - 0 \right) \\ &- |K| R_\nu(\cdot, (\frac{u_{1K}}{\overline{u}_{1K}}, \dots, \frac{u_{\nu-1K}}{\overline{u}_{\nu-1K}}, 0, \frac{u_{\nu+1K}}{\overline{u}_{\nu+1K}}, \dots, \frac{u_{mK}}{\overline{u}_{mK}})) \leq 0, \end{aligned} \tag{3.16}$$

which means that zero concentrations are raised by the system.

Lemma 1 *Let $\tilde{\boldsymbol{u}} \in \widehat{\mathcal{U}} + \boldsymbol{U}$ with $\tilde{\boldsymbol{u}} > \mathbf{0}$. And let (3.14), (3.15) be fulfilled. Then for all $s > 0$, there exists an $\boldsymbol{u} \in \mathbb{R}^{Mm}$ such that*

$$\boldsymbol{u} = \tilde{\boldsymbol{u}} - s \widehat{B} \boldsymbol{u}, \tag{3.17}$$

and $\boldsymbol{u} > \mathbf{0}$. Furthermore $\boldsymbol{u} \in \widehat{\mathcal{U}} + \boldsymbol{U}$.

Proof In the following, we use Bouwer's fixed point theorem to deduce the existence of a solution. We define the set of all densities which fulfill the same invariants as the initial concentration $\boldsymbol{U}$

$$\mathcal{C} := \left\{ \boldsymbol{u} \in \mathbb{R}^{mM} : \boldsymbol{u} \geq \boldsymbol{0} \wedge \boldsymbol{u} \in \widehat{\mathcal{U}} + \boldsymbol{U} \right\}.$$

The main point of the proof is to show that the fixed point is positive. Since $\mathcal{C}$ is the intersection of an affine space with Mm half spaces of nonnegative densities, the space $\mathcal{C}$ is convex. From (3.15), we deduce the existence of a vector $\boldsymbol{s}^{\perp} \in \mathcal{S}^{\perp}$, with only positive entries. As a consequence of the definition of $\widehat{\mathcal{U}}^{\perp}$, we conclude the existence of $\boldsymbol{w}^{\perp} \in \widehat{\mathcal{U}}^{\perp}$, with only positive entries. From $\langle \boldsymbol{u} - \boldsymbol{U}, \boldsymbol{w}^{\perp} \rangle_{\mathbb{R}^{Mm}} = 0$ for all $\boldsymbol{u} \in \mathcal{C}$, we conclude the boundedness of $\mathcal{C}$.

We define $\theta : \mathcal{C} \times [0, \infty) \to \mathbb{R}$ by

$$\theta(\boldsymbol{u}, s) := \sup_{\tau \in [0,s]} \left\{ \tau : \tilde{\boldsymbol{u}} - \tau \widehat{B} \boldsymbol{u} \in \mathcal{C} \right\}.$$

Since $\tilde{\boldsymbol{u}} \in \mathcal{C}$ holds, and $\mathcal{C}$ is bounded, the function θ is well defined. Using

$$\left\langle \tilde{\boldsymbol{u}} - \tau \widehat{B} \boldsymbol{u}, \boldsymbol{v}^{\perp} \right\rangle_{\mathbb{R}^{Mm}} = \langle \boldsymbol{U}, \boldsymbol{v}^{\perp} \rangle_{\mathbb{R}^{Mm}} \, \forall \boldsymbol{v}^{\perp} \in \widehat{\mathcal{U}}^{\perp}$$

and the convexity of $\mathcal{C}$, we deduce the continuity of θ. Hence, the function $\varphi_s : \mathcal{C} \to \mathcal{C}$ with

$$\varphi_s(\boldsymbol{u}) = \tilde{\boldsymbol{u}} - \theta(\boldsymbol{u}, s) \widehat{B} \boldsymbol{u} \tag{3.18}$$

is continuous for every $s > 0$, and the function $\theta(\boldsymbol{u}, s)$ ensures that $\varphi_s(\boldsymbol{u}) \in \mathcal{C}$ holds. Using Brouwer's fixed point theorem, we conclude the existence of a nonnegative fixed point $\boldsymbol{u}$ of φ_s for all $s > 0$. Assuming one or more components of $\boldsymbol{u}$ are zero, then by (3.14) and (3.16) we find that these components of $-\theta(\boldsymbol{u}, s) \widehat{B} \boldsymbol{u}$ are nonnegative, which leads to a contradiction with $\tilde{\boldsymbol{u}} > \boldsymbol{0}$. Therefore, the fixed point is not only nonnegative, but positive. But then, the fixed point is not on the boundary of $\mathcal{C}$ and $\theta(\boldsymbol{u}, s) = s$ must hold. This means that the fixed point of (3.18) is also fixed point of (3.17). □

By induction we conclude:

Theorem 1 *Let $\boldsymbol{U} = \boldsymbol{u}(t_0) > \boldsymbol{0}$ and let* (3.14), (3.15) *fulfilled. For all $t_n > 0$ there exists at least one solution $\boldsymbol{u}(t_n) > \boldsymbol{0}$ with $\boldsymbol{u}(t_n) \in \widehat{\mathcal{U}} + \boldsymbol{U}$ of the nonlinear equation $(P_{\widetilde{D}})$.*

This implies:

Theorem 2 *Let $\boldsymbol{U} = \boldsymbol{u}(t_0) > \boldsymbol{0}$ and let* (3.14) *as well as* (3.15) *be fulfilled. Then there exists a solution $(\boldsymbol{u}(t_n), \boldsymbol{v}(t_n))$ of the discrete Problem (P_D). Moreover there exists a unique stationary solution $(\boldsymbol{u}^*, \boldsymbol{v}^*)$ of (P_D) with $\boldsymbol{u}^* \in \widehat{\mathcal{U}} + \boldsymbol{U}$ and $0 < c \leq \boldsymbol{u}^*$.*

Proof Since $\boldsymbol{u}(t_n) > 0$ and $\boldsymbol{v}(t_n) = \ln \boldsymbol{u}(t_n) / \overline{\boldsymbol{u}}$, the solution of (3.17) delivers a solution to (P_D), too. From [13, Theorem 2.1] we conclude the existence and uniqueness of the stationary solution. We remind you that in our case the diffusion coefficients may depend on the state in contrast to [13]. But a carefully inspection of the proof given there, shows the validity of the result for this situation, too. □

Remark 1 Local existence results for systems with reaction terms not fulfilling (3.14) and (3.15) can be proven by investigating a "regularized" problem which arises from (P_D) by cutting off the nonlinearities in a suitable way at a certain level and using the theory of pseudomonotone operators, see [9, 18, 25]. Similarly, in the proof of Lemma 1 we cut off the time step s by using the function $\theta(\cdot, \cdot)$.

3.3 Physically motivated estimates

In this section we show that physical motivated arguments lead to a priori estimates for the solution to (P_D). We introduce the free energy being a convex functional. Since we consider an isolated process we only expect the decay along trajectories. In the literature the term free energy is often denoted as entropy [2,3]. All results are based on the articles [14,13]. We also refer to [4] for basic notation and results from convex analysis.

First we define the discrete potential $\widehat{\Phi} : \mathbb{R}^{Mm} \to \mathbb{R}$ by

$$\widehat{\Phi}(\boldsymbol{v}) = \sum_{\nu=1}^{m} \sum_{K \in \mathcal{V}} \bar{u}_{\nu K}(\mathrm{e}^{v_{\nu K}} - 1)|K|.$$

Due to $\boldsymbol{u} = \widehat{E}\boldsymbol{v}$, it holds $\boldsymbol{u} = \widehat{\Phi}'(\boldsymbol{v})$. The conjugate functional of $\widehat{\Phi}$ is defined by $\widehat{F} : \mathbb{R}^{Mm} \to \bar{\mathbb{R}}$,

$$\widehat{F}(\boldsymbol{u}) := \sup_{\boldsymbol{v} \in \mathbb{R}^{Mm}} \left\{ \langle \boldsymbol{u}, \boldsymbol{v} \rangle_{\mathbb{R}^{Mm}} - \widehat{\Phi}(\boldsymbol{v}) \right\}. \tag{3.19}$$

For a given argument $\boldsymbol{u} \in \mathbb{R}^{Mm}$ the value of $\widehat{F}(\boldsymbol{u})$ can be interpreted as the *free energy* of the state $\boldsymbol{u}$. Together with $\boldsymbol{u} = \widehat{E}\boldsymbol{v}$ we find

$$\widehat{F}(\boldsymbol{u}) = \left\langle \widehat{E}\boldsymbol{v}, \boldsymbol{v} \right\rangle_{\mathbb{R}^{Mm}} - \widehat{\Phi}(\boldsymbol{v}) = \sum_{\nu=1}^{m} \sum_{K \in \mathcal{V}} \left(u_{\nu K}(v_{\nu K} - 1) + \bar{u}_{\nu K} \right) |K|.$$

Using the elementary inequality $\ln s \geq 1 - 1/s$, $s > 0$ we observe the nonnegativity of the free energy

$$\widehat{F}(\boldsymbol{u}) = \sum_{\nu=1}^{m} \sum_{K \in \mathcal{V}} \left(u_{\nu K}(\ln \frac{u_{\nu K}}{\bar{u}_{\nu K}} - 1) + \bar{u}_{\nu K} \right) |K|.$$

Finally we introduce the discrete dissipation as functional $\widehat{D} : \mathbb{R}^{Mm} \to \mathbb{R}$ by

$$\widehat{D}(\boldsymbol{v}) := \left\langle \widehat{A}\boldsymbol{v}, \boldsymbol{v} \right\rangle_{\mathbb{R}^{Mm}}, \quad \boldsymbol{v} \in \mathbb{R}^{Mm}.$$

As a consequence of (3.10) we mention that for all $v \in \mathbb{R}^{Mm}$

$$\left\langle \widehat{A}\boldsymbol{v}, \boldsymbol{v} \right\rangle_{\mathbb{R}^{Mm}} = \sum_{\nu=1}^{m} \sum_{\sigma = K|L \in \mathcal{E}_{int}} T_{\sigma} Y_{\nu}^{\sigma} Z^{\sigma} (v_{\nu L} - v_{\nu K})^2$$
$$+ \sum_{K \in \mathcal{V}} |K| \sum_{(\boldsymbol{\alpha}, \boldsymbol{\beta}) \in \mathcal{R}} k_{(\boldsymbol{\alpha}, \boldsymbol{\beta})} \left(\mathrm{e}^{\boldsymbol{\alpha} \cdot \boldsymbol{v}_k} - \mathrm{e}^{\boldsymbol{\beta} \cdot \boldsymbol{v}_k} \right) (\boldsymbol{\alpha} - \boldsymbol{\beta}) \cdot \boldsymbol{v}_K \geq 0,$$

which provides that for all $\boldsymbol{v} \in \mathbb{R}^{Mm}$ the dissipation is nonnegative, see [13,14].

Lemma 2 (Monotonicity of the free energy, see [13, Lemma 3.1]) *Let $(\boldsymbol{u}, \boldsymbol{v})$ be a solution to (P_D) on a Voronoi mesh $\mathcal{M}$ and let $(A1)$ be fulfilled. Then for $0 \leq t_{n_1} < t_{n_2} \in \mathbb{R}_+$ holds*

$$\widehat{F}(\boldsymbol{u}(t_{n_2})) - \widehat{F}(\boldsymbol{u}(t_{n_1})) \leq - \sum_{n=n_1+1}^{n_2} t_{\delta}^{(n)} \widehat{D}(\boldsymbol{v}(t_n)),$$

i.e., the free energy decays along all solutions to (P_D). Moreover, it holds

$$\sum_{\nu=1}^{m} \|u_{\nu,h}(t_n)\|_{L^1, \mathcal{M}, V} \leq 2 \left(\widehat{F}(\boldsymbol{U}) + \sum_{\nu=1}^{m} \|\bar{u}_{\nu,h}\|_{L^1, \mathcal{M}, V} \right) \quad \forall n \geq 1.$$

Proof For $\boldsymbol{u} = \widehat{E}\boldsymbol{v}$, $\boldsymbol{v} \in \mathbb{R}^{Mm}$, $\widehat{F}'(\boldsymbol{u}) = \boldsymbol{v}$ and $\widehat{G}'(\boldsymbol{v}) = \boldsymbol{u}$ hold. Therefore, using the subdifferential property of $\widehat{F}$ (see [12, Eq. (3.9)]) it holds

$$\widehat{F}(\boldsymbol{u}) - \widehat{F}(\boldsymbol{w}) \leq \left\langle \boldsymbol{u} - \boldsymbol{w}, \widehat{F}'(\boldsymbol{u}) \right\rangle_{\mathbb{R}^{Mm}} \quad \forall \boldsymbol{w} \in \mathbb{R}^{Mm}.$$

As a consequence we find

$$
\begin{aligned}
\widehat{F}(\boldsymbol{u}(t_{n_2})) - \widehat{F}(\boldsymbol{u}(t_{n_1})) &= \sum_{n=n_1+1}^{n_2} \widehat{F}(\boldsymbol{u}(t_n)) - \widehat{F}(\boldsymbol{u}(t_{n-1})) \\
&\leq \sum_{n=n_1+1}^{n_2} \langle \boldsymbol{u}(t_n) - \boldsymbol{u}(t_{n-1}), \boldsymbol{v}(t_n) \rangle_{\mathbb{R}^{Mm}} \\
&= -\sum_{n=n_1+1}^{n_2} t_\delta^{(n)} \widehat{D}(\boldsymbol{v}(t_n)) \leq 0
\end{aligned}
$$

and by using the elementary inequalities

$$(x/2 - y) \leq (\sqrt{x} - \sqrt{y})^2 \leq x \ln x/y - x + y \qquad \forall x \geq 0, y > 0 \qquad (3.20)$$

we get

$$
\begin{aligned}
\widehat{F}(\boldsymbol{U}) \geq \widehat{F}(\boldsymbol{u}(t_n)) &= \sum_{\nu=1}^{m} \sum_{K \in \mathcal{V}} |K| \left\{ u_{\nu K}(t_n) \left(\ln \frac{u_{\nu K}(t_n)}{\overline{u}_{\nu K}} - 1 \right) + \overline{u}_{\nu K} \right\} \\
&\geq \sum_{\nu=1}^{m} \left\{ \frac{1}{2} \|u_{\nu,h}(t_n)\|_{L^1,\mathcal{M},V} - \|\overline{u}_{\nu,h}\|_{L^1,\mathcal{M},V} \right\}.
\end{aligned}
$$

$\square$

Remark 2 If there exists a vector $\boldsymbol{s}^\perp \in \mathcal{S}^\perp$ with $s_\nu^\perp > 0$, $\nu = 1, \dots, m$ one can obtain a priori bounds in L^1 without using the free energy of the system. Summing up all equations of (P_D) weighted by $s_\nu^\perp$ and integrating in space and time one gets for $N \geq 1$

$$
\begin{aligned}
0 &= \sum_{\nu=1}^{m} \sum_{n=1}^{N} \sum_{K \in \mathcal{V}} |K| t_\delta^{(n)} s_\nu^\perp \frac{u_{\nu,h}(t_n) - u_{\nu,h}(t_{n-1})}{t_\delta^{(n)}} \\
&= \sum_{\nu=1}^{m} \sum_{n=1}^{N} t_\delta^{(n)} s_\nu^\perp \frac{\|u_{\nu,h}(t_n)\|_{L^1,\mathcal{M},V} - \|u_{\nu,h}(t_{n-1})\|_{L^1,\mathcal{M},V}}{t_\delta^{(n)}} \\
&= \sum_{\nu=1}^{m} s_\nu^\perp \left(\|u_{\nu,h}(t_N)\|_{L^1,\mathcal{M},V} - \|U_{\nu,h}\|_{L^1,\mathcal{M},V} \right).
\end{aligned}
$$

Since we have Neumann boundary conditions, the diffusive flux is zero. We refer to [24] for more examples of systems which fulfill this property and for generalisations.

3.4 Global upper bounds

In this section we want to prove upper bounds for the densities that are uniform in time and space. In order to establish the new results in the following sections we need some additional assumptions on the domain and the mesh:

(A2) We assume that all Voronoi boxes $K \in \mathcal{V}$ can be covered by outer circles with radius $r_{K,out}$ and the radii of these circles can be estimated by the radii of inner circles (with radius $r_{K,in}$) with a uniform constant C. We define $r_{out} := \max_{K \in \mathcal{V}} r_{K,out}$ and $r_{in} = \min_{K \in \mathcal{V}} r_{K,in}$. Then, $r_{out} \leq C r_{in}$ holds.

This assumption also guarantees the validity of (A.41), see Remark 3. For obtaining the global bounds, we use a technique introduced by Moser, see [8].

Theorem 3 (Upper bounds) *Let* $(A1)$ *fulfilled and let a class of Voronoi finite volume discretizations* $\mathcal{M} = (\mathcal{P}, \mathcal{V}, \mathcal{E})$ *fulfill* $(A2)$. *Then there exists a constant* $c_1 > 0$ *only depending on the data and not on* $\mathcal{M}$ *such that for every solution* (u_h, v_h) *to* (P_D)

$$\sum_{\nu=1}^{m} \|u_{\nu,h}(t_N)/\overline{u}_{\nu,h}\|_{L^2,\mathcal{M},V} \le c_1 \quad \forall N \ge 1$$

holds uniformly for all Voronoi finite volume discretizations $\mathcal{M}$. *Furthermore there exists a second constant* $c_2 > 0$ *only depending on the data and not on* $\mathcal{M}$ *such that*

$$\|u_{\nu,h}(t_N)/\overline{u}_{\nu,h}\|_{L^\infty,\mathcal{M},V} \le c_2 \quad \forall N \ge 1, \quad \nu = 1,\dots,m$$

holds uniformly for all Voronoi finite volume discretizations $\mathcal{M}$.

Proof First we mention that

$$e^{t_{n-1}} \le \frac{e^{t_n} - e^{t_{n-1}}}{t_\delta^{(n)}} \le e^{t_n} = e^{t_{n-1}+t_\delta^{(n)}} \le e^{\overline{t}_\delta} e^{t_{n-1}}. \tag{3.21}$$

We introduce $z_{\nu,h} = (e^{v_{\nu,h}} - \kappa)^+$ with

$$\kappa := \max_{\nu=1,\dots,m} \|U_\nu/\overline{u}_\nu\|_{L^\infty}$$

and $w_{\nu,h} = z_{\nu,h}^{p/2}$, $p \ge 2$. The constant κ is chosen in such a way that $z_{\nu,h}(t_0) = (U_{\nu,h}/\overline{u}_{\nu,h} - \kappa)^+ = 0$. Now, we test (P_D) with test functions $pe^{t_{n-1}} z_{\nu,h}^{p-1}(t_n)$, $p \ge 2$, and estimate

$$S_1 := \sum_{n=1}^{N} t_\delta^{(n)} p\, e^{t_{n-1}} \left\langle \frac{\boldsymbol{u}(t_n) - \boldsymbol{u}(t_{n-1})}{t_\delta^{(n)}}, \boldsymbol{z}^{p-1}(t_n) \right\rangle_{\mathbb{R}^{Mm}}$$

$$= -\sum_{n=1}^{N} t_\delta^{(n)} p\, e^{t_{n-1}} \left\langle \widehat{A}\boldsymbol{v}(t_n), \boldsymbol{z}^{p-1}(t_n) \right\rangle_{\mathbb{R}^{Mm}} = S_2 + S_3$$

with

$$S_2 := -\sum_{\nu=1}^{m} \sum_{n=1}^{N} p t_\delta^{(n)} e^{t_{n-1}} \sum_{\sigma=K|L\in\mathcal{E}_{int}} T_\sigma Y_\nu^\sigma Z^\sigma (v_{\nu L} - v_{\nu K})(z_{\nu L}^{p-1} - z_{\nu K}^{p-1})$$

$$S_3 := \sum_{n=1}^{N} t_\delta^{(n)} p\, e^{t_{n-1}} \sum_{K\in\mathcal{V}} |K| \sum_{\nu=1}^{m} z_{\nu K}^{p-1}(t_n) R_\nu (e^{\boldsymbol{v}_K(t_n)}).$$

For that purpose we proceed in three steps.

Time derivative: For the term S_1 we write

$$S_1 = p \sum_{\nu=1}^{m} \sum_{n=1}^{N} e^{t_{n-1}} \sum_{K\in\mathcal{V}} |K| z_{\nu K}^{p-1}(t_n)(u_{\nu K}(t_n) - u_{\nu K}(t_{n-1}))$$

$$= p \sum_{\nu=1}^{m} \sum_{n=1}^{N} e^{t_{n-1}} \sum_{K\in\mathcal{V}} |K| \overline{u}_{\nu K} z_{\nu K}^{p-1}(t_n) \Big((z_{\nu K}(t_n) - z_{\nu K}(t_{n-1}))$$

$$+ (e^{v_{\nu K}(t_{n-1})} - \kappa)^- \Big).$$

We denote by

$$\delta_{\overline{u}} = \min_{\nu=1,\dots,m} \inf_{\boldsymbol{x}\in\Omega} \overline{u}_\nu(\boldsymbol{x}) \tag{3.22}$$

the lower bound of the reference densities. Using (B.51) and the fact that

$z_{\nu K}^{p-1}(t_n)(\mathrm{e}^{v_{\nu K}(t_{n-1})} - \kappa)^- \geq 0$ holds, we get

$$S_1 \geq \sum_{\nu=1}^m \sum_{n=1}^N \mathrm{e}^{t_{n-1}} \sum_{K \in \mathcal{V}} |K| \overline{u}_{\nu K} (z_{\nu K}^p(t_n) - z_{\nu K}^p(t_{n-1}))$$

$$= \sum_{\nu=1}^m \sum_{n=1}^N \sum_{K \in \mathcal{V}} |K| \overline{u}_{\nu K} \Big\{ \big(e^{t_n} z_{\nu K}^p(t_n) - \mathrm{e}^{t_{n-1}} z_{\nu K}^p(t_{n-1}) \big)$$

$$- (\mathrm{e}^{t_n} - \mathrm{e}^{t_{n-1}}) z_{\nu K}^p(t_n) \Big\}$$

$$\geq \sum_{\nu=1}^m \bigg\{ \mathrm{e}^{t_N} \, \delta_{\overline{u}} \| z_{\nu,h}(t_N) \|_{L^p, \mathcal{M}, V}^p$$

$$- \sum_{n=1}^N t_\delta^{(n)} \, \mathrm{e}^{\overline{t}_\delta} \, \mathrm{e}^{t_{n-1}} \, \| \overline{u}_{\nu,h} \|_{L^\infty, \mathcal{M}, V} \| z_{\nu,h} \|_{L^p, \mathcal{M}, V}^p \bigg\}.$$

In the last line we used $z_{\nu,h}(t_0) = 0$ and (3.21).

Diffusion term: Now, we consider the diffusion term S_2. Applying the definition (3.9) to

$$Z^\sigma(v_{\nu L} - v_{\nu K}) z_{\nu K}^{p-1} = (z_{\nu L} - z_{\nu K}) z_{\nu K}^{p-1} - ((\mathrm{e}^{v_{\nu L}} - \kappa)^- - (\mathrm{e}^{v_{\nu K}} - \kappa)^-) z_{\nu K}^{p-1}$$

$$= (z_{\nu L} - z_{\nu K}) z_{\nu K}^{p-1} - (\mathrm{e}^{v_{\nu L}} - \kappa)^- z_{\nu K}^{p-1}$$

$$\leq (z_{\nu L} - z_{\nu K}) z_{\nu K}^{p-1},$$

and using inequality (B.50), we find

$$S_2 = \sum_{\nu=1}^m \sum_{n=1}^N p t_\delta^{(n)} \, \mathrm{e}^{t_{n-1}} \sum_{K \in \mathcal{V}} \sum_{\sigma = K|L \in \mathcal{E}_K} T_\sigma Y_\nu^\sigma Z^\sigma(v_{\nu L} - v_{\nu K}) z_{\nu K}^{p-1}$$

$$\leq - \sum_{\nu=1}^m \sum_{n=1}^N p t_\delta^{(n)} \, \mathrm{e}^{t_{n-1}} \sum_{\sigma = K|L \in \mathcal{E}_{int}} T_\sigma Y_\nu^\sigma (z_{\nu L} - z_{\nu K})(z_{\nu L}^{p-1} - z_{\nu K}^{p-1})$$

$$\leq \sum_{\nu=1}^m \sum_{n=1}^N p t_\delta^{(n)} \, \mathrm{e}^{t_{n-1}} \widetilde{D}_{\nu,p} \left(-\| w_{\nu,h} \|_{H^1, \mathcal{M}}^2 + \| z_{\nu,h} \|_{L^p, \mathcal{M}, V}^p \right).$$

In the last line we extend the H^1 semi-norm to the full H^1 norm, and introduce $\widetilde{D}_{\nu,p} = \frac{4(p-1)}{p^2} \delta_{D_\nu \overline{u}_\nu}$ and

$$\delta_{D_\nu \overline{u}_\nu} = \min_{\boldsymbol{x} \in \Omega, \boldsymbol{y} \in \mathbb{R}^m} D_\nu(\boldsymbol{x}, \boldsymbol{y}) \overline{u}_\nu(\boldsymbol{x}).$$

Reaction terms: Together with (5), the calculation

$$\mathrm{e}^{2v_{\nu K}} \leq (z_{\nu K} + \kappa)^2 \leq 2(z_{\nu K}^2 + \kappa^2),$$

and Muirhead's inequality

$$\sum_{\nu,j=1}^m z_{jK}^2 z_{\nu K}^{p-1} \leq m \sum_{\nu=1}^m z_{\nu K}^{p+1},$$

we can estimate the reaction terms by

$$
\begin{aligned}
S_3 \leq & C_1 \sum_{\nu=1}^{m} \sum_{n=1}^{N} p t_\delta^{(n)} \, \mathrm{e}^{t_{n-1}} \sum_{K \in \mathcal{V}} |K| z_{\nu K}^{p-1} \left(1 + \sum_{j=1}^{m} e^{2v_{jK}} \right) \\
\leq & 2 C_1 \sum_{\nu=1}^{m} \sum_{n=1}^{N} p t_\delta^{(n)} \, \mathrm{e}^{t_{n-1}} \Bigg\{ (1 + m\kappa^2) \|z_{\nu,h}\|_{L^{p-1},\mathcal{M},V}^{p-1} \\
& + \sum_{j=1}^{m} \sum_{K \in \mathcal{V}} |K| z_{jK}^2 z_{\nu K}^{p-1} \Bigg\} \\
\leq & C_2 \sum_{n=1}^{N} t_\delta^{(n)} p \, \mathrm{e}^{t_{n-1}} \sum_{\nu=1}^{m} \left(\|z_{\nu,h}\|_{L^{p+1},\mathcal{M},V}^{p+1} + 1 \right)
\end{aligned}
$$

with two constants C_1, $C_2 > 0$.

The tested equation: Combining all parts, we find with a constant $C_3 > 0$

$$
\begin{aligned}
S_4 = & \sum_{\nu=1}^{m} \mathrm{e}^{t_N} \, \delta_{\overline{u}} \|z_{\nu,h}(t_N)\|_{L^p,\mathcal{M},V}^p \\
\leq & S_2 + S_3 + \sum_{n=1}^{N} t_\delta^{(n)} \, \mathrm{e}^{\overline{t}_\delta} \, \mathrm{e}^{t_{n-1}} \sum_{\nu=1}^{m} \|\overline{u}_{\nu,h}\|_{L^\infty,\mathcal{M},V} \|z_{\nu,h}\|_{L^p,\mathcal{M},V}^p \\
\leq & \sum_{n=1}^{N} p t_\delta^{(n)} \, \mathrm{e}^{t_{n-1}} \sum_{\nu=1}^{m} \Big\{ -\widetilde{D}_{\nu,p} \|w_{\nu,h}\|_{H^1,\mathcal{M}}^2 + C_2 (\|z_{\nu,h}\|_{L^{p+1},\mathcal{M},V}^{p+1} + 1) \\
& + (\widetilde{D}_{\nu,p} + \mathrm{e}^{\overline{t}_\delta} / p \|\overline{u}_{\nu,h}\|_{L^\infty,\mathcal{M},V}) \|z_{\nu,h}\|_{L^p,\mathcal{M},V}^p \Big\} \\
\leq & \sum_{n=1}^{N} p t_\delta^{(n)} \, \mathrm{e}^{t_{n-1}} \sum_{\nu=1}^{m} \Big\{ -\widetilde{D}_{\nu,p} \|w_{\nu,h}\|_{H^1,\mathcal{M}}^2 + C_3 \left(\|z_{\nu,h}\|_{L^{p+1},\mathcal{M},V}^{p+1} + 1 \right) \Big\} .
\end{aligned}
\tag{3.23}
$$

The constant C_3 can be chosen such that it depends on the largest possible time step (see Definition 3) and the data, but not on p.

Bounds in L^2: For obtaining the L^2 bound, we set $p = 2$. In order to control the last term in (3.23) (the L^3 norm of $z_{\nu,h}$), we use the discrete Gagliardo-Nirenberg inequality (A.48) to obtain

$$
\begin{aligned}
\|z_{\nu,h}\|_{L^3,\mathcal{M},V}^3 \leq & \epsilon C_{\mathcal{M},2,3} \|z_{\nu,h} \ln z_{\nu,h}\|_{L^1,\mathcal{M},V} \|z_{\nu,h}\|_{H^1,\mathcal{M},V}^2 \\
& + c_{\epsilon,3} C_{\mathcal{M},3,3} \|z_{\nu,h}\|_{L^1,\mathcal{M},V},
\end{aligned}
\tag{3.24}
$$

with constants $C_{\mathcal{M},2,3}$ and $C_{\mathcal{M},3,3}$ as given by Theorem A.5. From Lemma 2 and $z_{\nu,h} \leq a_{\nu,h}$ we deduce the boundedness of $\|z_{\nu,h}\|_{L^1,\mathcal{M},V}$. Using Lemma 2 once more and

$$
\begin{aligned}
\widehat{F}(\boldsymbol{U}) + \sum_{\nu=1}^{m} \|u_{\nu,h}\|_{L^1,\mathcal{M},V} \geq & \sum_{\nu=1}^{m} \sum_{K \in \mathcal{V}} |K| \overline{u}_{\nu K} \left(a_{\nu K} \ln a_{\nu K} + 1 \right) \\
\geq & \sum_{\nu=1}^{m} \sum_{\substack{K \in \mathcal{V}, \\ u_{\nu K} > \kappa \overline{u}_{\nu K}}} |K| \overline{u}_{\nu K} (a_{\nu K} - \kappa) \ln(a_{\nu K} - \kappa) \\
= & \sum_{\nu=1}^{m} \|z_{\nu,h} \ln z_{\nu,h}\|_{L^1,\mathcal{M},V},
\end{aligned}
$$

we can control $z_{\nu,h} \ln z_{\nu,h}$ in L^1 from above.

The constant $\epsilon > 0$ in (3.24) is now chosen such that the term in front of the H^1-norm in (3.23) fulfills

$$-\widetilde{D}_{2,\nu} + \epsilon C_3 C_{\mathcal{M},2,3} \|z_{\nu,h} \ln z_{\nu,h}\|_{L^1,\mathcal{M},V} = 0.$$

From (3.21) we get

$$\sum_{n=1}^{N} t_\delta^{(n)} \mathrm{e}^{t_{n-1}} \leq \sum_{n=1}^{N} \mathrm{e}^{t_n} - \mathrm{e}^{t_{n-1}} = e^{t_N} - 1$$

and we can, therefore, derive the boundedness of

$$\sum_{\nu=1}^{m} \delta_{\overline{u}} \|z_{\nu,h}(t_N)\|_{L^2,\mathcal{M},V}^2 \leq C_4, \quad N \geq 1 \tag{3.25}$$

by a constant $C_4 > 0$. The first result of the Theorem follows by using $u_{\nu K}/\overline{u_{\nu K}} \leq z_{\nu,K} + \kappa$ together with the monotonicity of x^2, $x \geq 0$.

Moser iteration for $p \geq 4$: For $p \geq 4$ let $r = \frac{2(p+1)}{p}$ be introduced . Using discrete Gagliardo-Nirenberg inequality (A.47) the estimate (3.23) can be written as

$$\begin{aligned}
S_4 &= \sum_{\nu=1}^{m} \mathrm{e}^{t_N} \delta_{\overline{u}} \|w_{\nu,h}(t_N)\|_{L^2,\mathcal{M},V}^2 \\
&\leq \sum_{n=1}^{N} p t_\delta^{(n)} \mathrm{e}^{t_{n-1}} \sum_{\nu=1}^{m} \left\{ -\widetilde{D}_{\nu,p} \|w_{\nu,h}\|_{H^1,\mathcal{M}}^2 + C_3 \left(\|w_{\nu,h}\|_{L^r,\mathcal{M},V}^r + 1 \right) \right\} \\
&\leq \sum_{n=1}^{N} p t_\delta^{(n)} \mathrm{e}^{t_{n-1}} \sum_{\nu=1}^{m} \left\{ -\widetilde{D}_{\nu,p} \|w_{\nu,h}\|_{H^1,\mathcal{M}}^2 \right. \\
&\quad \left. + C_3 c_r^r C_{\mathcal{M},1,r} \|w_{\nu,h}\|_{L^1,\mathcal{M},V} \|w_{\nu,h}\|_{H^1,\mathcal{M}}^{r-1} + C_3 \right\}.
\end{aligned} \tag{3.26}$$

For $r \in [2, 5/2]$ the constants appearing in (A.47) can be bounded by $c_r \leq \max(c_2, c_{5/2}, 1)^{1/2}$ and

$$2\frac{\max(\overline{C}_D, \overline{C}_D^{3/2})}{\underline{C}_D} \leq C_{\mathcal{M},1,r} \leq \frac{21}{8} \frac{\max(\overline{C}_D, \overline{C}_D^{7/4})}{\underline{C}_D}.$$

Therefore, by Young's inequality with $p' = \frac{2p}{p+2}$, $q' = \frac{2p}{p-2}$ and $\epsilon > 0$ we get

$$\|w_{\nu,h}\|_{L^1,\mathcal{M},V} \|w_{\nu,h}\|_{H^1,\mathcal{M}}^{r-1} \leq \frac{\epsilon}{p'} \|w_{\nu,h}\|_{H^1,\mathcal{M}}^2 + \frac{\epsilon^{-q'/p'}}{q'} \|w_{\nu,h}\|_{L^1,\mathcal{M},V}^{q'}.$$

The constant $\epsilon > 0$ is chosen such that

$$\left(-\widetilde{D}_{\nu,p} + C_3 c_r^r C_{\mathcal{M},1,r} \frac{\epsilon}{p'} \right) \|w_{\nu,h}\|_{H^1,\mathcal{M}}^2 = 0$$

meaning

$$\epsilon = \frac{\widetilde{D}_{\nu,p} p'}{C_3 c_r^r C_{\mathcal{M},1,r}}.$$

Then (3.26) can be estimated by

$$S_4 \leq \sum_{n=1}^{N} p t_\delta^{(n)} \mathrm{e}^{t_{n-1}} \sum_{\nu=1}^{m} C_3 \left(c_r^r C_{\mathcal{M},1,r} \frac{\epsilon^{-q'/p'}}{q'} \|w_{\nu,h}\|_{L^1,\mathcal{M},V}^{q'} + 1 \right).$$

The term in front of the L^1 norm is bounded from above by some constant C_4, namely

$$C_3 c_r^r C_{\mathcal{M},1,r} \frac{\epsilon^{-q'/p'}}{q'} \leq p C_4$$

and we proceed with

$$\mathrm{e}^{-t_N} S_4 = \sum_{\nu=1}^{m} \delta_{\overline{u}} \| z_{\nu,h}(t_N) \|_{L^p,\mathcal{M},V}^{p}$$

$$\leq \sum_{n=1}^{N} \mathrm{e}^{-t_N} t_\delta^{(n)} \mathrm{e}^{t_{n-1}} \sum_{\nu=1}^{m} p^2 C_4 \left(\| w_{\nu,h} \|_{L^1,\mathcal{M},V}^{q'} + 1 \right)$$

$$\leq p^2 C_4 \sum_{\nu=1}^{m} \sup_{n=0,\ldots,N} \left(\| z_{\nu,h}(t_n) \|_{L^{p/2},\mathcal{M},V}^{p^2/(p-2)} + 1 \right).$$

Therefore, with some constant $C_5 > 1$ we get

$$\mathrm{e}^{-t_N} S_4 + 1 \leq p^2 C_5 \left\{ \sum_{\nu=1}^{m} \sup_{n=0,\ldots,N} \left(\| z_{\nu,h}(t_n) \|_{L^{p/2},\mathcal{M},V}^{p/2} + 1 \right) \right\}^{2p/(p-2)}.$$

Iteratively using this inequality and setting $p = 2^k$, $k \in \mathbb{N}_+$ and

$$b_k := \sum_{\nu=1}^{m} \sup_{n=0,\ldots,N} \| z_{\nu,h}(t_n) \|_{L^{2^k},\mathcal{M},V}^{2^k} + 1$$

we find for $k \in \mathbb{N}_+$, $k \geq 2$ the recursion formula $b_k \leq C_5 4^k b_{k-1}^{\frac{4^k}{2^{k-1}-1}}$ and by induction

$$b_k \leq \left[(4)^{\sum_{i=0}^{k-2}(k-i)2^i} (C_5)^{\sum_{i=0}^{k-2} 2^i} b_1^{2^{k-1}} \right]^{\prod_{j=1}^{k-1} \frac{2^j}{2^j-1}}.$$

Again by induction one can prove

$$\sum_{i=0}^{k-2} 2^i \leq 2^{k-1} \leq 2^k, \qquad \sum_{i=0}^{k-2} (k-i)2^i \leq 2^{k+1}, \qquad k \geq 2, \qquad (3.27)$$

see [18, p. 112]. The product $\theta = \prod_{j=1}^{\infty} \frac{1}{1-2^{-j}}$ is finite and $b_k \leq (16 C_5 b_1)^{\theta 2^k}$. Since b_1 is bounded from above by (3.25) we obtain for $k \geq 2$

$$\sum_{\nu=1}^{m} \| z_{\nu,h}(t_N) \|_{L^{2^k},\mathcal{M},V} \leq \sqrt{m} \left\{ 16 C_5 \left(\sum_{\nu=1}^{m} \sup_{n=0,\ldots,N} \| z_{\nu,h}(t_n) \|_{L^2,\mathcal{M},V}^{2} + 1 \right) \right\}^{\theta}$$

and finally with [22, Theorem 2.11.5]

$$\sum_{\nu=1}^{m} \| z_{\nu,h}(t_N) \|_{L^\infty,\mathcal{M},V} \leq \sqrt{m} \left\{ 16 C_5 \left(\sum_{\nu=1}^{m} \sup_{n=0,\ldots,N} \| z_{\nu,h}(t_n) \|_{L^2,\mathcal{M},V}^{2} + 1 \right) \right\}^{\theta}$$

for $k \to \infty$. From $u_{\nu,h}/\overline{u}_{\nu,h} \leq z_{\nu,h} + \kappa$ the result follows. $\qquad \square$

3.5 Asymptotics

In this section we will extend the result of Lemma 2. We mention the result of [13] where it is proved that the free energy decays exponentially along trajectories. We also note that in special situations an explicit rate of convergence is proven, see [2].

Lemma 3 (Exponential decay, see [13, Theorem 3.2/3.3]) *Let a class of Voronoi finite volume discretizations $\mathcal{M} = (\mathcal{P}, \mathcal{V}, \mathcal{E})$ fulfill (A2), moreover let $(\boldsymbol{u}^*, \boldsymbol{v}^*)$ be the thermodynamic equilibrium to (P_D). Assuming that (A1) is fulfilled, then there exist constants $\lambda > 0$ and $c > 0$, such that*

$$\widehat{F}(\boldsymbol{u}(t_N)) - \widehat{F}(\boldsymbol{u}^*) \leq \mathrm{e}^{-\lambda t_N} (\widehat{F}(\boldsymbol{U}) - \widehat{F}(\boldsymbol{u}^*)), \qquad N \geq 1,$$

$$\left\| \sqrt{u_{\nu,h}(t_N)} - \sqrt{u_{\nu,h}^*} \right\|_{L^1,\mathcal{M},V} \leq c\,\mathrm{e}^{-\lambda t_N}, \qquad N \geq 1$$

hold uniformly for all Voronoi finite volume discretizations $\mathcal{M}$.

Using the L^∞ bounds from Lemma 3 we can prove the following result. The continuous can be found in [17, Theorem 5.5].

Corollary 1 (Asymptotics of the solution) *Let a class of Voronoi finite volume discretizations $\mathcal{M} = (\mathcal{P}, \mathcal{V}, \mathcal{E})$ fulfill $(A2)$, moreover let $(\boldsymbol{u}^*, \boldsymbol{v}^*)$ be the thermodynamic equilibrium to (P_D). Assuming that $(A1)$ is fulfilled, then there exist constants $c > 0$ and $\lambda > 0$ such that for every solution $(\boldsymbol{u}, \boldsymbol{v})$ to (P_D) and for all $\nu = 1, \ldots, m$ and $p \in [1, +\infty)$ the estimate*

$$\sum_{\nu=1}^m \left\| u_{\nu,h}(t_N) - u_{\nu,h}^* \right\|_{L^p, \mathcal{M}, V} \leq c\, \mathrm{e}^{-\lambda t_N/2}, \quad N \geq 1 \tag{3.28}$$

holds uniformly for all Voronoi finite volume discretizations $\mathcal{M}$.

Proof Using Hölder's inequality we find

$$\left\| u_{\nu,h}(t_n) - u_{\nu,h}^* \right\|_{L^p, \mathcal{M}, V}^p \leq \left\| u_{\nu,h}(t_n) - u_{\nu,h}^* \right\|_{L^1, \mathcal{M}, V} \left\| u_{\nu,h}(t_n) - u_{\nu,h}^* \right\|_{L^\infty, \mathcal{M}, V}^{p-1}.$$

As a consequence of Theorem 3, we obtain the boundedness of

$$\left\| u_{\nu,h}(t_n) - u_{\nu,h}^* \right\|_{L^\infty, \mathcal{M}, V}^{p-1} \leq \left(\left\| u_{\nu,h}(t_n) \right\|_{L^\infty, \mathcal{M}, V} + \left\| u_{\nu,h}^* \right\|_{L^\infty, \mathcal{M}, V} \right)^{p-1}.$$

Using $(x - 1) = (\sqrt{x} - 1)(2 + (\sqrt{x} - 1)) \ \forall x \geq 0$ we get for all $\nu = 1, \ldots, m$

$$\begin{aligned}
\left\| u_{\nu K} - u_{\nu K}^* \right\|_{L^1, \mathcal{M}, V} \leq & \left\| \overline{u}_{\nu,h} \right\|_{L^\infty, \mathcal{M}, V} \left\{ 2 \left\| \sqrt{u_{\nu,h}/u_{\nu,h}^*} - 1 \right\|_{L^1, \mathcal{M}, V} \right. \\
& \left. + \left\| \sqrt{u_{\nu,h}/u_{\nu,h}^*} - 1 \right\|_{L^2, \mathcal{M}, V}^2 \right\}.
\end{aligned} \tag{3.29}$$

Again using Hölder's inequality we estimate

$$\left\| \sqrt{u_{\nu,h}/u_{\nu,h}^*} - 1 \right\|_{L^1, \mathcal{M}, V} \leq C \left\| \sqrt{u_{\nu,h}/u_{\nu,h}^*} - 1 \right\|_{L^2, \mathcal{M}, V}, \quad C > 0, \tag{3.30}$$

and by Lemma 3 we conclude (3.28). □

3.6 Global lower bounds

Now, we intend to show global lower bounds of the densities or in other words upper bounds of the negative part of the chemical potentials. In the continuous setting, this was done in [9] and [18, p. 18]. In a first step we need lower bounds in L^1 which provide a suitable start for the Moser iteration.

Lemma 4 (Lower bounds in L^1) *Let the assumptions of Theorem 3 be fulfilled. Then there exists a constant $c_1 > 0$ only depending on the data such that for every solution $(\boldsymbol{u}, \boldsymbol{v})$ to (P_D)*

$$\left\| v_{\nu,h}^-(t_N) \right\|_{L^1, \mathcal{M}, V} \leq c_1 \quad \forall N \geq 1, \quad \nu = 1, \ldots, m$$

hold uniformly for all $\mathcal{M}$.

Proof Following [18, p. 18] we define the convex and lower semicontinuous functional $\widehat{\Theta} : \mathbb{R}^m \to \bar{\mathbb{R}}$ by

$$\widehat{\Theta}(\boldsymbol{w}) = \sum_{K \in \mathcal{V}} |K| u_{\nu K}^* \vartheta(w_K), \qquad \vartheta(y) := \begin{cases} -\ln(1 - y), & \text{for } y \leq 0, \\ +\infty & \text{for } y > 0, \end{cases}$$

and its conjugate functional

$$\widehat{G}(\boldsymbol{u}_\nu) = \sup_{\boldsymbol{w} \in \mathbb{R}^M} \{ \langle \boldsymbol{u}_\nu, \boldsymbol{w} \rangle - \widehat{\Theta}(\boldsymbol{w}) \}. \tag{3.31}$$

Introducing $\overline{z}_{\nu,h} := (1 - u^*_{\nu,h}/u_{\nu,h})^-$ and determining the supremum by differentiating $\widehat{G}(\boldsymbol{u}_\nu)$ with respect to $\boldsymbol{w}$, we observe that $-\overline{z}_{\nu,h} \in \partial\widehat{G}(\boldsymbol{u}_\nu)$. If $(\boldsymbol{u}, \boldsymbol{v})$ is a solution to (P_D), then by inserting $-\overline{z}_{\nu,h}$ for $\boldsymbol{w}$ in (3.31) we obtain

$$\widehat{G}(\boldsymbol{u}_\nu) = \sum_{K \in \mathcal{V}} |K| \left\{ u^*_\nu \left(\ln \frac{u_{\nu K}}{u^*_{\nu K}} \right)^- - (u_{\nu K} - u^*_{\nu K})^- \right\} \tag{3.32}$$

and by using the convexity of $\widehat{G}$ we find

$$\begin{aligned}
\widehat{G}(\boldsymbol{u}_\nu(t_N)) - \widehat{G}(\boldsymbol{U}_\nu) &\leq -\sum_{n=1}^{N} t_\delta^{(n)} \left\langle \frac{\boldsymbol{u}_\nu(t_n) - \boldsymbol{u}_\nu(t_{n-1})}{t_\delta^{(n)}}, \overline{\boldsymbol{z}}_\nu \right\rangle_{\mathbb{R}^M} \\
&= \sum_{n=1}^{N} t_\delta^{(n)} \left\langle \widehat{A}\boldsymbol{v}, (0, \ldots, 0, \overline{\boldsymbol{z}}_\nu, 0, \ldots, 0,) \right\rangle_{\mathbb{R}^{Mm}} \\
&= S_1 + S_2
\end{aligned} \tag{3.33}$$

with

$$S_1 := \sum_{\sigma = K|L \in \mathcal{E}_{\text{int}}} T_\sigma Y^\sigma_\nu Z^\sigma (v_{\nu L} - v_{\nu K})(\overline{z}_{\nu L} - \overline{z}_{\nu K}),$$

$$S_2 := -\sum_{K \in \mathcal{V}} |K| R_\nu(\mathrm{e}^{\boldsymbol{v}_K})\overline{z}_{\nu K}.$$

Now we decompose the mesh into

$$\Omega_+(t_n) = \{K \in \mathcal{V} : u_{\nu K}(t_n) \geq u^*_{\nu K}\}, \qquad \Omega_-(t_n) = \{K \in \mathcal{V} : u_{\nu K}(t_n) < u^*_{\nu K}\}.$$

In a first step we show that the diffusion term S_1 is negative. We remark $\overline{z}_{\nu K} = 0$ for all $K \in \Omega_+(t_n)$. Using $v^*_{\nu K} \equiv \text{const} \; \forall K \in \mathcal{V}$ we write

$$\begin{aligned}
S_1 = &\sum_{\substack{\sigma = K|L \in \mathcal{E}_{int} \\ K,L \in \Omega_-(t_n)}} T_\sigma Y^\sigma_\nu (\mathrm{e}^{v_{\nu L}} - \mathrm{e}^{v_{\nu K}})(\mathrm{e}^{-v_{\nu L}} - \mathrm{e}^{-v_{\nu K}}) \mathrm{e}^{v^*_{\nu K}} \\
&- \sum_{\substack{\sigma = K|L \in \mathcal{E}_{int} \\ K \in \Omega_-(t_n), L \in \Omega_+(t_n)}} T_\sigma Y^\sigma_\nu ((a_{\nu L} - a^*_{\nu L}) + (a^*_{\nu K} - a_{\nu K}))\overline{z}_{\nu K}
\end{aligned} \tag{3.34}$$

Since $(x - y)(1/x - 1/y) \leq 0$, $x, y > 0$ the first sum in (3.34) is less than or equal to zero. From $K \in \Omega_-(t_n)$ we conclude $a^*_{\nu K} - a_{\nu K} > 0$ and from $L \in \Omega_+(t_n)$ we obtain $a_{\nu L} - a^*_{\nu L} > 0$, hence the second sum in (3.34) is less than or equal to zero.

Therefore S_1 is negative and we get from (3.33)

$$\widehat{G}(\boldsymbol{u}_\nu(t_N)) \leq \widehat{G}(\boldsymbol{U}_\nu) + S_2.$$

Now we consider the term S_2. On Ω_+ reaction terms multiplied by the test function vanish. Since $(\boldsymbol{\alpha} - \boldsymbol{\beta}) \cdot \boldsymbol{v}^*_K = 0 \; \forall K \in \mathcal{V}$, we get on Ω_-

$$\begin{aligned}
-R_\nu(\mathrm{e}^{\boldsymbol{v}_K})\overline{z}_{\nu K} &= \sum_{(\boldsymbol{\alpha},\boldsymbol{\beta}) \in \mathcal{R}} \mathrm{e}^{\boldsymbol{\alpha} \cdot \boldsymbol{v}^*_K} \left(\mathrm{e}^{\boldsymbol{\alpha} \cdot (\boldsymbol{v}_K - \boldsymbol{v}^*_K)} - \mathrm{e}^{\boldsymbol{\beta} \cdot (\boldsymbol{v}_K - \boldsymbol{v}^*_K)} \right) (\alpha_\nu - \beta_\nu)\overline{z}_{\nu K} \\
&= -\sum_{(\boldsymbol{\alpha},\boldsymbol{\beta}) \in \mathcal{R}} \mathrm{e}^{\boldsymbol{\alpha} \cdot \boldsymbol{v}^*_K} \left(\mathrm{e}^{\boldsymbol{\alpha} \cdot (\boldsymbol{v}_K - \boldsymbol{v}^*_K)} - \mathrm{e}^{\boldsymbol{\beta} \cdot (\boldsymbol{v}_K - \boldsymbol{v}^*_K)} \right) (\alpha_\nu - \beta_\nu) \\
&\quad \sum_{(\boldsymbol{\alpha},\boldsymbol{\beta}) \in \mathcal{R}} \mathrm{e}^{\boldsymbol{\alpha} \cdot \boldsymbol{v}^*_K} \left(\mathrm{e}^{\boldsymbol{\alpha} \cdot (\boldsymbol{v}_K - \boldsymbol{v}^*_K)} - \mathrm{e}^{\boldsymbol{\beta} \cdot (\boldsymbol{v}_K - \boldsymbol{v}^*_K)} \right) (\alpha_\nu - \beta_\nu) \frac{u^*_{\nu K}}{u_{\nu K}}.
\end{aligned} \tag{3.35}$$

Having in mind that

$$\mathrm{e}^{\boldsymbol{\alpha} \cdot (\boldsymbol{v}_K - \boldsymbol{v}^*_K)} = \prod_{j=1}^{m} \left(\frac{u_{jK}}{u^*_{jK}} \right)^{\alpha_j}$$

holds, the second line of (3.35), i.e.

$$\left(e^{\boldsymbol{\alpha}\cdot(\boldsymbol{v}_K - \boldsymbol{v}_K^*)} - e^{\boldsymbol{\beta}\cdot(\boldsymbol{v}_K - \boldsymbol{v}_K^*)} \right)(\alpha_\nu - \beta_\nu).$$

is Lipschitz continuous in $(\boldsymbol{u}_K / \boldsymbol{u}_K^*)$ on $[0, R]^m$, $R > 0$ and has at $(1)_{\nu=1}^m$ the value 0. Using the global boundedness of $(\boldsymbol{u}_K / \boldsymbol{u}_K^*)$ we can estimate

$$|\alpha_\nu - \beta_\nu| \left| e^{\boldsymbol{\alpha}\cdot(\boldsymbol{v}_K - \boldsymbol{v}_K^*)} - e^{\boldsymbol{\beta}\cdot(\boldsymbol{v}_K - \boldsymbol{v}_K^*)} \right| \leq C_1 \sum_{\nu=1}^m \left| \frac{u_{\nu K}}{u_{\nu K}^*} - 1 \right|.$$

For $\alpha_\nu > \beta_\nu$ the second line of (3.35) can be written as

$$\left(e^{\boldsymbol{\alpha}\cdot(\boldsymbol{v}_K - \boldsymbol{v}_K^*)} - e^{\boldsymbol{\beta}\cdot(\boldsymbol{v}_K - \boldsymbol{v}_K^*)} \right)(\alpha_\nu - \beta_\nu)\frac{u_{\nu K}^*}{u_{\nu K}}$$

$$\leq \left((\frac{u_{\nu K}}{u_{\nu K}^*})^{(\alpha_\nu - 1)} \prod_{\substack{j=1, \\ j\neq\nu}}^m \left(\frac{u_{jK}}{u_{jK}^*} \right)^{\alpha_j} - \prod_{j=1}^m \left(\frac{u_{jK}}{u_{jK}^*} \right)^{\beta_j} \right).$$

Again the term is Lipschitz continuous in $(\boldsymbol{u}_K / \boldsymbol{u}_K^*)$ on $[0, R]^m$, $R > 0$ and has at $(1)_{\nu=1}^m$ the value 0. Using the global boundedness of $(\boldsymbol{u}_K / \boldsymbol{u}_K^*)$ we conclude

$$\left(e^{\boldsymbol{\alpha}\cdot(\boldsymbol{v}_K - \boldsymbol{v}_K^*)} - e^{\boldsymbol{\beta}\cdot(\boldsymbol{v}_K - \boldsymbol{v}_K^*)} \right)(\alpha_\nu - \beta_\nu)\frac{u_{\nu K}^*}{u_{\nu K}} \leq C_2 \sum_{\nu=1}^m \left| \frac{u_{\nu K}}{u_{\nu K}^*} - 1 \right|.$$

Similar estimates are obtained for $\alpha_\nu < \beta_\nu$. So, we continue to estimate (3.35) with a constant $C_3 > 0$ by

$$S_2 \leq C_3 \sum_{\nu=1}^m \left\| u_{\nu,h} / u_{\nu,h}^* - 1 \right\|_{L^1, \mathcal{M}, V}. \tag{3.36}$$

From Corollary 1 and Lemma 3 we conclude that

$$\left\| \frac{u_{\nu,h}}{u_{\nu,h}^*} - 1 \right\|_{L^1, \mathcal{M}, V} \leq C_4\, e^{-\lambda t_n / 2}$$

with the constant λ given in Lemma 3. Hence there exists a constant $C_5 > 0$ such that $\widehat{G}(\boldsymbol{u}_\nu(t_N)) \leq C_5$. Let $\delta_{u^*} = \inf_{x\in\Omega} u_\nu^*(x)$. Together with

$$\left\| (u_{\nu,h} - u_{\nu,h}^*)^- \right\|_{L^1, \mathcal{M}, V} \leq \left\| u_{\nu,h}^* \right\|_{L^1, \mathcal{M}, V}$$

and the the definition of $\widehat{G}$ in (3.32) we find

$$\delta_{u^*} \left\| (v_{\nu,h} - v_{\nu,h}^*)^- \right\|_{L^1, \mathcal{M}, V} \leq \widehat{G}(\boldsymbol{u}_\nu) + \left\| u_{\nu,h}^* \right\|_{L^1, \mathcal{M}, V}$$

from which the bounds in L^1 follow.   □

Now, we show global lower bounds for the chemical potentials by Moser iteration.

Theorem 4 (Lower bounds in L^∞) *Let the assumptions of Theorem 3 be fulfilled. Then there exists a constant $c > 0$, only depending on the data, such that for every solution (u_h, v_h) of (P_D)*

$$\left\| v_{\nu,h}^-(t_N) \right\|_{L^\infty, \mathcal{M}, V} \leq c \quad \forall N \geq 1, \quad \nu = 1, \ldots, m$$

holds uniformly for all Voronoi finite volume discretizations $\mathcal{M}$.

Proof Let $z_{\nu,h} = (v_{\nu,h} + \kappa)^-$ and $w_{\nu,h} = z_{\nu,h}^{p/2}$. The constant κ is defined by

$$\kappa := \max_{\nu=1,\dots,m} \left\| (v_{\nu,h}(t_0))^- \right\|_{L^\infty}.$$

For $p \geq 2$ we test (P_D) with test functions which have the ν-th component

$$-p \, e^{t_{n-1}} \, z_{\nu,h}^{p-1}(t_n) \, e^{-v_{\nu,h}(t_n)},$$

the other components are zero. We want to estimate

$$S_1 := -p \sum_{n=1}^N t_\delta^{(n)} e^{t_{n-1}} \left\langle \frac{\boldsymbol{u}(t_n) - \boldsymbol{u}(t_{n-1})}{t_\delta^{(n)}}, \boldsymbol{z}^{p-1}(t_n) e^{-\boldsymbol{v}_{\nu,h}(t_n)} \right\rangle_{\mathbb{R}^{Mm}}$$

$$= p \sum_{n=1}^N t_\delta^{(n)} e^{t_{n-1}} \left\langle \widehat{A} \boldsymbol{v}(t_n), \boldsymbol{z}^{p-1}(t_n) e^{-\boldsymbol{v}_{\nu,h}(t_n)} \right\rangle_{\mathbb{R}^{Mm}} = S_2 + S_3.$$

Defining

$$S_2 := \sum_{n=1}^N t_\delta^{(n)} p \, e^{t_{n-1}} \sum_{\sigma = K|L \in \mathcal{E}_{\mathrm{int}}} T_\sigma Y_\nu^\sigma Z^\sigma (v_{\nu L} - v_{\nu K})(z_{\nu L}^{p-1} e^{-v_{\nu L}} - z_{\nu K}^{p-1} e^{-v_{\nu K}})$$

$$S_3 := -p \sum_{K \in \mathcal{V}} |K| \sum_{n=1}^N t_\delta^{(n)} e^{t_{n-1}} z_{\nu K}^{p-1}(t_n) e^{-v_{\nu K}(t_n)} R_\nu(e^{\boldsymbol{v}_K})$$

we will proceed in three steps.

Time derivative: Since $e^x - e^y = e^\xi (x - y)$ for some $\xi \in [x, y] \subset \mathbb{R}$ we find

$$I = -p \, e^{t_{n-1}} z_{\nu K}^{p-1}(t_n) e^{-v_{\nu K}(t_n)} (u_{\nu K}(t_n) - u_{\nu K}(t_{n-1}))$$

$$\geq p \, e^{t_{n-1}} z_{\nu K}^{p-1}(t_n) \overline{u}_{\nu K} \, e^{\xi_{\nu K} - v_{\nu K}(t_n)} (z_{\nu K}(t_n) - z_{\nu K}(t_{n-1})),$$

since $z_{\nu K}^{p-1}(t_n)(v_{\nu K}(t_n) - \kappa)^+ = 0$. In the following we consider the two cases:

1. From $u_{\nu K}(t_n) > u_{\nu K}(t_{n-1})$ we get $z_{\nu K}(t_n) \leq z_{\nu K}(t_{n-1})$ and $e^{\xi_{\nu K}} < e^{v_{\nu K}(t_n)}$, hence

$$I \geq p \, e^{t_{n-1}} z_{\nu K}^{p-1}(t_n) \overline{u}_{\nu K} (z_{\nu K}(t_n) - z_{\nu K}(t_{n-1})).$$

2. From $u_{\nu K}(t_n) < u_{\nu K}(t_{n-1})$ we find $z_{\nu K}(t_n) \geq z_{\nu K}(t_{n-1})$ and $e^{\xi_{\nu K}} > e^{v_{\nu K}(t_n)}$, hence

$$I \geq p \, e^{t_{n-1}} z_{\nu K}^{p-1}(t_n) \overline{u}_{\nu K} (z_{\nu K}(t_n) - z_{\nu K}(t_{n-1})).$$

Together with (B.51), (3.22) and (3.21) we can estimate S_1 by

$$\begin{aligned}
S_1 &= \sum_{n=1}^N \sum_{K \in \mathcal{V}} |K| I \\
&\geq \sum_{n=1}^N \sum_{K \in \mathcal{V}} |K| \overline{u}_{\nu K} \left\{ (e^{t_n} z_{\nu K}(t_n)^p - e^{t_{n-1}} z_{\nu K}(t_{n-1})^p) \right. \\
&\quad \left. - (e^{t_n} - e^{t_{n-1}}) z_{\nu K}(t_n)^p \right\} \\
&\geq e^{t_N} \delta_{\overline{u}} \| z_{\nu,h}(t_N) \|_{L^p, \mathcal{M}, V}^p \\
&\quad - \sum_{n=1}^N t_\delta^{(n)} e^{\overline{t}_\delta} e^{t_{n-1}} \| \overline{u}_{\nu,h} \|_{L^\infty, \mathcal{M}, V} \| z_{\nu,h}(t_n) \|_{L^p, \mathcal{M}, V}^p.
\end{aligned}$$

(3.37)

Diffusion term: A short calculation gives for $\sigma = K|L$ and $x := v_{\nu L} - v_{\nu K}$

$$Z^\sigma (v_{\nu L} - v_{\nu K})(z_{\nu L}^{p-1} \, \mathrm{e}^{-v_{\nu L}} - z_{\nu K}^{p-1} \, \mathrm{e}^{-v_{\nu K}}) = A + B$$

with

$$A := \frac{(\mathrm{e}^x - 1)(\mathrm{e}^{-x} + 1)}{2x} x(z_{\nu L}^{p-1} - z_{\nu K}^{p-1}),$$

$$B := \frac{(\mathrm{e}^x - 1)(\mathrm{e}^{-x} - 1)}{x^2} \frac{x^2}{2}(z_{\nu L}^{p-1} + z_{\nu K}^{p-1}).$$

Using Lemma B.7, inequality (B.50) and the auxiliary calculation with $x_{\nu L} = (v_{\nu L} + \kappa)^+$ and $x_{\nu K} = (v_{\nu K} + \kappa)^+$

$$
\begin{aligned}
(v_{\nu L} - v_{\nu K})(z_{\nu L}^{p-1} - z_{\nu K}^{p-1}) =& (x_{\nu L} - x_{\nu K})(z_{\nu L}^{p-1} - z_{\nu K}^{p-1}) \\
&- (z_{\nu L} - z_{\nu K})(z_{\nu L}^{p-1} - z_{\nu K}^{p-1}) \\
=& -(x_{\nu L} z_{\nu K}^{p-1} + x_{\nu K} z_{\nu L}^{p-1}) \\
&- (z_{\nu L} - z_{\nu K})(z_{\nu L}^{p-1} - z_{\nu K}^{p-1}) \\
\leq& -(z_{\nu L} - z_{\nu K})(z_{\nu L}^{p-1} - z_{\nu K}^{p-1}),
\end{aligned}
$$

we can estimate A from above by

$$A \leq -\frac{4(p-1)}{p^2}\left(z_{\nu L}^{p/2} - z_{\nu K}^{p/2}\right)^2.$$

Together with Lemma B.7, inequality (B.52) and the auxiliary calculation

$$
\begin{aligned}
x^2 = (v_{\nu L} - v_{\nu K})^2 =& ((x_{\nu L} - x_{\nu K}) - (z_{\nu L} - z_{\nu K}))^2 \\
=& (x_{\nu L} - x_{\nu K})^2 + 2(x_{\nu L} z_{\nu K} + x_{\nu K} z_{\nu L}) + (z_{\nu L} - z_{\nu K})^2 \\
\geq& (z_{\nu L} - z_{\nu K})^2,
\end{aligned}
$$

we can bound the term B by

$$B \leq -(z_{\nu L} - z_{\nu K})^2 \frac{(z_{\nu L}^{p-1} + z_{\nu K}^{p-1})}{2} \leq -\frac{1}{(p+1)^2}\left(z_{\nu L}^{\frac{p+1}{2}} - z_{\nu K}^{\frac{p+1}{2}}\right)^2.$$

Therefore we can bound S_2 with some constant

$$\delta_{D_\nu \overline{u}_\nu} = \min_{\boldsymbol{x} \in \Omega, \boldsymbol{y} \in \mathbb{R}^m} D_\nu(\boldsymbol{x}, \boldsymbol{y}) \overline{u}_\nu(\boldsymbol{x})$$

by

$$
\begin{aligned}
S_2 \leq& -\sum_{n=1}^N t_\delta^{(n)} p \, \mathrm{e}^{t_{n-1}} \, 4\delta_{\overline{u}_\nu D_\nu} \left(\frac{p-1}{p^2}\left|z_{\nu,h}^{p/2}\right|^2_{H^1,\mathcal{M}} + \frac{1}{4(p+1)^2}\left|z_{\nu,h}^{\frac{p+1}{2}}\right|^2_{H^1,\mathcal{M}}\right) \\
\leq& -\sum_{n=1}^N t_\delta^{(n)} p \, \mathrm{e}^{t_{n-1}} \, 4\delta_{\overline{u}_\nu D_\nu} \frac{p-1}{p^2}\left|z_{\nu,h}^{p/2}\right|^2_{H^1,\mathcal{M}}.
\end{aligned}
$$

The last term in the first line of the above inequalities can be neglected, since we only need the first H^1-seminorm in the following Moser iteration.

Reaction terms: The reaction terms multiplied by the test function can be written as

$$-R_\nu(\mathrm{e}^{\boldsymbol{v}_K}) z_{\nu K}^{p-1} \, \mathrm{e}^{-v_{\nu K}} = R_{(\boldsymbol{\alpha},\boldsymbol{\beta})}(\mathrm{e}^{\boldsymbol{v}_K})(\alpha_\nu - \beta_\nu) z_{\nu K}^{p-1} \, \mathrm{e}^{-v_{\nu K}}.$$

Using the L^∞ bounds of Theorem 3 we deduce for $\alpha_\nu > \beta_\nu$ that

$$R_{(\boldsymbol{\alpha},\boldsymbol{\beta})}(\mathrm{e}^{\boldsymbol{v}_K}) \, \mathrm{e}^{-v_{\nu K}} = k_{(\boldsymbol{\alpha},\boldsymbol{\beta})}\left(a_{\nu K}^{(\alpha_\nu - 1)} \prod_{\substack{j=1 \\ j \neq \nu}}^m a_{\nu K}^{\alpha_j} - a_{\nu K}^{(\beta_\nu - 1)} \prod_{\substack{j=1 \\ j \neq \nu}}^m a_{\nu K}^{\beta_j}\right) \leq C_1,$$

hence $-R_\nu(\mathrm{e}^{\boldsymbol{v}_K}) z_{\nu K}^{p-1} \, \mathrm{e}^{-v_{\nu K}} \leq C_1 z_{\nu K}^{p-1}$. A similar estimate holds for $\alpha_\nu < \beta_\nu$ and therefore we get with $C_2 > 0$

$$S_3 \leq C_2 \sum_{n=1}^N p t_\delta^{(n)} \, \mathrm{e}^{t_{n-1}} \|z_{\nu K}\|^{p-1}_{L^{p-1},\mathcal{M},V}.$$

Moser iteration: From $S_1 = S_2 + S_3$ we conclude

$$S_4 = e^{t_N} \delta_{\overline{u}} \|z_{\nu,h}(t_N)\|^p_{L^p,\mathcal{M},V}$$

$$\leq \sum_{n=1}^N t_\delta^{(n)} p \, e^{t_{n-1}} \left\{ -\delta_{\overline{u}_\nu D_\nu} \frac{4(p-1)}{p^2} \|w_{\nu,h}\|^2_{H^1,\mathcal{M},V} + G \right\}.$$

The expression G can be bounded by

$$G := \left(\frac{e^{\bar{t}_\delta}}{p} + \delta_{\overline{u}_\nu D_\nu} \frac{4(p-1)}{p^2} \right) \|z_{\nu,h}\|^p_{L^p,\mathcal{M},V} + C_2 \|z_{\nu,h}\|^{p-1}_{L^{p-1},\mathcal{M},V}$$

$$\leq C_3(\|w_{\nu,h}\|^2_{L^2,\mathcal{M},V} + 1)$$

with some constant $C_3 > 0$ independent of p. Using Gagliardo-Nirenberg's inequality (A.47) and Young's inequality with ($p' = 2$, $q' = 2$) we can estimate

$$\|w_{\nu,h}\|^2_{L^2,\mathcal{M},V} \leq c_2^2 C_{\mathcal{M},1,2} \|w_{\nu,h}\|_{L^1,\mathcal{M},V} \|w_{\nu,h}\|_{H^1,\mathcal{M},V}$$

$$\leq \frac{c_2^2 C_{\mathcal{M},1,2}}{2} \left(\epsilon \|w_{\nu,h}\|^2_{H^1,\mathcal{M},V} + \epsilon^{-1} \|w_{\nu,h}\|^2_{L^1,\mathcal{M},V} \right).$$

The constant ϵ is chosen in such a way that

$$-\delta_{\overline{u}_\nu D_\nu} \frac{4(p-1)}{p^2} + \epsilon \frac{C_3 c_2^2 C_{\mathcal{M},1,2}}{2} = 0 \tag{3.38}$$

holds, namely

$$\epsilon = 8 \frac{\delta_{\overline{u}_\nu D_\nu}}{C_3 c_2^2 C_{\mathcal{M},1,2}} \frac{p-1}{p^2}.$$

Therefore with $C_4 > 0$ we find

$$S_4 = e^{t_N} \delta_{\overline{u}} \|z_{\nu,h}(t_N)\|^p_{L^p,\mathcal{M},V}$$

$$\leq \sum_{n=1}^N t_\delta^{(n)} p \, e^{t_{n-1}} \frac{C_3 c_2^2 C_{\mathcal{M},1,2}}{2} \epsilon^{-1} \|w_{\nu,h}\|^2_{L^1,\mathcal{M},V} + C_3$$

$$\leq C_4 p^2 \left(\sum_{n=1}^N t_\delta^{(n)} e^{t_{n-1}} \|z_{\nu,h}\|^p_{L^{p/2},\mathcal{M},V} + 1 \right).$$

Now we proceed in a similar way as in the proof of Theorem 3. We set

$$b_k = \sup_{n=1,\dots,N} \|z_{\nu,h}\|^{2^k}_{L^{2^k},\mathcal{M},V} + 1, \quad k \geq 0.$$

Moreover let $p = 2^k$ for $k \geq 1$. Together with $C_5 > 0$

$$\|z_{\nu,h}(t_N)\|^p_{L^p,\mathcal{M},V} + 1 \leq C_5 p^2 \sup_{n=1,\dots,N} \left(\|z_{\nu,h}\|^{p/2}_{L^{p/2},\mathcal{M},V} + 1 \right)^2, \quad p \geq 2,$$

we find for all $k \geq 1$ the recursion formula

$$b_k \leq 2^{2k} C_5 (b_{k-1})^2 \leq \left\{ (4)^{\sum_{i=0}^{k-2}(k-i)2^i} (C_5)^{\sum_{i=0}^{k-2} 2^i} b_0^{2^{k-1}} \right\}^{2^{k-1}}.$$

Applying (3.27) we conclude $b_k \leq (16 C_5 b_0)^{2^{k-1}}$ and

$$\|z_{\nu,h}(t_N)\|_{L^{2^k},\mathcal{M},V} \leq (16 C_5 b_0)^{2^{-1}}, \quad k \geq 1, \, n = 1,\dots,N.$$

The term b_0 is bounded by Lemma 4. Passing to the limit $k \to \infty$ we obtain

$$\|z_{\nu,h}(t_N)\|_{L^\infty,\mathcal{M},V} \leq (16 C_5 b_0)^{2^{-1}} \leq C_8.$$

The procedure can be done for $\nu = 1,\dots,m$ and the result of the theorem follows with $v_{\nu,h}^- \leq z_{\nu,h} + v_{\nu,h}^- + \kappa$ and Theorem 3. $\qquad \square$

A Discrete Gagliardo-Nirenberg inequality

In the following, we prove a discrete version of the Gagliardo-Nirenberg inequality [23] on Voronoi finite volume meshes. The proof is based on the equivalence of the Voronoi finite volume L^p-norm, the Donald box finite volume L^p-norm (for the definition of a Donald box see [21]), and the linear finite element L^p-norm. First, we introduce the following notations, see also Figure 2 : The dual of a Voronoi mesh $\mathcal{M} = (\mathcal{P}, \mathcal{V}, \mathcal{E})$ is given by a tuple $(\mathcal{P}, \mathcal{T})$, where $\mathcal{T}$ is a family of triangles T spanned by $(x_K, x_L, x_M) \in \mathcal{P}^3$ fulfilling $\overline{K} \cap \overline{L} \cap \overline{M} \neq \emptyset$, $K, L, M \in \mathcal{V}$. Furthermore by $\mathcal{N}_T(K)$ we denote the set of all triangle sharing sharing x_K as common vertex.
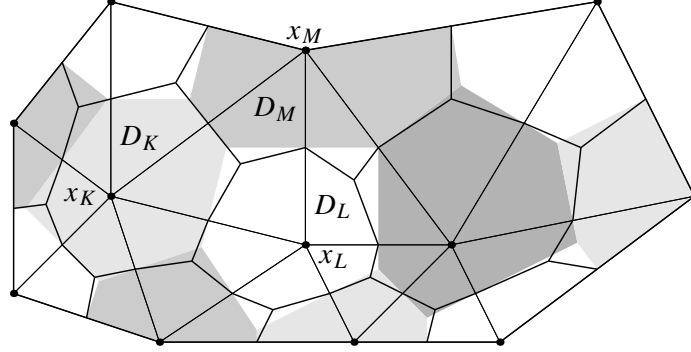
Figure 2: Notation of the dual Voronoi mesh and the Donald box mesh. Voronoi boxes (gray areas), triangles (thin lines), Donald boxes (thick lines)

A *Donald box* $D_K = D(x_K)$ around a node $x_K \in \mathcal{P}$ is constructed by intersecting the barycenters of all neighboring triangles. The area of a triangle $T \in \mathcal{T}$ is denoted by $|T|$ and the area of a Donald box is given by $|D_K \cap T| = 1/3|T|$, see [21]. By $X_D(\mathcal{M})$ we denote the set of all piecewise constant functions from Ω to $\mathbb{R}$ which are constant on every Donald box D_K. The discrete Donald box finite volume L^p-norm is then introduced by

$$\|w_D\|_{L^p, \mathcal{M}, D} = \left(\sum_{K \in \mathcal{V}} |D_K| |w_K|^p \right)^{1/p} \quad \forall w_D \in X_D(\mathcal{M}). \tag{A.39}$$

Let $w_T(\boldsymbol{x})$ the linear function on a triangle $T \in \mathcal{T}$ with nodes $(x_K, x_L, x_M) \in \mathcal{P}^3$ and values $w_T(x_K) = f_K$, $w_T(x_L) = w_L$, $w_T(x_M) = w_M$, where w_K, resp. is the value in the node $x_K \in \mathcal{P}$. The set of all these functions is denoted by $P_1(\mathcal{M})$. The finite element L^p-norm is then defined by

$$\|w_T\|_{L^p, \mathcal{M}, FEM} = \left(\sum_{T \in \mathcal{T}} \int_T |w_T(\boldsymbol{x})|^p \, d\boldsymbol{x} \right)^{1/p} \quad \forall w_T \in P_1(\mathcal{M}). \tag{A.40}$$

We make the following assumption on the mesh: There exists two constants $\underline{C}_D > 0$, $\overline{C}_D \geq 1$ such that for all $x_K \in \mathcal{P}$ the area of the Donald box around x_K can be estimated by the area of the area of the Voronoi box K, i.e., it holds

$$\underline{C}_D |K| \leq |D_K| \leq \overline{C}_D |K| \qquad \forall K \in \mathcal{V}. \tag{A.41}$$

Remark 3 Such an inequality holds for all uniform FEM-meshes, where the largest edge $l_{\max}$ of all triangles $T \in \mathcal{T}$ can be bounded by the smallest edge $l_{\min}$ and some constant $C > 1$. In this case we can cover the area of the Voronoi box and the Donald box by the area of a circle with radius $l_{\min}/2$ and $l_{\max}$, i.e.

$$\frac{\pi l_{\min}^2}{4} \leq |K|, |D_K| \leq \pi l_{\max}^2 \leq \pi C^2 l_{\min}^2.$$

Therefore, we have

$$\frac{1}{4C^2} |K| \leq |D_K| \leq 4C^2 |K|.$$

We make the following observation:

Lemma A.5 *Let Ω be an open, bounded, polyhedral subset of $\mathbb{R}^2$ and $\mathcal{M} = (\mathcal{P}, \mathcal{V}, \mathcal{E})$ a given Voronoi mesh and $(\mathcal{P}, \mathcal{T})$ its dual fulfilling (A.41). The following statements hold:*

1. *For all* $w_h \in X_{\mathcal{V}}(\mathcal{M})$, $w_D \in X_D(\mathcal{M})$ *and* $p \in \mathbb{N}$, $w_h \geq 0$ *the estimate*

$$\underline{C}_D^{1/p}\|w_h\|_{L^p,\mathcal{M},V} \leq \|w_D\|_{L^p,\mathcal{M},D} \leq \overline{C}_D^{1/p}\|w_h\|_{L^p,\mathcal{M},V} \tag{A.42}$$

   holds.
2. *Furthermore there exist two constants* $\underline{C}_{FEM,p} = \frac{6}{(p+1)(p+2)} \leq 1$ *and* $\overline{C}_{FEM} = 1$ *such that for* $w_D \in X_D(\mathcal{M})$ *and* $w_T \in P_1(\mathcal{M})$, $w_D \geq 0$

$$\underline{C}_{FEM,p}^{1/p}\|w_D\|_{L^p,\mathcal{M},D} \leq \|w_T\|_{L^p,\mathcal{M},FEM} \leq \overline{C}_{FEM}\|w_D\|_{L^p,\mathcal{M},D} \tag{A.43}$$

   holds.

Proof In order to simplify the following notation, we assume that $w_K \geq 0$ holds for all $K \in \mathcal{V}$. The proof of (A.42) follows immediately from (A.41) together with

$$\|w_D\|_{L^p,\mathcal{M},D} = \left(\sum_{K \in \mathcal{V}} |D_K|w_K^p\right)^{1/p} \leq \left(\sum_{K \in \mathcal{V}} \overline{C}_D|K|w_K^p\right)^{1/p} = \overline{C}_D^{1/p}\|w_h\|_{L^p,\mathcal{M},V}.$$

Similar, the estimate from above is derived.

For the second second assertion (A.40) we observe together with $|D_K \cap T| = 1/3|T|$

$$\|w_D\|_{L^p,\mathcal{M},D} = \left(\sum_{K \in \mathcal{V}} \sum_{T \in \mathcal{N}_T(K)} \frac{|T|}{3}w_K^p\right)^{1/p} = \sum_{T \in \mathcal{T}} \frac{|T|}{3}(w_K + w_L + w_M) \tag{A.44}$$

with $T = (\boldsymbol{x}_K, \boldsymbol{x}_L, \boldsymbol{x}_M)$. It remains to show that for every triangle the identities

$$\frac{\underline{C}_{FEM,p}|T|}{3}\left(w_K^p + w_L^p + w_M^p\right) \leq \int_T w_T(\boldsymbol{x})^p \, d\boldsymbol{x} \leq \frac{\overline{C}_{FEM,p}|T|}{3}\left(w_K^p + w_L^p + w_M^p\right)$$

with constants $\underline{C}_{FEM,p}$ and $\overline{C}_{FEM,p}$ hold. In a first step we transform the triangle $T = (\boldsymbol{x}_K, \boldsymbol{x}_L, \boldsymbol{x}_M)$ to the reference triangle $\widehat{T} = (P_1, P_2, P_3)$ with vertices $P_1 = (0,0)$, $P_2 = (1,0)$, $P_3 = (0,1)$ using

$$\boldsymbol{x} = \boldsymbol{x}_K + (\boldsymbol{x}_L - \boldsymbol{x}_K)\xi + (\boldsymbol{x}_M - \boldsymbol{x}_K)\rho$$

with $\xi \in [0,1]$ and $\rho \in [0,\xi]$. The transformed function reads as

$$\widehat{w}(\xi,\rho) = w_T(\boldsymbol{x}_K + (\boldsymbol{x}_L - \boldsymbol{x}_K)\xi + (\boldsymbol{x}_M - \boldsymbol{x}_K)\rho)$$
$$= w_K + (w_L - w_K)\xi + (w_M - w_K)\rho$$

and its functional determinant is given by $\det(J) = 2|T|$. The integral over the simplex T can be written in the form

$$I = \int_T (w_T(\boldsymbol{x}))^p \, d\boldsymbol{x} = 2|T| \int_0^1 \int_0^{1-\xi} (\widehat{w}(\xi,\rho))^p \, d\rho \, d\xi$$
$$= \frac{2|T|}{(p+1)(w_M - w_K)} \int_0^1 (w_M + (w_L - w_M)\xi)^{p+1} - (w_K + (w_L - w_K)\xi)^{p+1} \, d\xi$$
$$= \frac{2|T|}{(p+2)(p+1)(w_M - w_K)} \left(\frac{w_M^{p+2} - w_L^{p+2}}{w_M - w_L} - \frac{w_L^{p+2} - w_K^{p+2}}{w_L - w_K}\right).$$

To continue the estimate, we use $0 \leq (v^a - 1)(v^b - 1)$ for all $v \geq 1$ and $a,b \geq 0$. Let $v = x/y$ with nonnegative real numbers x, y. Using

$$x^a y^b + y^a x^b \leq x^{a+b} + y^{a+b} \tag{A.45}$$

we can bound the cyclic sum

$$\sum_{cycl} x^i y^j z^k := x^i(y^j z^k + y^k z^j) + y^i(x^j z^k + x^k z^j) + z^i(x^j y^k + y^k x^j)$$

by $\sum_{cycl} x^i y^j z^k \leq 2(z^{i+j+k} + x^{i+j+k} + y^{i+j+k})$.

Now, using the binomial theorem we obtain for $p \in \mathbb{N}$ the identity

$$\frac{w_M^{p+2} - w_L^{p+2}}{w_M - w_L} = \sum_{i=0}^{p+1} w_M^i w_L^{p+1-i}.$$

Therefore

$$I = \frac{2|T|}{(p+1)(p+2)} \sum_{\substack{i,j,k\geq 0 \\ i+j+k=p}} w_M^i w_L^j w_K^k = \frac{2|T|}{(p+1)(p+2)} \sum_{\substack{i,j,k\geq 0 \\ i+j+k=p}} \frac{1}{6} \sum_{cycl} w_M^i w_L^j w_K^k$$

$$\leq \frac{4|T|}{6(p+1)(p+2)} \left(w_M^p + w_L^p + w_K^p\right) \sum_{\substack{i,j,k\geq 0 \\ i+j+k=p}} 1 = \frac{|T|}{3} \left(w_M^p + w_L^p + w_K^p\right)$$

holds. In the last line we used

$$\sum_{\substack{i,j,k\geq 0 \\ i+j+k=p}} 1 = \sum_{i=0}^{p} \left(1 + \sum_{j=0}^{i-1} 1\right) = \sum_{i=0}^{p} i + 1 = \frac{(p+2)(p+1)}{2}.$$

Since the term $w_M^p + w_L^p + w_K^p$, $w_M, w_L, w_K > 0$ is contained in $\sum_{\substack{i,j,k\geq 0 \\ i+j+k=p}} w_M^i w_L^j w_K^k$, the lower bound of I follows. □

Theorem A.5 (Discrete Gagliardo-Nirenberg inequality) *Under the assumptions of Lemma A.5 the following statements hold:*

– For every $p \in \mathbb{N}$ there exist constants $c_p > 0$ and

$$C_{\mathcal{M},1,p} = \frac{\max(\overline{C}_D, \overline{C}_D^{(p+1)/2})}{\underline{C}_D \underline{C}_{FEM,p}} \tag{A.46}$$

such that

$$\|w_h\|_{L^p,\mathcal{M},V} \leq c_p C_{\mathcal{M},1,p}^{1/p} \|w_h\|_{L^1,\mathcal{M},V}^{1/p} \|w_h\|_{H^1,\mathcal{M},V}^{1-1/p} \quad \forall w_h \in X(\mathcal{M}). \tag{A.47}$$

Especially, for p from a compact interval $[p_1, p_2]$ the constant c_p can be bounded by $c_p \leq \max(c_{p_1}, c_{p_2}, 1)^{1/p_1}$.

– Additionally, for every $\epsilon > 0$ and $p \in \mathbb{N}$, $p > 1$ there exist a constant $c_{\epsilon,p} > 0$ such that for all $w_h \in X(\mathcal{M})$

$$\|w_h\|_{L^p,\mathcal{M},V}^p \leq \epsilon C_{\mathcal{M},2,p} \|w_h \ln |w_h|\|_{L^1,\mathcal{M},V} \|w_h\|_{H^1,\mathcal{M},V}^{p-1}$$
$$+ c_{\epsilon,p} C_{\mathcal{M},3,p} \|w_h\|_{L^1,\mathcal{M},V} \tag{A.48}$$

with the two constants

$$C_{\mathcal{M},2,p} = \frac{\max(\overline{C}_D, \overline{C}_D^{(p+1)/2})}{\underline{C}_D \underline{C}_{FEM,p}}, \qquad C_{\mathcal{M},3,p} = \frac{\overline{C}_D}{\underline{C}_D \underline{C}_{FEM,p}}.$$

The constants $C_{\mathcal{M},i,p}$, $i = 1, 2, 3$ are the only difference to the continuous version in [18].

Proof As a consequence of Lemma A.5 we can use the continuous version to prove the discrete inequalities. From Lemma A.5 we conclude that

$$\|w_h\|_{L^p,\mathcal{M},V} \leq \frac{1}{(\underline{C}_D \underline{C}_{FEM,p})^{1/p}} \|w_T\|_{L^p,\mathcal{M},FEM},$$

$$\|w_T\|_{L^p,\mathcal{M},FEM} \leq \overline{C}_D^{1/p} \|w_h\|_{L^p,\mathcal{M},V},$$

$$\|w_T\|_{H^1,\mathcal{M},FEM} \leq \max(1, \overline{C}_D^{1/2}) \|w_h\|_{H^1,\mathcal{M},V}$$

hold. Using the continuous Gagliardo-Nirenberg inequality [18, (1.8)] the assertion

$$\|w_h\|_{L^p,\mathcal{M},V} \leq c_p C_{\mathcal{M},1,p}^{1/p} \|w_h\|_{L^1,\mathcal{M},V}^{1/p} \|w_h\|_{H^1,\mathcal{M},V}^{1-1/p},$$

holds with a constant $C_{\mathcal{M},1,p}$ defined above.

We mention that $x \ln x$, $x \geq 0$ is convex and therefore the the linear interpolation of $w_T \ln w_T$ denoted by $(w_T \ln w_T)_T$ is greater or equal $w_T \ln w_T$. Hence,

$$\int_T w_T \ln w_T \, d\boldsymbol{x} \leq \int_T (w_T \ln w_T)_T \, d\boldsymbol{x}. \tag{A.49}$$

Together with the continuous Gagliardo-Nirenberg inequality [18, (1.9)] we get

$$\|w_h\|_{L^p,\mathcal{M},V}^p \leq \epsilon \frac{1}{\underline{C}_D \underline{C}_{FEM,p}} \|(w_T \ln w_T)_T\|_{L^1,\mathcal{M},FEM} \|w_T\|_{H^1,\mathcal{M},FEM}^{p-1}$$
$$+ c_{\epsilon,p} \|w_T\|_{L^1,\mathcal{M},FEM}$$
$$\leq \epsilon C_{\mathcal{M},2,p} \|w_h \ln |w_h|\|_{L^1,\mathcal{M},V} \|w_h\|_{H^1,\mathcal{M},V}^{p-1} + c_{\epsilon,p} C_{\mathcal{M},3,p} \|w_h\|_{L^1,\mathcal{M},V}.$$

□

Remark 4 Of course, the discrete Gagliardo-Nirenberg inequality can be proven in a direct manner on much more general mesh families, but the special case needed here can be proven in a much shorter way. For a similar proof of a discrete Sobolev inequality, see [15, Theorem 2.2].

B Technical lemmas

In this part we collect some auxiliary results, which we use in the proof of Lemma 3 and in Section 3.4.

Lemma B.6 *Let $x, y, p \in \mathbb{R}$, $x, y > 0$.*

1. *For $p \geq 2$ the following inequalities hold:*

$$\frac{4(p-1)}{p^2} \left(x^{p/2} - y^{p/2} \right)^2 \leq (x-y)(x^{p-1} - y^{p-1}) \leq \left(x^{p/2} - y^{p/2} \right)^2 . \tag{B.50}$$

2. *For $p \geq 1$, we have*

$$\frac{1}{p}(x^p - y^p) \leq x^{p-1}(x-y). \tag{B.51}$$

3. *Finally, for $p \geq 2$ the inequalities*

$$\frac{2}{p^2}(x^{p/2} - y^{p/2})^2 \leq (x^{p-2} + y^{p-2})(x-y)^2 \leq 2(x^{p/2} - y^{p/2})^2 \tag{B.52}$$

are fulfilled.

Proof   1. For $z \geq 1$, we consider the function

$$f(z) = (z-1)(z^{p-1} - 1) - \frac{4(p-1)}{p^2}(z^{p/2} - 1)^2.$$

The first and second derivatives of f are given by

$$\frac{d}{dz}f(z) = \frac{(p-2)^2}{p}z^{p-1} - (p-1)z^{p-2} + \frac{4(p-1)}{p}z^{p/2-1} - 1,$$

$$\frac{d^2}{dz^2}f(z) = \frac{(p-2)(p-1)}{p}\left(((p-2)z - p)z^{p-3} + 2z^{p/2-2}\right).$$

It is easy to see that $f(1) = 0$, $f'(1) = 0$ and $f''(1) = 0$. Further, we deduce from $f''(z) > 0$ for $z > 1$ that $f'(z) > 0$ and $f(z) > 0$. With $z = x/y$, $x \geq y > 0$ we find

$$0 \leq f(x/y) = (x-y)(x^{p-1} - y^{p-1}) - \frac{4(p-1)}{p^2}\left(x^{p/2} - y^{p/2}\right)^2$$

and finally by using Muirhead's inequality

$$\left(x^{p/2} - y^{p/2}\right)^2 - (x-y)(x^{p-1} - y^{p-1}) = x^{p-1}y + xy^{p-1} - 2x^{p/2}y^{p/2} \geq 0$$

holds. The case $y = 0$ is trivial.

2. For the second statement we consider for $z \geq 1$ the function

$$f(z) = \frac{p-1}{p}z^p - z^{p-1} + \frac{1}{p}.$$

Since $f(1) = 0$, the first derivative of f

$$\frac{d}{dz}f(z) = (p-1)z^{p-2}(z-1) \geq 0$$

implies $f(z) \geq 0$. Setting $z = x/y$, $x \geq y > 0$ we find

$$0 \leq y^p f(x/y) = \left(\frac{p-1}{p}\frac{x^p}{y^p} - \frac{x^{p-1}}{y^{p-1}} + \frac{1}{p}\right)y^p = x^{p-1}(x-y) - \frac{1}{p}(x^p - y^p).$$

For $x \leq y$ it results

$$\frac{1}{p}(x^p - y^p) \leq (x^p - y^p) \leq x^{p-1}(x - yx^{-p+1}) \leq x^{p-1}(x-y).$$

3. Now let

$$f(z) = (z^{p-2} + 1)(z-1)^2 - \frac{2}{p^2}(z^{p/2} - 1)^2.$$

The first and second derivatives are given by

$$\frac{d}{dz}f(z) = 2(z-1)(z^{p-2} + 1) + (p-2)(z-1)^2 z^{p-3} - \frac{2}{p}(z^{p/2} - 1)z^{p/2-1},$$

$$\frac{d^2}{dz^2}f(z) = \frac{1}{p}\left(2p + (p-2)z^{p/2-2} + z^{p-4}g(z)\right)$$

with

$$g(z) = (p-3)(p-2)p - 2(p-2)(p-1)pz + (p-1)(p^2-2)z^2,$$
$$g'(z) = 2(p-1)\left((p^2-2)z - (p-2)p\right),$$
$$g''(z) = 2(p-1)(p^2-2).$$

From $g''(z) > 0$ for $z > 1$ and $p \geq 2$ we see that $g(z)$ is a convex function. Furthermore $f(z)$ is convex since $g'(1) = 4(p-1)^2 > 0$, $g(1) = 2$ and $f''(z) > 0$. Using $f'(1) = f(1) = 0$ we get $f(z) > 0$ and with $z = x/y$, $x \geq y > 0$ the first inequality of (B.52).

The last assertion follows from

$$(x^{p/2} - y^{p/2})^2 - \frac{1}{2}(x^{p-2} + y^{p-2})(x-y)^2 = \frac{1}{2}\left(x^p + y^p - x^{p-2}y^2 - x^2 y^{p-2}\right)$$
$$+ \left(x^{p-1}y + xy^{p-1} - 2x^{p/2}y^{p/2}\right)$$

together with Muirhead's inequality for the term

$$x^p + y^p \geq x^{p-2}y^2 + x^2 y^{p-2}, \qquad x^{p-1}y + xy^{p-1} \geq 2x^{p/2}y^{p/2}.$$

$\square$

Lemma B.7 *Let x be a real number. Then*

$$f(x) = \frac{(e^x - 1)(e^{-x} + 1)}{2x} \geq 1, \qquad g(x) = \frac{(e^x - 1)(e^{-x} - 1)}{x^2} \leq -1$$

hold. We define the value of the functions at $x = 0$ as limit $x \to 0$.

Proof For $x + \epsilon > 0$ we get

$$f(x + \epsilon) = \frac{(e^{x+\epsilon} - 1)(e^{-(x+\epsilon)} + 1)}{2(x+\epsilon)} > \frac{(e^{x+\epsilon} - 1)(e^{-x} + 1)}{2x} > f(x), \qquad (B.53)$$

this means $f(x)$ is strictly increasing. Since $f(x) = -f(-x)$, the function $f(x)$ is strictly decreasing for $x < 0$. Hence there exists a global minimum at $x = 0$ with value

$$\lim_{x \to 0} f(x) = \lim_{x \to 0} \cosh(x) = 1.$$

With similar arguments the second inequality follows. $\square$

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